



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:16 AM UTC

PDB ID : 9FMD / pdb_00009fmd
EMDB ID : EMD-4525
Title : Integrative model of the human post-catalytic spliceosome (P-complex)
Authors : Rothe, P.; Plaschka, C.; Vorlaender, M.K.
Deposited on : 2024-06-05
Resolution : 3.30 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:

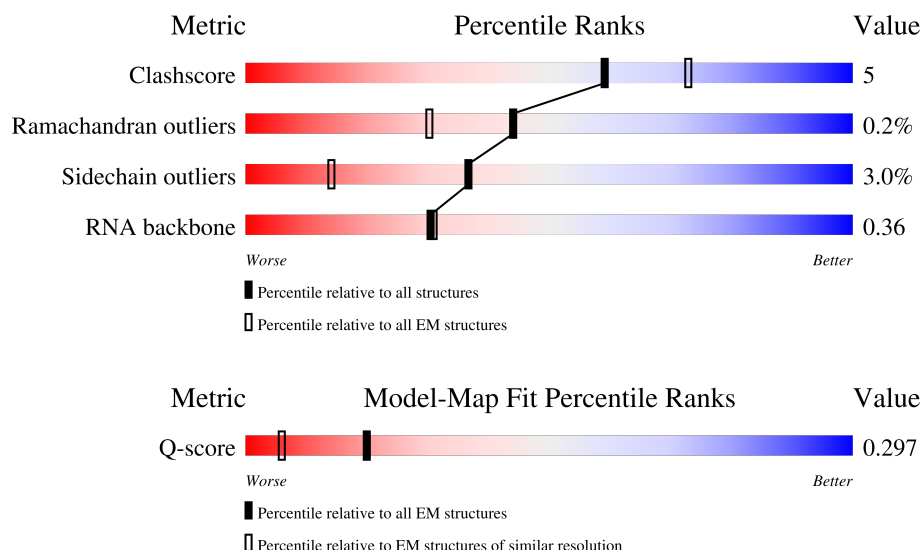
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.30 Å.

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



Metric	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	15087 (2.80 - 3.80)

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	1	184	35% 59% 8% 33%
2	2	187	36% 36% 21% 6% 36%
3	3	476	16% 17% 83%

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Mol	Chain	Length	Quality of chain
4	32	112	
5	5	116	
6	50	339	
7	56	222	
8	6	106	
9	7	411	
10	8	174	
11	9	146	
12	A	2335	
13	B	2136	
14	C	972	
15	D	285	
16	E	357	
17	EX	14	
18	F	758	
19	H	908	
20	I	855	
21	IN	113	
22	J	848	
23	K	225	
24	L	802	
25	M	243	
26	N	144	
27	NO	301	
28	O	420	

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Mol	Chain	Length	Quality of chain
29	P	229	
30	Q	1485	
31	R	536	
32	S	166	
33	SR	2752	
34	T	514	
35	U	586	
36	V	1220	
37	W	579	
38	X	451	
39	Z	166	
40	a	126	
40	h	126	
41	b	240	
41	i	240	
42	c	119	
42	j	119	
43	d	118	
43	k	118	
44	e	92	
44	l	92	
45	f	86	
45	m	86	
46	g	76	
46	n	76	

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Mol	Chain	Length	Quality of chain
47	o	255	
48	p	225	
49	q	504	
49	r	504	
49	s	504	
49	t	504	
50	w	646	
51	x	289	
52	y	301	
53	z	415	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 120489 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 PRKR-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	123	Total	C	N	O	S	0	0
			1013	635	193	180	5		

- Molecule 2 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	120	Total	C	N	O	P	0	0
			2535	1135	428	852	120		

- Molecule 3 is a protein called Splicing factor ESS-2 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	82	Total	C	N	O	0	0
			408	244	82	82		

- Molecule 4 is a protein called Protein FAM32A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	32	60	Total	C	N	O	S	0	0
			504	314	96	92	2		

- Molecule 5 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	92	Total	C	N	O	P	0	0
			1936	867	322	655	92		

- Molecule 6 is a protein called Protein FAM50A.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	50	226	Total	C	N	O	0	0
			1124	671	226	227		

- Molecule 7 is a protein called STING ER exit protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	56	101	Total	C	N	O	0	0
			498	296	101	101		

- Molecule 8 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	6	97	Total	C	N	O	P	0	0
			2075	928	381	669	97		

- Molecule 9 is a protein called Eukaryotic initiation factor 4A-III.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	7	390	Total	C	N	O	0	0
			1928	1147	390	391		

- Molecule 10 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	8	91	Total	C	N	O	0	0
			445	263	91	91		

- Molecule 11 is a protein called Protein mago nashi homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	9	144	Total	C	N	O	0	0
			712	423	144	145		

- Molecule 12 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	2250	Total	C	N	O	S	0	0
			17802	11405	3151	3176	70		

- Molecule 13 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	1864	Total	C	N	O	S	0	0
			15004	9583	2569	2775	77		

- Molecule 14 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	894	Total	C	N	O	S	0	0
			7069	4521	1178	1336	34		

- Molecule 15 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	D	72	Total	C	N	O	0	0
			358	214	72	72		

- Molecule 16 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E	303	Total	C	N	O	S	0	0
			2370	1489	416	452	13		

- Molecule 17 is a RNA chain called Exon.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	EX	14	Total	C	N	O	P	0	0
			296	132	52	98	14		

- Molecule 18 is a protein called Splicing factor Cactin.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F	122	Total	C	N	O	S	0	0
			1089	714	197	176	2		

- Molecule 19 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	H	459	Total	C	N	O	S	0	0
			2932	1827	533	560	12		

- Molecule 20 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	I	727	Total	C	N	O	0	0
			3610	2156	727	727		

- Molecule 21 is a RNA chain called INTRON.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	IN	42	Total	C	N	O	P	0	0
			893	400	158	293	42		

- Molecule 22 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	J	602	Total	C	N	O	0	0
			2998	1794	602	602		

- Molecule 23 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	K	189	Total	C	N	O	0	0
			941	563	189	189		

- Molecule 24 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	L	555	Total	C	N	O	S	0	0
			3642	2233	706	695	8		

- Molecule 25 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	M	224	Total	C	N	O	0	0
			1115	666	224	225		

- Molecule 26 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	N	144	Total	C	N	O	S	0	0
			1189	748	218	211	12		

- Molecule 27 is a protein called Nitric oxide synthase-interacting protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	NO	174	Total	C	N	O	0	0
			864	516	174	174		

- Molecule 28 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	O	289	Total	C	N	O	S	0	0
			2327	1459	416	432	20		

- Molecule 29 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	P	106	Total	C	N	O	S	0	0
			889	544	174	169	2		

- Molecule 30 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Q	1322	Total	C	N	O		0	0
			6554	3910	1322	1322			

- Molecule 31 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	R	328	Total	C	N	O	P	S	0	0
			2618	1634	479	489	2	14		

- Molecule 32 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S	164	Total	C	N	O	S	0	0
			1271	810	220	234	7		

- Molecule 33 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SR	70	Total	C	N	O	S	0	0
			412	251	80	80	1		

- Molecule 34 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	T	363	Total	C	N	O	S	0	0
			2881	1820	525	526	10		

- Molecule 35 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	U	295	Total	C	N	O	S	0	0
			2425	1525	431	461	8		

- Molecule 36 is a protein called ATP-dependent RNA helicase DHX8.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	V	733	Total	C	N	O		0	0
			3629	2163	733	733			

- Molecule 37 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	W	513	Total	C	N	O	S	0	0
			4158	2643	719	772	24		

- Molecule 38 is a protein called Splicing regulator SDE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	X	66	Total	C	N	O		0	0
			328	196	66	66			

- Molecule 39 is a protein called Coiled-coil domain-containing protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Z	53	Total	C	N	O		0	0
			265	159	53	53			

- Molecule 40 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	a	84	Total	C	N	O	S	0	0
			658	412	116	124	6		
40	h	83	Total	C	N	O	S	0	0
			652	409	115	122	6		

- Molecule 41 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	b	87	Total	C	N	O	S	0	0
			654	412	120	115	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	82	Total	C	N	O	S	0	0
			664	419	121	117	7		

- Molecule 42 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	c	80	Total	C	N	O	S	0	0
			634	404	111	115	4		
42	j	80	Total	C	N	O	S	0	0
			634	404	111	115	4		

- Molecule 43 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	d	89	Total	C	N	O	S	0	0
			723	454	133	131	5		
43	k	95	Total	C	N	O	S	0	0
			774	486	141	142	5		

- Molecule 44 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	e	79	Total	C	N	O	S	0	0
			651	413	115	118	5		
44	l	81	Total	C	N	O	S	0	0
			669	424	119	121	5		

- Molecule 45 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	f	72	Total	C	N	O	S	0	0
			562	364	93	100	5		
45	m	72	Total	C	N	O	S	0	0
			562	364	93	100	5		

- Molecule 46 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	g	73	Total	C	N	O	S	0	0
			568	358	102	102	6		
46	n	73	Total	C	N	O	S	0	0
			568	358	102	102	6		

- Molecule 47 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	162	Total	C	N	O	S	0	0
			1282	820	219	240	3		

- Molecule 48 is a protein called U2 small nuclear ribonucleoprotein B''.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	92	Total	C	N	O	S	0	0
			745	480	130	130	5		

- Molecule 49 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	q	103	Total	C	N	O	0	0
			514	308	103	103		
49	r	119	Total	C	N	O	0	0
			594	356	119	119		
49	s	132	Total	C	N	O	0	0
			659	395	132	132		
49	t	103	Total	C	N	O	0	0
			514	308	103	103		

- Molecule 50 is a protein called Peptidylprolyl isomerase domain and WD repeat-containing protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	w	528	Total	C	N	O	0	0
			2605	1548	528	529		

- Molecule 51 is a protein called Splicing factor C9orf78.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	x	128	Total	C	N	O	0	0
			636	379	128	129		

- Molecule 52 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	y	79	Total	C	N	O	0	0
			318	160	79	79		

- Molecule 53 is a protein called NF-kappa-B-activating protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	z	70	Total	C	N	O	S	0	0
			430	259	83	86	2		

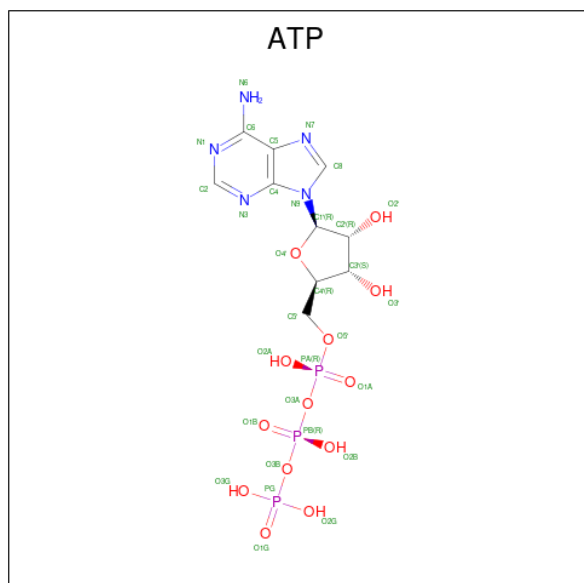
- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	6	5	Total	Mg	0
			5	5	
54	7	1	Total	Mg	0
			1	1	

- Molecule 55 is POTASSIUM ION (CCD ID: K) (formula: K).

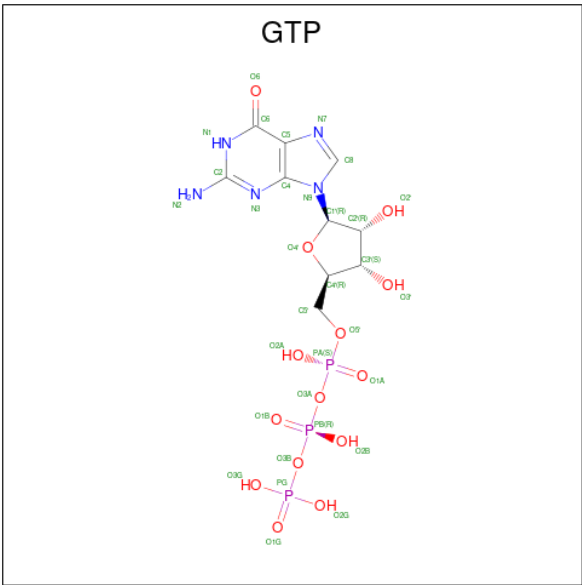
Mol	Chain	Residues	Atoms		AltConf
55	6	1	Total	K	0
			1	1	

- Molecule 56 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
56	7	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 57 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

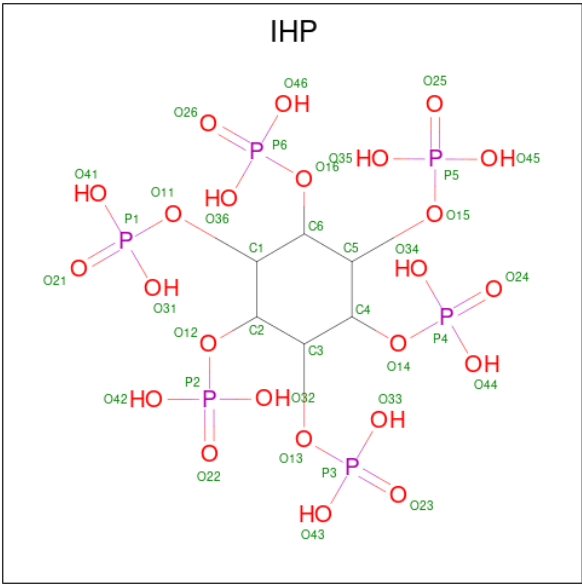


Mol	Chain	Residues	Atoms					AltConf
57	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

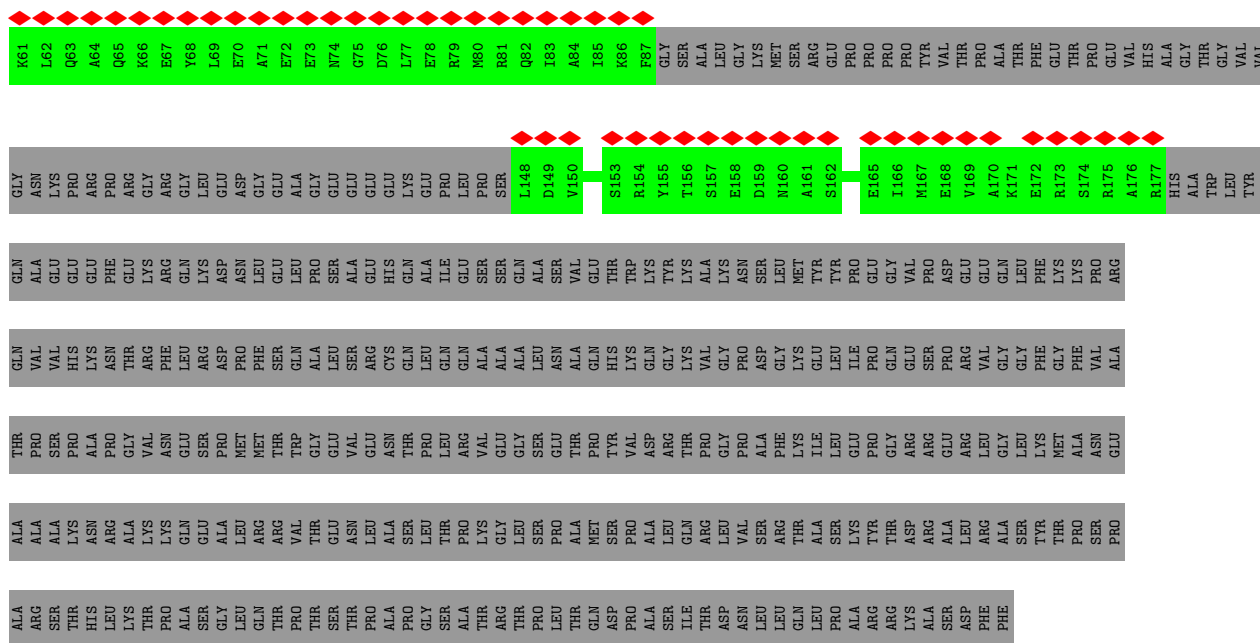
- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	N	3	Total	Zn	0
			3	3	
58	O	3	Total	Zn	0
			3	3	

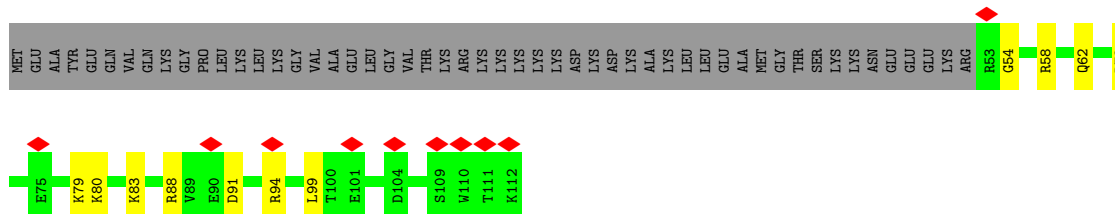
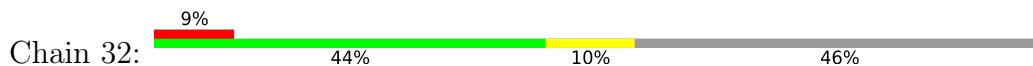
- Molecule 59 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



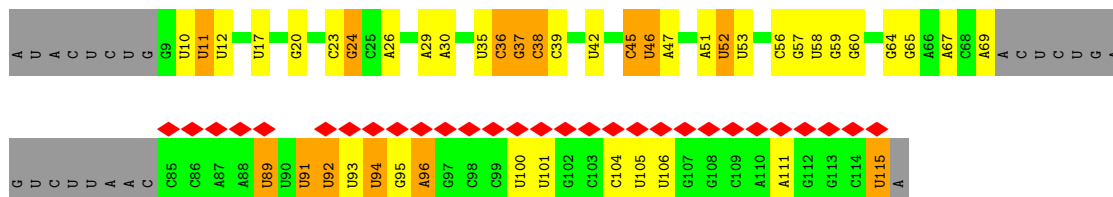
Mol	Chain	Residues	Atoms				AltConf
59	U	1	Total	C	O	P	0
			36	6	24	6	



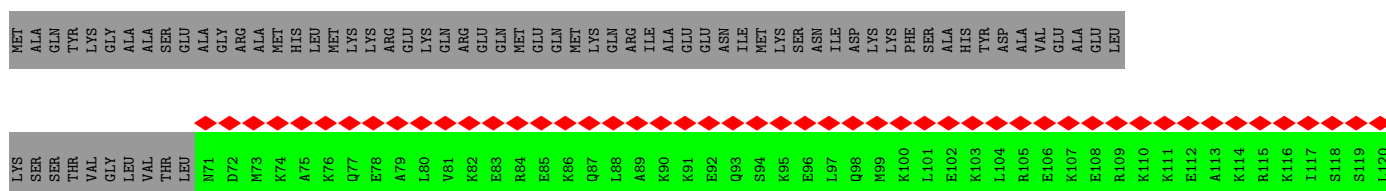
- Molecule 4: Protein FAM32A



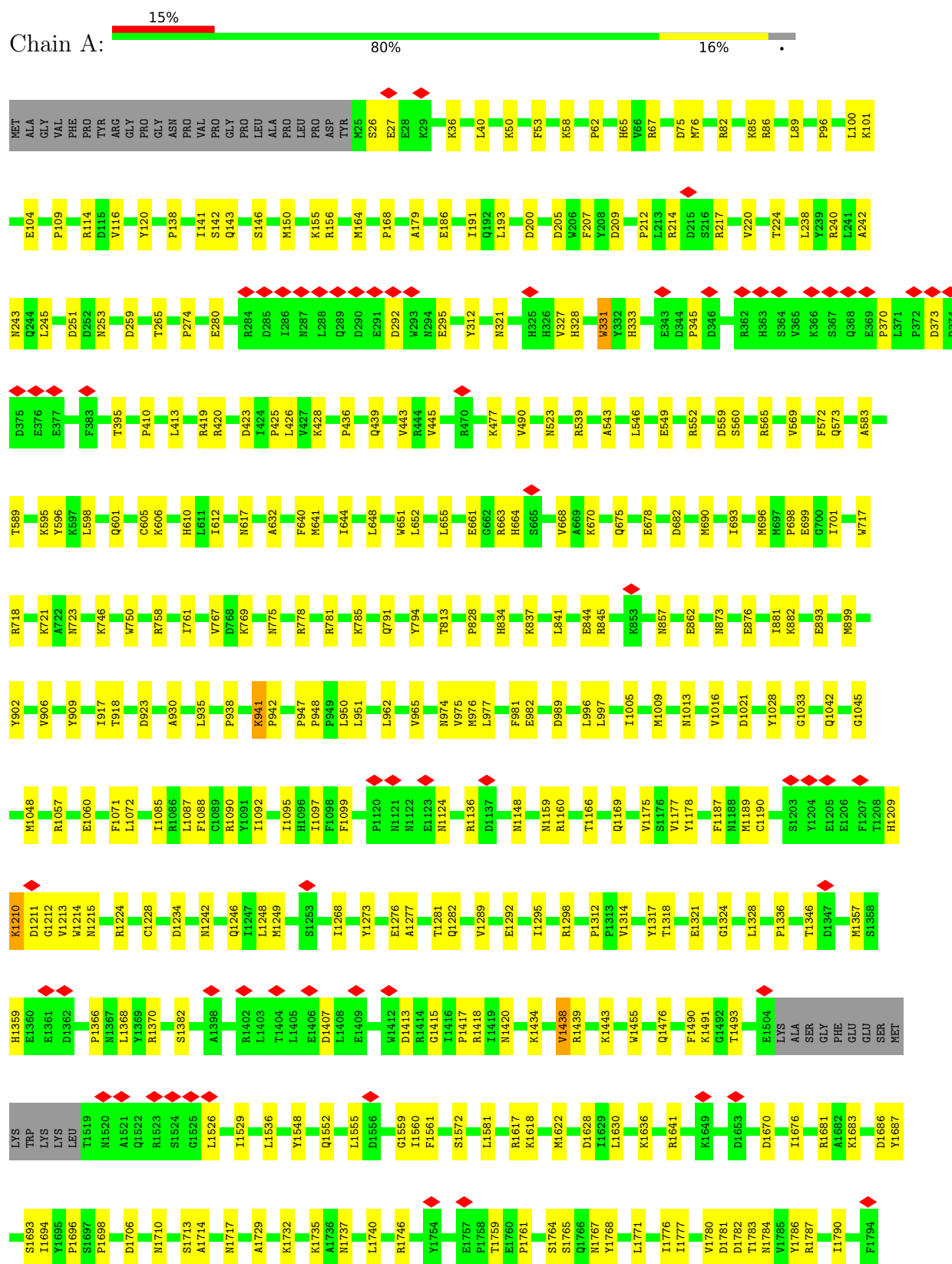
- Molecule 5: U5 snRNA



- Molecule 6: Protein FAM50A

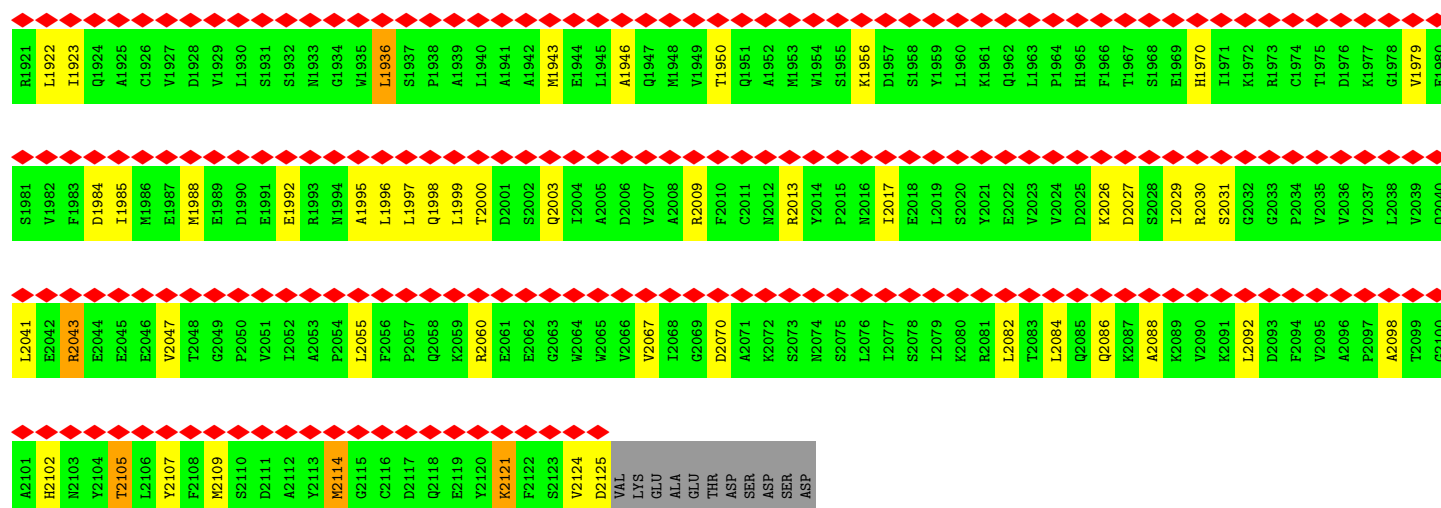


• Molecule 12: Pre-mRNA-processing-splicing factor 8

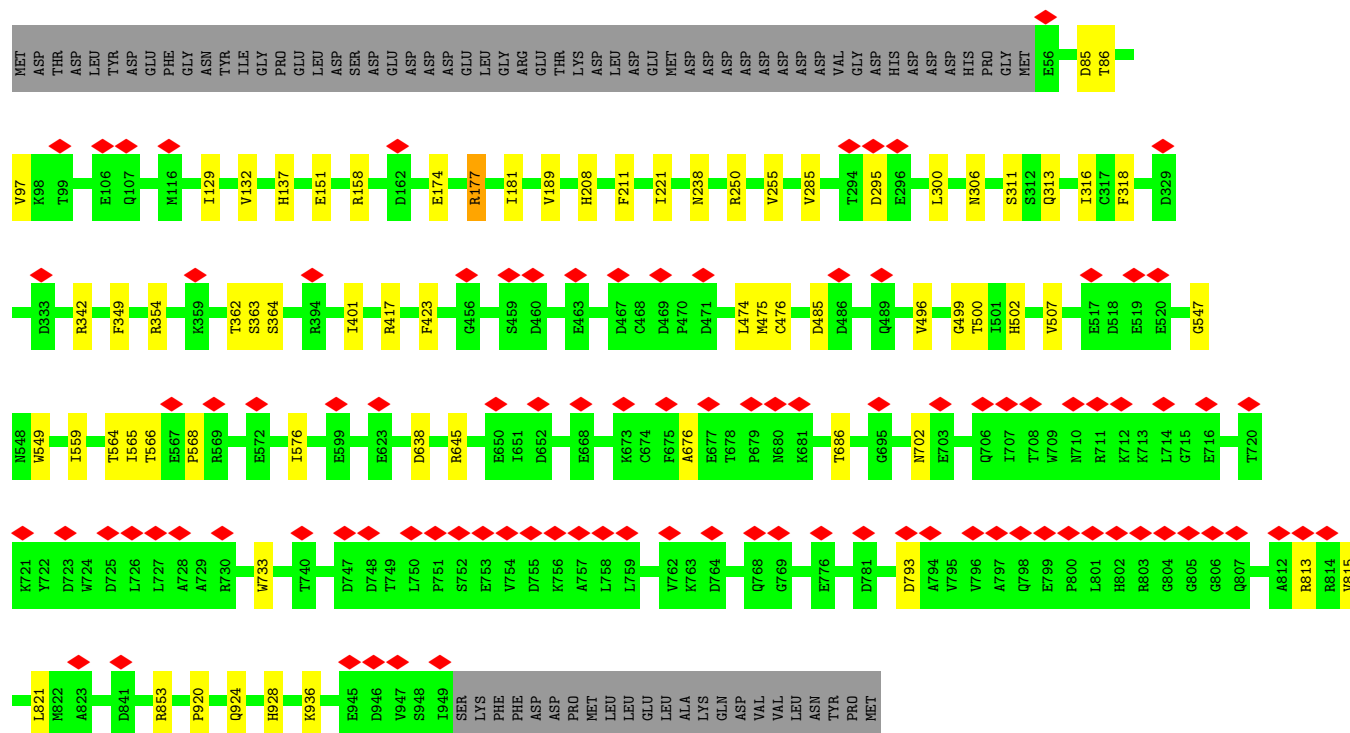
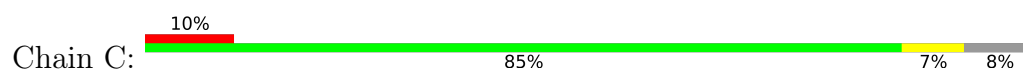


TTR	GLN	LEU	HIS	GLU	THR	GLU	LYS	GLU	ASP	LEU	ILE	ARG	GLU	ARG	GLU	ARG	ARG	ARG	VAL	ARG	GLN	SER	SER	ARG	MET	ASP	THR	ASP	LEU	GLU	GLU	GLY	GLU	ALA	LEU	A404	P405	R406	Q407	V408	L409	D410	L411	E412	D413	L414	V415	F416	T417	Q418	G419	S420																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
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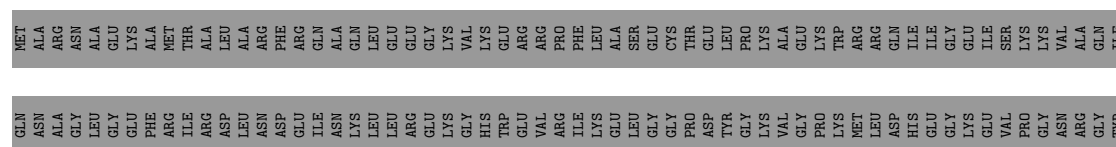
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H1862	I1802	T1742	Y1682	E1622	F1562	H1502	R1442	M1382	Q1322	L1262	L1202	K1142
E1863	S1803	K1743	D1683	G1623	V1563	W1503	K1443	E1383	D1323	P1263	L1203	I1143
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V1875	L1815	L1755	L1695	L1635	D1575	H1515	E1455	K1395	V1335	W1275	H1215	D1155
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R1901	K1841	L1781	P1721	V1661	L1601	S1541	I1481	K1421	E1361	L1301	L1241	F1181
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S1917	N1857	E1797	M1737	V1677	V1617	K1557	N1497	R1437	V1377	F1317	V1257	T1197
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A1919	P1859	S1799	E1739	Y1679	Y1619	V1559	D1499	W1439	I1379	F1259	K1199	K1999
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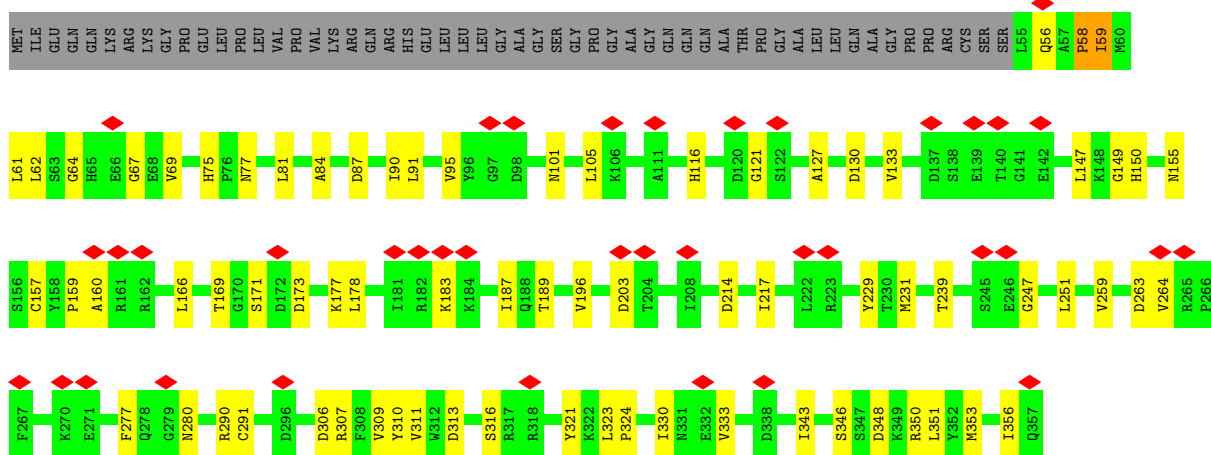
- Molecule 14: 116 kDa U5 small nuclear ribonucleoprotein component



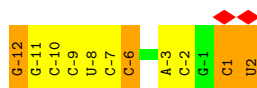
- Molecule 15: Pre-mRNA-splicing factor ISY1 homolog



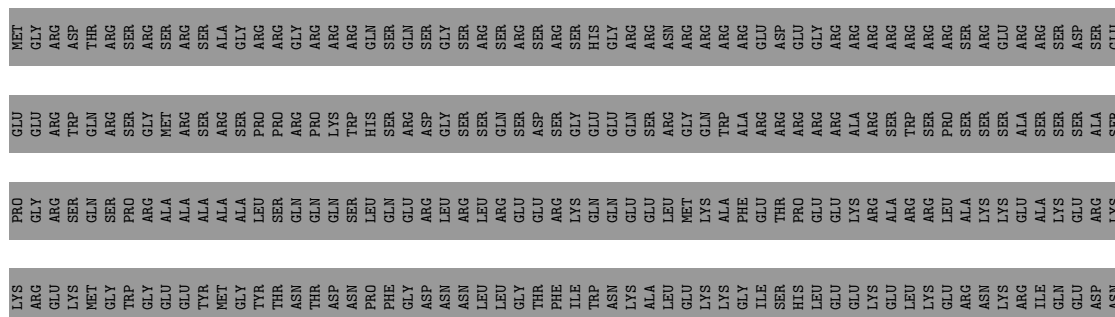
- Molecule 16: U5 small nuclear ribonucleoprotein 40 kDa protein

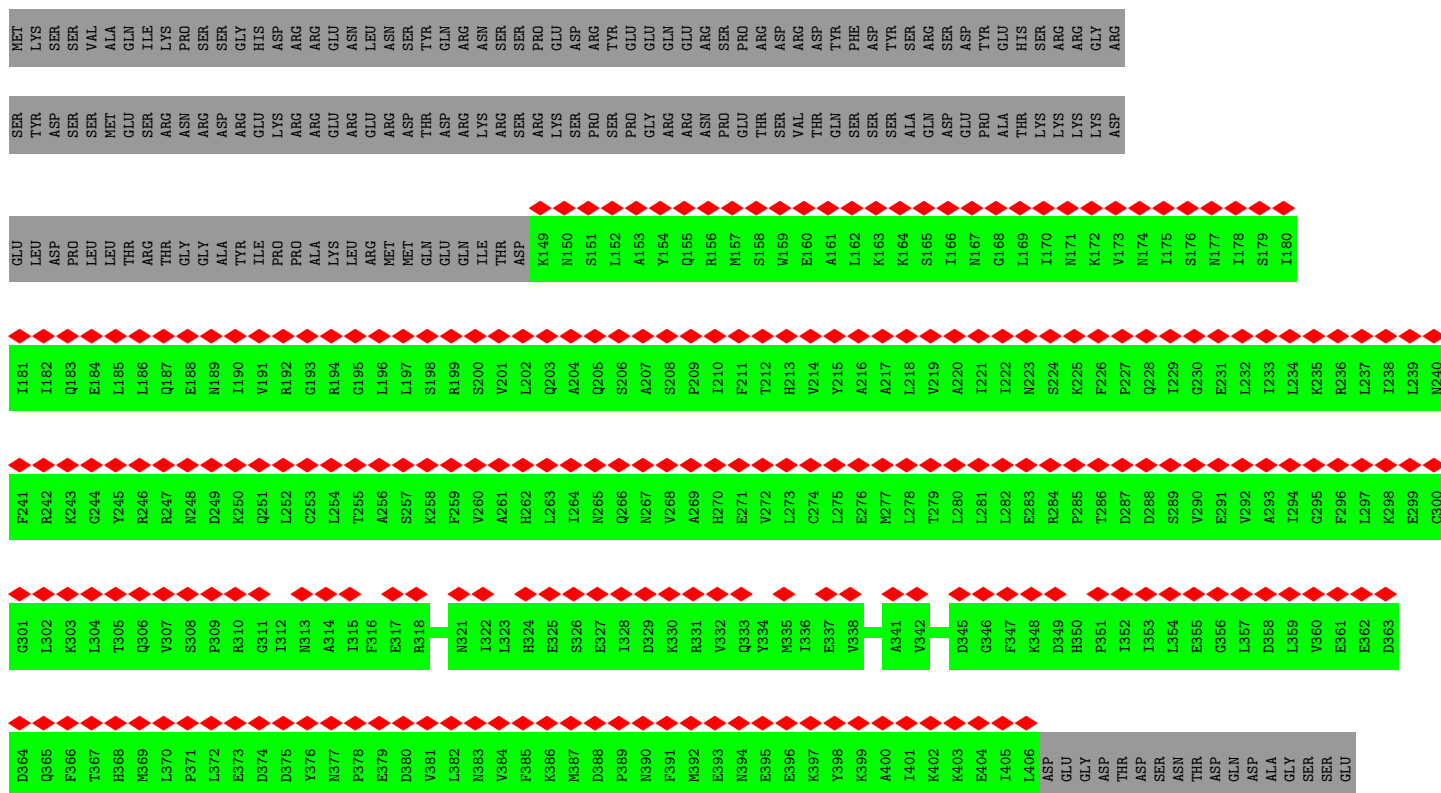


- Molecule 17: Exon

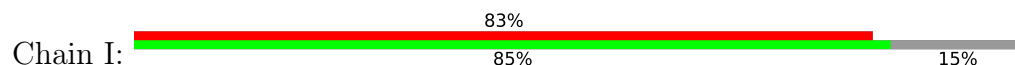


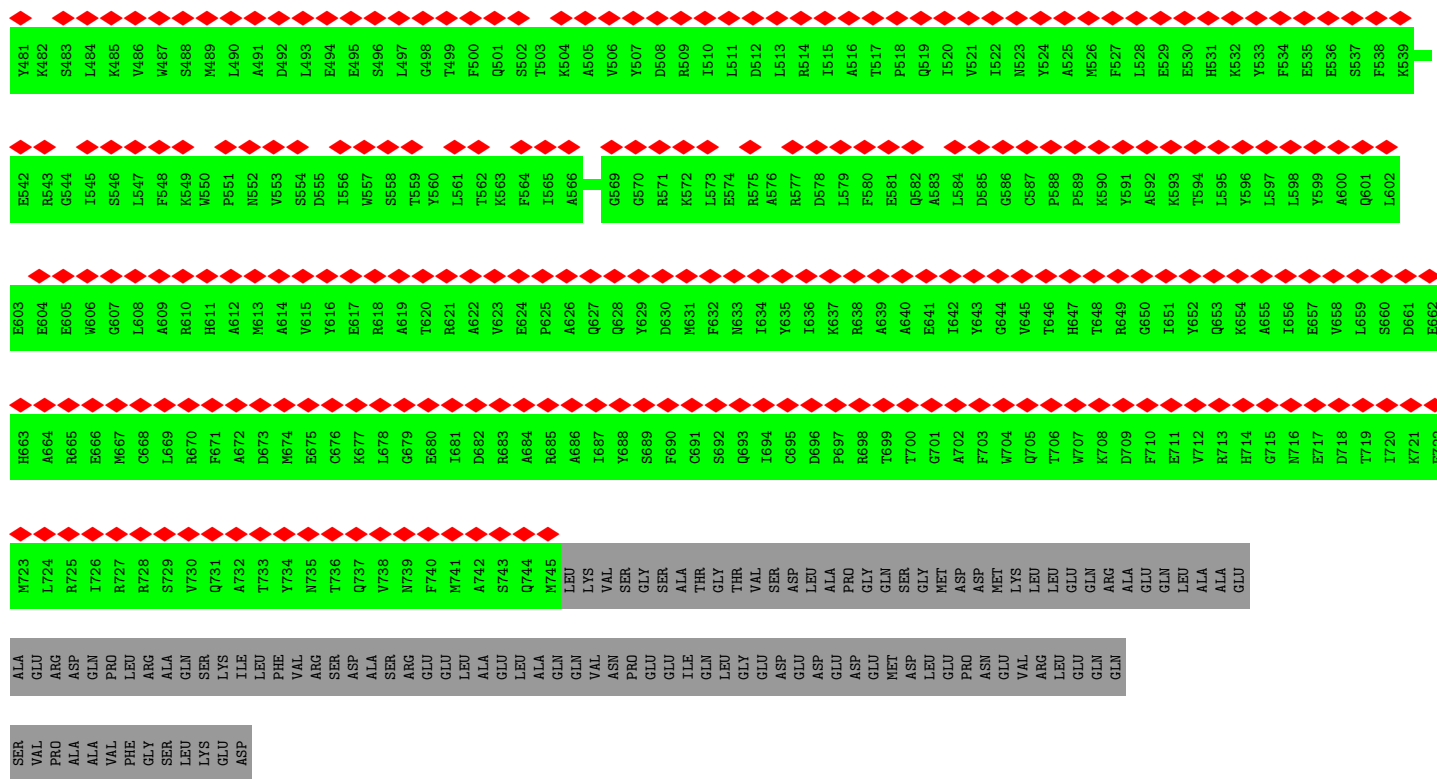
- Molecule 18: Splicing factor Cactin



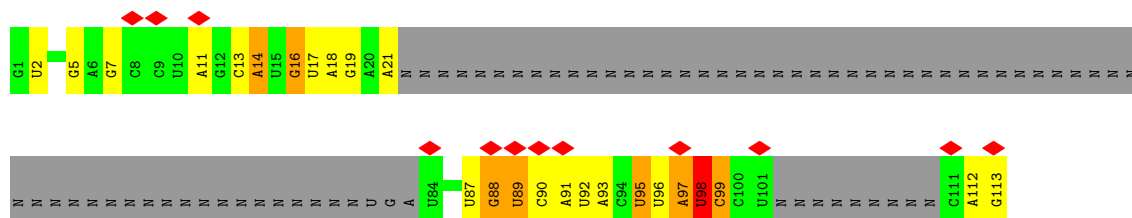


- Molecule 20: Pre-mRNA-splicing factor SYF1

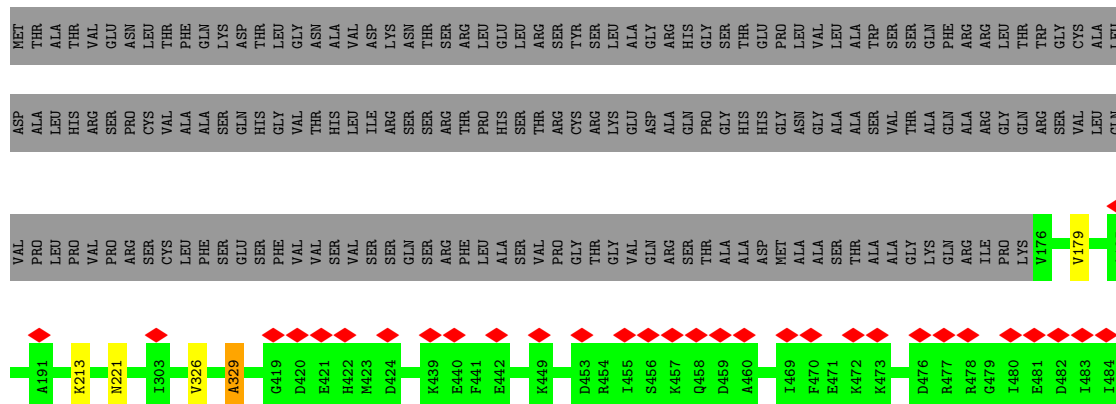
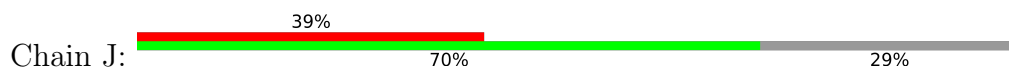


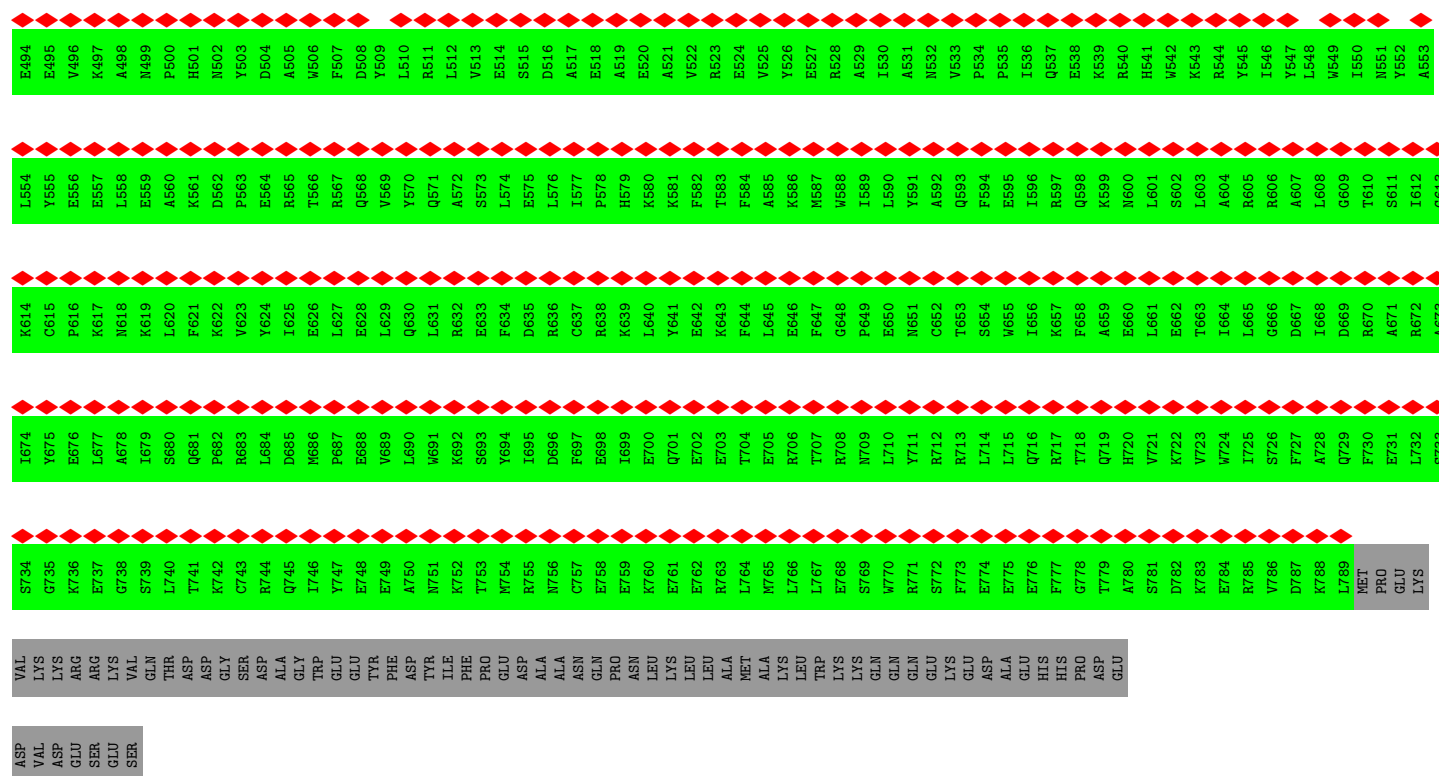


• Molecule 21: INTRON

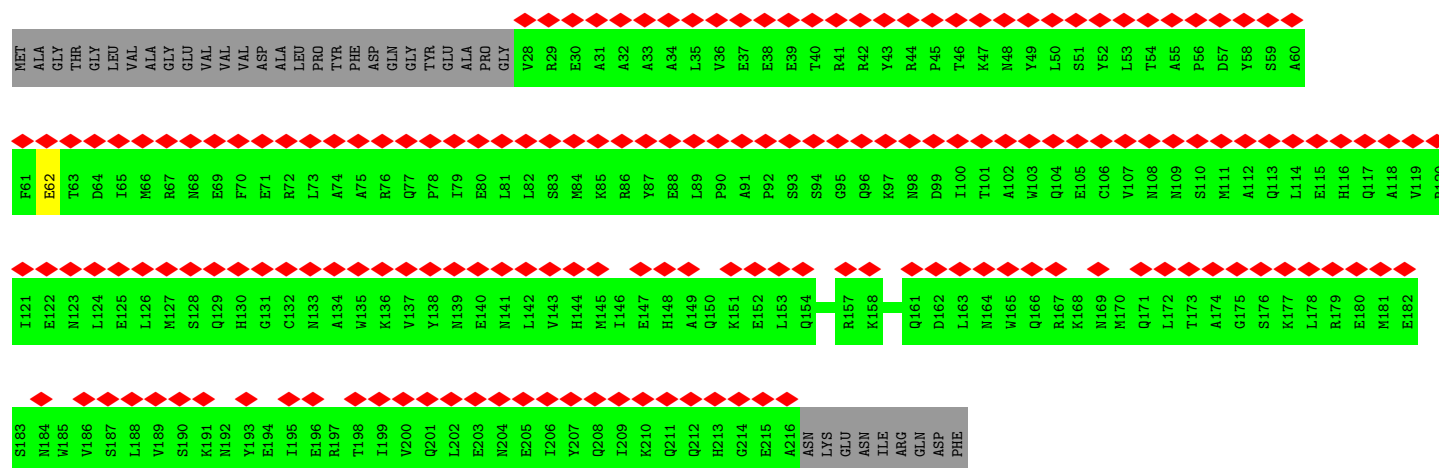
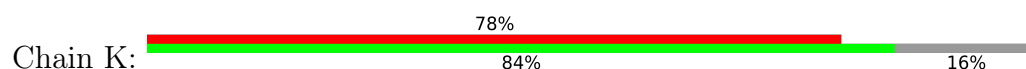


• Molecule 22: Crooked neck-like protein 1

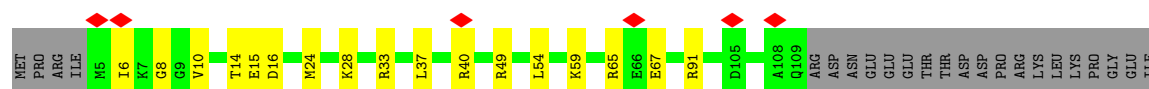




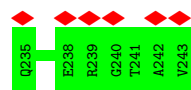
• Molecule 23: Pre-mRNA-splicing factor SPF27



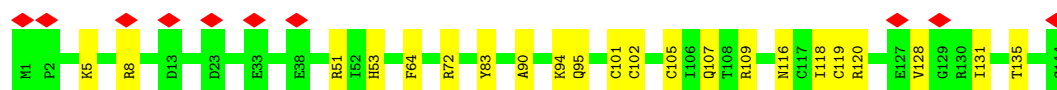
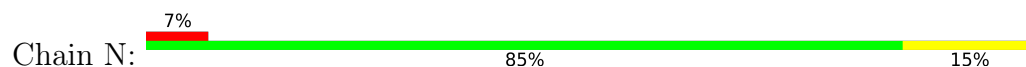
• Molecule 24: Cell division cycle 5-like protein



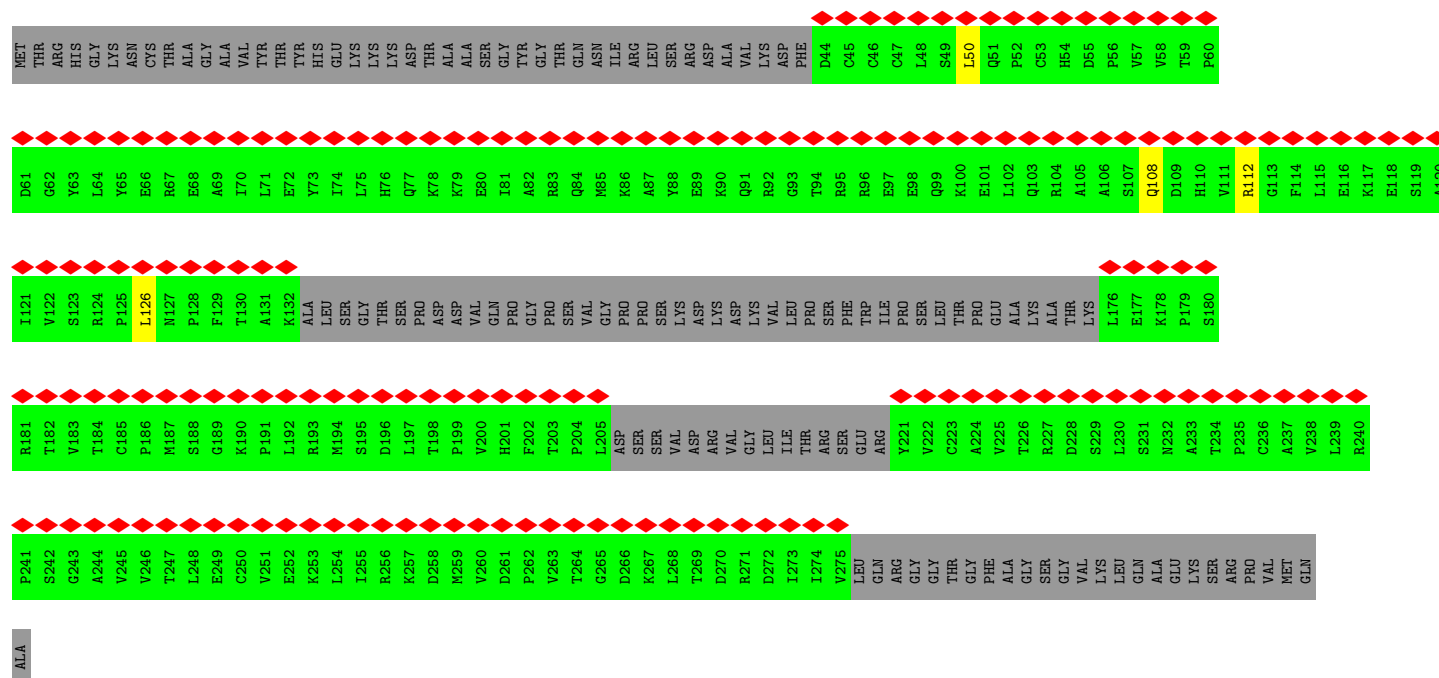




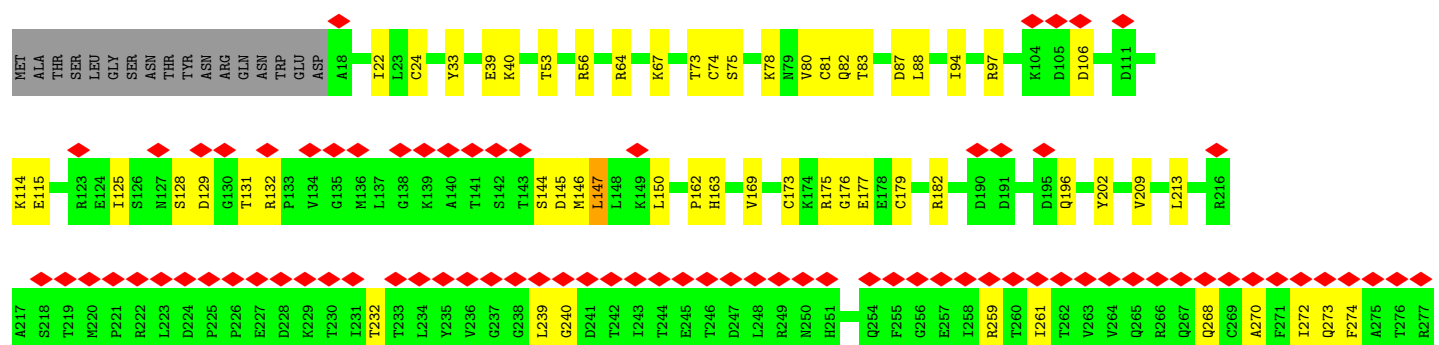
- Molecule 26: Protein BUD31 homolog

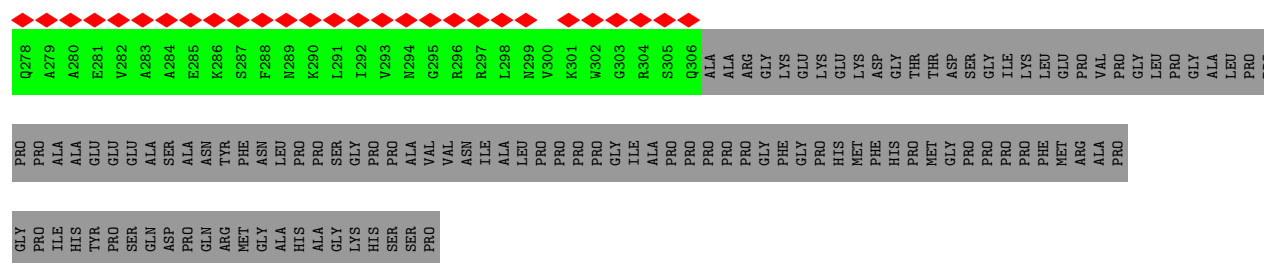


- Molecule 27: Nitric oxide synthase-interacting protein

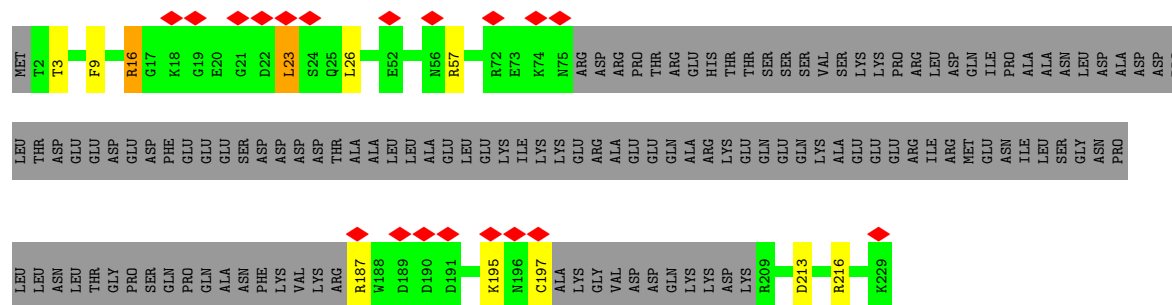
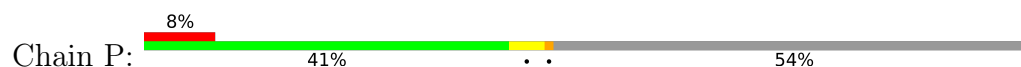


- Molecule 28: Pre-mRNA-splicing factor RBM22

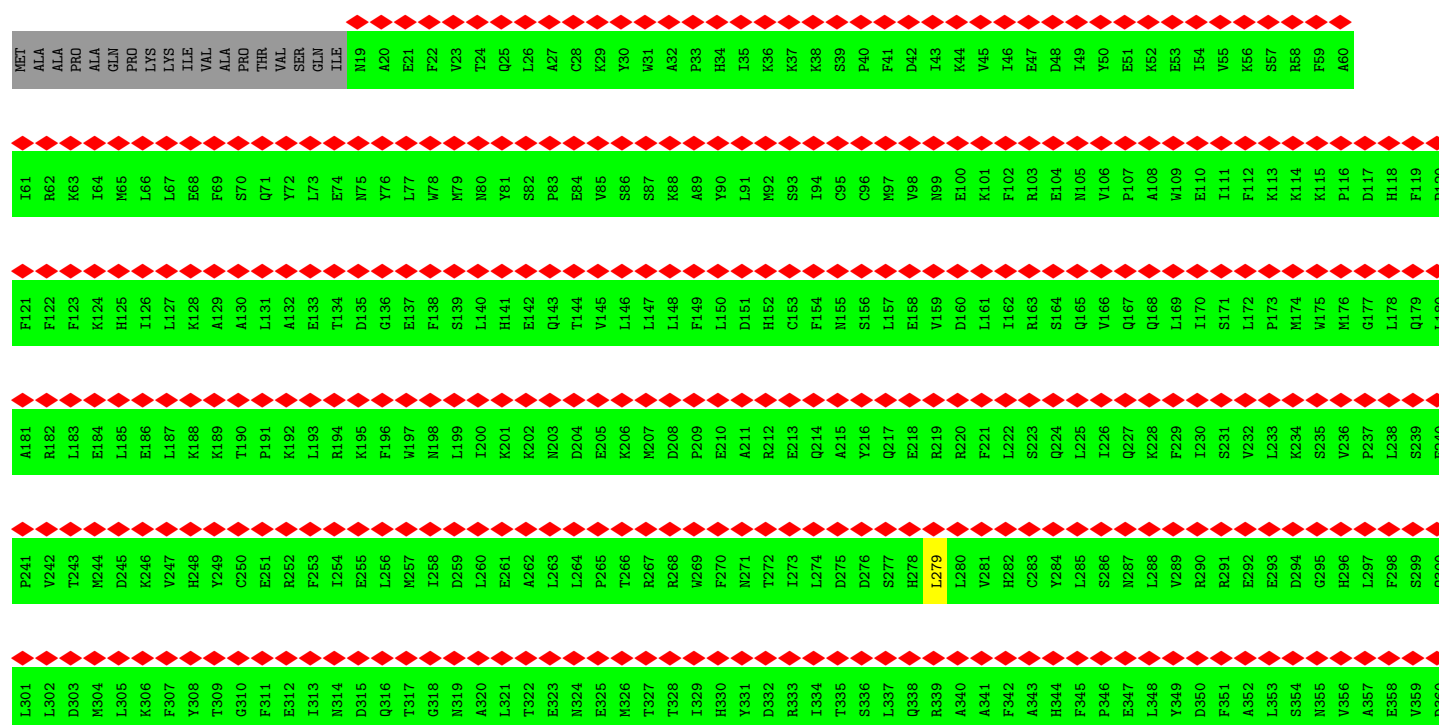
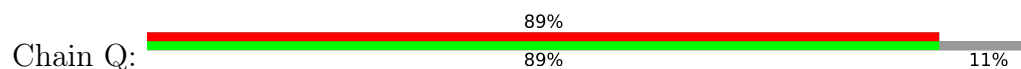




• Molecule 29: Spliceosome-associated protein CWC15 homolog



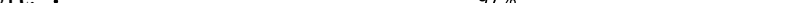
• Molecule 30: Intron-binding protein aquarius

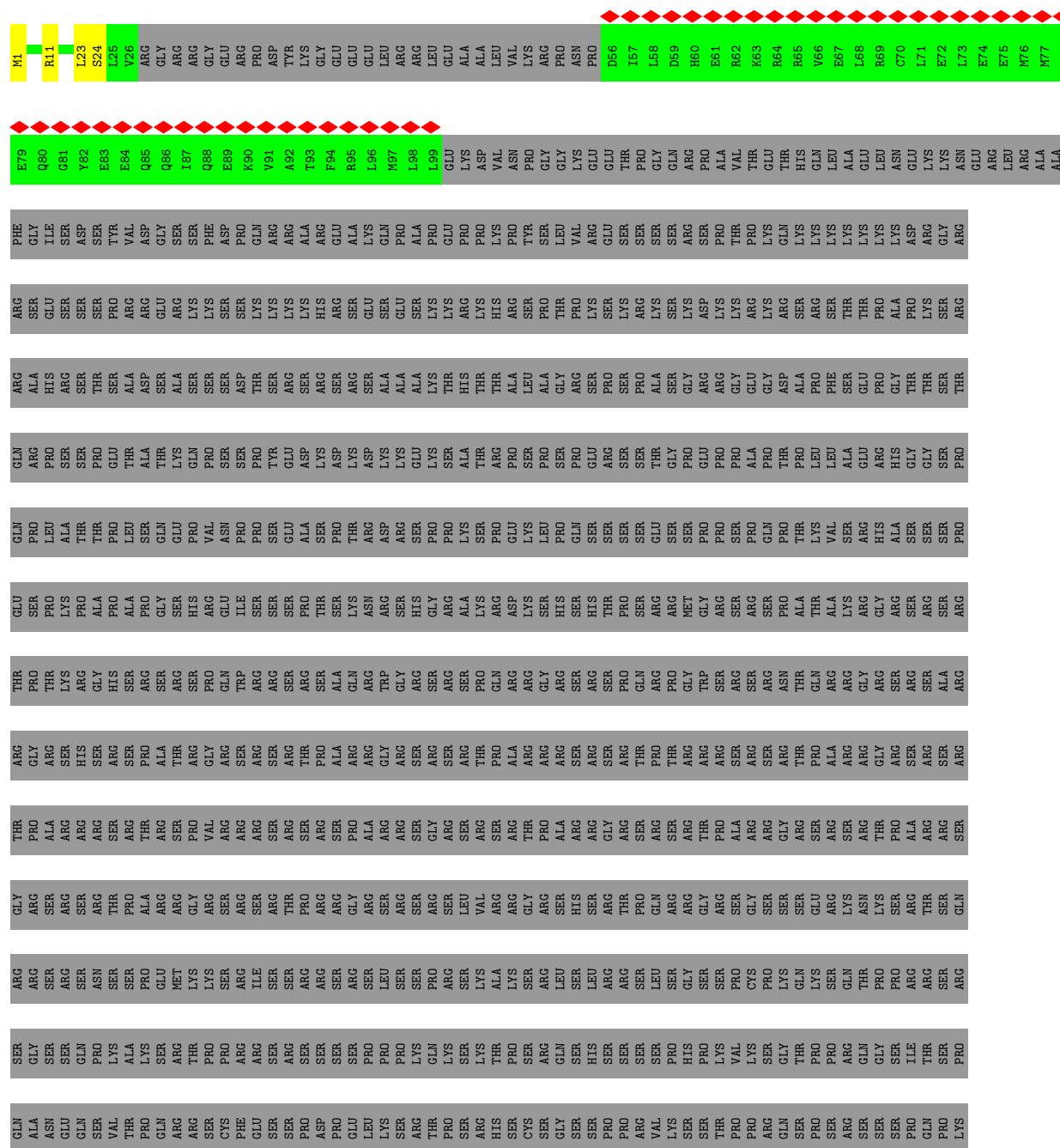


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G1084	S1024	R1023	R1023	E963	N843	V783	H723	E663	D603	L542	Q483	Q423	E363
F1085	S1024	R1023	S1024	V964	F844	I784	L724	N664	K604	N544	D484	M424	S364
S1086	Y1026	R905	R905	S965	P845	P785	K725	N665	G605	V545	I485	P425	L365
R1087	Y1027	R906	R906	T966	E846	N786	A726	P666	G606	R546	E486	L426	V366
L1088	L1027	R907	R907	T967	Q847	R787	S727	K667	V607	D547	D487	Y427	K367
R1089	L1028	R908	R908	F968	R848	G788	F728	A668	I608	H548	S488	P428	F368
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I1092	E1031	E911	E911	H971	L851	P791	H731	E671	PRO	D551	R491	K431	P371
M1093	A1032	V912	V912	E972	V852	Y792	N732	T672	GLU	E552	M492	I432	L372
I1094	K1033	R913	R913	Y973	T853	N793	K733	I673	P614	W553	K493	I433	S373
G1095	R914	R914	R914	F974	H854	Q794	V734	R674	R615	E554	P494	W434	S374
D1096	L915	L915	L915	A975	S855	P795	V735	N675	P616	G555	W495	D435	N375
H1097	Q916	Q916	Q916	N976	N856	K796	T736	L476	N617	L556	Q496	E436	T376
H1098	R917	R917	R917	Q857	Q857	R797	V737	M677	L618	R557	N437	N437	L377
Q1099	S918	S918	S918	A858	A858	N798	E738	N678	R619	K558	I438	I438	H378
L1100	L919	L919	L919	L859	L859	T799	D739	T679	G620	H559	V439	V439	Q379
P1101	G920	G920	G920	N860	N860	I800	P740	D680	E621	D560	P440	P440	V380
P1102	V921	V921	V921	Q861	Q861	Q801	A741	C681	S622	V561	T441	T441	A381
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Q1110	C929	C929	C929	L869	L869	A909	I750	D689	D630	R509	C449	C449	T389
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A1114	G933	G933	G933	R874	R874	M814	ARG	G693	Y634	P513	P453	P453	N393
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E1116	F936	F936	F936	L876	L876	P816	LYS	D696	D637	V515	L455	L455	D395
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V1126	Q1066	Q1066	Q1066	E887	E887	G526	THR	P706	E647	N526	L466	L466	E405
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V1128	L1008	L1008	L1008	E889	E889	K628	E773	Q708	V649	G528	L467	L467	L407
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G1137	THR	THR	THR	R897	R897	I837		T717	R658	A537	E476	E476	S416
R1138	LEU	LEU	LEU	V898	V898	S838		T718	R658	D538	T477	T477	I418
A1139	P959	P959	P959	N899	N899	N639		L719	K660	V539	Y479	Y479	Q419
R1140	D960	D960	D960	T840	T840			S720		M600			Q420



- Molecule 33: Serine/arginine repetitive matrix protein 2

Chain SR: 





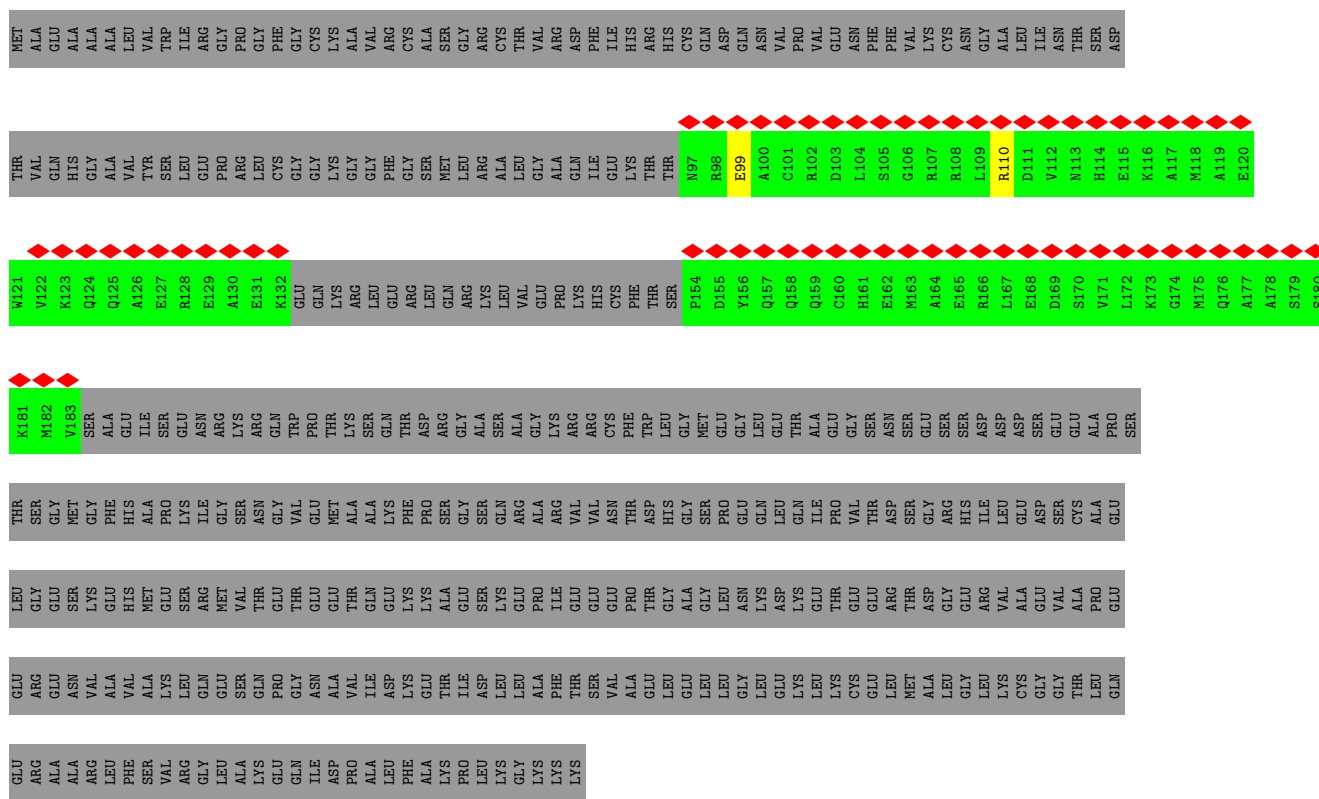


- Molecule 37: Pre-mRNA-processing factor 17

Chain W:

- Molecule 38: Splicing regulator SDE2

Chain X:

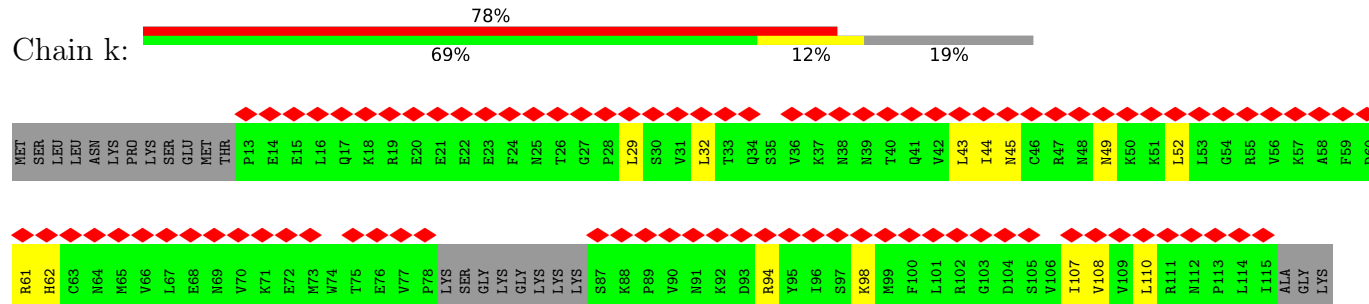


Chain Z: 32% 31% 68%

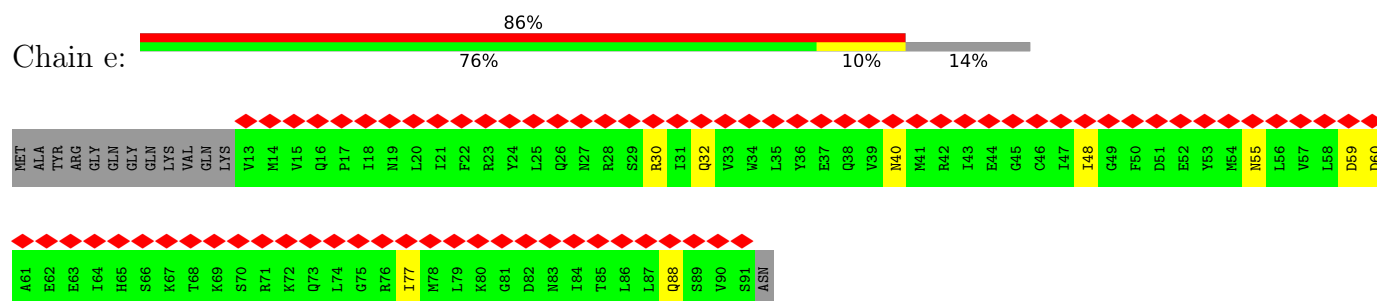


R61	H62	C63	M64	M65	V66	L67	E68	N69	V70	K71	T72	M73	W74	T75	E76	V77	P78	LYS	SER	GLY	LYS	GLY	LYS	LYS	LYS	S87	K88	P89	V90	N91	K92	D93	R94	Y95	I96	S97	K98	M99	F100	L101	R102	G103	D104	S105	V106	I107	V108	V109	L110	R111	N112	P113	L114	I115	ALA	GLY	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----

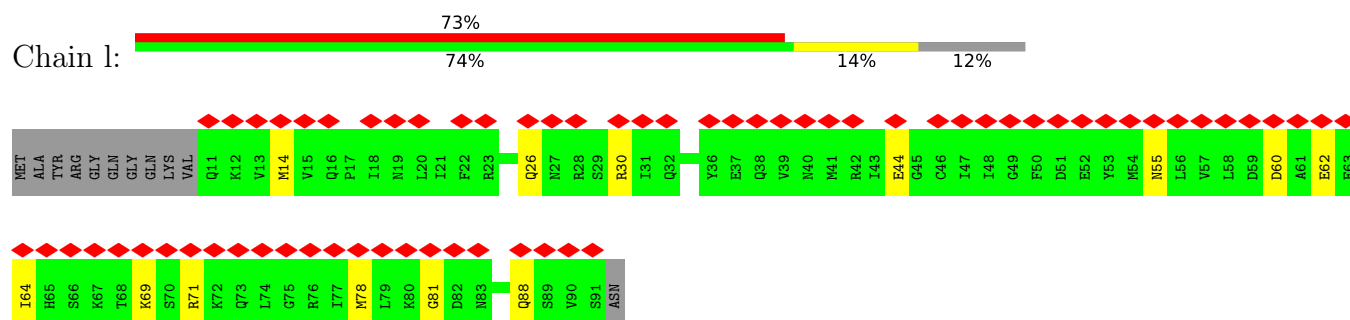
- Molecule 43: Small nuclear ribonucleoprotein Sm D2



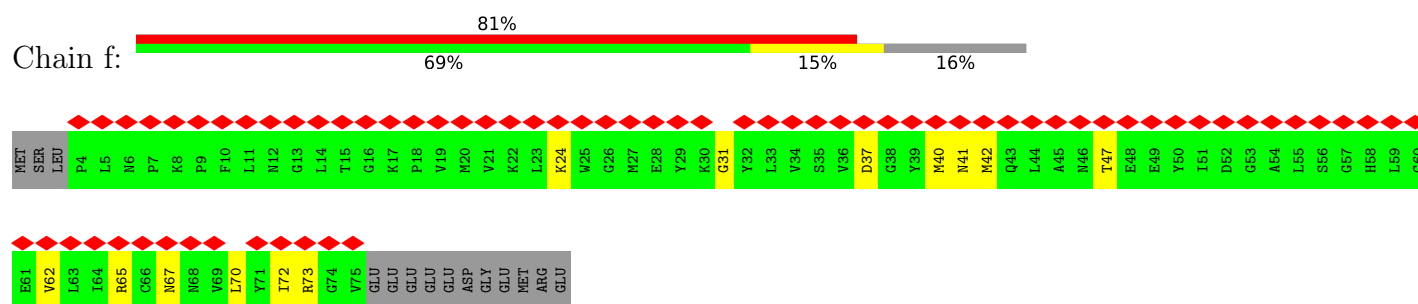
- Molecule 44: Small nuclear ribonucleoprotein E



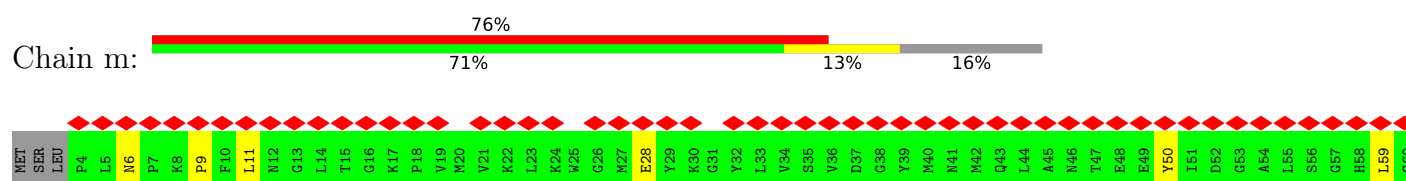
- Molecule 44: Small nuclear ribonucleoprotein E



- Molecule 45: Small nuclear ribonucleoprotein F

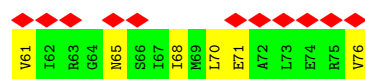
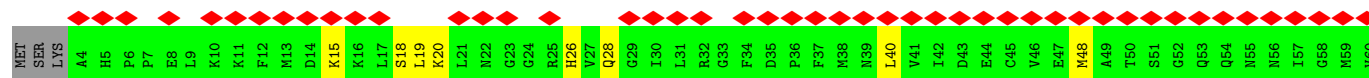
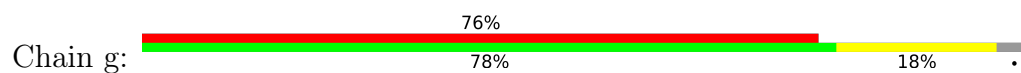


- Molecule 45: Small nuclear ribonucleoprotein F

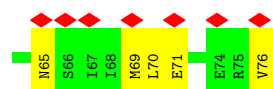
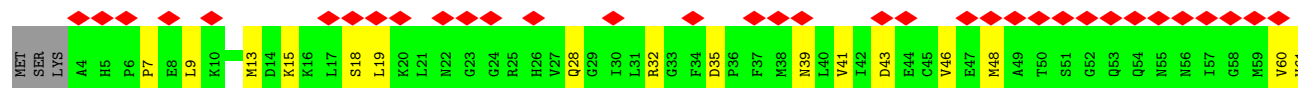




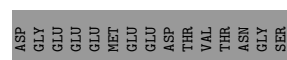
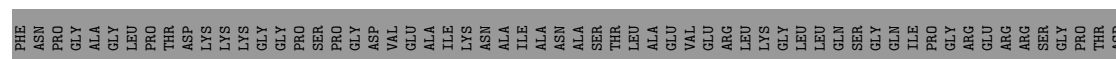
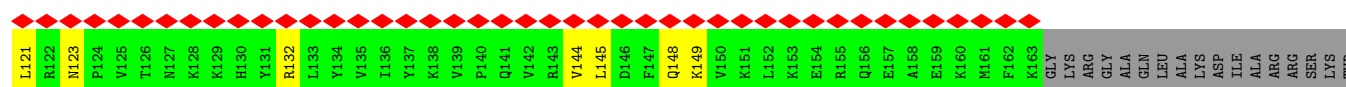
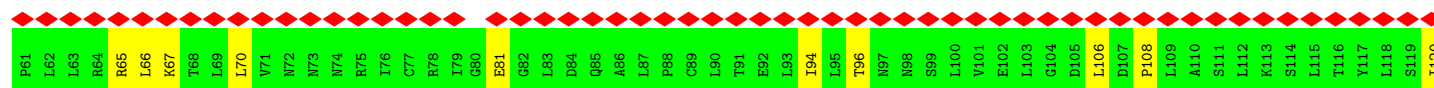
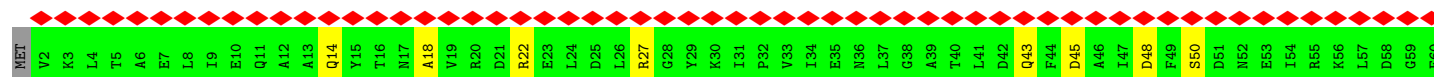
- Molecule 46: Small nuclear ribonucleoprotein G



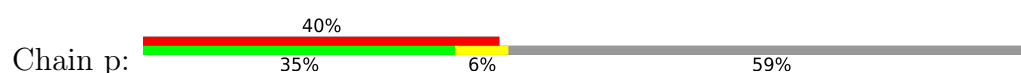
- Molecule 46: Small nuclear ribonucleoprotein G



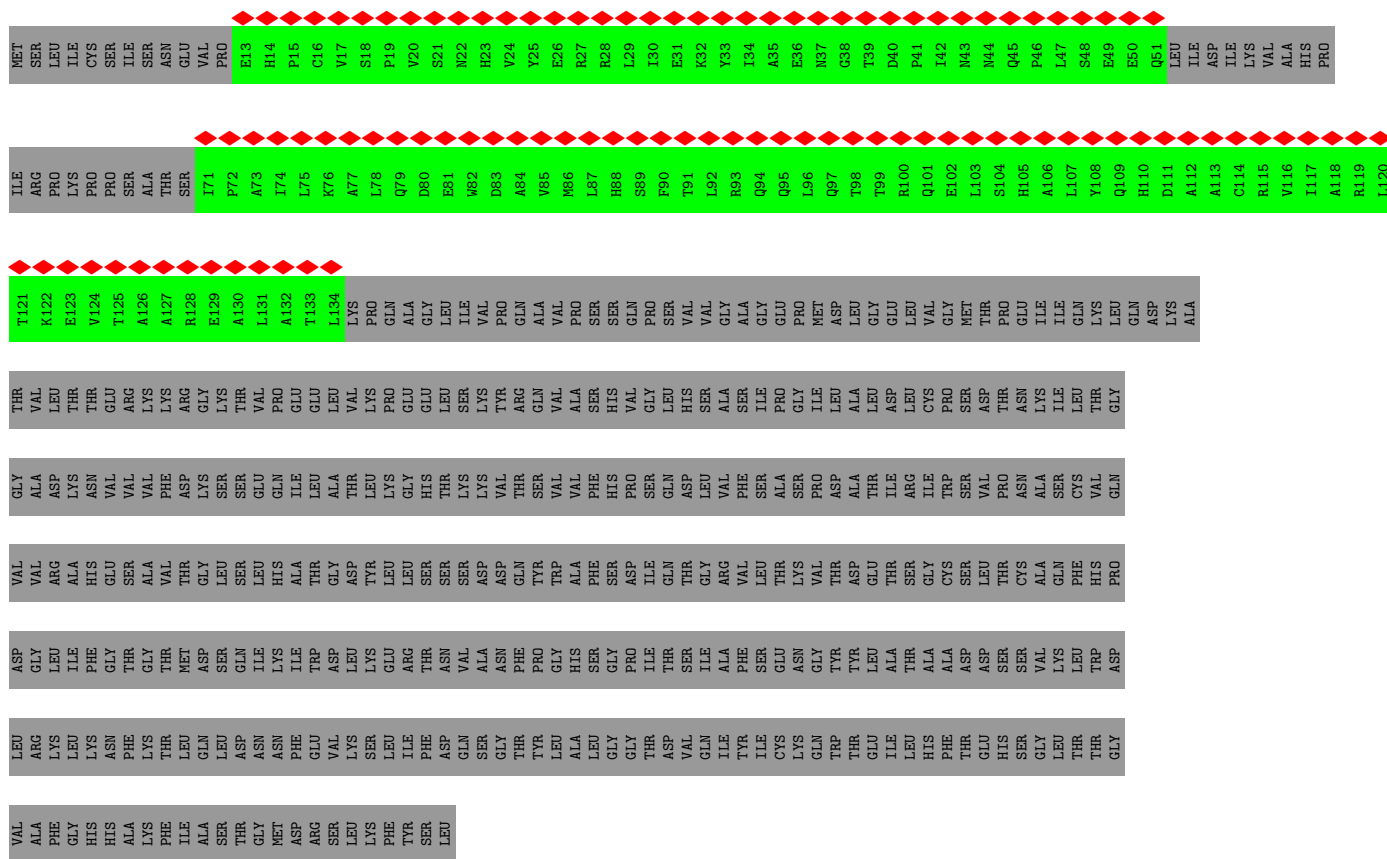
- Molecule 47: U2 small nuclear ribonucleoprotein A'



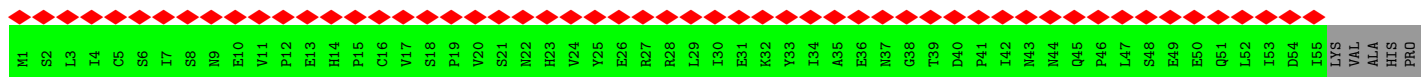
- Molecule 48: U2 small nuclear ribonucleoprotein B''



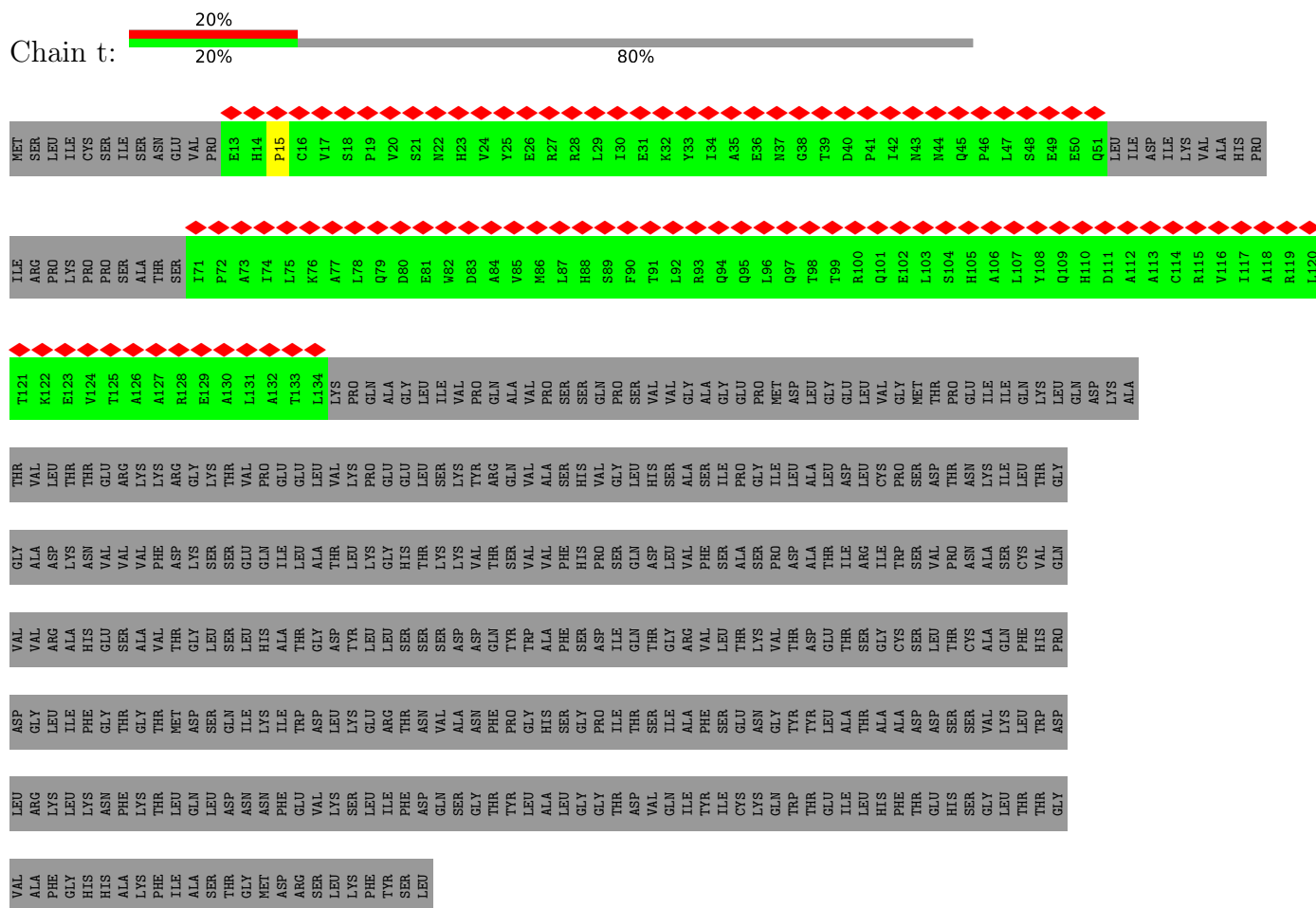
- Molecule 49: Pre-mRNA-processing factor 19



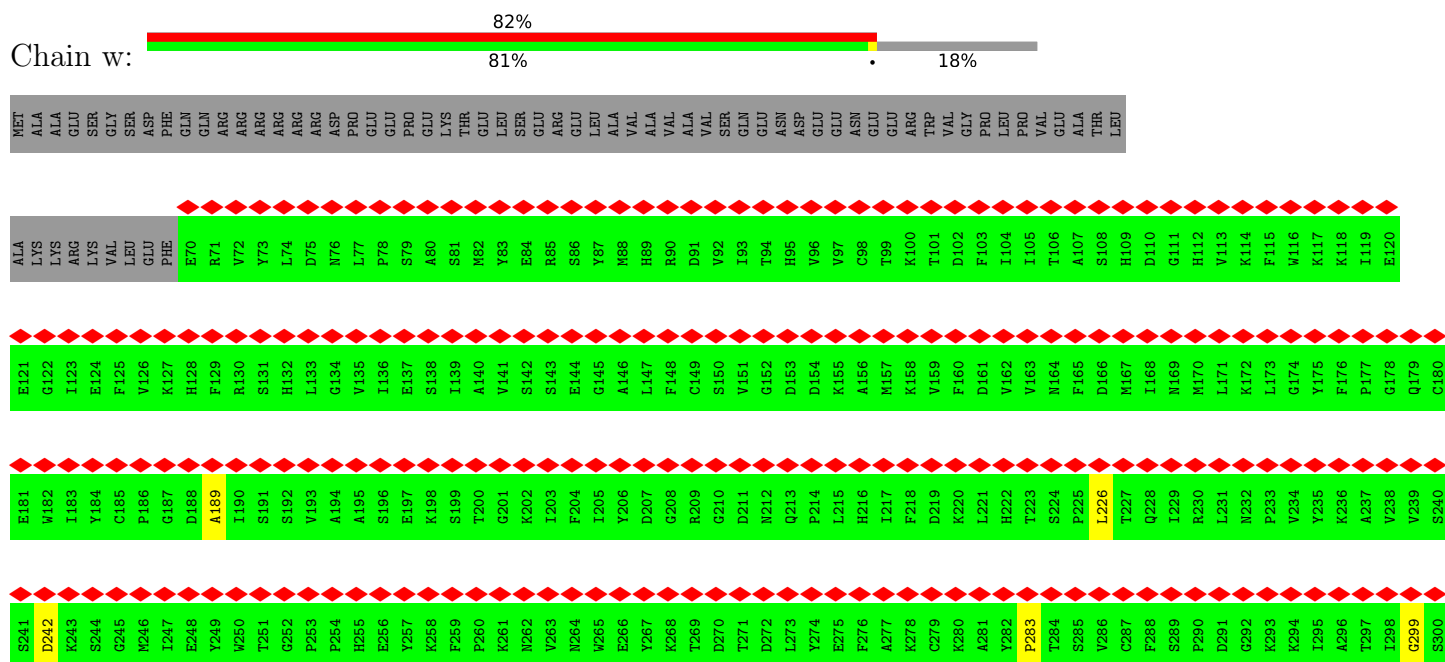
- Molecule 49: Pre-mRNA-processing factor 19



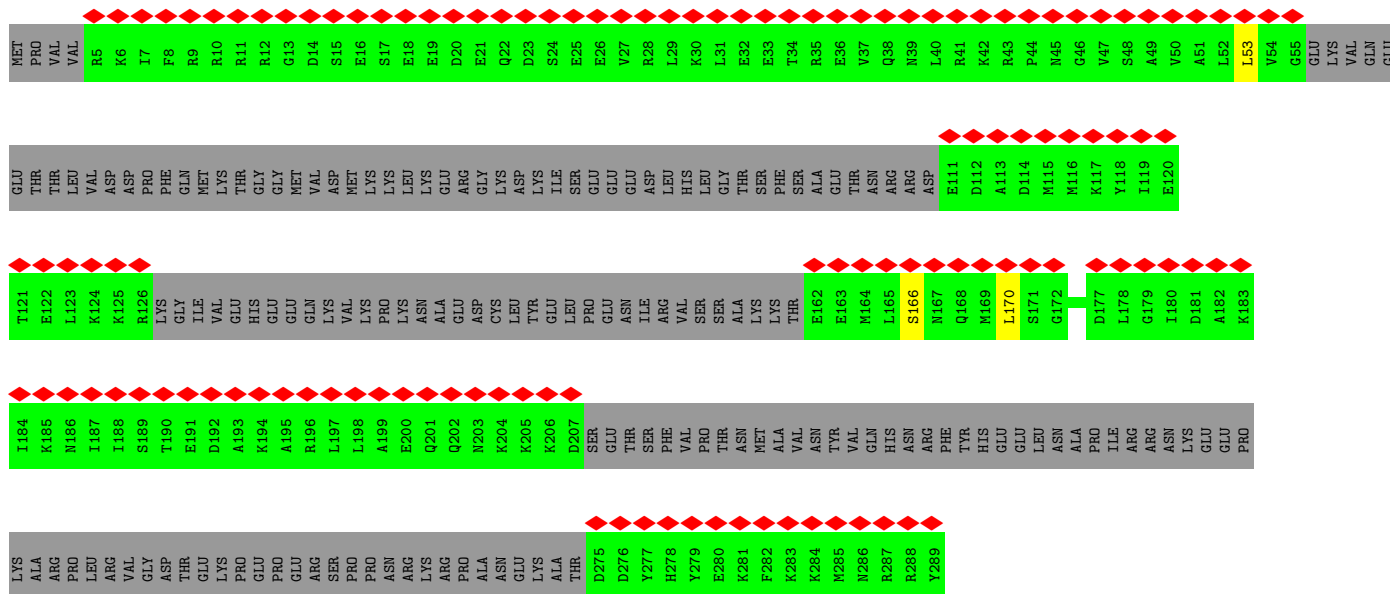
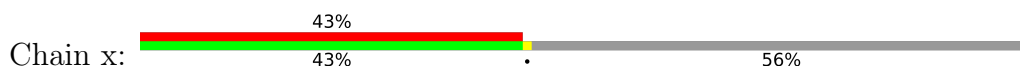
• Molecule 49: Pre-mRNA-processing factor 19



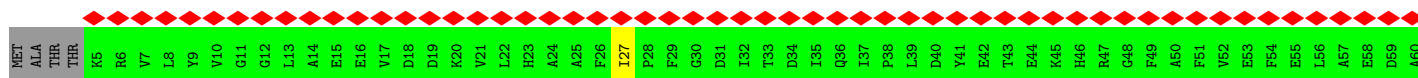
• Molecule 50: Peptidylprolyl isomerase domain and WD repeat-containing protein 1

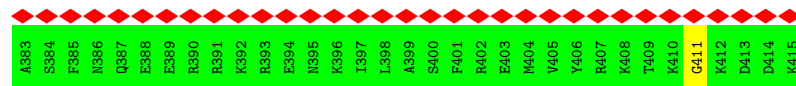


- Molecule 51: Splicing factor C9orf78



- Molecule 52: Peptidyl-prolyl cis-trans isomerase E





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103860	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.177	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	492.00003, 492.00003, 492.00003	wwPDB
Map dimensions	410, 410, 410	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, MG, GTP, K, ATP, ZN, SEP

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	1	0.33	0/1030	0.67	0/1371
2	2	0.38	0/2827	0.60	2/4393 (0.0%)
3	3	0.32	0/406	0.83	0/564
4	32	0.34	0/513	0.66	0/683
5	5	0.54	0/2157	0.79	6/3351 (0.2%)
6	50	0.63	0/1122	1.40	4/1562 (0.3%)
7	56	0.26	0/497	0.65	0/690
8	6	0.54	0/2323	0.66	1/3619 (0.0%)
9	7	0.35	0/1927	1.00	0/2681
10	8	0.34	0/444	0.91	0/614
11	9	0.38	0/711	0.94	0/987
12	A	0.58	0/18250	0.71	3/24798 (0.0%)
13	B	0.36	0/15311	0.92	13/20733 (0.1%)
14	C	0.53	0/7228	0.91	2/9822 (0.0%)
15	D	0.38	0/356	0.87	0/494
16	E	0.59	1/2424 (0.0%)	0.78	7/3285 (0.2%)
17	EX	0.91	0/329	1.68	8/510 (1.6%)
18	F	0.38	0/1134	0.65	0/1530
19	H	0.41	0/2965	0.83	1/4049 (0.0%)
20	I	0.37	0/3609	0.99	0/5036
21	IN	0.39	0/996	0.81	4/1544 (0.3%)
22	J	0.42	0/2997	1.03	0/4187
23	K	0.38	0/940	0.97	0/1312
24	L	0.42	0/3674	0.78	0/4988
25	M	0.34	0/1114	0.81	0/1553
26	N	0.49	0/1215	0.72	0/1627
27	NO	0.37	0/861	0.88	0/1197
28	O	0.43	0/2375	0.59	0/3204
29	P	0.41	0/903	0.64	0/1201
30	Q	0.36	0/6545	0.88	0/9115
31	R	0.43	0/2647	0.72	0/3554
32	S	0.31	0/1305	0.56	0/1767

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	SR	0.48	0/414	0.73	0/568
34	T	0.66	0/2957	0.79	0/4023
35	U	0.43	0/2483	0.72	0/3341
36	V	0.34	0/3626	0.87	0/5050
37	W	0.47	0/4266	0.70	0/5761
38	X	0.29	0/326	0.87	0/452
39	Z	0.32	0/263	0.93	0/365
40	a	0.32	0/666	0.66	0/897
40	h	0.33	0/660	0.70	0/889
41	b	0.24	0/663	0.54	0/885
41	i	0.25	0/674	0.57	0/899
42	c	0.21	0/642	0.50	0/867
42	j	0.22	0/642	0.51	0/867
43	d	0.21	0/732	0.56	0/984
43	k	0.24	0/784	0.58	0/1053
44	e	0.24	0/659	0.63	0/885
44	l	0.26	0/677	0.63	0/908
45	f	0.32	0/574	0.71	0/775
45	m	0.29	0/574	0.65	0/775
46	g	0.29	0/575	0.63	0/768
46	n	0.27	0/575	0.60	0/768
47	o	0.25	0/1299	0.65	0/1761
48	p	0.22	0/759	0.50	0/1016
49	q	0.38	0/512	0.85	0/713
49	r	0.43	0/592	0.87	0/825
49	s	0.42	0/658	0.98	1/919 (0.1%)
49	t	0.40	0/512	0.96	0/713
50	w	0.33	0/2602	0.83	0/3615
51	x	0.33	0/632	0.90	0/874
52	y	0.25	0/317	0.77	1/396 (0.3%)
53	z	0.34	0/431	0.67	0/582
All	All	0.44	1/122881 (0.0%)	0.81	53/169215 (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
12	A	0	2
13	B	0	20
14	C	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	E	0	1
29	P	0	1
31	R	0	2
All	All	0	29

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	E	58	PRO	C-N	22.51	1.54	1.33

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	E	58	PRO	CA-C-N	13.57	138.10	122.36
16	E	58	PRO	C-N-CA	13.57	138.10	122.36
16	E	58	PRO	O-C-N	-13.42	104.26	122.24
6	50	196	SER	CA-C-N	13.16	139.56	120.87
6	50	196	SER	C-N-CA	13.16	139.56	120.87
16	E	59	ILE	N-CA-C	8.27	121.14	113.20
6	50	196	SER	O-C-N	-7.84	110.79	122.39
13	B	2124	VAL	CA-C-N	7.62	135.42	121.70
13	B	2124	VAL	C-N-CA	7.62	135.42	121.70
21	IN	98	U	O4'-C1'-N1	7.54	119.82	108.50
13	B	697	ALA	CA-C-N	7.54	132.99	120.62
13	B	697	ALA	C-N-CA	7.54	132.99	120.62
17	EX	-2	C	O4'-C1'-N1	7.49	119.73	108.50
21	IN	97	A	N9-C1'-C2'	-7.20	103.20	114.00
5	5	24	G	O4'-C1'-N9	-6.85	97.93	108.20
16	E	59	ILE	N-CA-CB	-6.66	102.48	112.67
16	E	59	ILE	CA-CB-CG2	6.43	121.44	110.50
5	5	51	A	N9-C1'-C2'	6.34	121.52	112.00
5	5	46	U	N1-C1'-C2'	6.29	121.44	112.00
49	s	65	PRO	N-CA-C	6.25	118.33	110.70
5	5	52	U	N1-C1'-C2'	6.21	121.32	112.00
17	EX	-10	C	O4'-C1'-C2'	5.99	111.79	105.80
12	A	598	LEU	CB-CG-CD1	-5.93	92.90	110.70
52	y	27	ILE	N-CA-C	5.92	121.68	108.88
13	B	1583	ASP	CA-C-N	5.90	132.59	121.97
13	B	1583	ASP	C-N-CA	5.90	132.59	121.97
5	5	37	G	N9-C1'-C2'	5.89	120.83	112.00
13	B	606	THR	CA-C-N	5.78	132.57	121.54
13	B	606	THR	C-N-CA	5.78	132.57	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	EX	-8	U	O4'-C1'-N1	5.75	117.13	108.50
17	EX	1	C	N1-C1'-C2'	5.70	120.55	112.00
12	A	331	TRP	CA-CB-CG	5.64	124.32	113.60
17	EX	-6	C	C4'-C3'-O3'	-5.62	100.96	109.40
17	EX	-12	G	C2'-C3'-O3'	5.62	122.13	113.70
21	IN	95	U	P-O3'-C3'	5.59	128.59	120.20
12	A	1417	PRO	N-CA-C	-5.58	100.97	112.47
17	EX	2	U	OP1-P-OP2	-5.51	103.06	119.60
2	2	102	U	P-O3'-C3'	5.48	128.42	120.20
2	2	105	G	P-O3'-C3'	5.39	128.29	120.20
13	B	1679	TYR	CA-CB-CG	5.31	123.45	113.90
14	C	733	TRP	CA-CB-CG	5.29	123.64	113.60
13	B	2098	ALA	CB-CA-C	-5.28	109.50	115.79
8	6	50	A	C2'-C3'-O3'	5.28	121.61	113.70
14	C	177	ARG	CA-CB-CG	5.24	124.58	114.10
13	B	1007	PRO	N-CA-C	5.20	121.35	113.81
19	H	575	THR	CA-CB-CG2	5.16	119.27	110.50
16	E	56	GLN	OE1-CD-NE2	-5.13	117.47	122.60
5	5	92	U	P-O3'-C3'	5.12	127.88	120.20
17	EX	-6	C	OP1-P-O3'	5.09	123.28	108.00
21	IN	95	U	C2'-C3'-O3'	5.08	117.13	109.50
6	50	288	VAL	N-CA-C	5.04	111.60	106.21
13	B	1053	GLU	CA-C-N	5.03	129.35	122.06
13	B	1053	GLU	C-N-CA	5.03	129.35	122.06

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	A	1418	ARG	Sidechain
12	A	941	LYS	Peptide
13	B	1030	ARG	Sidechain
13	B	1043	ARG	Sidechain
13	B	1274	ARG	Sidechain
13	B	129	ARG	Sidechain
13	B	1313	ARG	Sidechain
13	B	1375	ARG	Sidechain
13	B	1400	ARG	Sidechain
13	B	1438	ARG	Sidechain
13	B	1442	ARG	Sidechain
13	B	1566	ARG	Sidechain
13	B	1843	ARG	Sidechain

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Mol	Chain	Res	Type	Group
13	B	1901	ARG	Sidechain
13	B	2009	ARG	Sidechain
13	B	2013	ARG	Sidechain
13	B	2043	ARG	Sidechain
13	B	728	ARG	Sidechain
13	B	739	ARG	Sidechain
13	B	794	ARG	Sidechain
13	B	858	ARG	Sidechain
13	B	953	ARG	Sidechain
14	C	318	PHE	Peptide
14	C	342	ARG	Sidechain
14	C	813	ARG	Sidechain
16	E	307	ARG	Sidechain
29	P	16	ARG	Sidechain
31	R	332	ARG	Sidechain
31	R	9	ALA	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	1	1013	0	1058	10	0
2	2	2535	0	1281	29	0
3	3	408	0	181	0	0
4	32	504	0	509	11	0
5	5	1936	0	982	29	0
6	50	1124	0	485	31	0
7	56	498	0	220	0	0
8	6	2075	0	1048	29	0
9	7	1928	0	856	0	0
10	8	445	0	203	0	0
11	9	712	0	299	0	0
12	A	17802	0	17006	245	0
13	B	15004	0	15162	114	0
14	C	7069	0	7089	33	0
15	D	358	0	167	0	0
16	E	2370	0	2306	49	0
17	EX	296	0	153	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	F	1089	0	1023	25	0
19	H	2932	0	2204	17	0
20	I	3610	0	1639	0	0
21	IN	893	0	453	13	0
22	J	2998	0	1333	3	0
23	K	941	0	424	0	0
24	L	3642	0	2904	31	0
25	M	1115	0	513	0	0
26	N	1189	0	1192	17	0
27	NO	864	0	371	1	0
28	O	2327	0	2315	44	0
29	P	889	0	865	8	0
30	Q	6554	0	2828	1	0
31	R	2618	0	2664	36	0
32	S	1271	0	1244	17	0
33	SR	412	0	287	7	0
34	T	2881	0	2836	41	0
35	U	2425	0	2370	40	0
36	V	3629	0	1603	0	0
37	W	4158	0	4060	87	0
38	X	328	0	156	1	0
39	Z	265	0	114	1	0
40	a	658	0	675	17	0
40	h	652	0	670	15	0
41	b	654	0	667	18	0
41	i	664	0	690	14	0
42	c	634	0	680	14	0
42	j	634	0	680	14	0
43	d	723	0	750	12	0
43	k	774	0	802	13	0
44	e	651	0	671	7	0
44	l	669	0	692	11	0
45	f	562	0	574	9	0
45	m	562	0	574	11	0
46	g	568	0	590	9	0
46	n	568	0	590	13	0
47	o	1282	0	1305	15	0
48	p	745	0	767	9	0
49	q	514	0	236	0	0
49	r	594	0	270	0	0
49	s	659	0	299	1	0
49	t	514	0	236	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	w	2605	0	1124	3	0
51	x	636	0	276	10	0
52	y	318	0	88	0	0
53	z	430	0	321	3	0
54	6	5	0	0	0	0
54	7	1	0	0	0	0
55	6	1	0	0	0	0
56	7	31	0	12	0	0
57	C	32	0	12	0	0
58	N	3	0	0	0	0
58	O	3	0	0	0	0
59	U	36	0	6	1	0
All	All	120489	0	96660	985	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 5.

All (985) 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)
6:50:336:TYR:O	18:F:667:ASN:HB2	1.14	1.30
6:50:288:VAL:CB	51:x:170:LEU:CB	2.12	1.27
28:O:144:SER:OG	28:O:147:LEU:HB2	1.42	1.17
6:50:288:VAL:CB	51:x:170:LEU:CA	2.28	1.10
6:50:336:TYR:O	18:F:667:ASN:CB	2.07	1.01
6:50:294:ALA:HA	18:F:663:TYR:OH	1.62	0.99
6:50:293:ASP:O	12:A:2001:SER:OG	1.81	0.98
6:50:294:ALA:CB	18:F:658:TYR:HE2	1.80	0.95
6:50:294:ALA:CB	18:F:658:TYR:CE2	2.51	0.93
6:50:288:VAL:CB	51:x:170:LEU:HA	1.99	0.92
5:5:36:C:H42	5:5:46:U:H3	1.09	0.90
6:50:338:ILE:H	18:F:666:ASP:CB	1.86	0.89
28:O:144:SER:HG	28:O:147:LEU:HB2	1.41	0.86
6:50:294:ALA:HB3	18:F:658:TYR:CE2	2.10	0.85
6:50:294:ALA:HB2	18:F:658:TYR:HE2	1.39	0.84
6:50:288:VAL:H	51:x:170:LEU:CB	1.90	0.84
6:50:338:ILE:H	18:F:666:ASP:HB2	1.43	0.84
2:2:25:G:N1	8:6:52:U:O2	2.15	0.76
6:50:288:VAL:N	51:x:170:LEU:CB	2.48	0.76
2:2:153:A:H62	2:2:177:A:H2	1.32	0.75
6:50:294:ALA:HB2	18:F:658:TYR:CE2	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:153:A:N6	2:2:177:A:C2	2.57	0.73
5:5:36:C:N4	5:5:46:U:H3	1.85	0.73
34:T:216:ASN:HD21	34:T:472:GLN:H	1.37	0.73
8:6:40:U:H3	21:IN:7:G:H22	1.41	0.68
28:O:24:CYS:SG	28:O:81:CYS:HB2	2.34	0.68
6:50:292:SER:N	12:A:1996:ASN:O	2.27	0.67
2:2:153:A:N6	2:2:177:A:H2	1.91	0.66
12:A:67:ARG:HD3	12:A:179:ALA:HB2	1.78	0.66
34:T:314:ILE:HD12	34:T:324:HIS:HB2	1.76	0.66
12:A:1476:GLN:NE2	35:U:85:GLN:OE1	2.30	0.65
16:E:259:VAL:HB	16:E:277:PHE:HB2	1.79	0.65
12:A:156:ARG:HD3	35:U:153:GLU:HG2	1.78	0.65
16:E:101:ASN:HD22	41:b:105:GLY:H	1.45	0.64
46:g:18:SER:HG	46:g:26:HIS:HE2	1.43	0.64
32:S:15:TYR:HB2	32:S:163:TYR:HB2	1.79	0.64
6:50:336:TYR:C	18:F:667:ASN:HB2	2.16	0.64
31:R:62:GLY:HA3	32:S:131:ARG:HH11	1.63	0.63
41:i:26:ILE:HB	41:i:48:PHE:HB2	1.81	0.63
45:f:24:LYS:HA	45:f:70:LEU:HD12	1.81	0.63
40:a:19:THR:HB	40:a:72:ILE:HB	1.81	0.62
6:50:294:ALA:CA	18:F:663:TYR:OH	2.44	0.62
6:50:336:TYR:CB	18:F:667:ASN:OD1	2.47	0.62
22:J:213:LYS:O	24:L:189:ARG:NH2	2.33	0.62
16:E:62:LEU:HB2	16:E:351:LEU:HB2	1.82	0.62
12:A:209:ASP:HB2	12:A:212:PRO:HA	1.82	0.62
12:A:1771:LEU:HD22	12:A:1812:PRO:HG2	1.81	0.61
13:B:1819:ALA:HB2	13:B:1829:ILE:HD13	1.82	0.61
5:5:45:C:H4'	12:A:596:TYR:HB3	1.83	0.61
13:B:1353:GLY:O	13:B:1692:ASN:ND2	2.34	0.61
40:h:19:THR:HB	40:h:72:ILE:HB	1.82	0.60
12:A:909:TYR:HB2	12:A:1033:GLY:HA3	1.83	0.60
24:L:145:ASP:OD1	24:L:145:ASP:N	2.34	0.60
29:P:23:LEU:HA	29:P:26:LEU:HD23	1.83	0.60
26:N:101:CYS:SG	26:N:102:CYS:N	2.71	0.60
13:B:415:VAL:HG12	13:B:894:VAL:HB	1.84	0.60
16:E:91:LEU:HD22	16:E:101:ASN:HD21	1.65	0.60
8:6:21:U:O2'	37:W:130:ARG:NH2	2.35	0.60
37:W:524:ILE:HG22	37:W:534:ILE:HG12	1.83	0.60
42:c:22:GLY:HA3	42:c:48:LYS:HD2	1.84	0.60
12:A:443:VAL:HG12	12:A:610:HIS:HB3	1.83	0.60
34:T:349:SER:OG	34:T:351:ASP:OD1	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:U:51:GLU:HB2	35:U:59:ILE:HB	1.83	0.60
24:L:65:ARG:HG3	24:L:362:ILE:HD11	1.83	0.59
6:50:288:VAL:CB	51:x:170:LEU:N	2.65	0.59
2:2:22:U:OP1	12:A:717:TRP:NE1	2.35	0.59
12:A:549:GLU:OE1	12:A:552:ARG:NH1	2.35	0.59
12:A:899:MET:HE1	12:A:1246:GLN:HE22	1.66	0.59
32:S:52:LYS:HA	32:S:158:LYS:HA	1.84	0.59
43:d:70:VAL:HG21	43:d:99:MET:HG2	1.83	0.59
12:A:82:ARG:NH2	21:IN:16:G:N7	2.51	0.59
12:A:1581:LEU:HD22	12:A:1746:ARG:HH11	1.68	0.59
13:B:569:LEU:HD13	13:B:580:ILE:HG21	1.85	0.59
6:50:338:ILE:N	18:F:666:ASP:HB2	2.17	0.59
35:U:67:ILE:HG23	35:U:85:GLN:HE21	1.68	0.59
6:50:338:ILE:H	18:F:666:ASP:HB3	1.67	0.59
8:6:64:U:OP2	12:A:663:ARG:NH2	2.33	0.58
6:50:294:ALA:HB3	18:F:658:TYR:CZ	2.38	0.58
8:6:49:G:OP1	24:L:33:ARG:NH1	2.35	0.58
13:B:686:GLU:HB2	13:B:866:GLU:HG2	1.86	0.58
37:W:552:VAL:HG13	37:W:571:TRP:HD1	1.67	0.58
40:h:69:ARG:O	41:i:76:ASN:ND2	2.36	0.58
4:32:72:ARG:NH2	12:A:186:GLU:O	2.37	0.58
6:50:288:VAL:CA	51:x:170:LEU:CB	2.81	0.58
40:a:28:TYR:OH	46:g:20:LYS:NZ	2.36	0.58
43:k:107:ILE:HG22	43:k:108:VAL:HG23	1.86	0.58
31:R:205:ASP:HB3	31:R:208:GLU:HB2	1.86	0.58
14:C:300:LEU:HD13	14:C:306:ASN:HB3	1.85	0.58
28:O:64:ARG:HG3	28:O:162:PRO:HA	1.84	0.58
8:6:21:U:OP1	26:N:116:ASN:ND2	2.37	0.58
1:1:68:MET:HA	18:F:757:ARG:HE	1.69	0.57
12:A:205:ASP:N	12:A:205:ASP:OD1	2.35	0.57
31:R:189:ASN:HD21	31:R:195:ARG:HB3	1.69	0.57
50:w:283:PRO:HA	50:w:299:GLY:HA2	1.86	0.57
2:2:37:U:OP1	37:W:454:LYS:NZ	2.36	0.57
8:6:10:U:O2'	8:6:12:G:N7	2.35	0.57
12:A:321:ASN:O	14:C:645:ARG:NH2	2.36	0.57
37:W:479:GLN:NE2	37:W:525:SER:OG	2.37	0.57
41:b:26:ILE:HB	41:b:48:PHE:HB2	1.85	0.57
12:A:200:ASP:OD1	12:A:240:ARG:NH2	2.36	0.57
13:B:493:LEU:O	13:B:519:ARG:NH1	2.37	0.57
16:E:203:ASP:HB3	16:E:247:GLY:HA3	1.86	0.57
37:W:432:ARG:NH2	37:W:446:GLU:OE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:12:U:H3	5:5:65:G:H1	1.52	0.57
12:A:1214:TRP:HB2	12:A:1228:CYS:HB3	1.87	0.57
6:50:288:VAL:O	51:x:166:SER:O	2.23	0.57
6:50:336:TYR:CB	18:F:667:ASN:HA	2.34	0.57
26:N:105:CYS:HB3	26:N:119:CYS:SG	2.45	0.57
41:i:64:LYS:NZ	47:o:45:ASP:OD2	2.37	0.57
6:50:126:GLU:O	13:B:1442:ARG:NH1	2.37	0.57
8:6:14:C:H2'	8:6:15:A:H8	1.68	0.57
12:A:1984:LYS:HG3	35:U:345:ALA:HB1	1.85	0.57
16:E:177:LYS:HG2	16:E:189:THR:HG22	1.87	0.57
34:T:294:LEU:HD12	34:T:303:LEU:HD11	1.86	0.57
8:6:2:U:O2	26:N:95:GLN:NE2	2.38	0.57
37:W:434:VAL:HG22	37:W:444:VAL:HG22	1.85	0.57
5:5:105:U:C5	5:5:106:U:C5	2.93	0.57
12:A:40:LEU:HD11	37:W:124:MET:HE1	1.87	0.56
12:A:873:ASN:ND2	12:A:876:GLU:OE1	2.38	0.56
31:R:178:ARG:HB2	37:W:118:ALA:HB2	1.87	0.56
45:f:31:GLY:HA3	45:f:47:THR:HG22	1.87	0.56
28:O:56:ARG:HG2	28:O:67:LYS:HB3	1.86	0.56
34:T:399:LYS:HB3	34:T:404:SER:HB2	1.85	0.56
37:W:435:SER:HB3	37:W:445:TRP:HE1	1.70	0.56
2:2:32:U:O4	21:IN:99:C:N3	2.38	0.56
13:B:128:PRO:HD2	13:B:131:ILE:HD12	1.88	0.56
34:T:210:ILE:HG13	34:T:480:ALA:HB2	1.88	0.56
37:W:333:LYS:H	37:W:353:ASP:HB3	1.71	0.56
2:2:182:U:OP2	41:i:54:LYS:NZ	2.37	0.56
6:50:337:THR:HA	18:F:666:ASP:HB2	1.86	0.56
16:E:346:SER:OG	16:E:348:ASP:OD1	2.23	0.56
16:E:95:VAL:HG13	16:E:353:MET:HE1	1.87	0.56
41:i:52:LYS:HB2	41:i:54:LYS:HE3	1.87	0.56
12:A:981:PHE:O	12:A:1166:THR:OG1	2.24	0.56
12:A:1124:ASN:ND2	12:A:1148:ASN:OD1	2.37	0.56
12:A:243:ASN:O	35:U:131:LYS:NZ	2.37	0.56
42:j:5:ARG:HG3	42:j:8:MET:HE2	1.88	0.56
12:A:280:GLU:OE2	33:SR:11:ARG:NH1	2.39	0.55
5:5:46:U:O2	33:SR:11:ARG:NH2	2.38	0.55
8:6:20:A:O2'	26:N:120:ARG:NH2	2.39	0.55
16:E:59:ILE:HD11	37:W:82:ASN:H	1.71	0.55
28:O:131:THR:O	37:W:108:ARG:NH1	2.39	0.55
37:W:436:THR:HG21	37:W:464:MET:HB2	1.88	0.55
37:W:257:ILE:HD12	37:W:266:ARG:HE	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:678:GLU:OE2	12:A:778:ARG:NH2	2.39	0.55
12:A:1366:PRO:HA	19:H:465:SER:HA	1.89	0.55
31:R:44:TYR:HA	31:R:47:ARG:HD2	1.87	0.55
42:c:25:VAL:HG22	42:c:45:MET:HG3	1.89	0.55
44:l:30:ARG:NH2	44:l:60:ASP:O	2.40	0.55
12:A:601:GLN:HG2	12:A:640:PHE:HB2	1.87	0.55
12:A:881:ILE:HG23	12:A:918:THR:HG23	1.87	0.55
12:A:1214:TRP:NE1	12:A:1276:GLU:OE1	2.39	0.55
24:L:37:LEU:HD13	24:L:158:ARG:HD3	1.88	0.55
42:j:20:LYS:HD3	42:j:66:ARG:HG3	1.89	0.55
48:p:39:ASP:HB3	48:p:55:ILE:HD12	1.88	0.55
12:A:976:MET:HG2	12:A:1187:PHE:HB3	1.88	0.55
24:L:147:ASP:OD1	24:L:147:ASP:N	2.36	0.55
14:C:177:ARG:NH2	14:C:638:ASP:OD2	2.39	0.55
31:R:265:ASP:OD1	31:R:265:ASP:N	2.38	0.55
5:5:105:U:C5	5:5:106:U:C4	2.94	0.55
12:A:546:LEU:HD11	12:A:595:LYS:HB2	1.89	0.55
13:B:1093:ARG:NH2	13:B:1273:ASP:OD1	2.40	0.55
13:B:1456:VAL:HG22	13:B:1491:SER:HB2	1.89	0.55
28:O:240:GLY:H	28:O:268:GLN:HB2	1.71	0.55
37:W:390:LEU:HD22	37:W:402:GLN:HE21	1.72	0.55
2:2:170:C:H2'	48:p:44:LYS:HB3	1.88	0.55
12:A:552:ARG:NH1	12:A:589:THR:O	2.40	0.55
16:E:311:VAL:HB	16:E:321:TYR:HB2	1.89	0.55
28:O:78:LYS:O	28:O:97:ARG:NH2	2.40	0.55
12:A:141:ILE:HD12	12:A:410:PRO:HG3	1.89	0.54
35:U:122:ASN:ND2	35:U:133:CYS:SG	2.74	0.54
19:H:525:PHE:HA	19:H:528:ILE:HG22	1.89	0.54
37:W:126:GLU:HA	37:W:129:ARG:HG2	1.89	0.54
12:A:723:ASN:OD1	12:A:785:LYS:NZ	2.39	0.54
12:A:1042:GLN:HE22	12:A:1092:ILE:HA	1.72	0.54
32:S:25:LEU:HD23	32:S:98:LEU:HD21	1.88	0.54
37:W:259:GLN:HB3	40:h:11:HIS:HB3	1.89	0.54
4:32:99:LEU:HD22	12:A:1617:ARG:HD2	1.89	0.54
32:S:156:ASP:N	32:S:156:ASP:OD1	2.39	0.54
12:A:1009:MET:O	12:A:1013:ASN:ND2	2.40	0.54
22:J:221:ASN:O	24:L:211:ASN:ND2	2.41	0.54
43:d:70:VAL:HB	43:d:96:ILE:HB	1.89	0.54
35:U:342:HIS:HB3	35:U:345:ALA:HB3	1.89	0.54
43:d:47:ARG:HA	43:d:107:ILE:HD11	1.89	0.54
12:A:523:ASN:OD1	12:A:552:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1215:ASN:HB3	12:A:1224:ARG:HD3	1.90	0.54
34:T:210:ILE:HG12	34:T:221:THR:HG22	1.90	0.54
12:A:143:GLN:NE2	12:A:207:PHE:O	2.33	0.53
31:R:238:THR:HG23	31:R:241:GLU:H	1.74	0.53
41:b:79:SER:HB2	42:j:58:LEU:HD11	1.90	0.53
12:A:1536:LEU:HG	12:A:1572:SER:HB3	1.90	0.53
19:H:517:LEU:HD21	33:SR:24:SER:HA	1.89	0.53
44:e:55:ASN:ND2	45:f:40:MET:SD	2.81	0.53
28:O:162:PRO:HG2	28:O:182:ARG:HG3	1.91	0.53
32:S:26:GLU:OE1	32:S:131:ARG:NH2	2.41	0.53
37:W:255:LEU:HD21	37:W:362:GLU:HB3	1.90	0.53
13:B:1855:TYR:HB3	13:B:1891:THR:HG21	1.90	0.53
16:E:81:LEU:HD21	16:E:343:ILE:HD12	1.90	0.53
31:R:47:ARG:HA	31:R:50:TRP:HE1	1.73	0.53
5:5:11:U:O2'	12:A:217:ARG:NH2	2.42	0.53
12:A:1090:ARG:NH2	12:A:1092:ILE:O	2.42	0.53
41:b:16:ARG:HB3	41:b:84:GLY:HA3	1.90	0.53
12:A:214:ARG:HA	12:A:220:VAL:HG21	1.91	0.53
12:A:698:PRO:HB2	31:R:237:MET:HE1	1.91	0.53
12:A:1618:LYS:NZ	12:A:1628:ASP:OD2	2.36	0.53
16:E:64:GLY:HA3	41:b:105:GLY:HA2	1.91	0.53
37:W:404:ASP:HB3	37:W:407:SER:HB3	1.91	0.53
12:A:164:MET:HE1	12:A:560:SER:HA	1.90	0.53
12:A:698:PRO:HD2	12:A:701:ILE:HG13	1.90	0.53
12:A:1759:THR:HG21	53:z:358:ARG:HH12	1.74	0.53
13:B:844:LEU:HD11	13:B:849:ILE:HG23	1.90	0.53
42:j:7:LEU:HD23	42:j:32:VAL:HG11	1.91	0.53
1:1:133:LYS:NZ	2:2:175:G:OP2	2.38	0.53
12:A:1021:ASP:OD1	12:A:1021:ASP:N	2.39	0.53
24:L:178:GLU:OE2	24:L:181:ARG:NH1	2.42	0.53
24:L:250:GLU:OE1	24:L:258:ARG:NH2	2.42	0.53
47:o:148:GLN:NE2	48:p:73:PRO:O	2.39	0.53
12:A:109:PRO:HB2	12:A:191:ILE:HD12	1.90	0.53
24:L:33:ARG:O	24:L:158:ARG:NH2	2.41	0.53
43:d:57:LYS:HB2	43:d:66:VAL:HG23	1.90	0.53
42:j:16:THR:HB	42:j:69:ILE:HB	1.92	0.53
12:A:36:LYS:NZ	37:W:163:GLN:O	2.42	0.52
12:A:641:MET:HA	12:A:644:ILE:HG22	1.90	0.52
12:A:1946:ASN:HD22	12:A:1986:LEU:HD11	1.73	0.52
31:R:61:GLY:HA3	32:S:136:ILE:HG21	1.91	0.52
37:W:304:LEU:HD11	37:W:567:ILE:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1042:GLN:HA	12:A:1090:ARG:HH12	1.72	0.52
13:B:1985:ILE:HA	13:B:1988:MET:HG3	1.92	0.52
24:L:15:GLU:HG2	24:L:151:MET:HE1	1.91	0.52
47:o:121:LEU:O	47:o:123:ASN:ND2	2.43	0.52
12:A:1904:ASP:HB3	12:A:1908:LYS:HE2	1.90	0.52
2:2:101:U:O2'	42:c:61:ARG:NH2	2.42	0.52
8:6:35:A:N6	21:IN:11:A:OP2	2.42	0.52
12:A:1860:GLN:HG2	12:A:1883:VAL:HB	1.90	0.52
13:B:537:LYS:NZ	13:B:581:SER:O	2.42	0.52
43:k:43:LEU:HB3	43:k:110:LEU:HG	1.91	0.52
12:A:58:LYS:NZ	12:A:477:LYS:O	2.43	0.52
12:A:962:LEU:HB3	12:A:965:VAL:HB	1.92	0.52
12:A:1491:LYS:O	12:A:1710:ASN:ND2	2.41	0.52
13:B:1563:VAL:HG12	13:B:1664:MET:HE2	1.91	0.52
34:T:305:THR:OG1	34:T:315:TRP:NE1	2.40	0.52
37:W:173:LYS:NZ	37:W:175:THR:O	2.41	0.52
44:l:64:ILE:HG12	44:l:71:ARG:HG2	1.90	0.52
12:A:721:LYS:HB3	12:A:781:ARG:HD3	1.91	0.52
12:A:1780:VAL:HG22	12:A:1809:ILE:HG12	1.90	0.52
13:B:967:ASN:ND2	13:B:995:ASN:O	2.41	0.52
13:B:1570:ARG:HH11	13:B:1608:THR:HG21	1.74	0.52
12:A:331:TRP:CD1	12:A:333:HIS:H	2.26	0.52
12:A:1085:ILE:HD11	12:A:1160:ARG:HH12	1.74	0.52
24:L:176:LEU:HD22	37:W:440:LYS:HD3	1.90	0.52
35:U:189:ASP:HA	35:U:192:LYS:HB2	1.90	0.52
12:A:490:VAL:HG21	12:A:565:ARG:HG3	1.92	0.52
13:B:505:THR:HG22	13:B:509:LYS:HZ1	1.75	0.52
37:W:301:GLY:O	37:W:559:HIS:NE2	2.41	0.52
2:2:151:C:H2'	2:2:152:G:H8	1.75	0.52
5:5:67:A:H5''	26:N:90:ALA:HB1	1.90	0.52
31:R:107:SER:OG	31:R:108:LYS:N	2.43	0.52
34:T:347:THR:HG22	34:T:357:TRP:HE1	1.74	0.52
13:B:425:ASN:ND2	13:B:886:GLN:O	2.42	0.52
29:P:16:ARG:NH2	31:R:218:ILE:O	2.43	0.52
12:A:26:SER:OG	12:A:27:GLU:N	2.43	0.51
12:A:1777:ILE:HG12	12:A:1860:GLN:HB2	1.91	0.51
16:E:67:GLY:N	16:E:87:ASP:OD1	2.43	0.51
34:T:365:ARG:HH22	34:T:401:PRO:HB2	1.75	0.51
12:A:761:ILE:HD12	12:A:775:ASN:HD22	1.76	0.51
2:2:103:U:O2'	45:m:65:ARG:NH2	2.38	0.51
2:2:166:G:OP2	2:2:166:G:N2	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:6:58:G:H2'	8:6:59:G:C8	2.45	0.51
12:A:1559:GLY:HA3	12:A:1622:MET:HE3	1.93	0.51
13:B:1287:ARG:NH1	51:x:53:LEU:O	2.44	0.51
40:h:40:ASN:HD22	40:h:65:GLY:H	1.59	0.51
12:A:857:ASN:N	12:A:857:ASN:OD1	2.43	0.51
13:B:1099:VAL:HG13	13:B:1108:THR:HG22	1.92	0.51
13:B:1564:PRO:O	13:B:1648:ARG:NH1	2.44	0.51
46:g:28:GLN:NE2	46:g:48:MET:SD	2.84	0.51
13:B:1950:THR:OG1	13:B:2060:ARG:NH2	2.42	0.51
19:H:545:ARG:HA	19:H:585:ILE:HG21	1.93	0.51
5:5:12:U:H5'	12:A:224:THR:HG23	1.93	0.51
13:B:1083:TYR:O	13:B:1087:SER:OG	2.28	0.51
28:O:97:ARG:HA	28:O:147:LEU:HD11	1.93	0.51
28:O:176:GLY:HA2	37:W:206:ALA:HB2	1.93	0.51
31:R:177:ILE:HG22	37:W:117:PRO:HA	1.92	0.51
8:6:65:G:N7	12:A:663:ARG:NH1	2.50	0.51
12:A:664:HIS:HE1	31:R:214:ILE:HG22	1.76	0.51
13:B:1360:ALA:HB2	13:B:1490:LEU:HD11	1.93	0.51
34:T:371:HIS:NE2	34:T:389:SER:OG	2.37	0.51
37:W:103:GLN:NE2	37:W:111:LEU:O	2.43	0.51
46:g:15:LYS:HG3	46:g:76:VAL:HG12	1.92	0.51
12:A:86:ARG:HH21	21:IN:14:A:H5'	1.75	0.51
13:B:548:VAL:HG22	13:B:587:VAL:HG12	1.93	0.51
13:B:1130:ARG:HG3	13:B:1140:VAL:HG11	1.91	0.51
19:H:590:LEU:HD22	19:H:599:LEU:HD13	1.93	0.51
44:l:62:GLU:OE2	44:l:71:ARG:NH2	2.40	0.51
37:W:572:ASP:OD1	37:W:572:ASP:N	2.42	0.51
12:A:923:ASP:OD2	12:A:1439:ARG:NH1	2.44	0.51
12:A:1776:ILE:HB	12:A:1858:PRO:HA	1.92	0.51
40:a:72:ILE:HG12	41:b:70:VAL:HG22	1.93	0.51
6:50:294:ALA:HB3	18:F:658:TYR:OH	2.11	0.50
34:T:270:VAL:HB	34:T:284:TYR:HB2	1.93	0.50
34:T:392:PRO:HG3	34:T:415:ILE:HA	1.93	0.50
1:1:123:GLN:HB3	1:1:127:ARG:HH12	1.75	0.50
6:50:286:ASP:O	51:x:170:LEU:CB	2.59	0.50
12:A:539:ARG:NH1	17:EX:-3:A:O2'	2.45	0.50
12:A:975:VAL:HB	12:A:1099:PHE:HB2	1.93	0.50
13:B:999:GLN:NE2	13:B:1003:GLN:OE1	2.41	0.50
28:O:22:ILE:HD13	37:W:111:LEU:HD23	1.93	0.50
43:k:62:HIS:O	45:m:65:ARG:NH1	2.44	0.50
47:o:70:LEU:HA	47:o:94:ILE:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:65:HIS:ND1	12:A:120:TYR:OH	2.42	0.50
13:B:639:ILE:HD11	13:B:646:VAL:HB	1.94	0.50
14:C:151:GLU:O	14:C:158:ARG:NH1	2.44	0.50
16:E:166:LEU:HD23	16:E:178:LEU:HD11	1.93	0.50
32:S:17:GLU:HB3	32:S:22:ILE:HG12	1.91	0.50
34:T:312:ALA:HB3	34:T:326:LEU:HB2	1.92	0.50
12:A:445:VAL:HG21	17:EX:-9:C:H2'	1.93	0.50
41:b:35:ASP:OD2	41:b:39:ASN:ND2	2.44	0.50
12:A:1382:SER:HA	12:A:1415:GLY:HA2	1.93	0.50
37:W:286:GLY:HA3	37:W:316:TRP:HH2	1.76	0.50
5:5:94:U:OP2	45:f:65:ARG:NH1	2.39	0.50
13:B:790:THR:HG21	13:B:793:ASP:HB2	1.93	0.50
29:P:213:ASP:OD2	29:P:216:ARG:NH1	2.41	0.50
31:R:122:LYS:HD2	34:T:406:ILE:HD13	1.94	0.50
45:m:28:GLU:HB2	45:m:50:TYR:HB2	1.93	0.50
12:A:1555:LEU:HD22	12:A:1560:ILE:HD12	1.93	0.50
28:O:75:SER:OG	28:O:80:VAL:O	2.29	0.50
5:5:56:C:H4'	12:A:100:LEU:HD21	1.94	0.50
12:A:1268:ILE:HG22	12:A:1368:LEU:HD21	1.93	0.50
12:A:1686:ASP:OD1	35:U:169:ARG:NH1	2.45	0.50
12:A:1782:ASP:OD2	12:A:1865:ARG:NH1	2.45	0.50
13:B:2105:THR:HG23	13:B:2121:LYS:HG3	1.94	0.50
31:R:320:HIS:HA	31:R:323:LYS:HB3	1.94	0.50
12:A:769:LYS:HD3	12:A:1249:MET:HG2	1.93	0.50
13:B:1329:ASN:ND2	13:B:1354:SER:O	2.45	0.50
19:H:474:HIS:HD2	33:SR:23:LEU:H	1.59	0.50
34:T:221:THR:HG21	34:T:486:ILE:HG12	1.94	0.50
34:T:223:SER:OG	34:T:224:ALA:N	2.44	0.50
40:a:73:LEU:HB2	41:b:69:LEU:HD23	1.92	0.49
12:A:974:ASN:HB2	12:A:1178:TYR:HB3	1.94	0.49
12:A:1312:PRO:HG2	12:A:1314:VAL:HG12	1.94	0.49
13:B:569:LEU:HD22	13:B:586:ILE:HD12	1.93	0.49
14:C:564:THR:HG21	14:C:576:ILE:HA	1.94	0.49
28:O:261:ILE:HG12	28:O:272:ILE:HG23	1.94	0.49
40:a:25:GLY:HA2	40:a:69:ARG:HH12	1.78	0.49
40:a:26:GLU:HG2	40:a:50:TYR:HA	1.94	0.49
12:A:1926:THR:O	35:U:355:LYS:NZ	2.40	0.49
13:B:1943:MET:HE1	13:B:2067:VAL:HG21	1.95	0.49
28:O:87:ASP:OD1	28:O:88:LEU:N	2.44	0.49
28:O:175:ARG:HB2	28:O:179:CYS:HB2	1.92	0.49
34:T:406:ILE:HG22	34:T:407:GLN:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:115:U:OP2	44:e:40:ASN:ND2	2.45	0.49
12:A:1045:GLY:HA2	12:A:1048:MET:HE2	1.94	0.49
13:B:143:LEU:O	13:B:153:ARG:NH1	2.46	0.49
31:R:192:ALA:O	37:W:142:SER:OG	2.29	0.49
37:W:121:ASN:HB3	37:W:124:MET:HG2	1.93	0.49
44:e:48:ILE:HD11	44:e:59:ASP:HB2	1.94	0.49
12:A:690:MET:HA	12:A:693:ILE:HG12	1.94	0.49
40:h:74:PRO:HG2	40:h:77:LEU:HD13	1.94	0.49
12:A:1210:LYS:NZ	12:A:1211:ASP:OD1	2.33	0.49
26:N:64:PHE:HZ	26:N:72:ARG:HD2	1.76	0.49
46:g:19:LEU:HD13	46:g:70:LEU:HB3	1.94	0.49
2:2:150:U:H3	2:2:181:G:H1	1.60	0.49
5:5:23:C:H5'	5:5:24:G:H5''	1.95	0.49
12:A:75:ASP:N	12:A:75:ASP:OD1	2.43	0.49
12:A:1042:GLN:OE1	12:A:1090:ARG:NH1	2.46	0.49
12:A:1832:ARG:NH1	21:IN:2:U:OP1	2.46	0.49
16:E:183:LYS:HG3	16:E:187:ILE:HD11	1.93	0.49
19:H:636:LEU:HB3	19:H:639:LEU:HD13	1.94	0.49
26:N:51:ARG:NH2	37:W:192:PHE:O	2.46	0.49
47:o:18:ALA:HB1	48:p:40:ILE:HG12	1.95	0.49
2:2:107:A:O2'	43:k:49:ASN:ND2	2.42	0.49
12:A:862:GLU:HG3	24:L:6:ILE:HG23	1.94	0.49
13:B:739:ARG:NH2	13:B:776:ASP:OD2	2.45	0.49
21:IN:18:A:O2'	28:O:83:THR:O	2.29	0.49
28:O:106:ASP:OD1	28:O:106:ASP:N	2.45	0.49
46:n:19:LEU:HD13	46:n:70:LEU:HB3	1.95	0.49
47:o:27:ARG:HG2	47:o:50:SER:HB3	1.95	0.49
2:2:161:U:O2	2:2:163:G:N2	2.46	0.49
12:A:245:LEU:HD13	12:A:426:LEU:HB3	1.93	0.49
12:A:2328:ALA:HB3	13:B:788:GLY:HA2	1.93	0.49
14:C:676:ALA:HB2	14:C:815:VAL:HB	1.95	0.49
16:E:58:PRO:HG2	37:W:80:GLN:O	2.12	0.49
24:L:59:LYS:O	24:L:91:ARG:NH1	2.46	0.49
32:S:87:HIS:ND1	32:S:89:ASP:OD1	2.45	0.49
12:A:1641:ARG:HD2	35:U:175:PRO:HB2	1.94	0.49
12:A:1942:ALA:HB1	12:A:1986:LEU:HD23	1.93	0.49
13:B:538:ILE:HB	13:B:585:ILE:HG12	1.94	0.49
13:B:1538:ARG:NH1	13:B:1665:ASP:OD1	2.46	0.49
16:E:214:ASP:N	16:E:214:ASP:OD1	2.46	0.49
28:O:94:ILE:HD12	28:O:202:TYR:HA	1.93	0.49
29:P:57:ARG:NH2	34:T:215:GLY:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:d:102:ARG:NH1	42:j:62:GLY:O	2.45	0.49
12:A:146:SER:HB2	12:A:193:LEU:HD22	1.95	0.48
12:A:948:PRO:HD2	12:A:1455:TRP:HB2	1.95	0.48
31:R:52:PRO:HG2	31:R:71:GLN:HG2	1.95	0.48
37:W:484:GLN:HG2	37:W:503:LYS:HB3	1.95	0.48
40:h:23:ASN:OD1	40:h:69:ARG:NH2	2.46	0.48
47:o:65:ARG:O	47:o:67:LYS:NZ	2.45	0.48
47:o:132:ARG:HG3	47:o:145:LEU:HD23	1.95	0.48
8:6:57:U:H2'	8:6:58:G:C8	2.48	0.48
16:E:133:VAL:HG21	16:E:169:THR:HG21	1.94	0.48
33:SR:1:MET:SD	33:SR:1:MET:N	2.85	0.48
35:U:102:TYR:HB3	35:U:156:GLN:HE21	1.78	0.48
42:c:67:TYR:OH	43:k:94:ARG:NH2	2.46	0.48
1:1:125:ALA:HA	1:1:128:ARG:HB2	1.95	0.48
12:A:425:PRO:HB2	12:A:428:LYS:HB2	1.95	0.48
12:A:938:PRO:HB2	12:A:1071:PHE:HA	1.94	0.48
12:A:1095:ILE:HD12	12:A:1097:ILE:HD11	1.93	0.48
28:O:145:ASP:OD1	28:O:146:MET:N	2.46	0.48
43:k:44:ILE:HB	43:k:52:LEU:HB2	1.95	0.48
12:A:1552:GLN:HG2	12:A:1561:PHE:HB3	1.95	0.48
12:A:1670:ASP:OD1	12:A:1670:ASP:N	2.44	0.48
13:B:1998:GLN:NE2	13:B:2003:GLN:OE1	2.46	0.48
24:L:150:GLU:HA	24:L:153:SER:HB2	1.95	0.48
40:h:17:ILE:HA	40:h:31:LYS:HA	1.96	0.48
13:B:1186:LEU:HD13	13:B:1282:LEU:HD22	1.94	0.48
13:B:1837:ASN:O	13:B:1840:THR:OG1	2.31	0.48
32:S:149:SER:O	37:W:100:ARG:NH2	2.46	0.48
42:c:31:GLY:HA3	41:i:8:LYS:HE3	1.94	0.48
43:d:28:PRO:HD2	45:f:37:ASP:HB3	1.95	0.48
43:k:110:LEU:HD22	45:m:59:LEU:HB3	1.96	0.48
8:6:14:C:H2'	8:6:15:A:C8	2.49	0.48
8:6:29:A:N6	21:IN:16:G:O2'	2.42	0.48
12:A:1212:GLY:HA2	12:A:1276:GLU:HB3	1.95	0.48
19:H:536:ILE:HG23	19:H:544:LEU:HD21	1.96	0.48
28:O:40:LYS:HA	28:O:53:THR:HG23	1.96	0.48
35:U:102:TYR:HD1	35:U:156:GLN:HB3	1.78	0.48
37:W:210:GLU:HA	37:W:213:GLN:HB2	1.95	0.48
37:W:258:PRO:HD2	37:W:265:LEU:HD12	1.96	0.48
2:2:97:G:OP2	43:k:61:ARG:NH2	2.47	0.48
12:A:841:LEU:HA	12:A:844:GLU:HG2	1.95	0.48
12:A:1630:LEU:HD11	12:A:1696:PRO:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:964:LEU:HD22	13:B:969:LEU:HG	1.94	0.48
40:a:20:CYS:SG	40:a:21:GLU:N	2.87	0.48
14:C:474:LEU:HA	14:C:499:GLY:HA3	1.95	0.48
37:W:422:ASN:N	37:W:436:THR:O	2.45	0.48
37:W:442:LEU:HB2	37:W:456:ILE:HB	1.94	0.48
40:h:21:GLU:HG2	40:h:69:ARG:HB3	1.96	0.48
4:32:88:ARG:HB3	12:A:1694:ILE:HG12	1.95	0.48
8:6:24:A:N3	8:6:26:U:O2'	2.39	0.48
12:A:1292:GLU:OE2	12:A:1317:TYR:OH	2.29	0.48
12:A:1413:ASP:OD1	12:A:1420:ASN:ND2	2.47	0.48
12:A:2328:ALA:HB1	13:B:791:ARG:HH22	1.78	0.48
13:B:1456:VAL:HG11	13:B:1489:ALA:HB1	1.96	0.48
31:R:53:ARG:N	31:R:57:ASP:OD2	2.45	0.48
34:T:419:LEU:HD22	34:T:427:LEU:HD11	1.96	0.48
12:A:2015:GLU:OE1	18:F:758:ARG:NE	2.41	0.48
13:B:782:PHE:HB3	13:B:808:VAL:HB	1.95	0.48
37:W:534:ILE:HB	37:W:544:SER:HB3	1.96	0.48
45:f:42:MET:HE1	45:f:72:ILE:HG21	1.94	0.48
12:A:251:ASP:HB3	12:A:253:ASN:H	1.79	0.47
12:A:975:VAL:HG22	12:A:1177:VAL:HG22	1.96	0.47
13:B:603:ARG:HH22	13:B:907:LEU:HD22	1.79	0.47
31:R:69:VAL:O	31:R:71:GLN:NE2	2.47	0.47
37:W:280:GLN:NE2	37:W:282:HIS:O	2.46	0.47
12:A:1072:LEU:HD13	12:A:1087:LEU:HD13	1.95	0.47
12:A:1314:VAL:O	12:A:1318:THR:OG1	2.30	0.47
13:B:2067:VAL:HB	13:B:2107:TYR:HB2	1.94	0.47
14:C:86:THR:HG21	34:T:237:LYS:HE3	1.96	0.47
16:E:90:ILE:HB	16:E:105:LEU:HB2	1.96	0.47
26:N:107:GLN:OE1	26:N:109:ARG:NH1	2.43	0.47
37:W:384:ASP:O	37:W:388:GLN:NE2	2.45	0.47
53:z:329:LYS:HE3	53:z:342:GLU:HG3	1.96	0.47
5:5:12:U:O2	5:5:65:G:N2	2.43	0.47
12:A:76:MET:HB3	12:A:85:LYS:HG2	1.97	0.47
4:32:58:ARG:HD2	4:32:62:GLN:HB3	1.96	0.47
12:A:265:THR:OG1	12:A:328:HIS:O	2.32	0.47
12:A:569:VAL:HG13	12:A:573:GLN:HB2	1.96	0.47
12:A:1956:PRO:HD2	12:A:1960:THR:HG21	1.96	0.47
4:32:80:LYS:HA	4:32:88:ARG:HH22	1.80	0.47
5:5:89:U:H1'	46:g:65:ASN:HB3	1.97	0.47
12:A:312:TYR:OH	14:C:853:ARG:NH2	2.47	0.47
12:A:652:LEU:HD23	12:A:655:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1005:ILE:HG22	12:A:1009:MET:HE2	1.95	0.47
16:E:149:GLY:O	16:E:177:LYS:NZ	2.42	0.47
28:O:169:VAL:HA	37:W:216:LEU:HD13	1.97	0.47
40:a:21:GLU:O	40:a:69:ARG:N	2.45	0.47
12:A:1407:ASP:OD1	12:A:1407:ASP:N	2.44	0.47
13:B:986:ARG:O	13:B:990:HIS:ND1	2.47	0.47
40:h:2:SER:OG	40:h:3:ILE:N	2.46	0.47
44:l:55:ASN:OD1	44:l:81:GLY:N	2.42	0.47
1:1:62:GLU:O	12:A:1949:ARG:NH1	2.48	0.47
2:2:19:G:H21	29:P:9:PHE:HD2	1.62	0.47
5:5:96:A:H1'	43:d:47:ARG:HE	1.79	0.47
12:A:1790:ILE:HG22	12:A:1800:THR:HG22	1.97	0.47
14:C:250:ARG:NH1	14:C:295:ASP:OD2	2.48	0.47
40:a:73:LEU:HD11	41:b:71:LEU:HB2	1.95	0.47
40:h:23:ASN:N	40:h:67:LYS:O	2.48	0.47
8:6:34:G:N2	21:IN:13:C:O2	2.47	0.47
13:B:142:VAL:HG12	13:B:153:ARG:HG2	1.96	0.47
13:B:1003:GLN:HE21	50:w:189:ALA:HB3	1.80	0.47
16:E:171:SER:OG	16:E:173:ASP:OD1	2.32	0.47
35:U:307:VAL:HG12	35:U:309:TYR:H	1.80	0.47
48:p:88:SER:HG	48:p:91:ILE:H	1.62	0.47
2:2:151:C:H2'	2:2:152:G:C8	2.49	0.47
5:5:105:U:C6	5:5:106:U:C5	3.02	0.47
12:A:682:ASP:OD2	12:A:746:LYS:NZ	2.40	0.47
13:B:730:GLU:HA	13:B:733:LYS:HB2	1.97	0.47
14:C:137:HIS:HD2	14:C:238:ASN:H	1.63	0.47
14:C:686:THR:HG23	14:C:793:ASP:HB2	1.97	0.47
16:E:155:ASN:ND2	16:E:196:VAL:O	2.46	0.47
40:a:67:LYS:HG3	46:g:68:ILE:HA	1.97	0.47
12:A:794:TYR:OH	12:A:989:ASP:OD1	2.29	0.47
12:A:893:GLU:HG2	12:A:1016:VAL:HB	1.96	0.47
12:A:1209:HIS:HB3	12:A:1213:VAL:HG21	1.96	0.47
13:B:300:ARG:O	13:B:304:ASN:ND2	2.47	0.47
33:SR:24:SER:O	33:SR:24:SER:OG	2.30	0.47
37:W:428:ASP:OD2	37:W:431:ARG:NH1	2.45	0.47
40:a:23:ASN:O	40:a:69:ARG:NH2	2.48	0.47
46:n:15:LYS:HE2	46:n:76:VAL:HA	1.97	0.47
12:A:606:LYS:NZ	12:A:1548:TYR:O	2.41	0.46
12:A:1159:ASN:ND2	29:P:197:CYS:O	2.48	0.46
34:T:246:ILE:HG13	34:T:269:GLN:HE22	1.80	0.46
34:T:307:SER:OG	34:T:308:ARG:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:e:32:GLN:N	44:e:88:GLN:O	2.47	0.46
12:A:1900:GLU:OE1	12:A:1951:LYS:NZ	2.43	0.46
13:B:512:VAL:HA	13:B:515:MET:HE2	1.97	0.46
13:B:1671:GLY:HA3	13:B:1860:ILE:HB	1.96	0.46
16:E:84:ALA:HB2	16:E:90:ILE:HG23	1.97	0.46
28:O:33:TYR:OH	37:W:139:LEU:O	2.32	0.46
46:n:18:SER:HB3	46:n:71:GLU:HB3	1.96	0.46
5:5:58:U:H2'	5:5:59:G:H8	1.81	0.46
12:A:240:ARG:HG2	35:U:137:PRO:HB2	1.98	0.46
26:N:51:ARG:HH21	37:W:193:LEU:HD23	1.80	0.46
43:d:110:LEU:HA	45:f:62:VAL:HA	1.97	0.46
12:A:899:MET:HB3	12:A:906:VAL:HB	1.98	0.46
12:A:1282:GLN:NE2	12:A:1336:PRO:O	2.46	0.46
13:B:987:ILE:HG12	13:B:1097:GLU:HB3	1.97	0.46
28:O:150:LEU:HD13	28:O:213:LEU:HD23	1.96	0.46
37:W:358:LEU:HD23	37:W:367:ILE:HB	1.97	0.46
47:o:96:THR:HG23	47:o:121:LEU:HB2	1.97	0.46
12:A:419:ARG:NH2	12:A:423:ASP:O	2.49	0.46
12:A:930:ALA:HB1	12:A:935:LEU:HB3	1.97	0.46
12:A:1764:SER:H	12:A:1767:ASN:HB2	1.80	0.46
13:B:720:GLN:HG2	13:B:807:GLN:HA	1.97	0.46
14:C:507:VAL:HA	14:C:568:PRO:HD3	1.96	0.46
16:E:330:ILE:HG12	16:E:346:SER:HB3	1.97	0.46
31:R:251:ILE:HG21	31:R:262:ILE:HG21	1.98	0.46
44:e:30:ARG:HH12	44:e:60:ASP:HB2	1.81	0.46
43:k:110:LEU:HA	45:m:62:VAL:HA	1.97	0.46
12:A:997:LEU:HD13	12:A:1009:MET:HE3	1.98	0.46
12:A:1808:PHE:HE2	12:A:1893:PHE:HB3	1.80	0.46
13:B:987:ILE:HG21	13:B:1098:ILE:HG13	1.97	0.46
16:E:127:ALA:HB2	16:E:157:CYS:HB3	1.97	0.46
41:b:9:MET:HE2	42:j:39:HIS:HE1	1.80	0.46
41:b:16:ARG:HA	41:b:30:THR:HA	1.98	0.46
12:A:1248:LEU:O	12:A:1298:ARG:NH2	2.49	0.46
14:C:500:THR:OG1	14:C:502:HIS:NE2	2.48	0.46
31:R:3:LEU:HA	31:R:6:PHE:HB2	1.97	0.46
32:S:56:ILE:HG12	32:S:62:ILE:HG23	1.98	0.46
12:A:834:HIS:HA	12:A:837:LYS:HE3	1.98	0.46
13:B:827:ILE:HD11	13:B:870:ILE:HD11	1.97	0.46
13:B:1992:GLU:HA	13:B:1995:ALA:HB3	1.97	0.46
16:E:173:ASP:OD1	16:E:173:ASP:N	2.47	0.46
34:T:354:ILE:HB	34:T:368:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:23:C:H5''	5:5:24:G:H8	1.80	0.46
8:6:56:A:OP1	12:A:675:GLN:NE2	2.49	0.46
12:A:1827:TRP:O	12:A:1830:GLN:NE2	2.39	0.46
14:C:313:GLN:O	14:C:417:ARG:NH1	2.48	0.46
28:O:24:CYS:SG	28:O:81:CYS:CB	3.01	0.46
37:W:397:ASP:OD1	37:W:397:ASP:N	2.47	0.46
40:a:71:LEU:HB2	41:b:71:LEU:HB3	1.98	0.46
2:2:167:U:O4	48:p:24:LYS:NZ	2.48	0.46
12:A:164:MET:HE2	12:A:164:MET:HB3	1.80	0.46
12:A:1277:ALA:O	12:A:1281:THR:OG1	2.27	0.46
14:C:475:MET:HE3	14:C:566:THR:HB	1.98	0.46
21:IN:19:G:H21	28:O:196:GLN:HG3	1.79	0.46
35:U:125:ALA:HB2	35:U:150:ALA:HB3	1.97	0.46
46:n:32:ARG:HB3	46:n:41:VAL:HG12	1.98	0.46
5:5:91:U:O2'	42:j:61:ARG:NH2	2.49	0.45
12:A:1808:PHE:HB2	12:A:1817:LEU:HD11	1.98	0.45
13:B:1499:ASP:OD2	13:B:1763:ARG:NH1	2.45	0.45
24:L:276:PRO:HA	24:L:279:ILE:HG12	1.98	0.45
34:T:373:LYS:HD2	34:T:392:PRO:HB2	1.98	0.45
8:6:25:C:N4	28:O:39:GLU:OE2	2.47	0.45
13:B:807:GLN:H	13:B:807:GLN:HG2	1.53	0.45
14:C:401:ILE:HD11	14:C:423:PHE:HB2	1.98	0.45
24:L:192:ARG:NH2	24:L:197:GLU:OE2	2.50	0.45
4:32:54:GLY:O	35:U:174:ASN:ND2	2.47	0.45
12:A:1784:ASN:HD22	12:A:1897:LEU:HD12	1.82	0.45
13:B:1338:THR:O	13:B:1342:SER:OG	2.30	0.45
19:H:494:LEU:HD11	19:H:547:VAL:HG13	1.98	0.45
35:U:161:PHE:HB2	35:U:166:LYS:HG3	1.98	0.45
42:j:21:ASN:ND2	42:j:23:THR:OG1	2.50	0.45
8:6:19:C:H1'	26:N:95:GLN:HG3	1.99	0.45
13:B:2041:LEU:HB2	13:B:2088:ALA:HB3	1.97	0.45
19:H:544:LEU:HD11	19:H:578:SER:HB2	1.99	0.45
1:1:78:GLU:HA	1:1:81:VAL:HG22	1.99	0.45
13:B:1382:MET:HG3	13:B:1652:TRP:CG	2.51	0.45
14:C:85:ASP:OD1	14:C:85:ASP:N	2.49	0.45
14:C:924:GLN:HB3	14:C:928:HIS:HB2	1.97	0.45
24:L:28:LYS:HB2	24:L:28:LYS:HE3	1.71	0.45
24:L:67:GLU:OE1	24:L:91:ARG:NH2	2.45	0.45
35:U:124:GLY:HA3	35:U:149:ILE:HG23	1.99	0.45
43:k:43:LEU:HD23	43:k:110:LEU:HD21	1.99	0.45
44:l:88:GLN:HA	46:n:60:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:750:TRP:HH2	12:A:781:ARG:HB3	1.82	0.45
27:NO:108:GLN:O	27:NO:112:ARG:N	2.41	0.45
32:S:23:ILE:HD13	32:S:139:VAL:HG12	1.99	0.45
13:B:641:MET:HG3	13:B:1582:ALA:HB2	1.98	0.45
13:B:785:HIS:HB2	13:B:797:VAL:HG11	1.98	0.45
24:L:8:GLY:N	24:L:40:ARG:O	2.49	0.45
47:o:14:GLN:HE21	47:o:22:ARG:HH21	1.65	0.45
8:6:73:A:OP1	8:6:75:G:O2'	2.35	0.45
13:B:1678:ASP:OD1	13:B:1710:LYS:NZ	2.46	0.45
16:E:306:ASP:HA	37:W:143:LEU:HD22	1.99	0.45
31:R:199:MET:HE3	31:R:199:MET:HB3	1.77	0.45
34:T:435:THR:HG23	34:T:451:HIS:HD2	1.82	0.45
41:i:47:GLU:HG2	41:i:65:ARG:HB2	1.98	0.45
53:z:330:ARG:HH21	53:z:332:PRO:HA	1.82	0.45
4:32:83:LYS:HB2	4:32:83:LYS:HE3	1.80	0.45
4:32:91:ASP:OD1	4:32:94:ARG:NH2	2.44	0.45
13:B:1527:ILE:HD13	13:B:1715:LYS:HG2	1.98	0.45
16:E:58:PRO:CG	37:W:80:GLN:O	2.65	0.45
31:R:159:VAL:HG12	31:R:163:MET:HB2	1.99	0.45
37:W:505:HIS:HB2	37:W:527:ASP:HB3	1.98	0.45
40:a:23:ASN:N	40:a:67:LYS:O	2.49	0.45
14:C:295:ASP:N	14:C:295:ASP:OD1	2.50	0.45
26:N:5:LYS:NZ	26:N:83:TYR:OH	2.49	0.45
28:O:169:VAL:HG13	37:W:216:LEU:HD22	1.98	0.45
39:Z:124:LEU:O	39:Z:128:LYS:N	2.49	0.45
44:l:69:LYS:HD2	44:l:69:LYS:HA	1.82	0.45
12:A:50:LYS:HB3	12:A:53:PHE:HB2	1.99	0.44
12:A:1781:ASP:OD1	12:A:1864:THR:OG1	2.35	0.44
31:R:235:ARG:NH1	31:R:241:GLU:OE1	2.42	0.44
37:W:520:MET:HE3	37:W:520:MET:HB3	1.78	0.44
8:6:46:G:OP1	24:L:169:ARG:NH1	2.45	0.44
12:A:1057:ARG:NH1	12:A:1060:GLU:OE1	2.50	0.44
13:B:294:LYS:HE3	13:B:333:LEU:HD11	2.00	0.44
16:E:229:TYR:HE1	16:E:231:MET:HE3	1.82	0.44
38:X:99:GLU:O	38:X:110:ARG:N	2.49	0.44
41:b:40:LEU:HD12	41:b:72:LEU:HD23	1.98	0.44
41:i:41:ILE:HD11	41:i:71:LEU:HD12	1.99	0.44
5:5:12:U:OP1	12:A:224:THR:OG1	2.29	0.44
5:5:29:A:H2'	5:5:30:A:H8	1.82	0.44
12:A:718:ARG:NH1	31:R:252:SER:OG	2.50	0.44
12:A:1717:ASN:HD21	35:U:178:HIS:CE1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1530:PHE:O	13:B:1708:GLY:N	2.41	0.44
16:E:309:VAL:HB	16:E:323:LEU:HB2	1.99	0.44
31:R:58:PHE:HZ	31:R:71:GLN:HB3	1.82	0.44
42:c:23:THR:HG23	42:c:47:LEU:HA	1.99	0.44
2:2:104:G:OP2	45:m:67:ASN:ND2	2.51	0.44
12:A:1234:ASP:N	12:A:1234:ASP:OD1	2.48	0.44
12:A:1328:LEU:HB3	12:A:1368:LEU:HD13	1.99	0.44
13:B:1455:GLU:HG3	13:B:1457:HIS:CE1	2.52	0.44
14:C:362:THR:O	14:C:364:SER:N	2.49	0.44
42:j:47:LEU:HB2	42:j:50:ARG:HB2	1.99	0.44
12:A:62:PRO:HG3	26:N:53:HIS:CG	2.53	0.44
12:A:699:GLU:HG2	34:T:372:LYS:HD3	2.00	0.44
12:A:1880:PRO:O	35:U:285:TYR:OH	2.35	0.44
13:B:1432:TRP:HD1	13:B:1470:ILE:HD12	1.82	0.44
14:C:208:HIS:HB3	14:C:211:PHE:HD2	1.81	0.44
31:R:182:SER:O	31:R:182:SER:OG	2.34	0.44
41:b:30:THR:N	41:b:43:CYS:O	2.48	0.44
12:A:150:MET:HE3	12:A:572:PHE:HZ	1.83	0.44
12:A:265:THR:HG23	12:A:327:VAL:HG13	1.99	0.44
12:A:758:ARG:HA	12:A:758:ARG:HD2	1.69	0.44
12:A:1676:ILE:HD13	12:A:1706:ASP:HB2	2.00	0.44
13:B:787:ALA:HA	13:B:794:ARG:HD3	2.00	0.44
13:B:1120:LYS:HG2	13:B:1131:GLN:HG2	1.99	0.44
14:C:920:PRO:O	14:C:936:LYS:NZ	2.50	0.44
28:O:196:GLN:HE22	28:O:209:VAL:HG23	1.83	0.44
5:5:17:U:H3	5:5:60:G:H1	1.66	0.44
12:A:168:PRO:HG2	12:A:559:ASP:HB3	1.99	0.44
12:A:292:ASP:HB2	12:A:1136:ARG:HE	1.82	0.44
13:B:1313:ARG:HA	13:B:1313:ARG:HD2	1.91	0.44
16:E:75:HIS:ND1	16:E:77:ASN:OD1	2.51	0.44
16:E:160:ALA:HB3	16:E:166:LEU:H	1.83	0.44
16:E:231:MET:HE1	16:E:264:VAL:HG22	2.00	0.44
41:i:9:MET:HE3	41:i:9:MET:HB3	1.87	0.44
12:A:138:PRO:HB2	12:A:238:LEU:HD13	2.00	0.44
12:A:610:HIS:NE2	59:U:601:IHP:O21	2.50	0.44
12:A:1248:LEU:HD21	12:A:1295:ILE:HD13	2.00	0.44
13:B:1180:LEU:O	13:B:1215:HIS:NE2	2.49	0.44
13:B:1979:VAL:HG13	13:B:1984:ASP:HB2	2.00	0.44
16:E:69:VAL:HG11	16:E:351:LEU:HD21	2.00	0.44
42:c:61:ARG:NH1	42:c:63:ASN:OD1	2.51	0.44
46:n:41:VAL:HG22	46:n:61:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:o:81:GLU:HA	47:o:108:PRO:HB3	2.00	0.44
12:A:1681:ARG:NH2	35:U:170:TRP:O	2.45	0.44
12:A:1737:ASN:HB3	12:A:1740:LEU:HB2	2.00	0.44
12:A:1800:THR:HG21	21:IN:98:U:H5'	1.99	0.44
13:B:1342:SER:O	13:B:1486:ARG:NH2	2.51	0.44
28:O:145:ASP:OD1	28:O:145:ASP:N	2.51	0.44
37:W:527:ASP:OD1	37:W:531:LYS:N	2.51	0.44
46:g:19:LEU:HD11	46:g:40:LEU:HD12	2.00	0.44
12:A:612:ILE:HD11	12:A:632:ALA:HB3	1.99	0.43
13:B:514:LEU:HA	13:B:517:MET:HE2	2.00	0.43
14:C:496:VAL:O	14:C:547:GLY:N	2.47	0.43
26:N:94:LYS:HA	26:N:94:LYS:HD3	1.75	0.43
28:O:232:THR:HB	28:O:274:PHE:HB2	2.00	0.43
37:W:307:CYS:HB3	37:W:335:VAL:HG13	1.99	0.43
46:n:69:MET:HB3	46:n:69:MET:HE3	1.81	0.43
47:o:45:ASP:HA	47:o:66:LEU:HA	2.00	0.43
5:5:64:G:H2'	5:5:65:G:H8	1.83	0.43
13:B:1824:ILE:HD13	13:B:1922:LEU:HD23	2.00	0.43
13:B:1936:LEU:HD23	13:B:1936:LEU:HA	1.88	0.43
16:E:130:ASP:N	16:E:130:ASP:OD1	2.47	0.43
16:E:239:THR:O	16:E:290:ARG:NH1	2.50	0.43
24:L:270:LYS:HG3	24:L:278:ALA:HB2	2.00	0.43
35:U:318:THR:O	35:U:321:THR:OG1	2.36	0.43
2:2:15:U:H5'	2:2:16:U:H2'	2.00	0.43
28:O:259:ARG:HD2	28:O:273:GLN:HB3	2.00	0.43
35:U:285:TYR:HB2	35:U:292:MET:HE3	2.01	0.43
42:c:16:THR:HG23	42:c:26:HIS:HB2	2.00	0.43
42:c:74:LEU:O	43:k:98:LYS:NZ	2.50	0.43
42:j:33:ASP:OD1	42:j:33:ASP:N	2.51	0.43
47:o:48:ASP:HA	47:o:70:LEU:HB2	2.00	0.43
12:A:813:THR:HG21	12:A:996:LEU:HD22	2.01	0.43
16:E:251:LEU:HD23	16:E:291:CYS:HB3	1.99	0.43
43:k:29:LEU:HD23	43:k:32:LEU:HD12	2.00	0.43
5:5:37:G:H2'	5:5:38:C:C6	2.53	0.43
12:A:58:LYS:HE2	12:A:58:LYS:HB3	1.83	0.43
12:A:1318:THR:HB	12:A:1324:GLY:HA3	2.00	0.43
12:A:1892:PRO:HD3	12:A:1941:ARG:HH21	1.83	0.43
13:B:905:ILE:HG22	13:B:981:VAL:HG22	1.99	0.43
14:C:311:SER:HB3	14:C:316:ILE:HB	2.00	0.43
16:E:217:ILE:HB	16:E:231:MET:HB2	2.00	0.43
37:W:188:ASN:OD1	37:W:188:ASN:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:W:386:ASP:OD2	37:W:387:LYS:NZ	2.52	0.43
40:a:68:ILE:HG21	40:a:71:LEU:HD22	2.01	0.43
46:g:18:SER:N	46:g:71:GLU:O	2.48	0.43
12:A:1190:CYS:O	12:A:1273:TYR:OH	2.34	0.43
14:C:485:ASP:OD1	14:C:485:ASP:N	2.47	0.43
16:E:324:PRO:HG3	37:W:88:MET:HE1	2.00	0.43
31:R:103:ARG:NH1	31:R:110:LYS:O	2.52	0.43
43:d:87:SER:OG	43:d:88:LYS:N	2.52	0.43
43:k:45:ASN:HB2	43:k:107:ILE:HB	2.01	0.43
2:2:25:G:C6	8:6:52:U:O2	2.72	0.43
12:A:420:ARG:NH2	12:A:423:ASP:OD1	2.51	0.43
13:B:328:ILE:O	13:B:332:THR:OG1	2.37	0.43
24:L:130:PRO:HB2	24:L:131:ASN:H	1.69	0.43
28:O:261:ILE:HG23	28:O:272:ILE:HG12	2.00	0.43
37:W:270:PRO:HB3	37:W:518:PRO:HB3	2.01	0.43
12:A:259:ASP:OD1	12:A:259:ASP:N	2.51	0.43
24:L:192:ARG:HA	24:L:192:ARG:HD3	1.82	0.43
31:R:60:ASP:HB3	32:S:134:GLN:HA	2.01	0.43
34:T:267:ASP:HB3	34:T:269:GLN:HG2	1.99	0.43
37:W:190:ASP:OD1	37:W:190:ASP:N	2.42	0.43
37:W:313:ILE:HB	37:W:328:PHE:HB2	2.00	0.43
12:A:1490:PHE:O	12:A:1493:THR:OG1	2.36	0.43
12:A:1782:ASP:HB3	12:A:1841:THR:HG21	2.01	0.43
14:C:255:VAL:HG21	14:C:285:VAL:HG11	2.01	0.43
14:C:349:PHE:HZ	14:C:354:ARG:HD3	1.84	0.43
28:O:129:ASP:OD1	28:O:129:ASP:N	2.46	0.43
32:S:91:LYS:HA	32:S:91:LYS:HD3	1.92	0.43
35:U:106:VAL:HB	35:U:151:PRO:HB2	2.01	0.43
37:W:208:PRO:HG2	37:W:213:GLN:HG2	2.01	0.43
37:W:228:LYS:HD2	37:W:228:LYS:HA	1.86	0.43
42:c:17:ILE:HD12	42:c:40:LEU:HD11	2.01	0.43
41:i:39:ASN:OD1	41:i:74:GLY:N	2.51	0.43
4:32:79:LYS:O	4:32:88:ARG:NH2	2.50	0.43
4:32:80:LYS:NZ	35:U:184:GLU:OE2	2.40	0.43
12:A:947:PRO:HD2	12:A:950:LEU:HD23	2.01	0.43
12:A:1838:LYS:HB3	12:A:1871:PRO:HG2	2.00	0.43
13:B:1590:LEU:HD11	13:B:1597:LEU:HD11	2.01	0.43
13:B:2114:MET:HE3	13:B:2114:MET:HB3	1.92	0.43
16:E:313:ASP:HB3	16:E:316:SER:HB3	2.01	0.43
24:L:10:VAL:HG11	24:L:138:ARG:HD3	2.01	0.43
34:T:320:LYS:HE3	34:T:320:LYS:HB2	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:W:103:GLN:HG2	37:W:108:ARG:HD3	2.01	0.43
42:j:15:VAL:HG12	42:j:71:PRO:HD3	2.01	0.43
1:1:123:GLN:O	1:1:127:ARG:NH1	2.51	0.42
8:6:23:U:C5	26:N:118:ILE:HD12	2.54	0.42
12:A:965:VAL:O	12:A:974:ASN:ND2	2.49	0.42
12:A:1210:LYS:HE2	19:H:468:ASP:HA	2.01	0.42
12:A:1687:TYR:O	12:A:1693:SER:OG	2.31	0.42
13:B:442:TYR:HA	13:B:693:THR:H	1.84	0.42
16:E:150:HIS:CG	16:E:171:SER:HG	2.35	0.42
28:O:132:ARG:HG3	37:W:104:MET:HE1	2.00	0.42
37:W:506:MET:HE2	37:W:506:MET:HB2	1.68	0.42
41:b:48:PHE:HA	41:b:63:GLU:HA	2.01	0.42
41:i:16:ARG:HD2	41:i:16:ARG:HA	1.87	0.42
12:A:292:ASP:HB2	12:A:1136:ARG:HH21	1.84	0.42
12:A:373:ASP:OD1	12:A:373:ASP:N	2.52	0.42
12:A:977:LEU:HD22	12:A:1097:ILE:HD12	2.01	0.42
12:A:982:GLU:HG3	12:A:1169:GLN:H	1.84	0.42
13:B:1346:VAL:HG12	13:B:1510:SER:HB2	2.01	0.42
28:O:125:ILE:O	28:O:128:SER:OG	2.35	0.42
37:W:239:THR:HG21	37:W:364:GLY:HA3	2.01	0.42
12:A:101:LYS:NZ	12:A:104:GLU:OE2	2.41	0.42
12:A:1088:PHE:HD1	12:A:1097:ILE:HG23	1.84	0.42
12:A:1370:ARG:NH1	19:H:504:GLU:OE1	2.52	0.42
12:A:1783:THR:HG22	12:A:1865:ARG:HD2	2.02	0.42
12:A:1868:MET:HB3	12:A:1868:MET:HE3	1.75	0.42
16:E:116:HIS:HB3	16:E:159:PRO:HD3	2.01	0.42
30:Q:827:THR:HA	30:Q:1136:GLN:HA	2.02	0.42
31:R:272:GLY:O	31:R:276:GLN:NE2	2.50	0.42
37:W:284:TRP:HE1	37:W:322:ARG:HB3	1.84	0.42
37:W:398:LYS:HD2	37:W:418:LEU:HA	2.02	0.42
44:l:44:GLU:OE2	44:l:71:ARG:NH2	2.51	0.42
12:A:845:ARG:HD3	12:A:845:ARG:HA	1.83	0.42
35:U:122:ASN:HB2	35:U:130:LYS:HG3	2.01	0.42
42:c:70:LEU:HB3	42:c:74:LEU:HD12	2.02	0.42
40:h:73:LEU:HD11	41:i:71:LEU:HB2	2.02	0.42
1:1:44:LYS:O	44:l:26:GLN:NE2	2.47	0.42
12:A:1249:MET:HE3	12:A:1249:MET:HB2	1.89	0.42
12:A:1321:GLU:OE1	35:U:66:TYR:OH	2.31	0.42
16:E:133:VAL:HB	16:E:147:LEU:HB2	2.01	0.42
44:l:14:MET:HE3	44:l:14:MET:HB2	1.80	0.42
12:A:1698:PRO:HB2	35:U:182:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1761:PRO:HD2	35:U:293:ARG:HH12	1.83	0.42
14:C:221:ILE:O	14:C:549:TRP:NE1	2.51	0.42
26:N:131:ILE:HD12	28:O:177:GLU:HB3	2.02	0.42
37:W:297:PHE:HB2	37:W:303:LEU:HB2	2.01	0.42
34:T:214:PRO:HG3	34:T:256:THR:HG22	2.02	0.42
35:U:86:ARG:HA	35:U:86:ARG:HD3	1.81	0.42
37:W:137:TYR:OH	37:W:165:LEU:N	2.53	0.42
37:W:392:VAL:HG22	37:W:400:ILE:HG22	2.02	0.42
45:m:6:ASN:HB2	45:m:9:PRO:HD2	2.00	0.42
4:32:58:ARG:NH2	35:U:177:GLU:OE1	2.52	0.42
5:5:100:U:H2'	5:5:101:U:H6	1.85	0.42
12:A:436:PRO:HG2	12:A:439:GLN:HG3	2.01	0.42
12:A:1786:TYR:HE1	12:A:1802:PRO:HB3	1.85	0.42
13:B:711:LYS:HE2	13:B:868:ILE:HG12	2.00	0.42
14:C:137:HIS:HA	14:C:238:ASN:HB3	2.01	0.42
19:H:628:ILE:HA	19:H:640:THR:HG21	2.01	0.42
29:P:195:LYS:HA	29:P:195:LYS:HD3	1.91	0.42
32:S:76:SER:OG	32:S:77:ILE:N	2.53	0.42
44:e:77:ILE:HG22	45:f:73:ARG:HB3	2.01	0.42
46:n:18:SER:HA	46:n:28:GLN:HG2	2.02	0.42
12:A:155:LYS:NZ	12:A:617:ASN:OD1	2.38	0.42
12:A:1189:MET:HB2	12:A:1189:MET:HE3	1.77	0.42
13:B:690:VAL:HG13	13:B:870:ILE:HA	2.01	0.42
14:C:559:ILE:HD13	14:C:559:ILE:HG21	1.88	0.42
16:E:61:LEU:HD11	16:E:350:ARG:HD2	2.02	0.42
18:F:655:TRP:HB3	18:F:660:GLN:HE21	1.85	0.42
18:F:686:ILE:HG12	18:F:715:PRO:HB3	2.01	0.42
28:O:22:ILE:H	28:O:82:GLN:HE21	1.68	0.42
34:T:213:GLU:HG3	34:T:218:TRP:CE2	2.55	0.42
34:T:257:ARG:NE	34:T:301:ASP:OD2	2.51	0.42
34:T:270:VAL:HG21	34:T:305:THR:HG21	2.01	0.42
34:T:394:ASN:HB2	34:T:396:LYS:HZ2	1.85	0.42
35:U:135:GLU:OE1	35:U:138:ARG:NH1	2.52	0.42
42:c:9:LYS:HB3	42:c:9:LYS:HE3	1.87	0.42
44:e:30:ARG:NH2	44:e:60:ASP:O	2.42	0.42
45:m:66:CYS:SG	45:m:67:ASN:N	2.92	0.42
12:A:670:LYS:HB3	12:A:670:LYS:HE2	1.83	0.42
12:A:1764:SER:OG	12:A:1765:SER:N	2.52	0.42
12:A:1889:LEU:HD23	12:A:1891:LEU:HD11	2.01	0.42
13:B:1018:PHE:HB2	13:B:1092:MET:HE1	2.02	0.42
13:B:1572:THR:HB	13:B:1645:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:O:74:CYS:O	28:O:202:TYR:OH	2.32	0.42
34:T:346:ILE:HD12	34:T:356:LEU:HG	2.01	0.42
37:W:296:LEU:HD23	37:W:296:LEU:HA	1.90	0.42
42:c:25:VAL:HG11	42:c:60:ILE:HD11	2.01	0.42
2:2:168:A:C8	40:h:47:THR:HG21	2.55	0.41
12:A:583:ALA:HA	12:A:605:CYS:HB3	2.01	0.41
12:A:1784:ASN:HB3	12:A:1787:ARG:HD3	2.02	0.41
13:B:606:THR:HA	13:B:609:VAL:HG22	2.02	0.41
13:B:1651:CYS:O	13:B:1690:HIS:NE2	2.46	0.41
13:B:1777:SER:OG	13:B:1778:HIS:N	2.52	0.41
34:T:295:ASP:OD2	34:T:338:CYS:N	2.52	0.41
43:d:60:ASP:OD1	43:d:60:ASP:N	2.53	0.41
12:A:345:PRO:HG3	35:U:140:VAL:HG22	2.03	0.41
12:A:881:ILE:HD11	12:A:917:ILE:HG22	2.03	0.41
12:A:941:LYS:HG3	12:A:951:LEU:HD22	2.02	0.41
13:B:729:LYS:HD2	13:B:729:LYS:HA	1.88	0.41
13:B:1005:LEU:HD22	13:B:1107:LEU:HD21	2.02	0.41
34:T:399:LYS:HB2	34:T:406:ILE:HD11	2.02	0.41
45:m:11:LEU:HD23	45:m:11:LEU:HA	1.94	0.41
12:A:1526:LEU:HD12	12:A:1529:ILE:HD12	2.02	0.41
12:A:1768:TYR:OH	35:U:344:GLN:NE2	2.44	0.41
13:B:1072:LEU:HB2	13:B:1078:MET:HG2	2.02	0.41
14:C:476:CYS:HB3	14:C:565:ILE:HB	2.02	0.41
16:E:75:HIS:NE2	16:E:121:GLY:O	2.52	0.41
16:E:155:ASN:O	16:E:290:ARG:NH2	2.53	0.41
24:L:24:MET:HB3	31:R:261:THR:HG23	2.02	0.41
34:T:216:ASN:HD22	34:T:216:ASN:HA	1.62	0.41
1:1:130:LYS:HB2	1:1:130:LYS:HE2	1.86	0.41
12:A:89:LEU:HD23	12:A:89:LEU:HA	1.84	0.41
13:B:2043:ARG:HB3	13:B:2086:GLN:HA	2.02	0.41
26:N:8:ARG:HD2	26:N:8:ARG:HA	1.93	0.41
40:h:40:ASN:ND2	40:h:65:GLY:H	2.16	0.41
42:j:38:THR:HG21	42:j:68:PHE:HZ	1.86	0.41
2:2:159:U:H2'	2:2:160:A:H8	1.86	0.41
12:A:696:MET:HE3	12:A:696:MET:HB2	1.88	0.41
13:B:307:VAL:HG22	13:B:318:ILE:HD13	2.02	0.41
13:B:1034:LYS:HA	13:B:1037:LEU:HB2	2.02	0.41
13:B:1367:MET:HE2	13:B:1367:MET:HB3	1.99	0.41
28:O:73:THR:HG23	28:O:125:ILE:HD12	2.01	0.41
32:S:58:LYS:HE2	32:S:144:MET:HG2	2.02	0.41
35:U:130:LYS:HB3	35:U:130:LYS:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:W:443:ARG:NH1	37:W:452:ASP:OD2	2.50	0.41
41:b:86:PRO:HA	41:b:87:PRO:HD3	1.91	0.41
12:A:274:PRO:HG3	33:SR:1:MET:HB3	2.02	0.41
12:A:775:ASN:HA	12:A:778:ARG:HB2	2.02	0.41
12:A:791:GLN:OE1	12:A:1028:TYR:N	2.51	0.41
12:A:828:PRO:HB2	12:A:882:LYS:HE2	2.03	0.41
12:A:942:PRO:HG2	12:A:1438:VAL:HG22	2.03	0.41
12:A:1434:LYS:O	12:A:1439:ARG:NH2	2.51	0.41
13:B:502:CYS:HB3	13:B:654:THR:HA	2.02	0.41
13:B:898:PRO:HA	13:B:960:ALA:HB1	2.03	0.41
29:P:187:ARG:HA	29:P:187:ARG:HD3	1.91	0.41
37:W:552:VAL:HG13	37:W:571:TRP:CD1	2.52	0.41
40:a:82:MET:HB3	40:a:82:MET:HE2	1.81	0.41
43:d:46:CYS:HB3	43:d:50:LYS:HB2	2.03	0.41
40:h:69:ARG:NH1	41:i:23:ASP:OD2	2.54	0.41
47:o:144:VAL:HG22	47:o:149:LYS:HG3	2.03	0.41
12:A:661:GLU:HA	31:R:213:LYS:HA	2.02	0.41
12:A:1443:LYS:HA	12:A:1443:LYS:HD3	1.87	0.41
19:H:576:THR:H	19:H:579:SER:HB3	1.86	0.41
19:H:648:LYS:HA	19:H:648:LYS:HD3	1.89	0.41
28:O:114:LYS:HB3	28:O:114:LYS:HE2	1.88	0.41
32:S:6:PRO:O	32:S:37:LYS:NZ	2.54	0.41
48:p:45:THR:O	48:p:49:ARG:N	2.53	0.41
13:B:1011:GLU:HG2	13:B:1110:LYS:HG2	2.03	0.41
16:E:280:ASN:HA	16:E:310:TYR:HE2	1.85	0.41
24:L:214:ILE:HB	24:L:217:GLU:HB3	2.03	0.41
37:W:463:SER:HB3	37:W:481:MET:HE2	2.03	0.41
37:W:477:ALA:HA	37:W:487:ILE:HD13	2.03	0.41
40:a:28:TYR:HB3	40:a:46:ILE:HD12	2.02	0.41
45:f:67:ASN:OD1	45:f:67:ASN:N	2.53	0.41
12:A:96:PRO:HG3	12:A:648:LEU:HB3	2.02	0.41
12:A:1713:SER:OG	12:A:1714:ALA:N	2.54	0.41
16:E:321:TYR:OH	16:E:356:ILE:O	2.33	0.41
18:F:682:TYR:CZ	18:F:712:ALA:HB2	2.56	0.41
24:L:49:ARG:NH1	24:L:133:GLU:O	2.44	0.41
24:L:49:ARG:NH1	24:L:135:LYS:O	2.44	0.41
28:O:173:CYS:HB3	37:W:206:ALA:HB3	2.02	0.41
28:O:239:LEU:HD22	28:O:270:ALA:HB2	2.02	0.41
31:R:152:GLU:HA	31:R:155:VAL:HG22	2.03	0.41
31:R:158:LYS:NZ	34:T:322:SER:O	2.54	0.41
35:U:121:GLU:HG2	35:U:130:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:W:127:GLN:O	37:W:131:THR:OG1	2.30	0.41
37:W:476:LEU:HG	37:W:490:ALA:HB2	2.02	0.41
41:b:18:ARG:HB2	41:b:83:GLU:HB2	2.03	0.41
41:b:35:ASP:OD1	41:b:35:ASP:N	2.53	0.41
42:j:79:LEU:HD12	42:j:80:LEU:HG	2.01	0.41
46:n:13:MET:HE3	46:n:13:MET:HB3	1.85	0.41
12:A:114:ARG:HG2	12:A:116:VAL:HG13	2.02	0.41
12:A:1732:LYS:HG2	35:U:278:LEU:HA	2.02	0.41
13:B:1741:VAL:HG13	13:B:1817:MET:HE3	2.03	0.41
19:H:584:LYS:HG3	19:H:634:ILE:HG23	2.02	0.41
41:i:83:GLU:O	47:o:43:GLN:NE2	2.41	0.41
50:w:226:LEU:HA	50:w:242:ASP:HA	2.03	0.41
12:A:1735:LYS:HE2	12:A:1735:LYS:HB3	1.89	0.40
13:B:1542:MET:HE2	13:B:1542:MET:HB3	1.96	0.40
13:B:1550:ILE:HG23	13:B:1559:VAL:HG21	2.03	0.40
21:IN:18:A:OP2	28:O:163:HIS:NE2	2.46	0.40
44:l:78:MET:HB3	45:m:72:ILE:HG23	2.03	0.40
1:1:90:TYR:O	1:1:94:ASP:N	2.53	0.40
2:2:99:U:H1'	46:n:65:ASN:HB3	2.03	0.40
5:5:111:A:H5'	40:a:51:ARG:HH12	1.86	0.40
8:6:48:A:OP2	24:L:33:ARG:NH2	2.52	0.40
12:A:142:SER:HA	12:A:242:ALA:HB2	2.02	0.40
12:A:902:TYR:HB2	12:A:1242:ASN:HB3	2.03	0.40
12:A:1729:ALA:HA	35:U:278:LEU:HD22	2.03	0.40
13:B:725:VAL:HG12	13:B:727:SER:H	1.86	0.40
13:B:1534:HIS:CE1	13:B:1536:GLN:HB2	2.56	0.40
16:E:263:ASP:OD1	16:E:263:ASP:N	2.43	0.40
19:H:560:LEU:HD23	19:H:560:LEU:HA	1.91	0.40
21:IN:88:G:N7	21:IN:89:U:N3	2.69	0.40
22:J:326:VAL:HA	22:J:329:ALA:HB3	2.03	0.40
37:W:434:VAL:HG21	37:W:476:LEU:HD11	2.03	0.40
44:l:78:MET:HE2	45:m:11:LEU:HD11	2.02	0.40
2:2:22:U:H3	8:6:53:A:H61	1.69	0.40
2:2:24:A:H8	2:2:24:A:H2'	1.79	0.40
5:5:24:G:O2'	5:5:26:A:N7	2.54	0.40
12:A:543:ALA:HB2	12:A:651:TRP:HB3	2.03	0.40
12:A:1289:VAL:HG13	12:A:1357:MET:HG3	2.02	0.40
12:A:1683:LYS:HD3	12:A:1683:LYS:HA	1.74	0.40
13:B:696:LYS:HB3	13:B:698:ILE:HG12	2.04	0.40
13:B:1737:ASN:HB2	13:B:1796:LEU:HD21	2.04	0.40
13:B:1815:LEU:HD11	13:B:1833:SER:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:T:377:ALA:O	34:T:390:GLY:N	2.48	0.40
42:c:16:THR:HB	42:c:69:ILE:HB	2.02	0.40
40:h:46:ILE:HD13	40:h:46:ILE:HA	1.95	0.40
46:n:35:ASP:OD2	46:n:39:ASN:ND2	2.54	0.40
46:n:48:MET:HE2	46:n:48:MET:HB3	1.95	0.40
48:p:15:ASN:HD21	48:p:17:LYS:HB2	1.86	0.40
13:B:1923:ILE:HD13	13:B:1946:ALA:HA	2.03	0.40
14:C:174:GLU:HG2	14:C:181:ILE:H	1.87	0.40
31:R:316:GLU:HA	31:R:319:LYS:HG2	2.02	0.40
37:W:218:GLU:HG2	37:W:222:LYS:HE3	2.04	0.40
37:W:464:MET:HE1	37:W:486:LEU:HD12	2.03	0.40
37:W:513:GLN:HE22	37:W:557:VAL:HG22	1.87	0.40
43:d:43:LEU:HD23	43:d:110:LEU:HD21	2.01	0.40
46:n:7:PRO:HB2	46:n:9:LEU:HG	2.03	0.40
48:p:15:ASN:HD22	48:p:18:ILE:HG23	1.86	0.40
8:6:22:A:C4	37:W:130:ARG:HD2	2.56	0.40
8:6:40:U:H2'	8:6:41:A:H8	1.85	0.40
18:F:643:PRO:HD2	18:F:719:ILE:HD11	2.02	0.40
24:L:16:ASP:OD2	24:L:49:ARG:NH2	2.49	0.40
34:T:261:LEU:HB2	34:T:275:LEU:HD11	2.03	0.40
49:s:91:THR:O	49:s:95:GLN:N	2.46	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	1	121/184 (66%)	114 (94%)	6 (5%)	1 (1%)	16	45
3	3	78/476 (16%)	78 (100%)	0	0	100	100
4	32	58/112 (52%)	56 (97%)	2 (3%)	0	100	100
6	50	222/339 (66%)	214 (96%)	6 (3%)	2 (1%)	14	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	56	99/222 (45%)	98 (99%)	1 (1%)	0	100	100
9	7	388/411 (94%)	377 (97%)	10 (3%)	1 (0%)	36	65
10	8	89/174 (51%)	87 (98%)	1 (1%)	1 (1%)	11	39
11	9	142/146 (97%)	139 (98%)	3 (2%)	0	100	100
12	A	2244/2335 (96%)	2107 (94%)	134 (6%)	3 (0%)	48	75
13	B	1856/2136 (87%)	1785 (96%)	68 (4%)	3 (0%)	43	71
14	C	892/972 (92%)	816 (92%)	72 (8%)	4 (0%)	30	60
15	D	68/285 (24%)	67 (98%)	1 (2%)	0	100	100
16	E	301/357 (84%)	281 (93%)	20 (7%)	0	100	100
18	F	120/758 (16%)	109 (91%)	11 (9%)	0	100	100
19	H	455/908 (50%)	439 (96%)	15 (3%)	1 (0%)	43	71
20	I	725/855 (85%)	710 (98%)	15 (2%)	0	100	100
22	J	600/848 (71%)	572 (95%)	26 (4%)	2 (0%)	36	65
23	K	187/225 (83%)	174 (93%)	12 (6%)	1 (0%)	24	55
24	L	545/802 (68%)	524 (96%)	20 (4%)	1 (0%)	43	71
25	M	222/243 (91%)	215 (97%)	6 (3%)	1 (0%)	24	55
26	N	142/144 (99%)	131 (92%)	9 (6%)	2 (1%)	9	33
27	NO	168/301 (56%)	158 (94%)	8 (5%)	2 (1%)	10	37
28	O	287/420 (68%)	271 (94%)	16 (6%)	0	100	100
29	P	100/229 (44%)	94 (94%)	6 (6%)	0	100	100
30	Q	1304/1485 (88%)	1267 (97%)	34 (3%)	3 (0%)	43	71
31	R	322/536 (60%)	296 (92%)	25 (8%)	1 (0%)	36	65
32	S	162/166 (98%)	148 (91%)	14 (9%)	0	100	100
33	SR	66/2752 (2%)	59 (89%)	7 (11%)	0	100	100
34	T	359/514 (70%)	340 (95%)	16 (4%)	3 (1%)	16	45
35	U	291/586 (50%)	272 (94%)	18 (6%)	1 (0%)	36	65
36	V	727/1220 (60%)	708 (97%)	18 (2%)	1 (0%)	48	75
37	W	511/579 (88%)	462 (90%)	49 (10%)	0	100	100
38	X	62/451 (14%)	59 (95%)	3 (5%)	0	100	100
39	Z	49/166 (30%)	49 (100%)	0	0	100	100
40	a	82/126 (65%)	77 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	h	81/126 (64%)	76 (94%)	5 (6%)	0	100	100
41	b	81/240 (34%)	80 (99%)	1 (1%)	0	100	100
41	i	80/240 (33%)	74 (92%)	6 (8%)	0	100	100
42	c	78/119 (66%)	73 (94%)	5 (6%)	0	100	100
42	j	78/119 (66%)	76 (97%)	2 (3%)	0	100	100
43	d	85/118 (72%)	82 (96%)	3 (4%)	0	100	100
43	k	91/118 (77%)	88 (97%)	3 (3%)	0	100	100
44	e	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
44	l	79/92 (86%)	77 (98%)	2 (2%)	0	100	100
45	f	70/86 (81%)	70 (100%)	0	0	100	100
45	m	70/86 (81%)	69 (99%)	1 (1%)	0	100	100
46	g	71/76 (93%)	67 (94%)	4 (6%)	0	100	100
46	n	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
47	o	160/255 (63%)	146 (91%)	14 (9%)	0	100	100
48	p	90/225 (40%)	88 (98%)	2 (2%)	0	100	100
49	q	99/504 (20%)	98 (99%)	1 (1%)	0	100	100
49	r	115/504 (23%)	111 (96%)	4 (4%)	0	100	100
49	s	130/504 (26%)	125 (96%)	4 (3%)	1 (1%)	16	45
49	t	99/504 (20%)	96 (97%)	2 (2%)	1 (1%)	12	40
50	w	522/646 (81%)	504 (97%)	18 (3%)	0	100	100
51	x	120/289 (42%)	118 (98%)	2 (2%)	0	100	100
52	y	77/301 (26%)	75 (97%)	2 (3%)	0	100	100
53	z	66/415 (16%)	64 (97%)	1 (2%)	1 (2%)	8	32
All	All	16534/28198 (59%)	15754 (95%)	743 (4%)	37 (0%)	44	71

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	50	285	HIS
13	B	1584	ILE
30	Q	1078	LEU
49	s	65	PRO
9	7	340	GLY
10	8	115	GLY

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Mol	Chain	Res	Type
13	B	957	VAL
22	J	329	ALA
26	N	135	THR
27	NO	126	LEU
30	Q	279	LEU
30	Q	406	LEU
6	50	294	ALA
12	A	1636	LYS
13	B	831	THR
14	C	363	SER
22	J	179	VAL
24	L	215	PRO
34	T	456	PRO
14	C	702	ASN
27	NO	50	LEU
31	R	10	PRO
34	T	458	SER
14	C	821	LEU
19	H	501	ARG
23	K	62	GLU
36	V	640	GLN
53	z	411	GLY
12	A	295	GLU
25	M	117	ARG
26	N	128	VAL
12	A	370	PRO
49	t	15	PRO
14	C	97	VAL
1	1	47	PRO
35	U	267	ILE
34	T	32	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	106/157 (68%)	106 (100%)	0	100	100
4	32	54/99 (54%)	54 (100%)	0	100	100
12	A	1732/2108 (82%)	1721 (99%)	11 (1%)	78	81
13	B	1662/1908 (87%)	1496 (90%)	166 (10%)	7	27
14	C	109/866 (13%)	106 (97%)	3 (3%)	38	62
16	E	87/300 (29%)	86 (99%)	1 (1%)	65	76
18	F	100/655 (15%)	100 (100%)	0	100	100
24	L	233/709 (33%)	228 (98%)	5 (2%)	47	67
26	N	130/130 (100%)	130 (100%)	0	100	100
28	O	258/361 (72%)	256 (99%)	2 (1%)	73	79
29	P	94/203 (46%)	92 (98%)	2 (2%)	47	67
31	R	275/457 (60%)	275 (100%)	0	100	100
32	S	133/134 (99%)	132 (99%)	1 (1%)	73	79
33	SR	21/2432 (1%)	21 (100%)	0	100	100
34	T	316/441 (72%)	308 (98%)	8 (2%)	42	64
35	U	258/520 (50%)	251 (97%)	7 (3%)	39	63
37	W	451/502 (90%)	447 (99%)	4 (1%)	70	78
40	a	74/101 (73%)	74 (100%)	0	100	100
40	h	73/101 (72%)	73 (100%)	0	100	100
41	b	68/177 (38%)	67 (98%)	1 (2%)	57	72
41	i	75/177 (42%)	75 (100%)	0	100	100
42	c	75/101 (74%)	75 (100%)	0	100	100
42	j	75/101 (74%)	75 (100%)	0	100	100
43	d	85/110 (77%)	84 (99%)	1 (1%)	63	75
43	k	91/110 (83%)	91 (100%)	0	100	100
44	e	74/84 (88%)	74 (100%)	0	100	100
44	l	76/84 (90%)	76 (100%)	0	100	100
45	f	61/74 (82%)	60 (98%)	1 (2%)	55	72
45	m	61/74 (82%)	61 (100%)	0	100	100
46	g	63/66 (96%)	62 (98%)	1 (2%)	55	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	n	63/66 (96%)	61 (97%)	2 (3%)	34	60
47	o	139/218 (64%)	137 (99%)	2 (1%)	59	73
48	p	81/195 (42%)	81 (100%)	0	100	100
53	z	25/366 (7%)	25 (100%)	0	100	100
All	All	7278/14187 (51%)	7060 (97%)	218 (3%)	37	61

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	A	395	THR
12	A	413	LEU
12	A	668	VAL
12	A	767	VAL
12	A	1175	VAL
12	A	1210	LYS
12	A	1346	THR
12	A	1359	HIS
12	A	1438	VAL
12	A	1868	MET
12	A	2011	ILE
13	B	130	ASP
13	B	159	LEU
13	B	164	THR
13	B	172	LEU
13	B	290	LEU
13	B	332	THR
13	B	334	LEU
13	B	409	LEU
13	B	410	ASP
13	B	414	LEU
13	B	420	SER
13	B	436	ARG
13	B	446	HIS
13	B	447	VAL
13	B	451	LYS
13	B	464	VAL
13	B	467	LEU
13	B	481	LEU
13	B	488	LEU
13	B	495	THR
13	B	500	LEU

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Mol	Chain	Res	Type
13	B	501	LEU
13	B	505	THR
13	B	525	ILE
13	B	533	VAL
13	B	547	LEU
13	B	550	GLU
13	B	566	VAL
13	B	572	ASP
13	B	576	CYS
13	B	584	GLN
13	B	591	GLU
13	B	592	LYS
13	B	595	ILE
13	B	602	GLU
13	B	604	THR
13	B	614	LEU
13	B	643	GLN
13	B	659	GLU
13	B	673	LEU
13	B	690	VAL
13	B	693	THR
13	B	712	ILE
13	B	719	ASN
13	B	728	ARG
13	B	743	LEU
13	B	759	THR
13	B	772	LEU
13	B	773	GLU
13	B	782	PHE
13	B	791	ARG
13	B	806	ILE
13	B	807	GLN
13	B	810	VAL
13	B	815	LEU
13	B	820	ASN
13	B	849	ILE
13	B	850	LEU
13	B	852	MET
13	B	855	ARG
13	B	868	ILE
13	B	869	LEU
13	B	877	GLN

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Mol	Chain	Res	Type
13	B	885	GLN
13	B	887	LEU
13	B	894	VAL
13	B	897	LEU
13	B	900	MET
13	B	901	LEU
13	B	906	VAL
13	B	910	VAL
13	B	920	LEU
13	B	942	ASP
13	B	957	VAL
13	B	972	TYR
13	B	975	LYS
13	B	981	VAL
13	B	992	TYR
13	B	1016	ARG
13	B	1020	LEU
13	B	1023	GLU
13	B	1051	SER
13	B	1053	GLU
13	B	1062	LEU
13	B	1063	LEU
13	B	1087	SER
13	B	1100	LEU
13	B	1135	LEU
13	B	1143	ILE
13	B	1153	LEU
13	B	1165	ILE
13	B	1166	ARG
13	B	1186	LEU
13	B	1204	ILE
13	B	1224	LEU
13	B	1225	VAL
13	B	1228	VAL
13	B	1234	LEU
13	B	1240	LEU
13	B	1241	LEU
13	B	1242	LYS
13	B	1301	LEU
13	B	1312	LEU
13	B	1320	LEU
13	B	1368	LEU

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Mol	Chain	Res	Type
13	B	1380	THR
13	B	1408	LEU
13	B	1413	SER
13	B	1419	LEU
13	B	1421	LYS
13	B	1430	GLU
13	B	1436	SER
13	B	1442	ARG
13	B	1443	LYS
13	B	1455	GLU
13	B	1456	VAL
13	B	1474	MET
13	B	1477	ILE
13	B	1480	GLN
13	B	1481	ILE
13	B	1482	GLU
13	B	1492	SER
13	B	1494	LEU
13	B	1567	LYS
13	B	1655	ASN
13	B	1682	TYR
13	B	1707	GLN
13	B	1728	LEU
13	B	1734	ASP
13	B	1742	THR
13	B	1762	ARG
13	B	1781	LEU
13	B	1788	LEU
13	B	1796	LEU
13	B	1817	MET
13	B	1829	ILE
13	B	1831	LEU
13	B	1834	MET
13	B	1840	THR
13	B	1854	GLU
13	B	1865	ASP
13	B	1936	LEU
13	B	1956	LYS
13	B	1970	HIS
13	B	1996	LEU
13	B	1997	LEU
13	B	1999	LEU

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Mol	Chain	Res	Type
13	B	2000	THR
13	B	2017	ILE
13	B	2026	LYS
13	B	2027	ASP
13	B	2029	ILE
13	B	2030	ARG
13	B	2031	SER
13	B	2047	VAL
13	B	2055	LEU
13	B	2070	ASP
13	B	2082	LEU
13	B	2084	LEU
13	B	2092	LEU
13	B	2102	HIS
13	B	2105	THR
13	B	2109	MET
13	B	2114	MET
13	B	2121	LYS
13	B	2125	ASP
14	C	129	ILE
14	C	132	VAL
14	C	189	VAL
16	E	333	VAL
24	L	14	THR
24	L	54	LEU
24	L	142	ILE
24	L	147	ASP
24	L	208	VAL
28	O	115	GLU
28	O	147	LEU
29	P	3	THR
29	P	23	LEU
32	S	139	VAL
34	T	29	ASN
34	T	220	VAL
34	T	261	LEU
34	T	302	VAL
34	T	323	VAL
34	T	364	THR
34	T	418	THR
34	T	456	PRO
35	U	181	ILE

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Mol	Chain	Res	Type
35	U	321	THR
35	U	329	LEU
35	U	352	LEU
35	U	353	LEU
35	U	373	LEU
35	U	390	LEU
37	W	335	VAL
37	W	375	VAL
37	W	436	THR
37	W	552	VAL
41	b	114	ILE
43	d	31	VAL
45	f	41	ASN
46	g	61	VAL
46	n	43	ASP
46	n	46	VAL
47	o	106	LEU
47	o	120	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (132) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	116	ASN
12	A	160	HIS
12	A	270	ASN
12	A	512	ASN
12	A	664	HIS
12	A	691	HIS
12	A	755	HIS
12	A	775	ASN
12	A	792	HIS
12	A	793	ASN
12	A	834	HIS
12	A	884	HIS
12	A	994	ASN
12	A	1014	ASN
12	A	1023	ASN
12	A	1096	HIS
12	A	1121	ASN
12	A	1159	ASN
12	A	1169	GLN
12	A	1188	ASN

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Mol	Chain	Res	Type
12	A	1227	GLN
12	A	1246	GLN
12	A	1304	ASN
12	A	1337	GLN
12	A	1359	HIS
12	A	1363	GLN
12	A	1468	ASN
12	A	1476	GLN
12	A	1487	HIS
12	A	1563	HIS
12	A	1586	HIS
12	A	1599	GLN
12	A	1717	ASN
12	A	1835	GLN
12	A	1946	ASN
13	B	269	GLN
13	B	425	ASN
13	B	549	GLN
13	B	574	GLN
13	B	805	HIS
13	B	912	ASN
13	B	1101	ASN
13	B	1113	ASN
13	B	1191	GLN
13	B	1236	HIS
13	B	1337	ASN
13	B	1388	GLN
13	B	1449	ASN
13	B	1528	GLN
13	B	1568	GLN
13	B	1659	HIS
13	B	1692	ASN
13	B	1733	HIS
13	B	1747	ASN
13	B	1766	GLN
13	B	1772	ASN
13	B	1877	HIS
13	B	1880	ASN
13	B	1898	HIS
13	B	1998	GLN
13	B	2012	ASN
14	C	60	HIS

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Mol	Chain	Res	Type
14	C	82	GLN
14	C	137	HIS
14	C	175	GLN
18	F	656	ASN
18	F	660	GLN
24	L	161	ASN
24	L	175	GLN
28	O	82	GLN
28	O	289	ASN
29	P	56	ASN
31	R	84	ASN
31	R	133	GLN
31	R	194	GLN
31	R	320	HIS
32	S	10	GLN
32	S	140	ASN
32	S	148	ASN
32	S	150	GLN
33	SR	20	GLN
34	T	216	ASN
34	T	269	GLN
34	T	278	ASN
34	T	417	ASN
34	T	446	ASN
34	T	451	HIS
34	T	500	HIS
35	U	84	HIS
35	U	85	GLN
35	U	92	GLN
35	U	122	ASN
35	U	154	HIS
35	U	156	GLN
35	U	171	ASN
35	U	178	HIS
35	U	381	HIS
37	W	80	GLN
37	W	127	GLN
37	W	128	GLN
37	W	145	ASN
37	W	147	GLN
37	W	242	HIS
37	W	250	GLN

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Mol	Chain	Res	Type
37	W	402	GLN
37	W	412	GLN
37	W	462	HIS
37	W	479	GLN
37	W	513	GLN
37	W	533	ASN
41	b	76	ASN
43	d	69	ASN
43	d	91	ASN
46	g	53	GLN
40	h	16	HIS
40	h	40	ASN
40	h	45	ASN
40	h	60	GLN
41	i	76	ASN
42	j	21	ASN
42	j	54	GLN
42	j	64	ASN
43	k	49	ASN
43	k	62	HIS
45	m	43	GLN
45	m	68	ASN
46	n	26	HIS
46	n	55	ASN
46	n	56	ASN
47	o	14	GLN
47	o	72	ASN
48	p	15	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	EX	14/14 (100%)	5 (35%)	1 (7%)
2	2	117/187 (62%)	30 (25%)	5 (4%)
21	IN	39/113 (34%)	19 (48%)	3 (7%)
5	5	90/116 (77%)	23 (25%)	2 (2%)
8	6	96/106 (90%)	37 (38%)	5 (5%)
All	All	356/536 (66%)	114 (32%)	16 (4%)

All (114) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	16	U
2	2	17	U
2	2	19	G
2	2	20	G
2	2	24	A
2	2	25	G
2	2	29	A
2	2	30	A
2	2	32	U
2	2	40	C
2	2	41	U
2	2	46	U
2	2	47	U
2	2	51	A
2	2	53	U
2	2	54	U
2	2	96	A
2	2	97	G
2	2	99	U
2	2	100	U
2	2	101	U
2	2	102	U
2	2	103	U
2	2	104	G
2	2	105	G
2	2	106	A
2	2	109	U
2	2	157	G
2	2	171	U
2	2	178	A
5	5	10	U
5	5	11	U
5	5	20	G
5	5	35	U
5	5	36	C
5	5	38	C
5	5	39	C
5	5	42	U
5	5	45	C
5	5	47	A
5	5	52	U
5	5	53	U
5	5	57	G

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Mol	Chain	Res	Type
5	5	69	A
5	5	89	U
5	5	91	U
5	5	92	U
5	5	93	U
5	5	94	U
5	5	95	G
5	5	96	A
5	5	104	C
5	5	115	U
8	6	6	C
8	6	7	G
8	6	8	C
8	6	9	U
8	6	11	C
8	6	12	G
8	6	26	U
8	6	28	A
8	6	29	A
8	6	33	G
8	6	34	G
8	6	35	A
8	6	37	C
8	6	38	G
8	6	41	A
8	6	44	G
8	6	45	A
8	6	46	G
8	6	48	A
8	6	49	G
8	6	51	U
8	6	54	G
8	6	56	A
8	6	58	G
8	6	59	G
8	6	60	C
8	6	61	C
8	6	62	C
8	6	67	G
8	6	68	C
8	6	74	U
8	6	79	C

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Mol	Chain	Res	Type
8	6	81	C
8	6	84	A
8	6	85	U
8	6	87	C
8	6	88	G
17	EX	-11	G
17	EX	-7	C
17	EX	-6	C
17	EX	1	C
17	EX	2	U
21	IN	5	G
21	IN	14	A
21	IN	16	G
21	IN	17	U
21	IN	21	A
21	IN	87	U
21	IN	88	G
21	IN	89	U
21	IN	90	C
21	IN	91	A
21	IN	92	U
21	IN	93	A
21	IN	95	U
21	IN	96	U
21	IN	97	A
21	IN	98	U
21	IN	99	C
21	IN	112	A
21	IN	113	G

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	39	U
2	2	46	U
2	2	95	A
2	2	102	U
2	2	105	G
5	5	92	U
5	5	95	G
8	6	5	U
8	6	33	G

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Mol	Chain	Res	Type
8	6	37	C
8	6	50	A
8	6	58	G
17	EX	-12	G
21	IN	90	C
21	IN	95	U
21	IN	98	U

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

2 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	$\# Z > 2$
31	SEP	R	232	31	8,9,10	1.64	1 (12%)	7,12,14	1.06	0
31	SEP	R	224	31	8,9,10	1.52	1 (12%)	7,12,14	0.89	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
31	SEP	R	232	31	-	3/6/8/10	-
31	SEP	R	224	31	-	1/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R	232	SEP	P-O1P	3.52	1.61	1.50
31	R	224	SEP	P-O1P	3.21	1.60	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	R	232	SEP	CB-OG-P-O1P
31	R	232	SEP	CB-OG-P-O2P
31	R	232	SEP	CB-OG-P-O3P
31	R	224	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 13 are monoatomic - leaving 3 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$
59	IHP	U	601	-	36,36,36	1.38	6 (16%)	60,60,60	1.17	7 (11%)
56	ATP	7	501	54	32,33,33	0.53	1 (3%)	48,52,52	0.72	1 (2%)
57	GTP	C	1500	-	33,34,34	1.00	1 (3%)	50,54,54	1.72	10 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	IHP	U	601	-	-	6/30/54/54	0/1/1/1
56	ATP	7	501	54	-	0/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	GTP	C	1500	-	-	1/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	U	601	IHP	P3-O13	2.76	1.64	1.59
59	U	601	IHP	P6-O16	2.64	1.64	1.59
59	U	601	IHP	P2-O12	2.41	1.63	1.59
57	C	1500	GTP	C5-N7	-2.34	1.34	1.39
59	U	601	IHP	P5-O15	2.30	1.63	1.59
56	7	501	ATP	PB-O3B	-2.29	1.57	1.59
59	U	601	IHP	P1-O11	2.24	1.63	1.59
59	U	601	IHP	P4-O14	2.17	1.63	1.59

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	C	1500	GTP	C5-C4-N3	-5.09	120.29	128.39
57	C	1500	GTP	C2-N3-C4	4.37	119.83	112.30
57	C	1500	GTP	N9-C4-N3	3.58	133.11	125.95
57	C	1500	GTP	C2-N1-C6	-3.31	119.11	125.11
59	U	601	IHP	C6-C1-C2	-3.04	103.75	110.43
57	C	1500	GTP	O2G-PG-O3B	3.01	114.72	104.64
59	U	601	IHP	P3-O13-C3	-2.97	115.51	123.43
59	U	601	IHP	C5-C4-C3	2.95	116.89	110.43
57	C	1500	GTP	N9-C8-N7	-2.91	108.00	113.40
57	C	1500	GTP	O6-C6-C5	-2.90	118.88	126.53
57	C	1500	GTP	C5-C6-N1	2.81	120.40	113.25
56	7	501	ATP	O5'-PA-O1A	-2.79	97.88	108.94
57	C	1500	GTP	O2B-PB-O3A	2.77	114.76	107.27
57	C	1500	GTP	C8-N7-C5	2.57	108.84	104.26
59	U	601	IHP	P1-O11-C1	-2.46	116.87	123.43
59	U	601	IHP	P4-O14-C4	-2.21	117.54	123.43
59	U	601	IHP	P6-O16-C6	-2.12	117.77	123.43
59	U	601	IHP	C4-C3-C2	2.06	114.95	110.43

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	U	601	IHP	C5-O15-P5-O25

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Mol	Chain	Res	Type	Atoms
59	U	601	IHP	C1-O11-P1-O31
59	U	601	IHP	C2-O12-P2-O42
59	U	601	IHP	C6-O16-P6-O46
59	U	601	IHP	C1-O11-P1-O41
59	U	601	IHP	C6-O16-P6-O26
57	C	1500	GTP	PB-O3A-PA-O2A

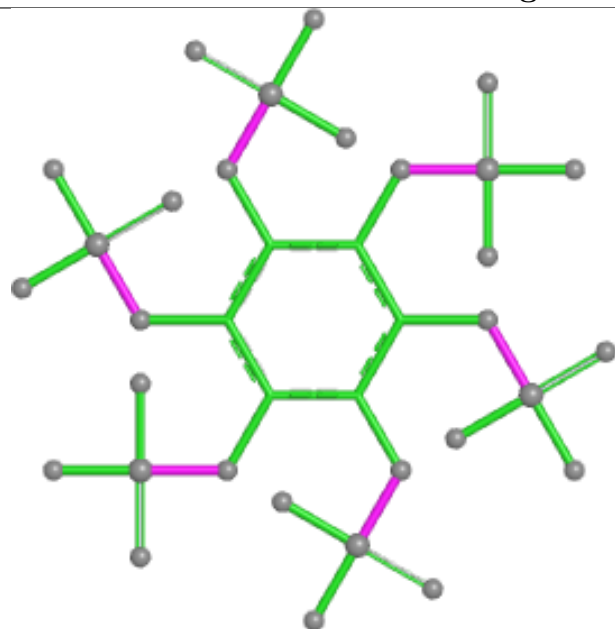
There are no ring outliers.

1 monomer is involved in 1 short contact:

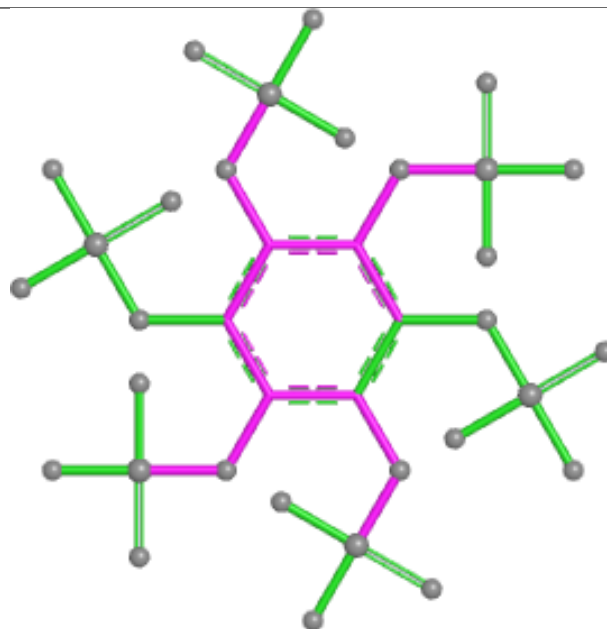
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	U	601	IHP	1	0

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.

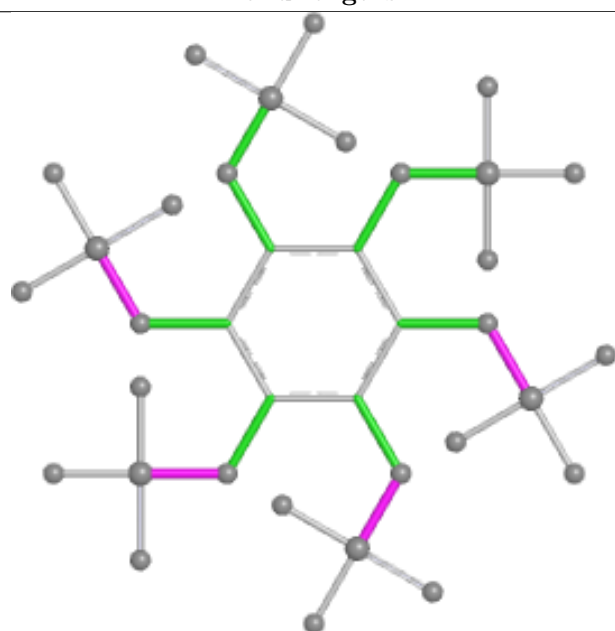
Ligand IHP U 601



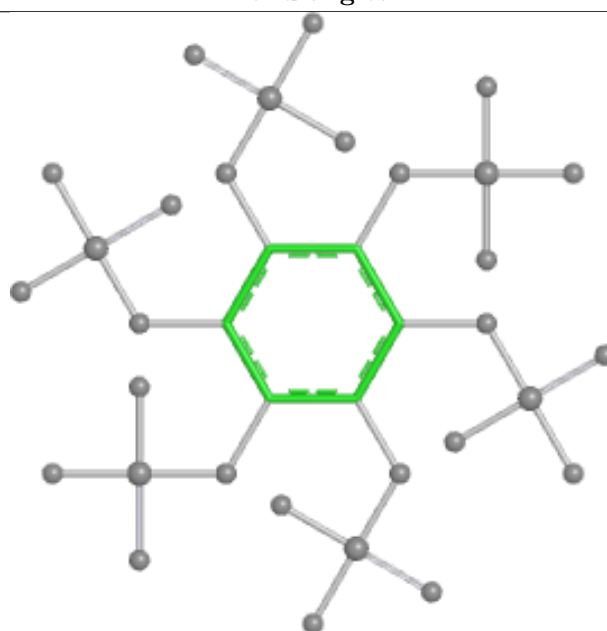
Bond lengths



Bond angles

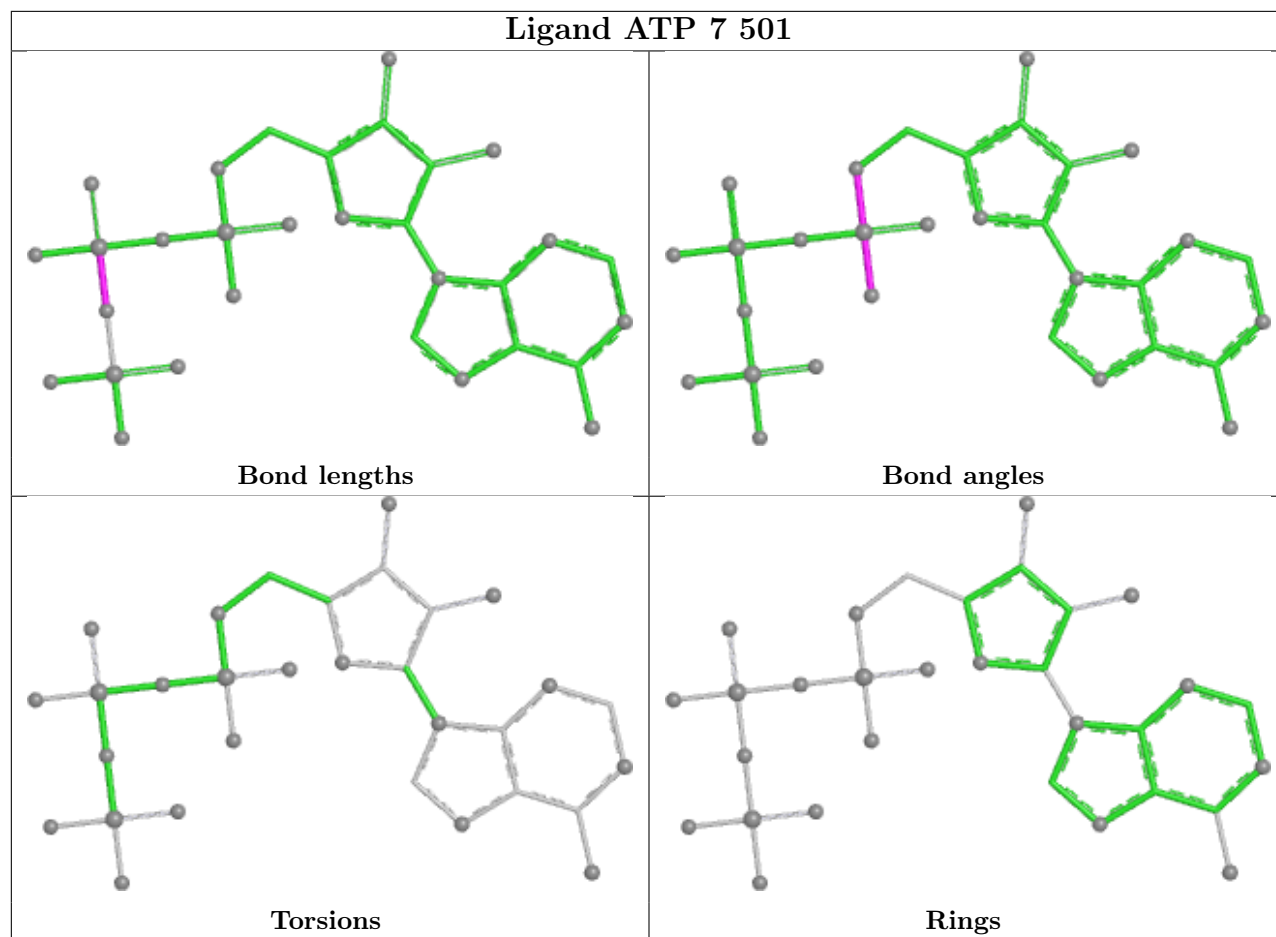


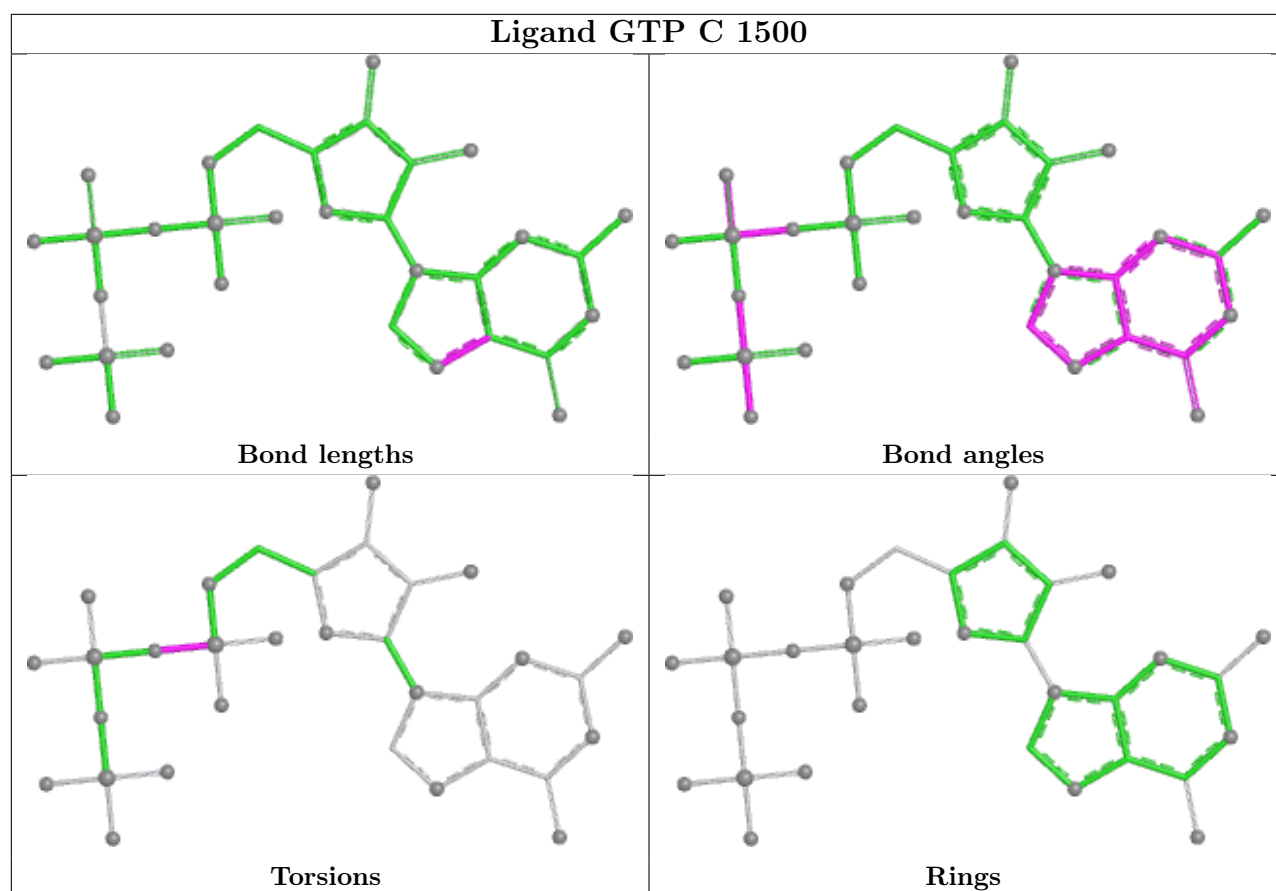
Torsions



Rings

Ligand ATP 7 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

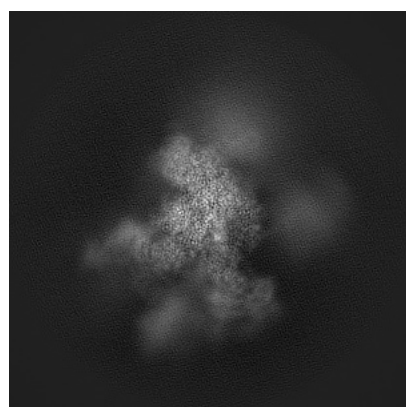
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4525. These allow visual inspection of the internal detail of the map and identification of artifacts.

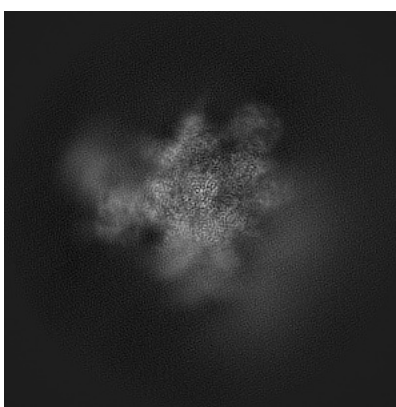
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

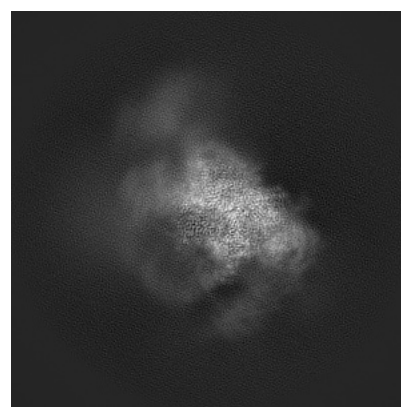
6.1.1 Primary map



X



Y

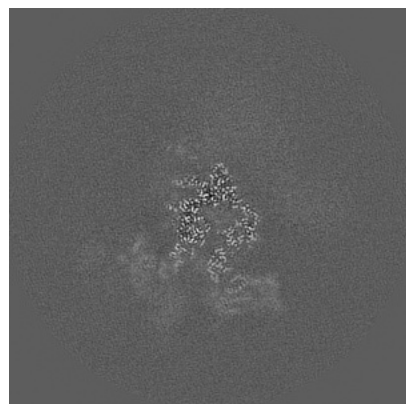


Z

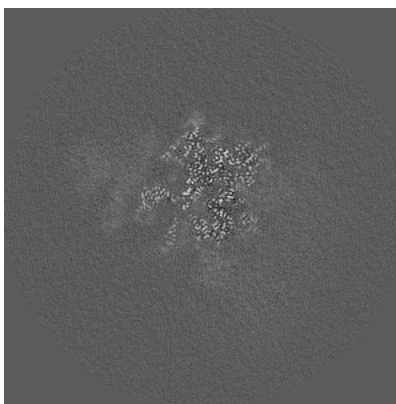
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

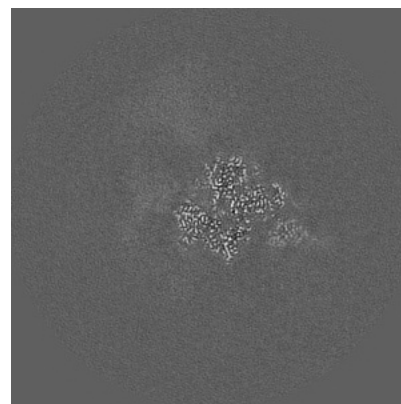
6.2.1 Primary map



X Index: 205



Y Index: 205

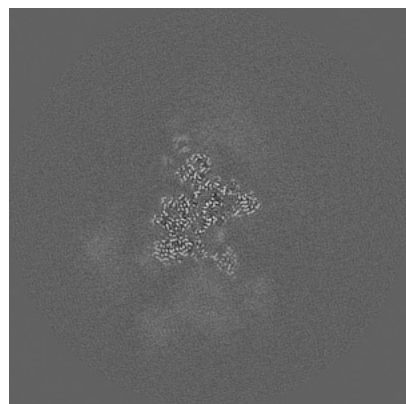


Z Index: 205

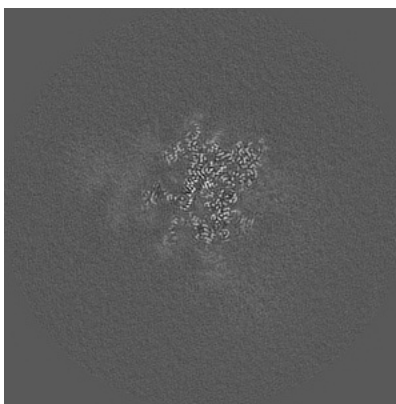
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

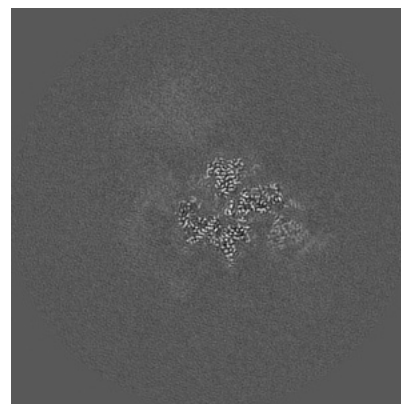
6.3.1 Primary map



X Index: 231



Y Index: 203

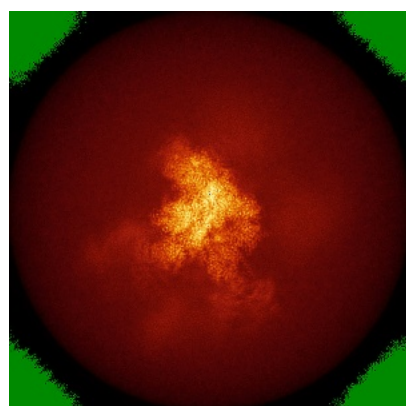


Z Index: 202

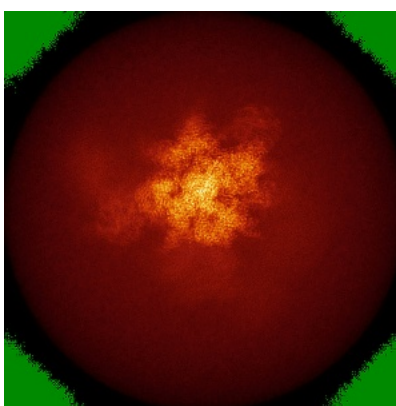
The images above show the largest variance slices of the map in three orthogonal directions.

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

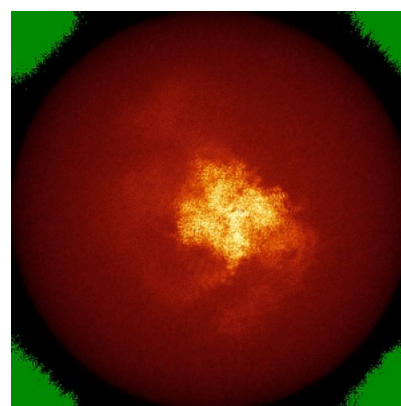
6.4.1 Primary map



X



Y



Z

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 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

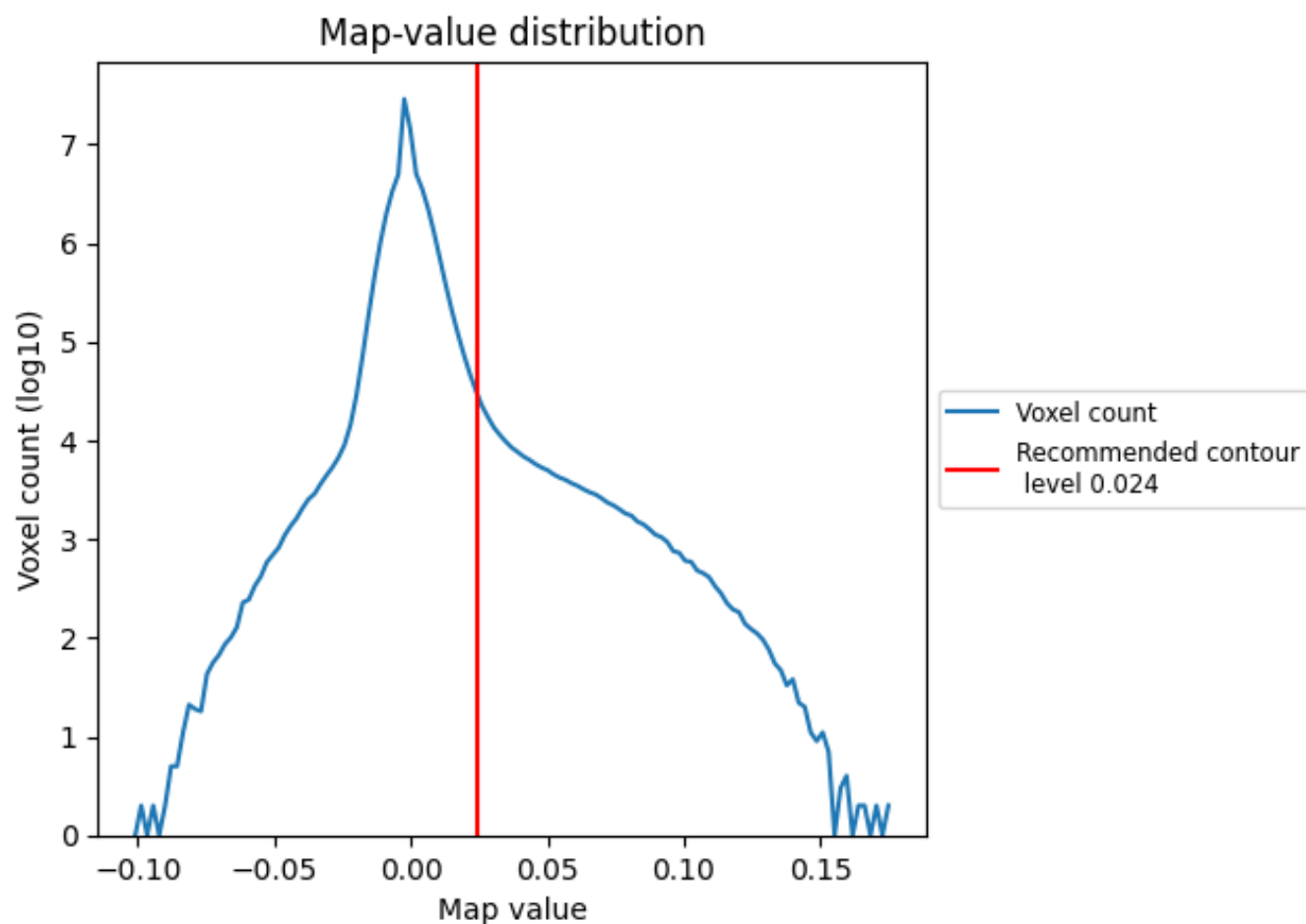
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

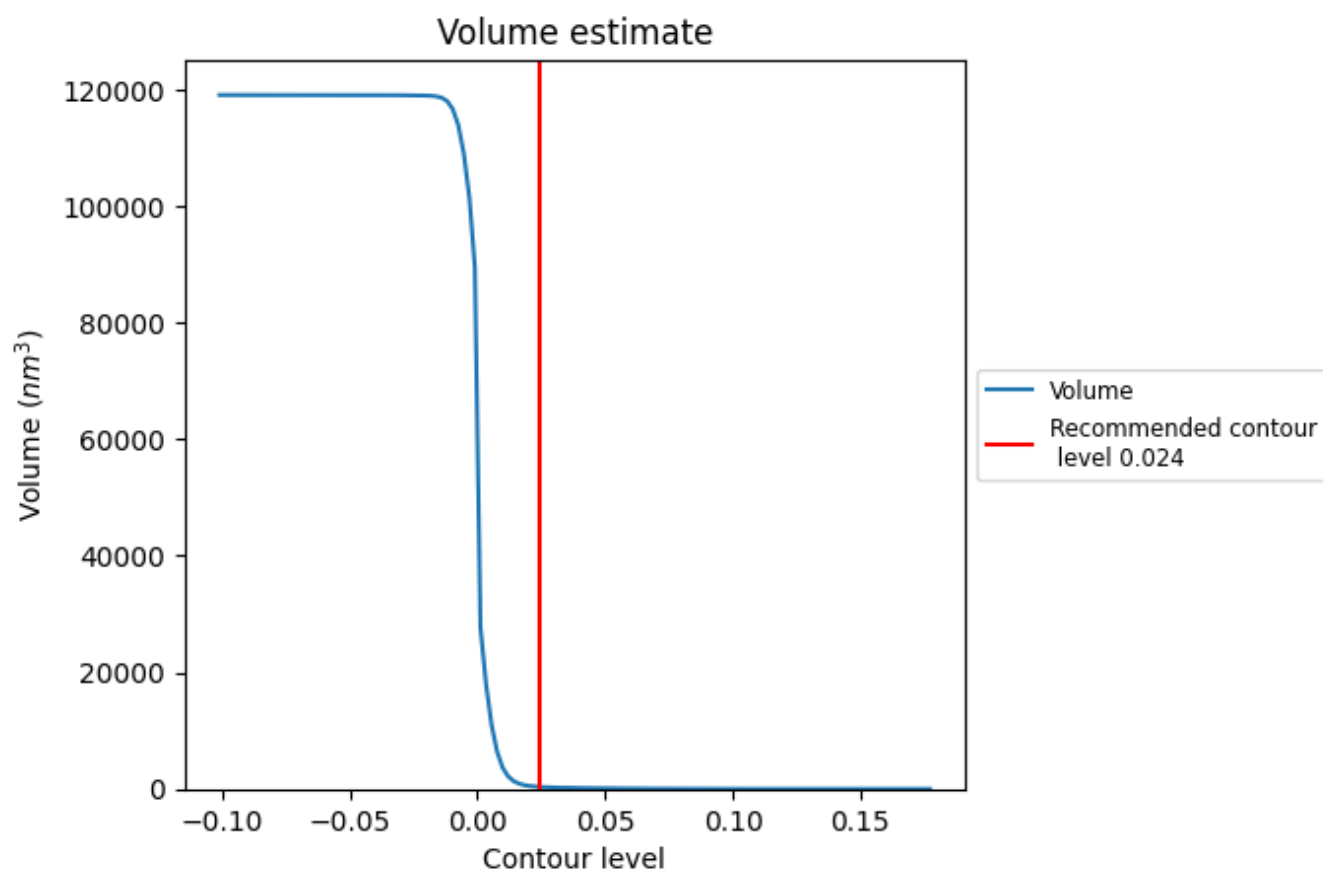
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

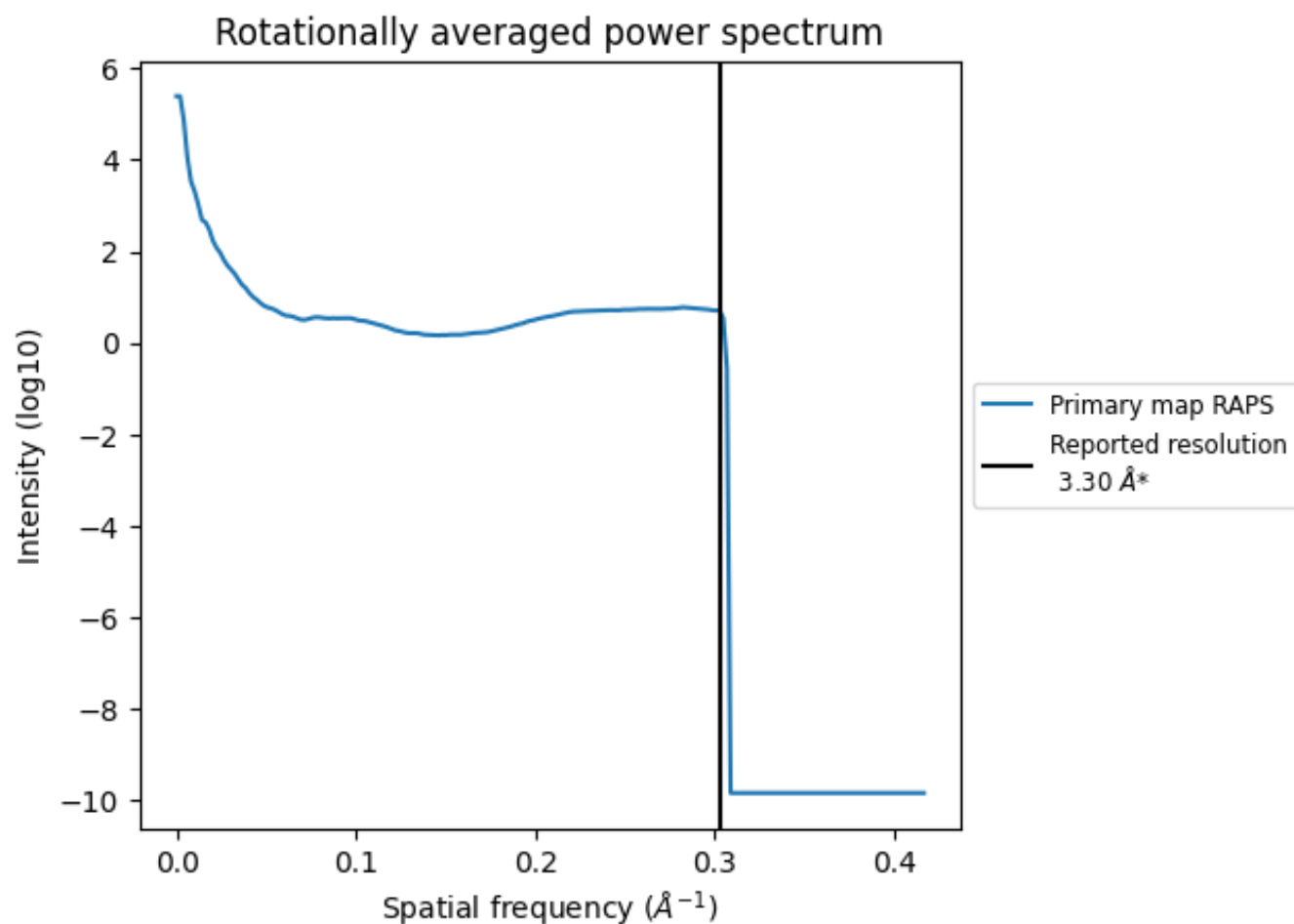
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 356 nm³; this corresponds to an approximate mass of 321 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 ⓘ

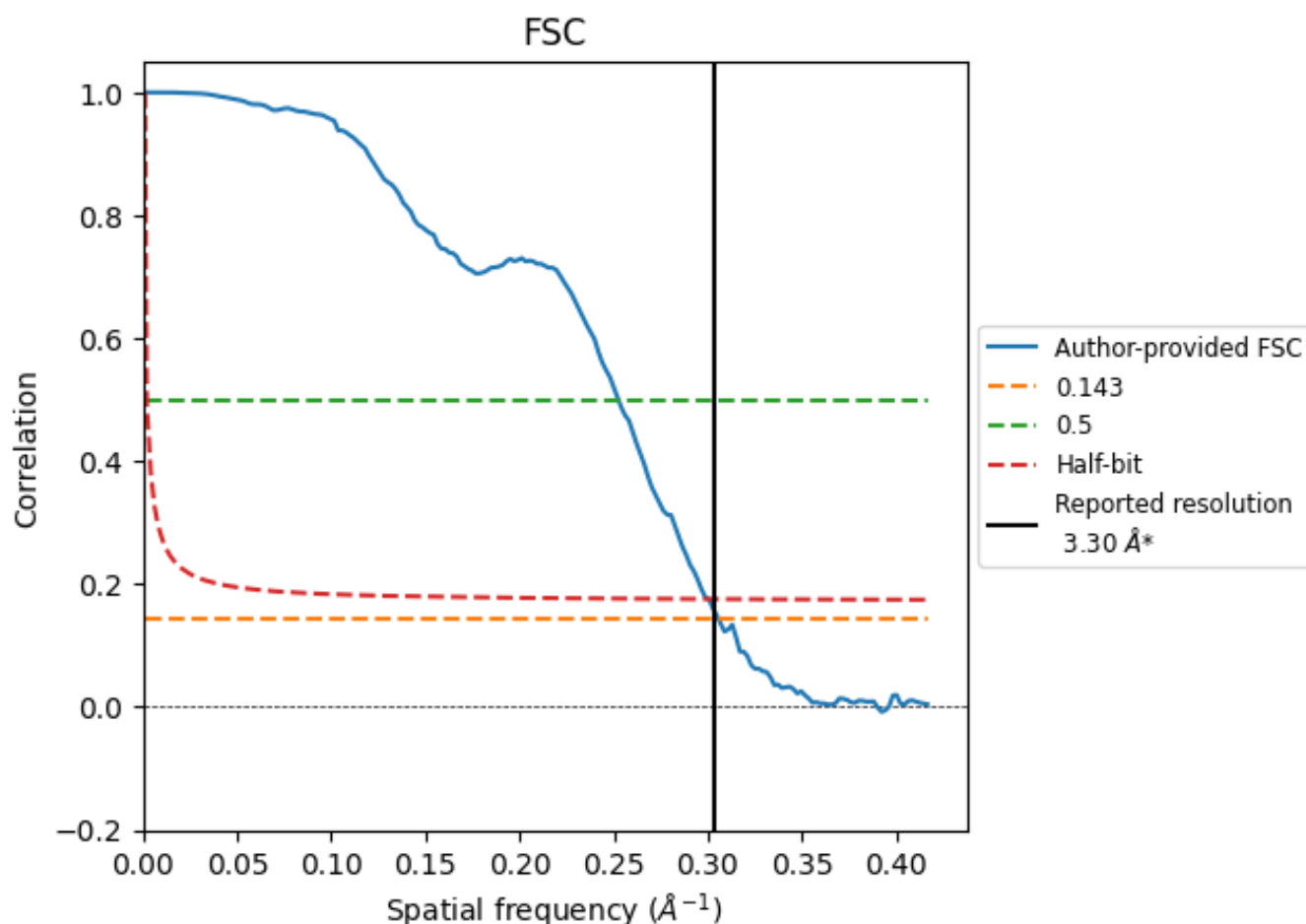


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

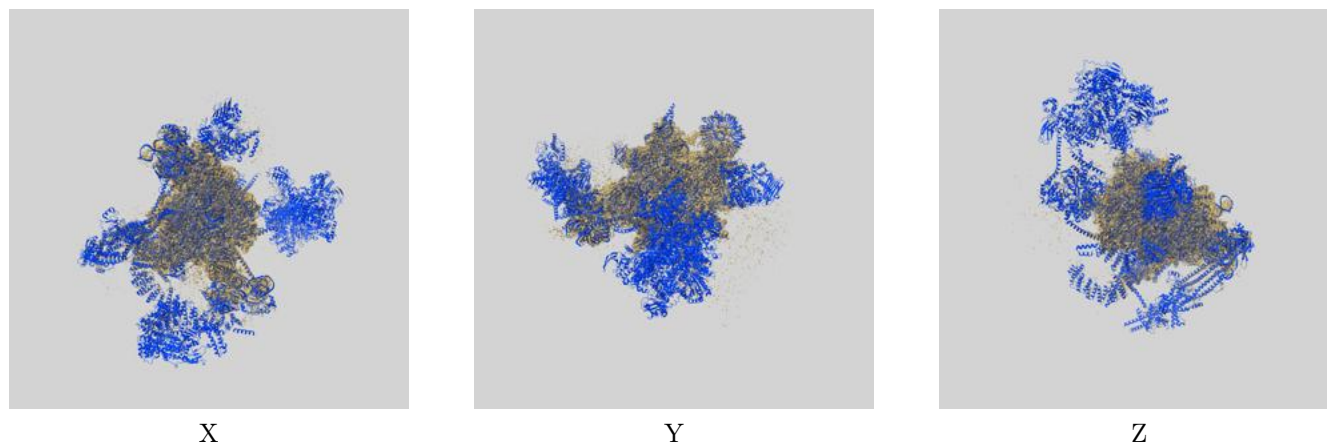
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.96	3.33
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

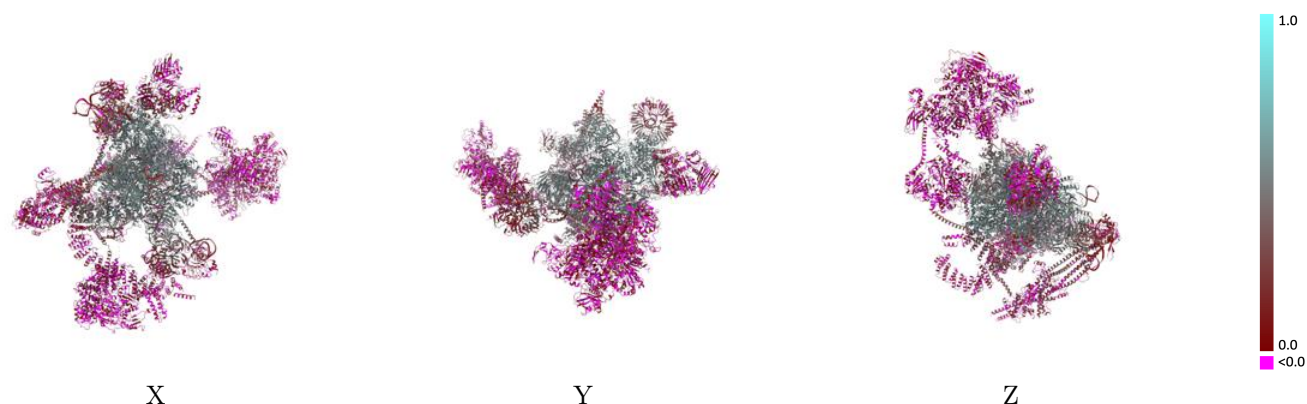
This section contains information regarding the fit between EMDB map EMD-4525 and PDB model 9FMD. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.024 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](#)

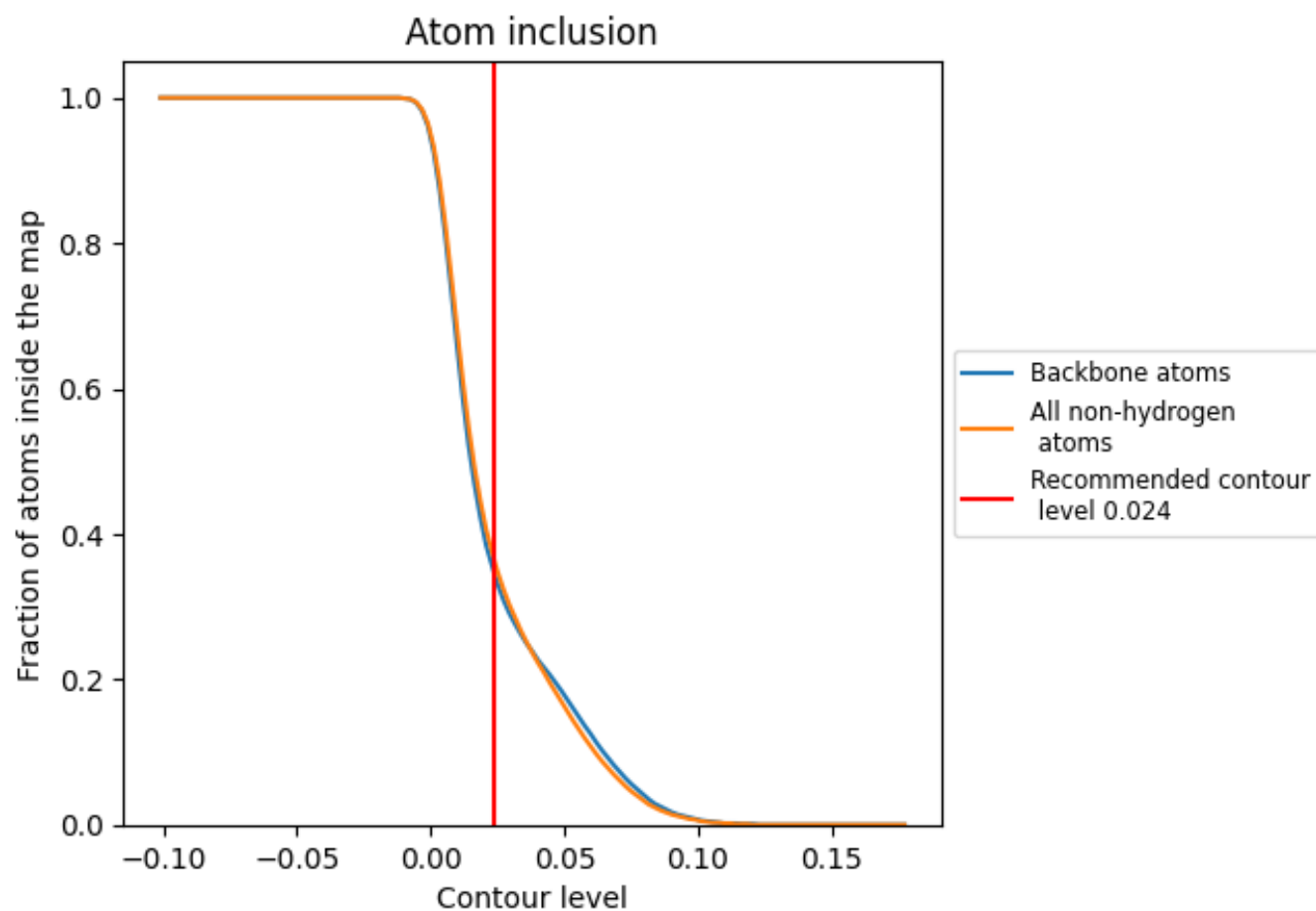


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 34% of all backbone atoms, 36% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3610	 0.2970
1	 0.4060	 0.3790
2	 0.4230	 0.3010
3	 0.1450	 0.2540
32	 0.5850	 0.5090
5	 0.6140	 0.3800
50	 0.0160	 0.0940
56	 0.0000	 -0.0080
6	 0.7320	 0.4560
7	 0.0070	 0.1120
8	 0.0000	 0.0520
9	 0.0000	 0.0410
A	 0.7230	 0.5070
B	 0.0010	 0.0490
C	 0.6930	 0.4900
D	 0.0000	 0.0980
E	 0.6300	 0.4760
EX	 0.8110	 0.5290
F	 0.6270	 0.4680
H	 0.4160	 0.3540
I	 0.0520	 0.1010
IN	 0.5690	 0.3790
J	 0.3950	 0.2850
K	 0.1140	 0.1850
L	 0.4040	 0.3650
M	 0.4950	 0.3800
N	 0.7540	 0.5330
NO	 0.0010	 0.1280
O	 0.5190	 0.4460
P	 0.6500	 0.5200
Q	 0.0020	 0.0540
R	 0.5290	 0.4400
S	 0.5720	 0.4560
SR	 0.4090	 0.3340
T	 0.7370	 0.5080



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Chain	Atom inclusion	Q-score
U	 0.5840	 0.4550
V	 0.0500	 0.0800
W	 0.6700	 0.5010
X	 0.0150	 0.1510
Z	 0.0150	 0.0570
a	 0.4280	 0.4140
b	 0.3330	 0.3340
c	 0.1390	 0.2060
d	 0.0680	 0.1490
e	 0.0870	 0.1940
f	 0.0470	 0.1550
g	 0.2180	 0.3330
h	 0.3940	 0.3510
i	 0.2460	 0.2900
j	 0.1200	 0.2020
k	 0.0810	 0.1590
l	 0.2390	 0.2770
m	 0.1380	 0.1770
n	 0.3620	 0.3680
o	 0.0250	 0.1130
p	 0.0560	 0.1370
q	 0.0430	 0.1160
r	 0.0180	 0.0870
s	 0.0290	 0.1440
t	 0.0120	 0.0880
w	 0.0000	 0.0340
x	 0.0270	 0.1330
y	 0.0060	 0.1250
z	 0.3540	 0.2970