



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 04:03 PM UTC

PDB ID : 8RO1 / pdb_00008ro1
EMDB ID : EMD-19398
Title : Structure of the C. elegans Intron Lariat Spliceosome double-primed for dis-assembly (ILS")
Authors : Vorlaender, M.K.; Rothe, P.; Plaschka, C.
Deposited on : 2024-01-11
Resolution : 3.00 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

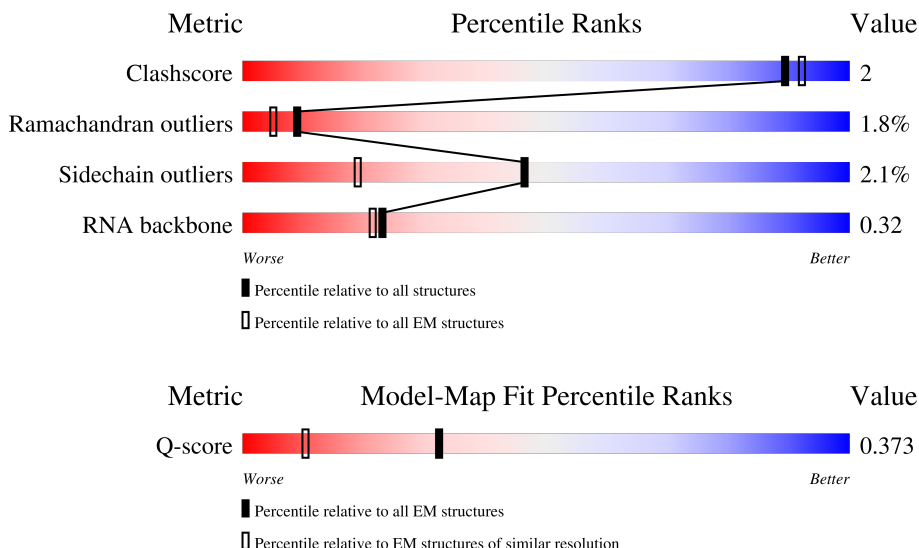
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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.



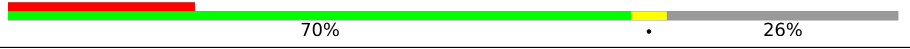
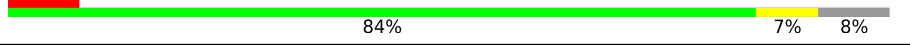
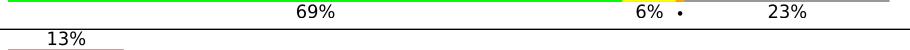
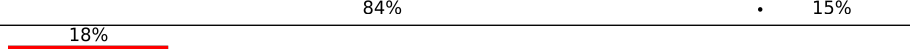
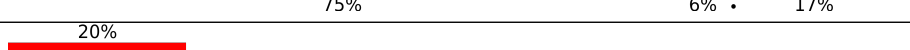
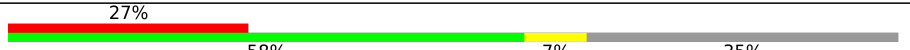
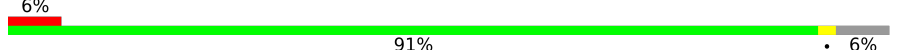
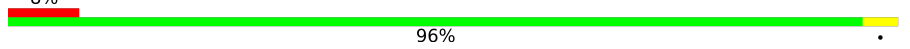
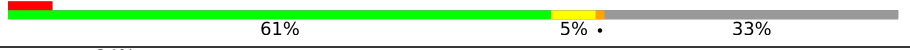
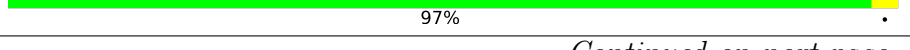
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	2	228	
2	5	112	
3	6	101	

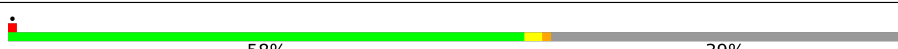
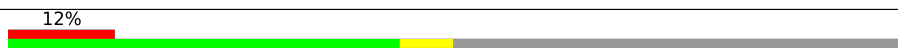
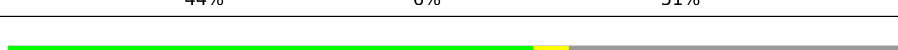
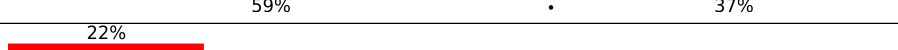
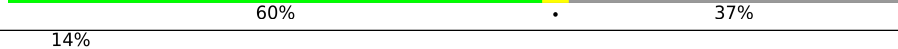
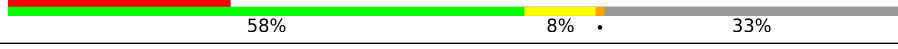
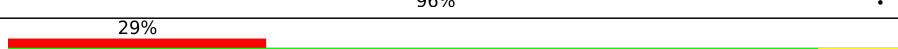
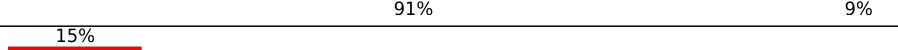
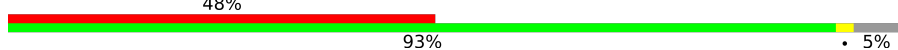
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Mol	Chain	Length	Quality of chain
4	A	2329	
5	C	974	
6	D	267	
7	DX	739	
8	E	331	
9	I	855	
10	IN	51	
11	J	744	
12	K	238	
13	L	755	
14	L1	533	
15	L2	460	
16	M	234	
17	N	147	
18	O	408	
19	P	230	
20	PX	809	
21	Q	1467	
22	R	535	
23	S	169	
24	T	494	
25	TF	830	
26	W	567	
27	X	500	
28	Z	69	

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Mol	Chain	Length	Quality of chain
29	a	136	
29	h	136	
30	b	160	
30	i	160	
31	c	127	
31	j	127	
32	d	118	
32	k	118	
33	e	90	
33	l	90	
34	f	85	
34	m	85	
35	g	77	
35	n	77	
36	o	253	
37	p	217	
38	q	492	
38	r	492	
38	s	492	
38	t	492	
39	y	79	

2 Entry composition [i](#)

There are 43 unique types of molecules in this entry. The entry contains 120201 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 RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	76	Total	C	N	O	P	0	0
			1268	554	140	498	76		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	111	Total	C	N	O	P	0	0
			2350	1052	405	782	111		

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	101	Total	C	N	O	P	0	0
			2153	965	391	696	101		

- Molecule 4 is a protein called Pre-mRNA-splicing factor 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	1982	Total	C	N	O	S	0	0
			16424	10576	2868	2904	76		

- Molecule 5 is a protein called Tr-type G domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	898	Total	C	N	O	S	0	0
			7153	4558	1211	1338	46		

- Molecule 6 is a protein called Protein isy-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	198	Total	C	N	O	S	0	0
			1629	1016	293	316	4		

- Molecule 7 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase ddx-15.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	DX	682	Total	C	N	O	S	0	0
			5465	3464	941	1026	34		

- Molecule 8 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	312	Total	C	N	O	S	0	0
			2445	1528	429	468	20		

- Molecule 9 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	747	Total	C	N	O	S	0	0
			6169	3916	1081	1128	44		

- Molecule 10 is a RNA chain called Intron lariat RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	IN	33	Total	C	N	O	P	0	0
			425	179	12	201	33		

- Molecule 11 is a protein called TPR_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	574	Total	C	N	O	S	0	0
			4895	3122	855	898	20		

- Molecule 12 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	203	Total	C	N	O	S	0	0
			1666	1041	298	310	17		

- Molecule 13 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	623	Total	C	N	O	S	0	0
			5030	3115	928	962	25		

- Molecule 14 is a protein called CWF19-like protein 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L1	472	Total	C	N	O	S	0	0
			3683	2345	616	701	21		

- Molecule 15 is a protein called CWF19-like protein 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L2	362	Total	C	N	O	S	0	0
			2974	1846	543	568	17		

- Molecule 16 is a protein called Pre-mRNA-splicing factor syf-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	196	Total	C	N	O	S	0	0
			1654	1021	308	319	6		

- Molecule 17 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	142	Total	C	N	O	S	0	0
			1163	731	212	208	12		

- Molecule 18 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	342	Total	C	N	O	S	0	0
			2721	1703	493	506	19		

- Molecule 19 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	150	Total	C	N	O	S	0	0
			1207	729	232	240	6		

- Molecule 20 is a protein called GCF C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	PX	472	Total	C	N	O	S	0	0
			3838	2396	695	720	27		

- Molecule 21 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	1378	Total	C	N	O	S	0	0
			11293	7218	1964	2064	47		

- Molecule 22 is a protein called Uncharacterized protein T27F2.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	282	Total	C	N	O	S	0	0
			2209	1379	404	416	10		

- Molecule 23 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	169	Total	C	N	O	S	0	0
			1303	818	233	245	7		

- Molecule 24 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	389	Total	C	N	O	S	0	0
			3082	1946	557	560	19		

- Molecule 25 is a protein called Septin and tuftelin-interacting protein 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	TF	559	Total	C	N	O	S	0	0
			4542	2908	769	838	27		

- Molecule 26 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	496	Total	C	N	O	S	0	0
			4072	2584	726	747	15		

- Molecule 27 is a protein called Replication stress response regulator SDE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	80	Total	C	N	O	S	0	0
			661	407	123	126	5		

- Molecule 28 is a protein called Coiled-coil domain-containing protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	69	Total	C	N	O	S	0	0
			569	356	104	107	2		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	81	Total	C	N	O	S	0	0
			635	396	113	120	6		
29	h	81	Total	C	N	O	S	0	0
			635	396	113	120	6		

- Molecule 30 is a protein called Probable small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	98	Total	C	N	O	S	0	0
			755	475	141	131	8		
30	i	79	Total	C	N	O	S	0	0
			639	405	117	111	6		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	80	Total	C	N	O	S	0	0
			622	396	109	113	4		
31	j	80	Total	C	N	O	S	0	0
			622	396	109	113	4		

- Molecule 32 is a protein called Probable small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	94	Total	C	N	O	S	0	0
			749	469	135	140	5		
32	k	79	Total	C	N	O	S	0	0
			632	398	118	111	5		

- Molecule 33 is a protein called Probable small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	80	Total	C	N	O	S	0	0
			665	424	118	121	2		
33	l	80	Total	C	N	O	S	0	0
			665	424	118	121	2		

- Molecule 34 is a protein called Probable small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	72	Total	C	N	O	S	0	0
			558	359	93	102	4		
34	m	72	Total	C	N	O	S	0	0
			558	359	93	102	4		

- Molecule 35 is a protein called Probable small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	77	Total	C	N	O	S	0	0
			608	379	107	115	7		
35	n	77	Total	C	N	O	S	0	0
			608	379	107	115	7		

- Molecule 36 is a protein called Probable U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	o	162	Total	C	N	O	S	0	0
			1335	849	236	243	7		

- Molecule 37 is a protein called RRM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	p	76	Total	C	N	O	S	0	0
			626	402	114	106	4		

- Molecule 38 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	q	121	Total	C	N	O	S	0	0
			941	585	165	186	5		
38	r	131	Total	C	N	O	S	0	0
			1004	621	179	199	5		
38	s	469	Total	C	N	O	S	0	0
			3571	2239	620	703	9		
38	t	128	Total	C	N	O	S	0	0
			993	620	173	195	5		

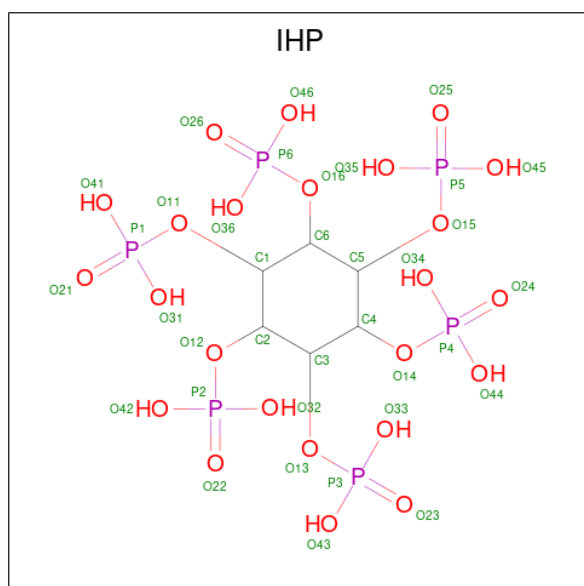
- Molecule 39 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	y	79	Total	C	N	O	S	0	0
			619	396	100	118	5		

- Molecule 40 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

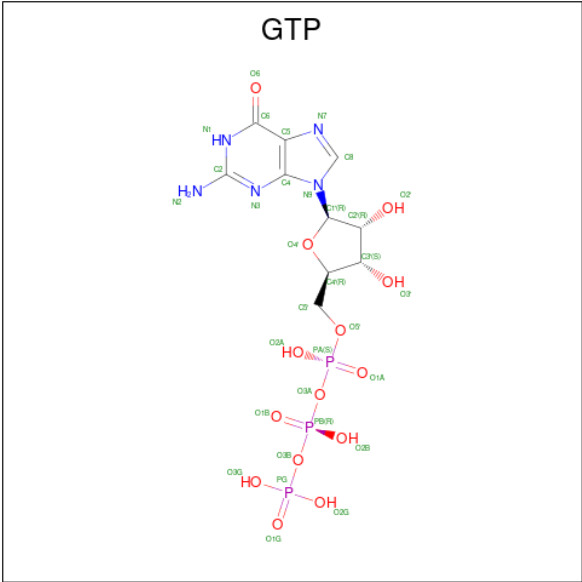
Mol	Chain	Residues	Atoms		AltConf
40	6	6	Total	Mg	0
			6	6	
40	C	1	Total	Mg	0
			1	1	

- Molecule 41 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



Mol	Chain	Residues	Atoms				AltConf
41	A	1	Total	C	O	P	0
			36	6	24	6	
41	J	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 42 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

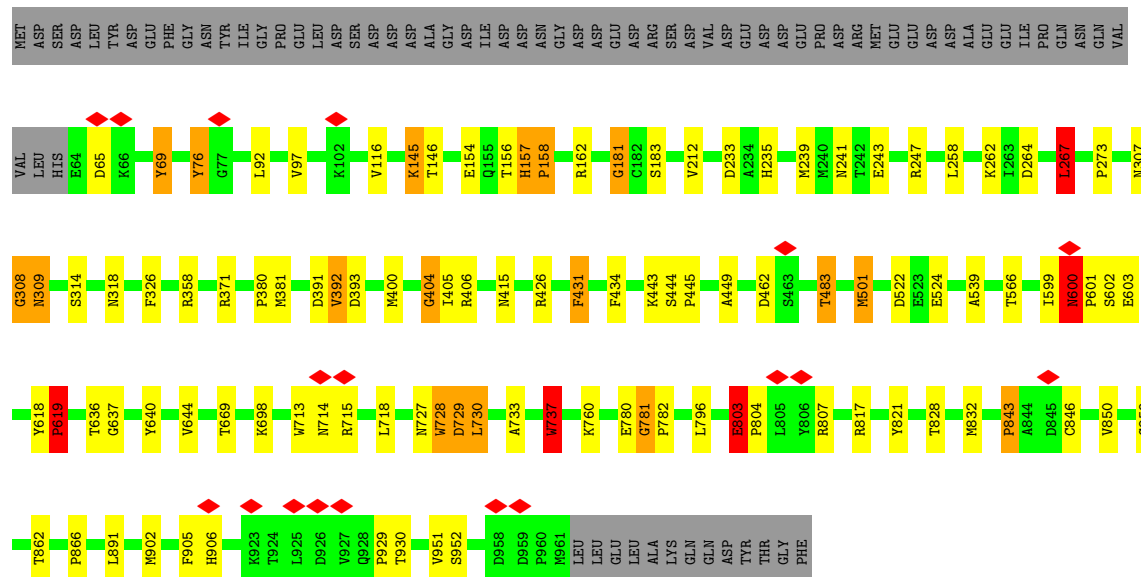
- Molecule 43 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
43	L2	1	Total	Zn	0
			1	1	
43	N	3	Total	Zn	0
			3	3	
43	O	3	Total	Zn	0
			3	3	



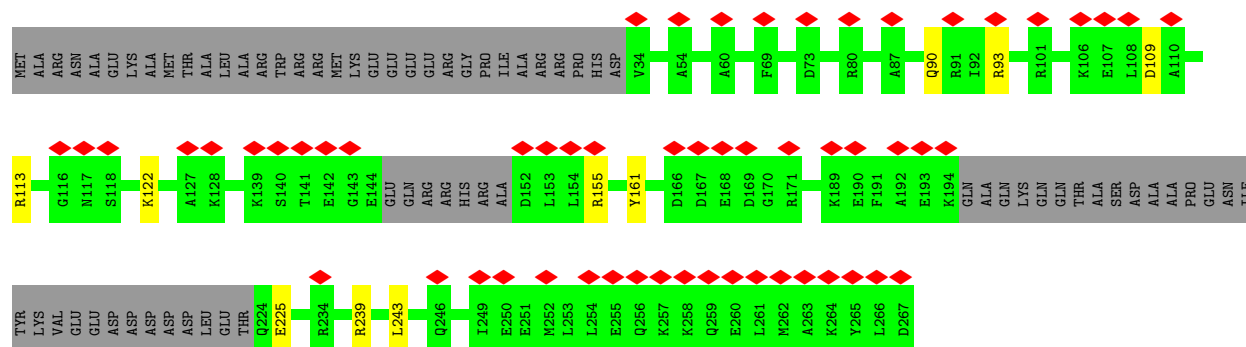
- Molecule 5: Tr-type G domain-containing protein

Chain C:



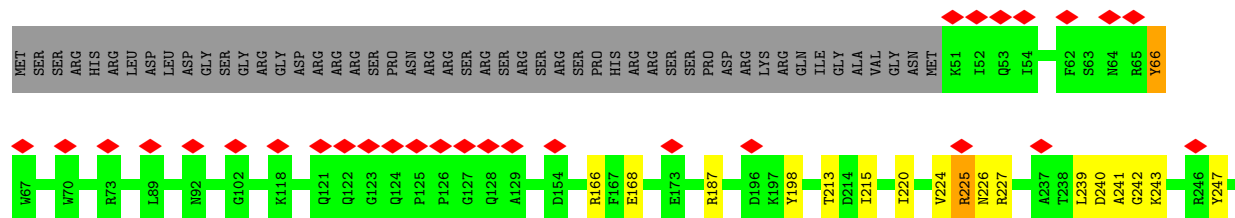
- Molecule 6: Protein isy-1

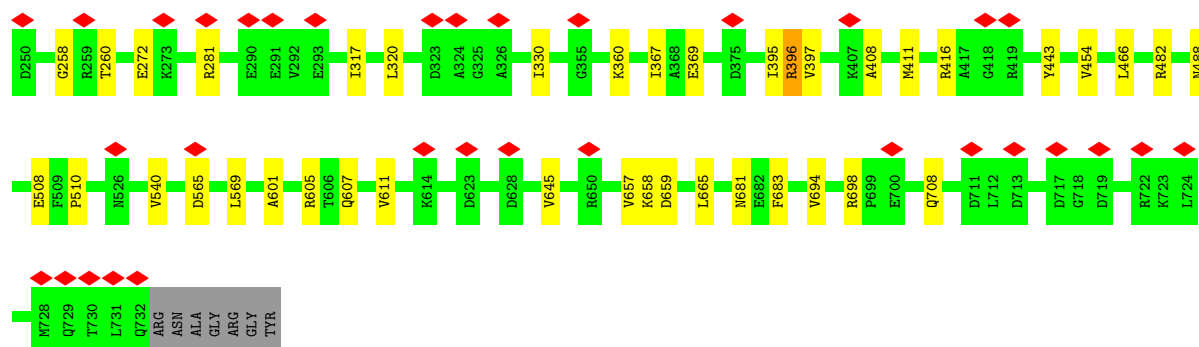
Chain D:



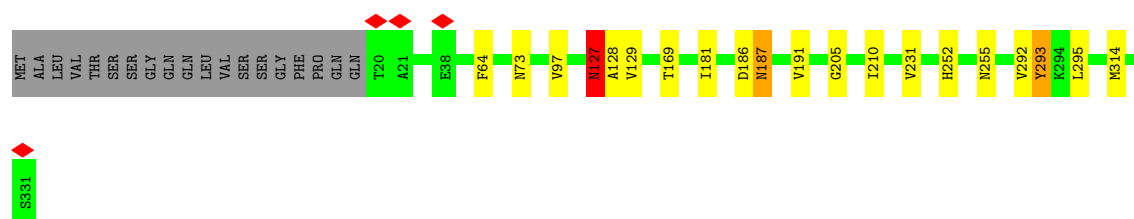
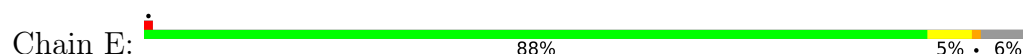
- Molecule 7: Pre-mRNA-splicing factor ATP-dependent RNA helicase ddx-15

Chain DX:

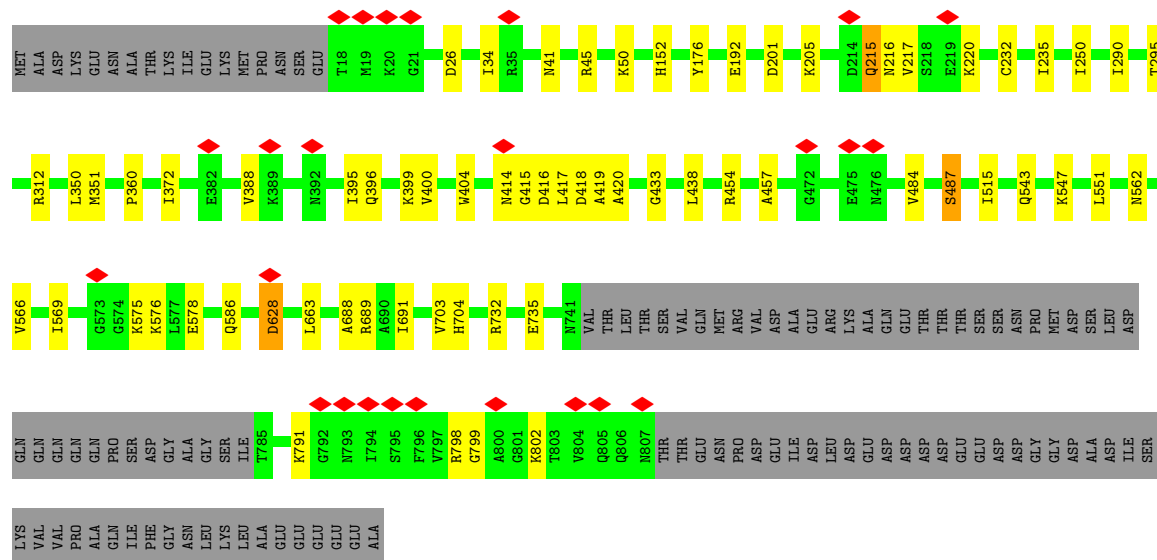
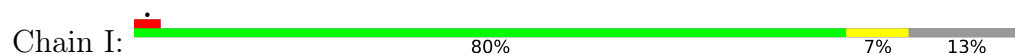




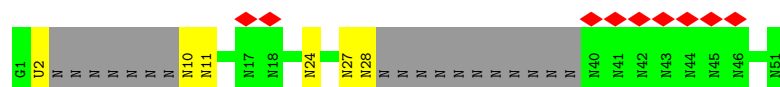
- Molecule 8: WD REPEATS REGION domain-containing protein



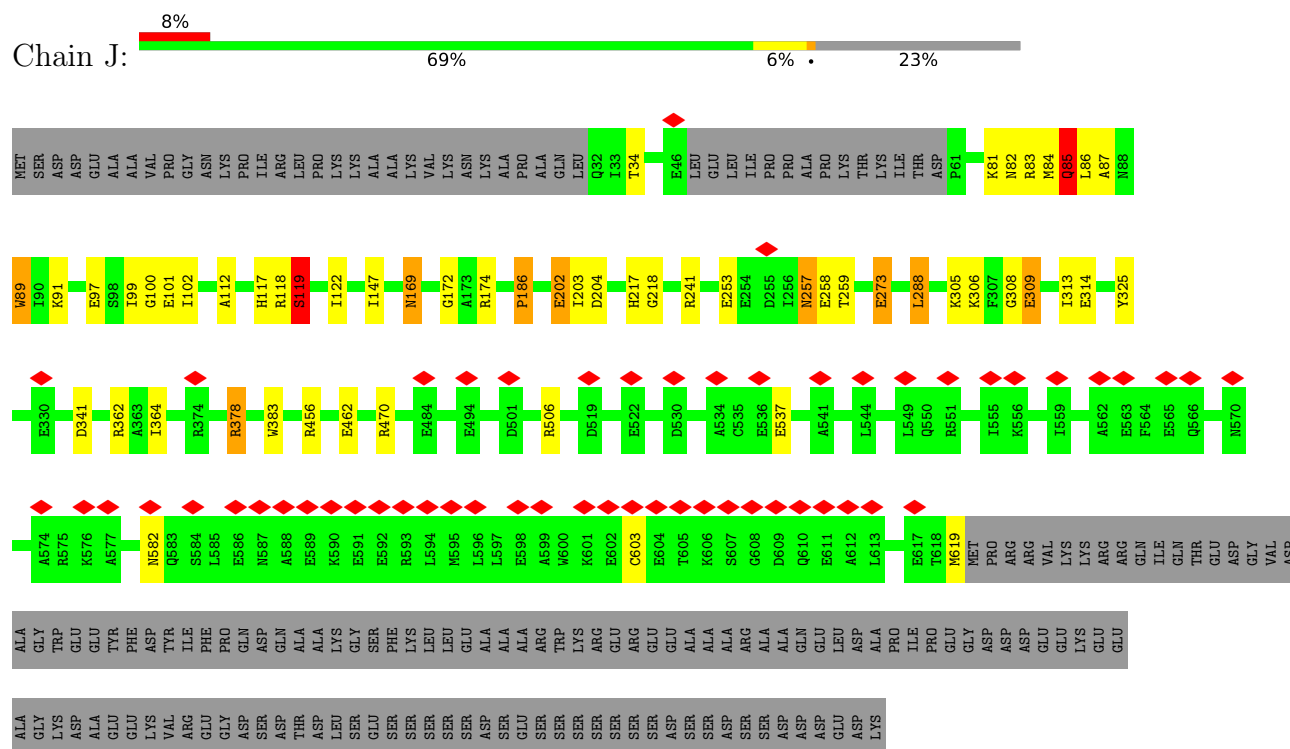
- Molecule 9: Pre-mRNA-splicing factor SYF1



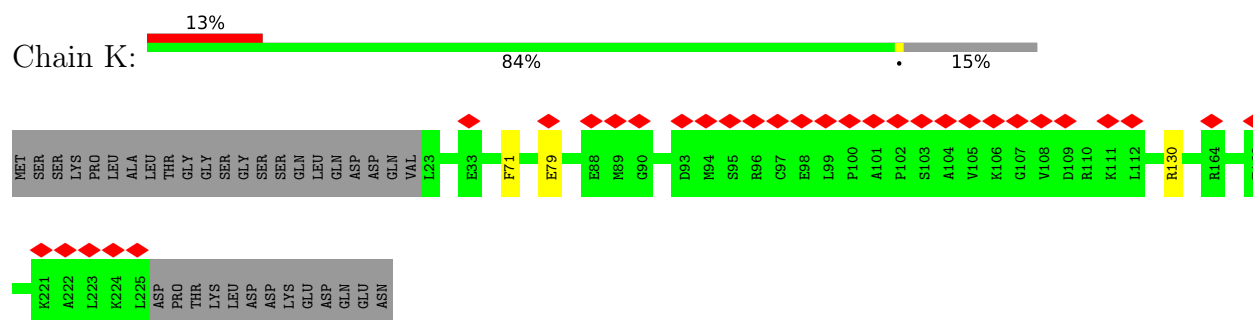
- Molecule 10: Intron lariat RNA



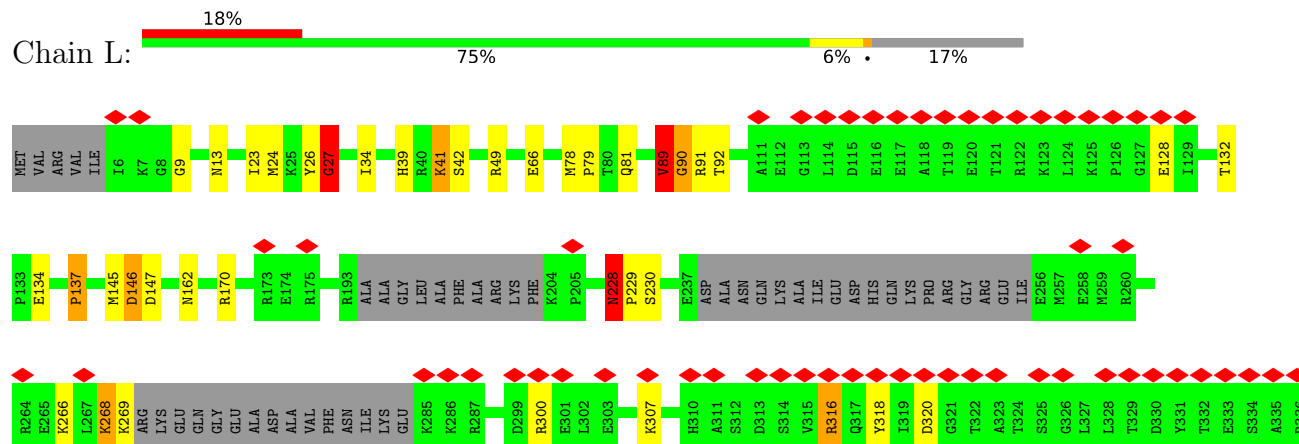
• Molecule 11: TPR_REGION domain-containing protein

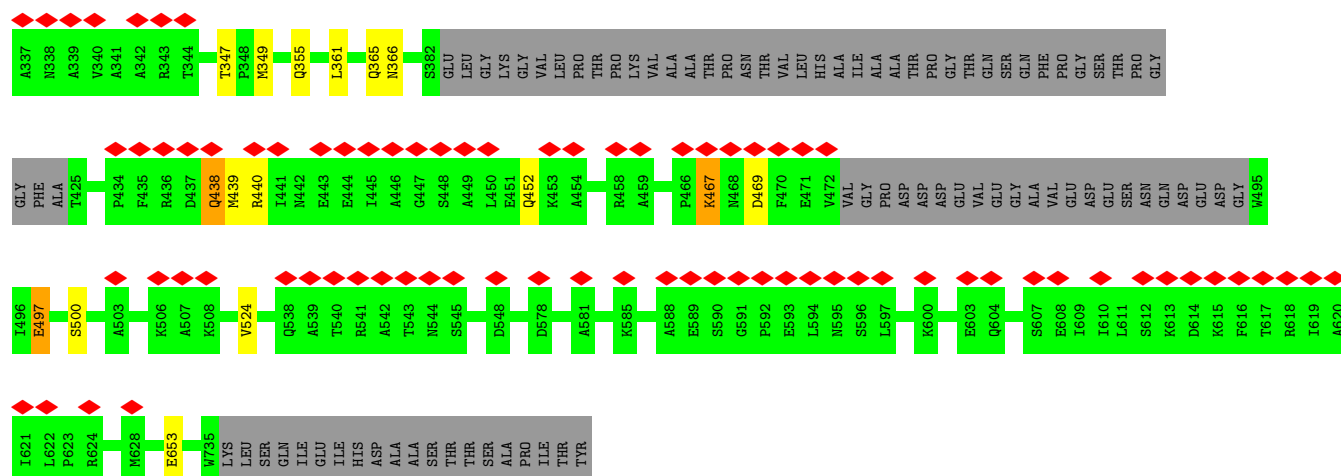


• Molecule 12: Pre-mRNA-splicing factor SPF27

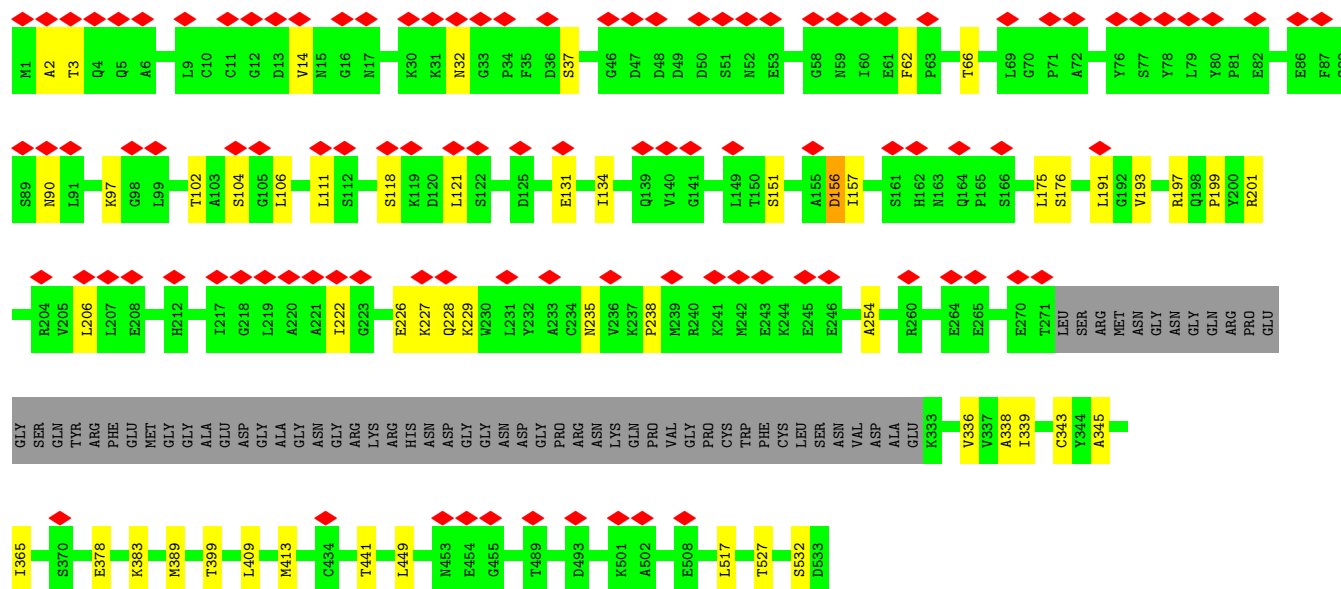
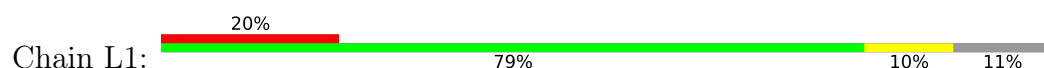


• Molecule 13: Cell division cycle 5-like protein

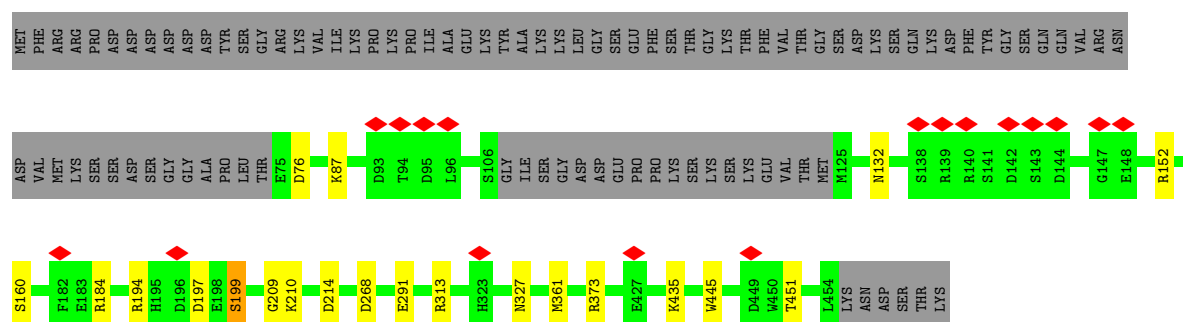
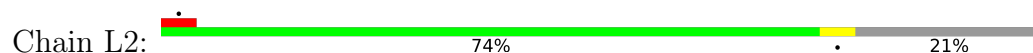




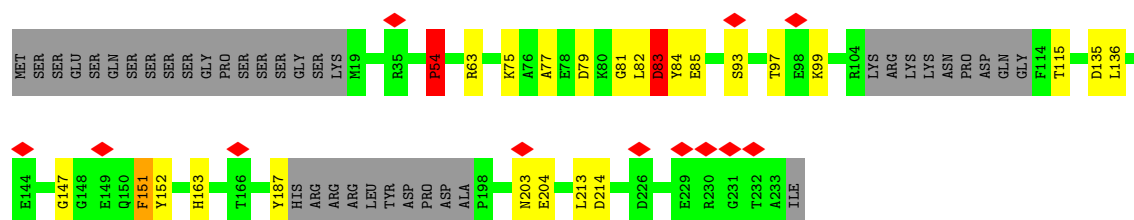
• Molecule 14: CWF19-like protein 1 homolog



• Molecule 15: CWF19-like protein 2 homolog



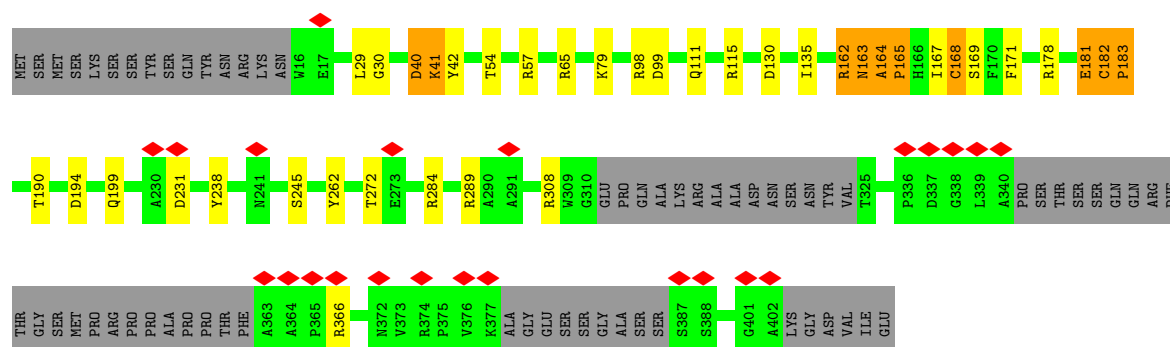
Chain M: 5% 73% 9% 16%



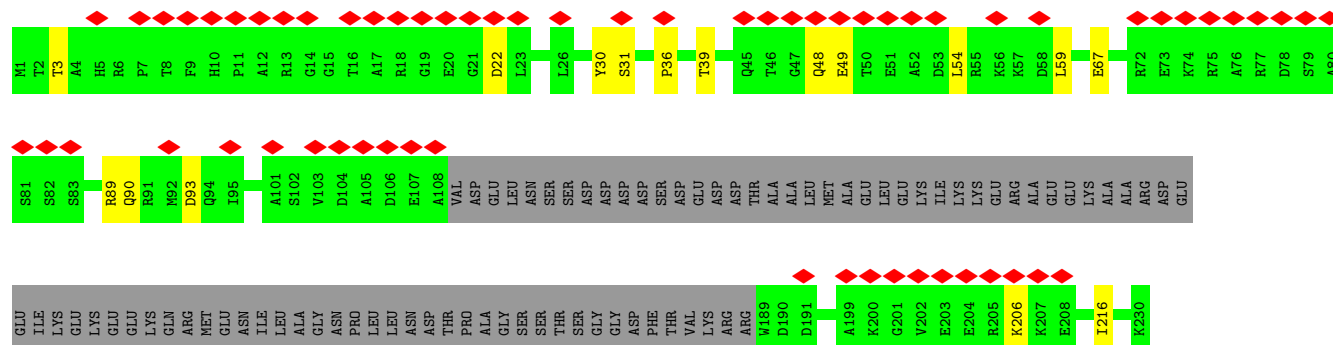
Chain N: 86% 8% ..



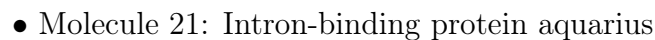
Chain O: 6% 74% 7% 16%

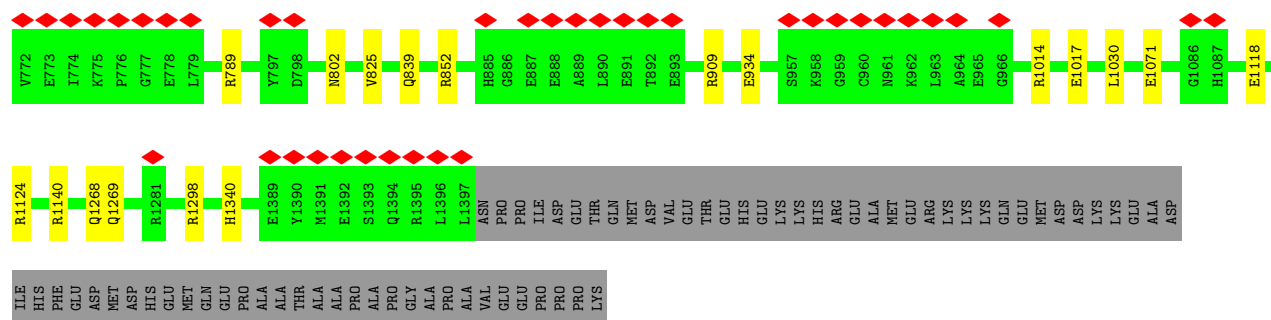


Chain P:

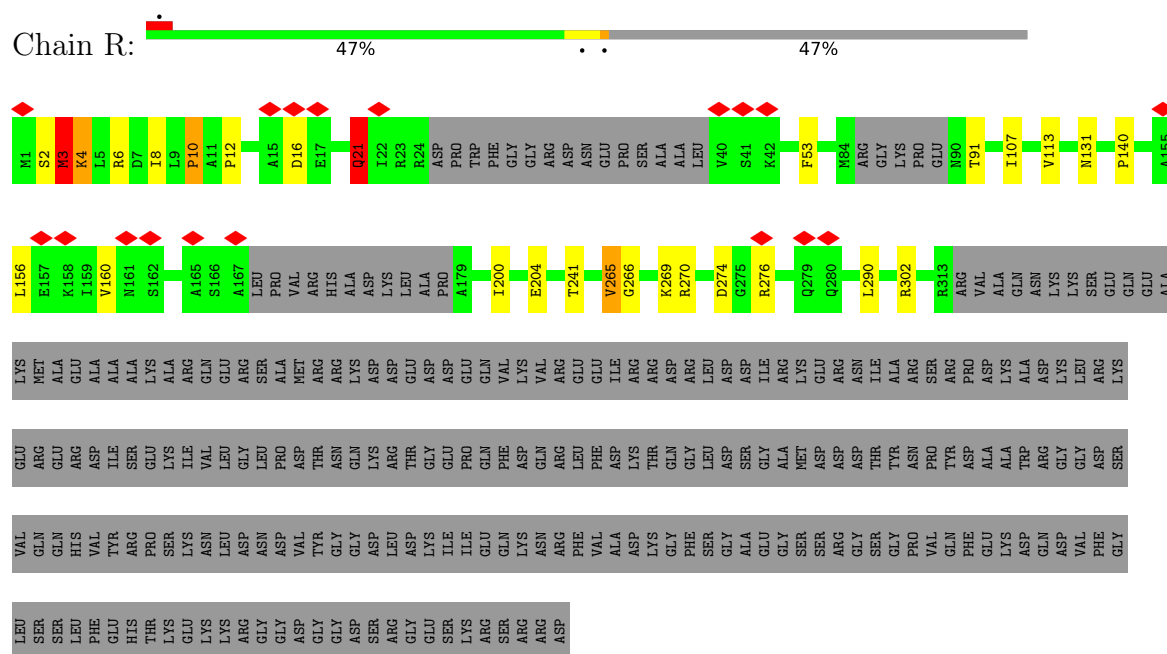


WORLDWIDE
PDB
PROTEIN DATA BANK

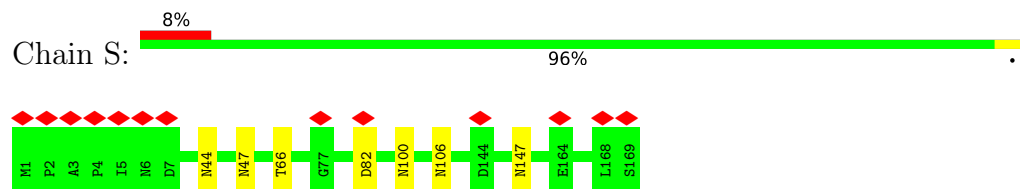




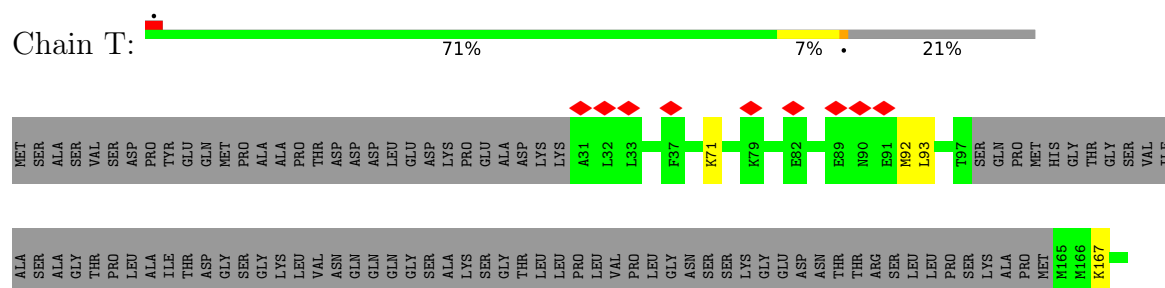
• Molecule 22: Uncharacterized protein T27F2.1

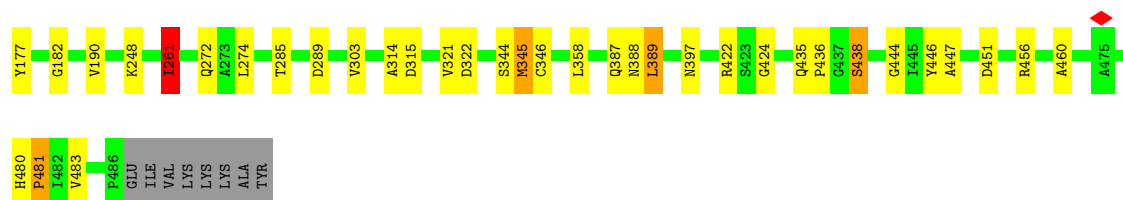


• Molecule 23: Peptidyl-prolyl cis-trans isomerase

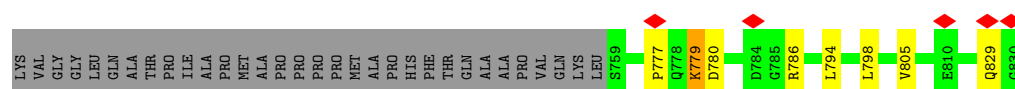
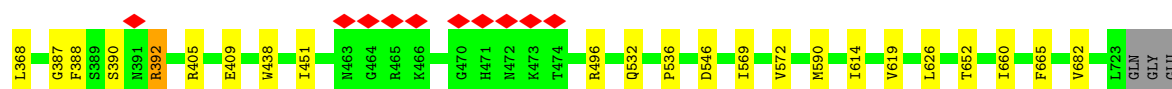
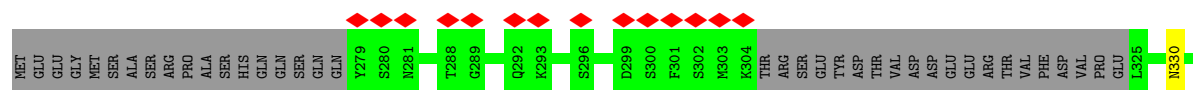
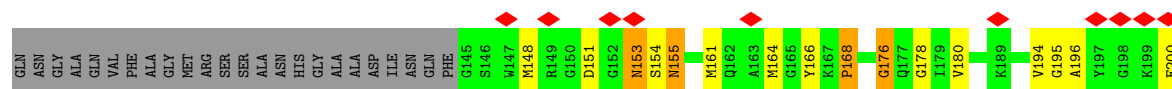
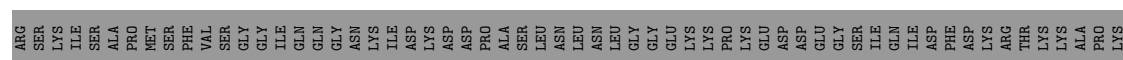
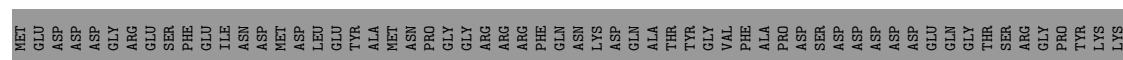


• Molecule 24: WD_REPEATS_REGION domain-containing protein

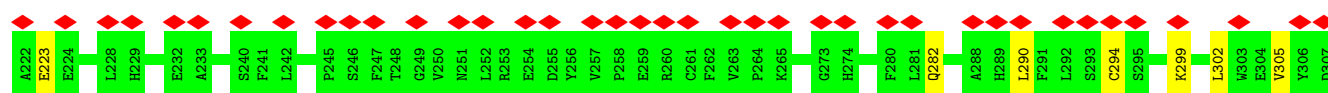
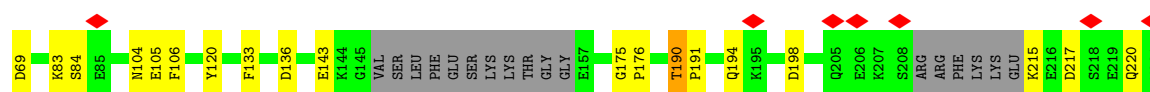
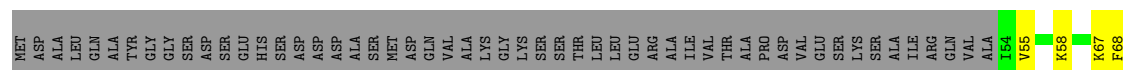
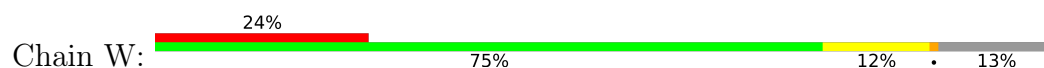




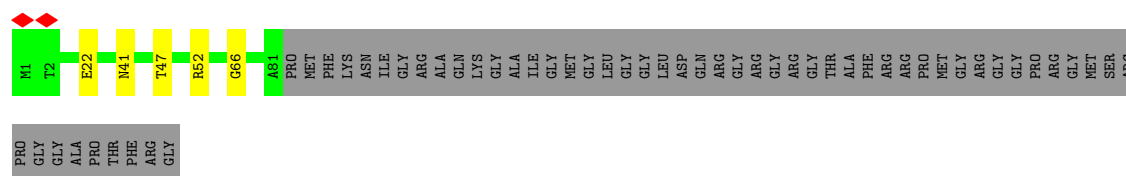
• Molecule 25: Septin and tuftelin-interacting protein 1 homolog



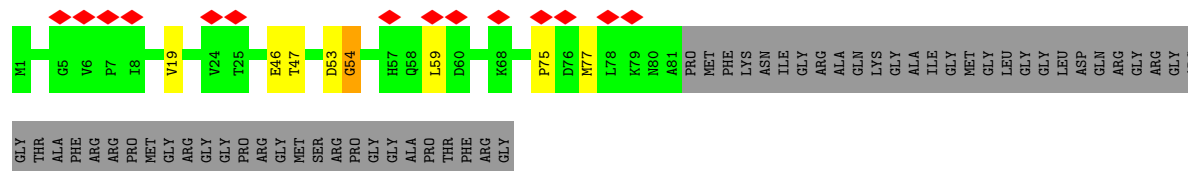
• Molecule 26: WD_REPEATS_REGION domain-containing protein



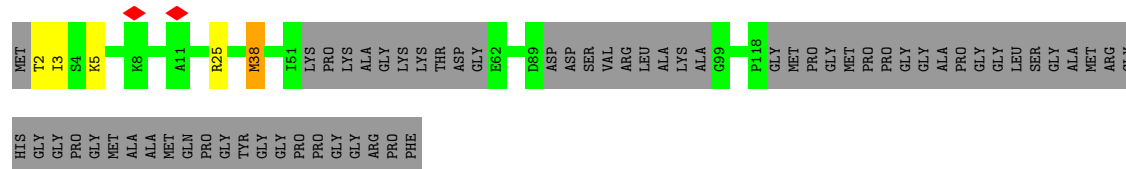




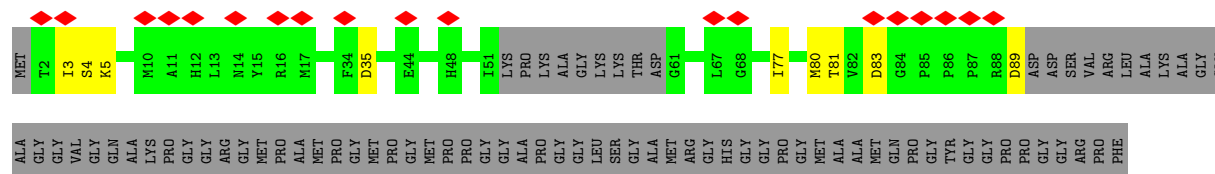
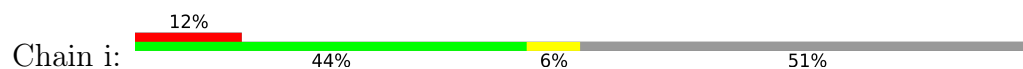
• Molecule 29: Small nuclear ribonucleoprotein Sm D3



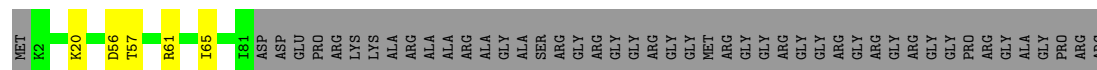
• Molecule 30: Probable small nuclear ribonucleoprotein-associated protein B



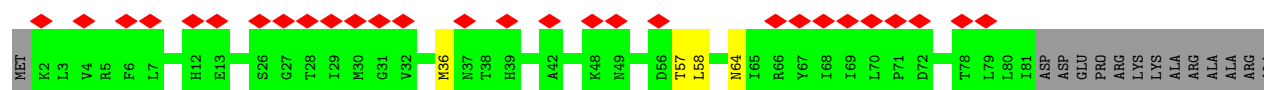
• Molecule 30: Probable small nuclear ribonucleoprotein-associated protein B

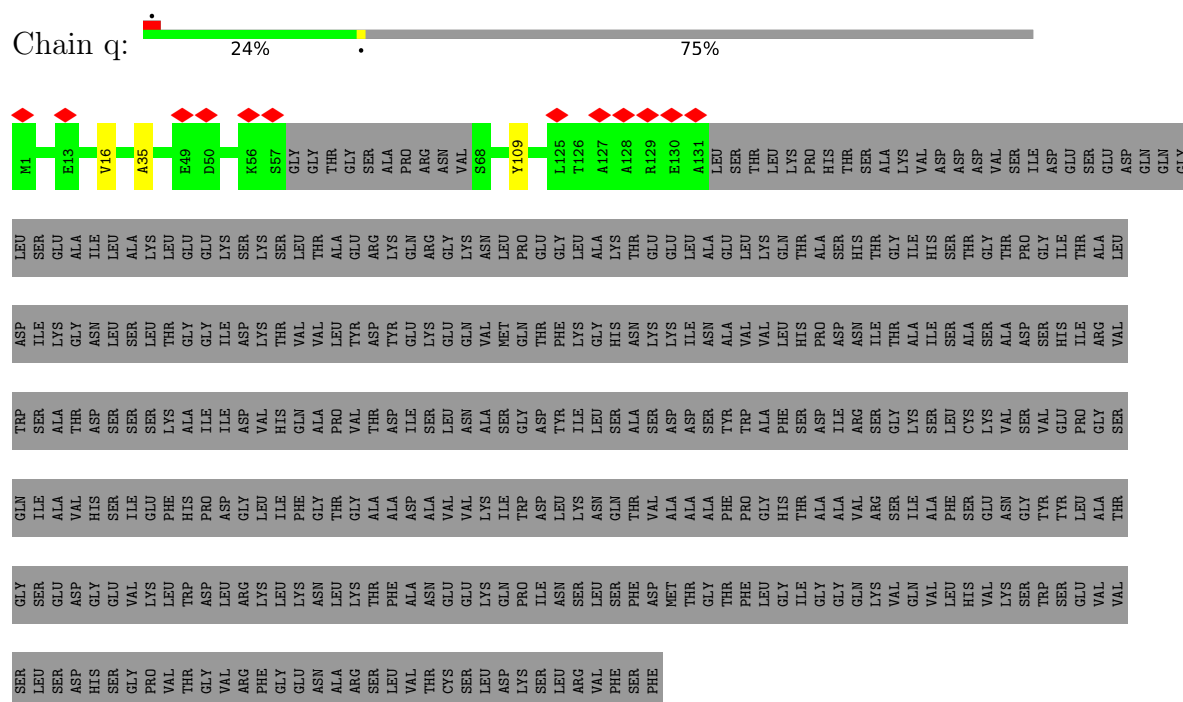


• Molecule 31: Small nuclear ribonucleoprotein Sm D1

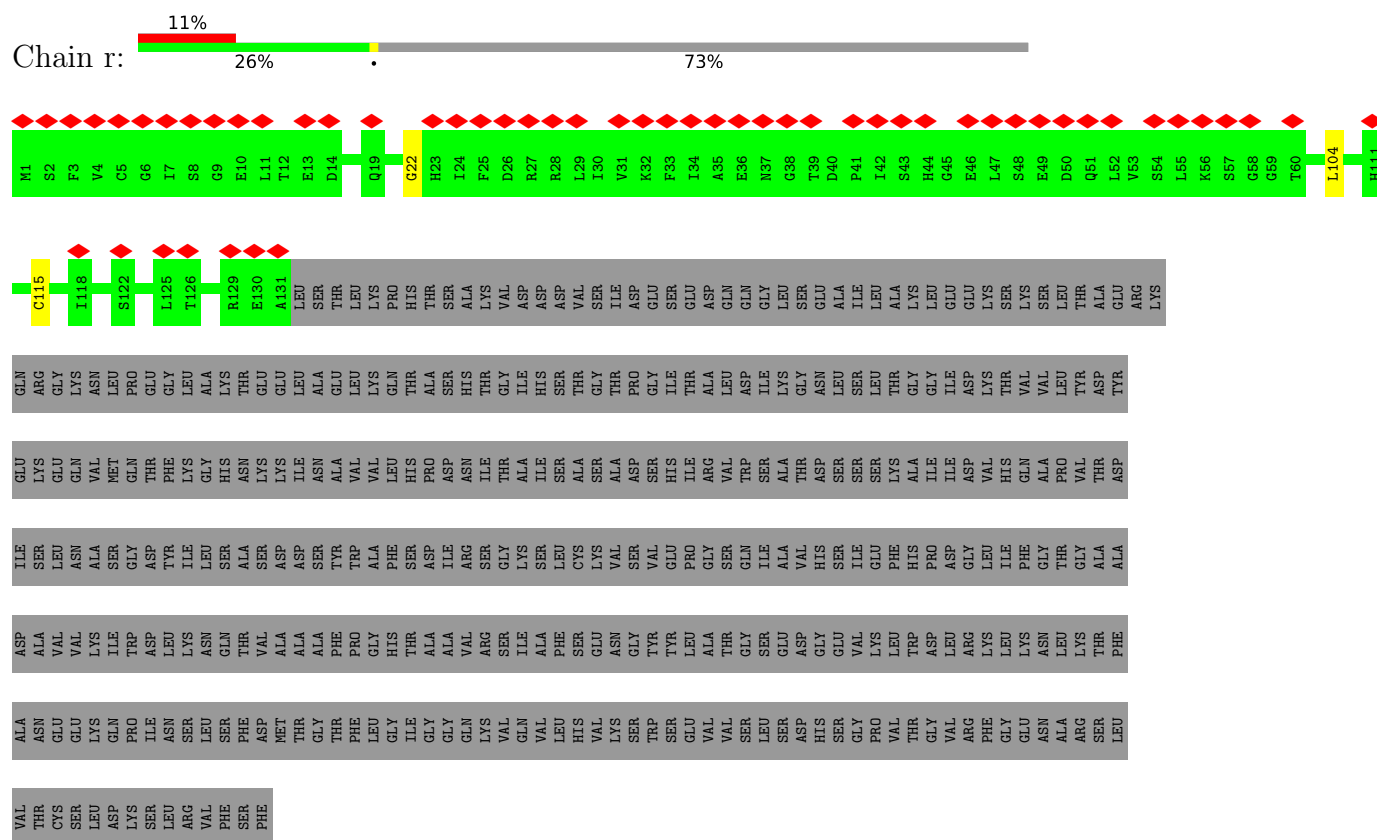


• Molecule 31: Small nuclear ribonucleoprotein Sm D1

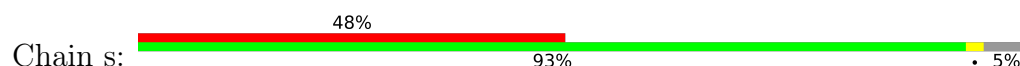


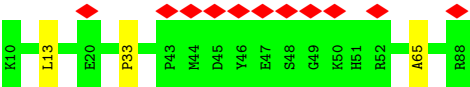


- Molecule 38: Pre-mRNA-processing factor 19



- Molecule 38: Pre-mRNA-processing factor 19





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	247908	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	10.125	Depositor
Minimum map value	0.000	Depositor
Average map value	0.070	Depositor
Map value standard deviation	0.281	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	258.9587, 300.6003, 307.1068	wwPDB
Map dimensions	199, 231, 236	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3013, 1.3013, 1.3013	Depositor

5 Model quality

5.1 Standard geometry

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

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	2	0.40	0/918	0.78	0/1424
2	5	0.58	0/2623	0.84	5/4079 (0.1%)
3	6	0.47	0/2410	0.83	3/3752 (0.1%)
4	A	0.44	0/16860	0.89	27/22857 (0.1%)
5	C	0.49	0/7310	0.91	25/9907 (0.3%)
6	D	0.25	0/1649	0.61	0/2202
7	DX	0.46	0/5577	0.80	1/7566 (0.0%)
8	E	0.40	0/2502	0.80	3/3385 (0.1%)
9	I	0.38	0/6307	0.73	2/8518 (0.0%)
10	IN	0.27	0/71	0.86	0/106
11	J	0.42	0/5008	0.85	5/6737 (0.1%)
12	K	0.25	0/1689	0.57	0/2261
13	L	0.32	0/5101	0.78	4/6840 (0.1%)
14	L1	0.30	0/3765	0.65	0/5090
15	L2	0.33	0/3024	0.73	0/4039
16	M	0.34	0/1680	0.92	6/2241 (0.3%)
17	N	0.53	0/1190	0.88	1/1597 (0.1%)
18	O	0.45	0/2783	0.85	11/3768 (0.3%)
19	P	0.34	0/1223	0.88	0/1626
20	PX	0.28	0/3893	0.64	0/5223
21	Q	0.35	0/11555	0.61	0/15627
22	R	0.40	0/2254	0.88	3/3042 (0.1%)
23	S	0.28	0/1332	0.65	0/1801
24	T	0.49	0/3161	0.87	2/4283 (0.0%)
25	TF	0.35	0/4656	0.73	2/6312 (0.0%)
26	W	0.37	0/4180	0.80	0/5639
27	X	0.23	0/666	0.59	0/879
28	Z	0.24	0/573	0.66	0/766
29	a	0.39	0/643	0.72	0/865
29	h	0.28	0/643	0.66	0/865
30	b	0.39	0/767	0.76	0/1022
30	i	0.26	0/649	0.67	0/866

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	c	0.36	0/628	0.72	0/849
31	j	0.30	0/628	0.66	0/849
32	d	0.35	0/757	0.65	0/1014
32	k	0.33	0/639	0.80	2/855 (0.2%)
33	e	0.36	0/676	0.66	0/910
33	l	0.28	0/676	0.66	0/910
34	f	0.35	0/569	0.63	0/770
34	m	0.32	0/569	0.66	0/770
35	g	0.33	0/616	0.71	0/821
35	n	0.27	0/616	0.65	0/821
36	o	0.27	0/1358	0.62	0/1837
37	p	0.27	0/638	0.66	0/850
38	q	0.27	0/953	0.53	0/1284
38	r	0.27	0/1018	0.59	0/1374
38	s	0.27	0/3633	0.55	0/4914
38	t	0.27	0/1006	0.54	0/1357
39	y	0.31	0/631	0.60	0/846
All	All	0.39	0/122273	0.77	102/166216 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	29
5	C	0	16
7	DX	0	5
8	E	0	3
9	I	0	5
11	J	0	8
13	L	0	9
15	L2	0	2
16	M	0	3
18	O	0	6
19	P	0	1
20	PX	0	1
22	R	0	4
24	T	0	7
25	TF	0	2
26	W	0	3
All	All	0	104

There are no bond length outliers.

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	781	GLY	N-CA-C	11.95	136.73	112.34
13	L	27	GLY	N-CA-C	11.35	140.09	113.18
4	A	790	GLY	N-CA-C	9.51	131.74	112.34
18	O	30	GLY	N-CA-C	8.44	133.17	113.18
18	O	182	CYS	N-CA-C	8.20	127.92	109.81
4	A	1311	PRO	N-CA-C	7.86	128.66	112.47
5	C	599	ILE	CA-C-N	7.69	140.55	121.80
5	C	599	ILE	C-N-CA	7.69	140.55	121.80
2	5	70	G	O5'-P-OP1	7.47	130.41	108.00
18	O	41	LYS	N-CA-C	-7.03	99.52	110.42
22	R	266	GLY	N-CA-C	6.95	129.65	113.18
4	A	1487	TYR	N-CA-C	6.78	125.24	110.80
4	A	1480	HIS	CA-CB-CG	6.62	120.42	113.80
4	A	581	THR	N-CA-C	6.52	124.68	110.80
2	5	25	C	C2'-C3'-O3'	6.51	123.47	113.70
5	C	158	PRO	CA-N-CD	-6.46	102.96	112.00
11	J	118	ARG	CA-C-N	6.42	133.80	121.54
11	J	118	ARG	C-N-CA	6.42	133.80	121.54
4	A	756	GLY	N-CA-C	6.39	128.32	113.18
16	M	147	GLY	N-CA-C	6.33	120.29	112.64
4	A	1489	PRO	N-CA-C	6.23	125.30	112.47
22	R	10	PRO	CA-N-CD	-6.21	103.30	112.00
5	C	618	TYR	N-CA-C	6.21	123.53	109.81
3	6	89	C	N1-C1'-C2'	6.15	121.23	112.00
4	A	1873	PRO	N-CA-C	6.15	125.13	112.47
11	J	378	ARG	NE-CZ-NH2	6.14	124.73	119.20
4	A	1939	ASN	N-CA-C	6.13	123.36	109.81
22	R	21	GLN	N-CA-C	6.11	123.81	110.80
5	C	308	GLY	N-CA-C	6.10	127.64	113.18
3	6	39	G	P-O3'-C3'	6.09	129.34	120.20
18	O	181	GLU	CA-C-N	6.09	136.66	121.80
18	O	181	GLU	C-N-CA	6.09	136.66	121.80
4	A	865	ASN	N-CA-C	6.08	123.24	109.81
24	T	480	HIS	N-CA-C	6.07	123.22	109.81
2	5	27	G	O4'-C1'-N9	-6.06	99.11	108.20
5	C	737	TRP	CA-CB-CG	6.05	125.09	113.60
18	O	183	PRO	CA-N-CD	-5.92	103.71	112.00
5	C	404	GLY	N-CA-C	5.89	127.14	113.18
3	6	39	G	C2'-C3'-O3'	5.86	118.30	109.50
5	C	157	HIS	N-CA-C	5.85	122.73	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	619	PRO	CA-N-CD	-5.80	103.88	112.00
4	A	1055	GLY	N-CA-C	5.79	124.15	112.34
4	A	1393	ASN	N-CA-C	5.75	123.06	110.80
4	A	1310	THR	C-N-CD	-5.74	101.46	125.00
5	C	803	GLU	N-CA-C	5.73	122.47	109.81
9	I	575	LYS	CA-C-N	5.71	132.45	121.54
9	I	575	LYS	C-N-CA	5.71	132.45	121.54
4	A	1311	PRO	N-CA-CB	-5.69	97.28	103.25
8	E	293	TYR	N-CA-C	-5.67	98.72	110.80
4	A	934	PRO	CA-N-CD	-5.63	104.11	112.00
4	A	1109	HIS	N-CA-C	5.62	122.22	109.81
17	N	124	VAL	N-CA-C	5.59	120.95	108.88
18	O	162	ARG	CD-NE-CZ	5.58	132.21	124.40
4	A	69	ARG	N-CA-C	5.51	122.55	110.80
18	O	182	CYS	C-N-CD	-5.50	102.43	125.00
4	A	1046	GLY	N-CA-C	5.50	119.29	112.64
2	5	21	U	O4'-C1'-N1	5.46	116.39	108.20
25	TF	779	LYS	N-CA-C	-5.45	101.65	110.32
5	C	69	TYR	N-CA-C	5.45	122.40	110.80
5	C	181	GLY	N-CA-C	5.43	126.06	113.18
4	A	1504	GLU	N-CA-C	5.42	122.33	110.80
5	C	619	PRO	N-CA-C	5.41	123.62	112.47
5	C	309	ASN	N-CA-C	5.41	122.32	110.80
13	L	90	GLY	N-CA-C	5.40	125.98	113.18
13	L	300	ARG	NE-CZ-NH2	5.38	124.04	119.20
18	O	167	ILE	CA-C-N	5.38	131.81	121.54
18	O	167	ILE	C-N-CA	5.38	131.81	121.54
32	k	116	GLN	CA-C-N	5.36	132.59	121.32
32	k	116	GLN	C-N-CA	5.36	132.59	121.32
5	C	267	LEU	CA-CB-CG	5.36	135.06	116.30
11	J	119	SER	N-CA-C	5.36	122.21	110.80
5	C	76	TYR	CA-CB-CG	5.35	123.53	113.90
5	C	843	PRO	N-CA-C	5.31	123.41	112.47
5	C	804	PRO	N-CA-C	5.30	123.39	112.47
24	T	481	PRO	N-CA-C	5.30	123.39	112.47
5	C	728	TRP	CA-C-N	5.29	131.64	121.54
5	C	728	TRP	C-N-CA	5.29	131.64	121.54
18	O	164	ALA	N-CA-C	5.28	119.35	112.17
16	M	151	PHE	CA-CB-CG	5.27	119.07	113.80
8	E	127	ASN	CA-C-N	5.22	131.52	121.54
8	E	127	ASN	C-N-CA	5.22	131.52	121.54
4	A	690	PRO	CA-N-CD	-5.21	104.71	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	637	GLY	N-CA-C	5.19	125.49	113.18
7	DX	66	TYR	CA-CB-CG	5.17	123.21	113.90
4	A	689	MET	N-CA-C	5.17	121.23	109.81
13	L	228	ASN	N-CA-C	5.16	121.22	109.81
4	A	881	ARG	N-CA-C	5.14	121.76	110.80
16	M	82	LEU	CA-C-N	5.12	131.31	121.54
16	M	82	LEU	C-N-CA	5.12	131.31	121.54
4	A	166	LEU	CA-C-N	5.09	131.27	121.54
4	A	166	LEU	C-N-CA	5.09	131.27	121.54
4	A	583	MET	CB-CA-C	-5.09	100.30	110.42
4	A	1872	PHE	N-CA-C	5.08	121.04	109.81
11	J	362	ARG	NE-CZ-NH2	5.07	123.77	119.20
5	C	951	VAL	CA-C-N	5.07	128.71	120.60
5	C	951	VAL	C-N-CA	5.07	128.71	120.60
16	M	136	LEU	N-CA-C	5.07	121.60	110.80
16	M	54	PRO	CA-N-CD	-5.07	104.91	112.00
2	5	69	A	C5'-C4'-C3'	-5.06	108.40	116.00
4	A	305	PRO	N-CA-C	5.02	122.81	112.47
25	TF	168	PRO	N-CA-C	5.02	122.81	112.47
5	C	600	ASN	N-CA-C	5.00	120.87	109.81

There are no chirality outliers.

All (104) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1045	LEU	Peptide
4	A	1054	ALA	Peptide
4	A	1078	ARG	Peptide
4	A	1109	HIS	Peptide
4	A	1310	THR	Peptide
4	A	1328	PRO	Peptide
4	A	1409	ILE	Peptide
4	A	1428	GLY	Peptide
4	A	1454	ASP	Peptide
4	A	1486	THR	Peptide
4	A	1504	GLU	Peptide
4	A	1668	ASP	Peptide
4	A	167	ASP	Peptide
4	A	1939	ASN	Peptide
4	A	1991	ASN	Peptide
4	A	239	VAL	Peptide
4	A	406	ARG	Sidechain

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Mol	Chain	Res	Type	Group
4	A	532	PHE	Peptide
4	A	533	GLY	Peptide
4	A	581	THR	Peptide
4	A	63	HIS	Peptide
4	A	68	SER	Peptide
4	A	76	ARG	Sidechain
4	A	760	ASP	Peptide
4	A	789	ASP	Peptide
4	A	865	ASN	Peptide
4	A	879	THR	Peptide
4	A	933	LYS	Peptide
4	A	990	ARG	Sidechain
5	C	307	ASN	Peptide
5	C	462	ASP	Peptide
5	C	483	THR	Peptide
5	C	501	MET	Peptide
5	C	600	ASN	Peptide
5	C	69	TYR	Peptide
5	C	713	TRP	Peptide
5	C	727	ASN	Peptide
5	C	729	ASP	Peptide
5	C	780	GLU	Peptide
5	C	781	GLY	Peptide
5	C	803	GLU	Peptide
5	C	862	THR	Peptide
5	C	905	PHE	Peptide
5	C	906	HIS	Peptide
5	C	952	SER	Peptide
7	DX	166	ARG	Sidechain
7	DX	225	ARG	Sidechain
7	DX	396	ARG	Sidechain
7	DX	482	ARG	Sidechain
7	DX	605	ARG	Sidechain
8	E	127	ASN	Peptide
8	E	169	THR	Peptide
8	E	292	VAL	Peptide
9	I	312	ARG	Sidechain
9	I	433	GLY	Peptide
9	I	628	ASP	Peptide
9	I	689	ARG	Sidechain
9	I	732	ARG	Sidechain
11	J	119	SER	Peptide

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Mol	Chain	Res	Type	Group
11	J	174	ARG	Sidechain
11	J	241	ARG	Sidechain
11	J	273	GLU	Peptide
11	J	288	LEU	Peptide
11	J	308	GLY	Peptide
11	J	378	ARG	Sidechain
11	J	85	GLN	Peptide
13	L	145	MET	Peptide
13	L	228	ASN	Peptide
13	L	26	TYR	Peptide
13	L	268	LYS	Peptide
13	L	27	GLY	Peptide
13	L	41	LYS	Peptide
13	L	497	GLU	Peptide
13	L	78	MET	Peptide
13	L	89	VAL	Peptide
15	L2	199	SER	Peptide
15	L2	313	ARG	Sidechain
16	M	115	THR	Peptide
16	M	135	ASP	Peptide
16	M	83	ASP	Peptide
18	O	163	ASN	Peptide
18	O	178	ARG	Peptide
18	O	181	GLU	Peptide
18	O	29	LEU	Peptide
18	O	41	LYS	Peptide
18	O	65	ARG	Sidechain
19	P	31	SER	Peptide
20	PX	469	ARG	Sidechain
22	R	265	VAL	Peptide
22	R	3	MET	Peptide
22	R	302	ARG	Sidechain
22	R	8	ILE	Peptide
24	T	177	TYR	Mainchain
24	T	261	ILE	Peptide
24	T	303	VAL	Peptide
24	T	314	ALA	Peptide
24	T	345	MET	Peptide
24	T	397	ASN	Peptide
24	T	438	SER	Peptide
25	TF	779	LYS	Peptide
25	TF	780	ASP	Peptide

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Mol	Chain	Res	Type	Group
26	W	175	GLY	Peptide
26	W	190	THR	Peptide
26	W	83	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	1268	0	715	9	0
2	5	2350	0	1189	18	0
3	6	2153	0	1088	17	0
4	A	16424	0	16438	89	0
5	C	7153	0	7141	34	0
6	D	1629	0	1627	5	0
7	DX	5465	0	5468	22	0
8	E	2445	0	2362	5	0
9	I	6169	0	6076	23	0
10	IN	425	0	274	4	0
11	J	4895	0	4774	23	0
12	K	1666	0	1707	1	0
13	L	5030	0	5111	19	0
14	L1	3683	0	3664	18	0
15	L2	2974	0	2960	10	0
16	M	1654	0	1626	10	0
17	N	1163	0	1142	5	0
18	O	2721	0	2661	13	0
19	P	1207	0	1182	3	0
20	PX	3838	0	3891	12	0
21	Q	11293	0	11206	17	0
22	R	2209	0	2212	11	0
23	S	1303	0	1282	3	0
24	T	3082	0	3042	10	0
25	TF	4542	0	4481	19	0
26	W	4072	0	3967	20	0
27	X	661	0	679	2	0
28	Z	569	0	603	1	0
29	a	635	0	643	3	0
29	h	635	0	643	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	b	755	0	772	4	0
30	i	639	0	655	5	0
31	c	622	0	673	3	0
31	j	622	0	673	4	0
32	d	749	0	764	3	0
32	k	632	0	662	7	0
33	e	665	0	666	5	0
33	l	665	0	666	4	0
34	f	558	0	560	0	0
34	m	558	0	560	8	0
35	g	608	0	624	2	0
35	n	608	0	624	2	0
36	o	1335	0	1367	5	0
37	p	626	0	646	7	0
38	q	941	0	941	2	0
38	r	1004	0	1003	0	0
38	s	3571	0	3573	5	0
38	t	993	0	1004	0	0
39	y	619	0	598	1	0
40	6	6	0	0	0	0
40	C	1	0	0	0	0
41	A	36	0	6	0	0
41	J	36	0	6	2	0
42	C	32	0	12	6	0
43	L2	1	0	0	0	0
43	N	3	0	0	0	0
43	O	3	0	0	0	0
All	All	120201	0	116909	422	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 2.

All (422) 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)
2:5:67:G:O2'	4:A:42:GLY:O	1.97	0.81
5:C:145:LYS:NZ	42:C:1101:GTP:O2G	2.14	0.80
1:2:20:A:OP1	3:6:77:A:N6	2.16	0.78
2:5:117:C:O2	35:g:24:ASN:ND2	2.18	0.77
3:6:59:U:OP2	4:A:655:ARG:NH1	2.18	0.76
37:p:65:ASN:OD1	37:p:68:ARG:NH1	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:p:14:ASN:ND2	37:p:79:PRO:O	2.18	0.75
32:k:69:ASN:ND2	32:k:118:GLU:OE1	2.20	0.75
9:I:586:GLN:OE1	11:J:305:LYS:NZ	2.19	0.75
3:6:60:G:N7	4:A:655:ARG:NH2	2.35	0.74
2:5:99:G:N2	32:d:64:ASN:OD1	2.21	0.73
22:R:2:SER:O	22:R:6:ARG:NH1	2.22	0.73
35:n:16:GLU:OE2	35:n:73:LYS:NZ	2.24	0.71
2:5:40:G:N2	2:5:48:C:O2	2.19	0.71
3:6:73:A:O4'	11:J:81:LYS:NZ	2.25	0.70
32:k:55:ARG:NH1	32:k:116:GLN:O	2.24	0.70
10:IN:28:N:O2'	18:O:190:THR:OG1	2.06	0.70
26:W:315:TYR:OH	26:W:348:THR:O	2.08	0.70
26:W:217:ASP:OD1	26:W:356:ARG:NH2	2.26	0.69
2:5:12:C:OP1	4:A:213:THR:OG1	2.08	0.68
7:DX:466:LEU:N	25:TF:164:MET:SD	2.67	0.68
21:Q:934:GLU:OE2	21:Q:1014:ARG:NH1	2.27	0.68
9:I:192:GLU:OE2	9:I:220:LYS:NZ	2.27	0.68
31:j:36:MET:SD	32:k:102:ARG:NH2	2.66	0.68
2:5:42:C:O2'	2:5:44:U:OP2	2.09	0.68
4:A:105:ASP:OD1	17:N:9:ARG:NH2	2.26	0.67
15:L2:445:TRP:NE1	15:L2:451:THR:OG1	2.28	0.67
2:5:10:U:O4	2:5:70:G:O6	2.13	0.66
9:I:543:GLN:NE2	11:J:306:LYS:O	2.28	0.66
1:2:170:N:OP2	37:p:45:ARG:NH2	2.28	0.66
6:D:109:ASP:OD1	6:D:122:LYS:NZ	2.28	0.66
4:A:1479:GLU:OE1	4:A:1484:ARG:NE	2.28	0.66
11:J:582:ASN:ND2	11:J:619:MET:SD	2.69	0.66
4:A:133:GLN:NE2	4:A:197:PHE:O	2.30	0.65
33:l:59:GLU:OE1	34:m:73:TYR:OH	2.13	0.64
13:L:27:GLY:HA2	13:L:34:ILE:HD11	1.79	0.64
9:I:26:ASP:OD2	9:I:50:LYS:NZ	2.30	0.64
14:L1:365:ILE:O	14:L1:409:LEU:N	2.29	0.64
18:O:231:ASP:O	18:O:284:ARG:NH1	2.31	0.64
38:s:422:GLU:OE1	38:s:424:GLN:NE2	2.31	0.64
33:l:73:ILE:HG22	34:m:75:GLY:HA3	1.80	0.63
36:o:29:GLN:N	36:o:52:ASN:OD1	2.32	0.63
4:A:824:TYR:OH	4:A:921:GLU:OE2	2.15	0.63
3:6:20:C:O4'	18:O:57:ARG:NH1	2.32	0.63
17:N:125:PRO:O	17:N:127:SER:N	2.33	0.62
2:5:27:G:OP1	2:5:61:U:O2'	2.17	0.61
4:A:68:SER:O	4:A:70:LYS:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:316:ARG:NH2	13:L:320:ASP:OD2	2.34	0.60
3:6:78:A:OP1	11:J:91:LYS:NZ	2.34	0.60
15:L2:291:GLU:OE2	15:L2:373:ARG:NH1	2.35	0.60
4:A:1857:THR:OG1	4:A:1858:ARG:NH2	2.35	0.60
5:C:154:GLU:OE1	5:C:162:ARG:NE	2.34	0.60
3:6:39:G:O2'	3:6:40:A:O5'	2.20	0.59
21:Q:802:ASN:ND2	21:Q:839:GLN:OE1	2.36	0.59
11:J:506:ARG:NH1	11:J:537:GLU:OE2	2.34	0.59
1:2:11:C:H42	3:6:82:C:H42	1.51	0.59
3:6:39:G:O3'	13:L:170:ARG:NH2	2.35	0.59
1:2:1:A:OP1	16:M:99:LYS:NZ	2.35	0.59
31:c:20:LYS:NZ	31:c:65:ILE:O	2.36	0.59
9:I:201:ASP:OD2	9:I:205:LYS:NZ	2.35	0.58
26:W:104:ASN:O	26:W:106:PHE:N	2.36	0.58
11:J:456:ARG:NH2	41:J:3000:IHP:O35	2.36	0.58
25:TF:438:TRP:O	25:TF:496:ARG:NH1	2.35	0.58
28:Z:87:ASP:OD2	28:Z:91:ARG:NH1	2.36	0.58
3:6:25:A:N1	10:IN:24:N:O2'	2.35	0.58
6:D:161:TYR:OH	9:I:152:HIS:ND1	2.32	0.58
7:DX:220:ILE:O	7:DX:224:VAL:HG23	2.03	0.57
4:A:1392:GLN:O	4:A:1394:ARG:N	2.36	0.57
25:TF:405:ARG:NH2	25:TF:409:GLU:OE1	2.36	0.57
4:A:1760:ASN:ND2	4:A:1881:GLU:OE2	2.37	0.57
2:5:116:G:OP1	29:a:52:ARG:NH2	2.37	0.57
33:e:11:VAL:HG22	33:e:12:GLN:O	2.05	0.57
24:T:71:LYS:NZ	38:q:35:ALA:O	2.38	0.56
24:T:315:ASP:OD2	24:T:358:LEU:N	2.36	0.56
5:C:145:LYS:NZ	42:C:1101:GTP:O1B	2.22	0.56
6:D:90:GLN:OE1	6:D:93:ARG:NH1	2.38	0.56
14:L1:343:CYS:N	14:L1:378:GLU:OE1	2.38	0.56
21:Q:724:ASP:OD2	21:Q:789:ARG:NH1	2.38	0.56
33:e:12:GLN:O	35:g:41:VAL:HG21	2.05	0.56
7:DX:396:ARG:NH1	7:DX:659:ASP:OD2	2.38	0.56
13:L:49:ARG:NH2	13:L:134:GLU:O	2.38	0.56
26:W:341:ARG:NH1	26:W:360:GLY:O	2.37	0.56
5:C:162:ARG:NH1	5:C:318:ASN:OD1	2.39	0.56
9:I:396:GLN:OE1	9:I:400:VAL:HG23	2.06	0.56
5:C:406:ARG:O	5:C:426:ARG:NH2	2.39	0.55
14:L1:336:VAL:HG11	14:L1:339:ILE:HD11	1.88	0.55
14:L1:383:LYS:HG2	14:L1:399:THR:HG21	1.89	0.55
1:2:13:G:H22	16:M:187:TYR:HD1	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:391:ASP:O	5:C:393:ASP:N	2.38	0.55
26:W:361:HIS:ND1	26:W:383:GLN:OE1	2.40	0.54
4:A:694:LYS:O	4:A:696:ASN:N	2.40	0.54
5:C:183:SER:N	42:C:1101:GTP:O3G	2.36	0.54
25:TF:388:PHE:O	25:TF:392:ARG:NH2	2.41	0.54
13:L:228:ASN:O	13:L:230:SER:N	2.39	0.54
21:Q:1140:ARG:NH2	21:Q:1269:GLN:OE1	2.40	0.54
4:A:1454:ASP:O	4:A:1456:LYS:N	2.40	0.54
20:PX:524:GLU:OE2	20:PX:534:ARG:NH1	2.40	0.54
30:i:77:ILE:O	31:j:64:ASN:ND2	2.41	0.54
4:A:545:LEU:HD13	4:A:577:VAL:CG2	2.37	0.54
4:A:793:ILE:HD13	4:A:984:LEU:HD22	1.89	0.54
26:W:120:TYR:OH	26:W:143:GLU:OE1	2.18	0.54
4:A:967:VAL:HG11	4:A:1145:VAL:HG21	1.90	0.54
7:DX:408:ALA:O	7:DX:411:MET:N	2.41	0.54
38:s:432:ASP:OD1	38:s:436:THR:N	2.40	0.54
12:K:130:ARG:NH1	13:L:653:GLU:OE1	2.38	0.53
4:A:1049:ARG:NH2	4:A:1052:GLU:OE1	2.41	0.53
5:C:483:THR:HG22	5:C:566:THR:HG22	1.91	0.53
22:R:131:ASN:OD1	24:T:422:ARG:NE	2.38	0.53
30:i:80:MET:O	31:j:58:LEU:HD12	2.08	0.53
1:2:163:N:OP2	37:p:20:LYS:NZ	2.36	0.53
18:O:79:LYS:O	18:O:98:ARG:NH2	2.39	0.53
18:O:366:ARG:NE	21:Q:1340:HIS:O	2.40	0.53
4:A:1048:ARG:NH2	4:A:1052:GLU:OE2	2.42	0.53
4:A:1328:PRO:O	4:A:1330:SER:N	2.41	0.53
5:C:262:LYS:HG2	42:C:1101:GTP:C6	2.44	0.53
7:DX:665:LEU:CD2	7:DX:694:VAL:HG11	2.38	0.53
26:W:215:LYS:NZ	26:W:223:GLU:OE1	2.32	0.53
3:6:95:A:O2'	3:6:96:A:OP1	2.25	0.53
26:W:359:THR:OG1	26:W:361:HIS:O	2.26	0.53
5:C:714:ASN:OD1	5:C:715:ARG:N	2.41	0.53
33:e:26:ARG:NH1	33:e:89:GLU:O	2.42	0.53
13:L:89:VAL:O	13:L:91:ARG:N	2.42	0.52
21:Q:1268:GLN:O	21:Q:1298:ARG:NH2	2.42	0.52
4:A:865:ASN:O	4:A:868:GLU:N	2.42	0.52
8:E:231:VAL:HG23	8:E:252:HIS:CE1	2.45	0.52
31:c:56:ASP:OD1	31:c:57:THR:N	2.42	0.52
8:E:181:ILE:HG13	8:E:191:VAL:HG13	1.91	0.52
36:o:96:THR:OG1	36:o:119:THR:OG1	2.27	0.52
37:p:48:LYS:O	37:p:52:GLN:NE2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:587:LYS:O	4:A:589:LYS:N	2.43	0.52
1:2:14:C:OP1	4:A:694:LYS:NZ	2.30	0.52
29:h:47:THR:N	29:h:59:LEU:O	2.42	0.52
13:L:266:LYS:O	13:L:269:LYS:NZ	2.37	0.52
21:Q:909:ARG:NH2	21:Q:1017:GLU:OE2	2.43	0.52
7:DX:565:ASP:HB2	7:DX:569:LEU:HD12	1.92	0.52
11:J:119:SER:O	11:J:122:ILE:N	2.41	0.51
13:L:23:ILE:HA	13:L:27:GLY:HA3	1.92	0.51
18:O:164:ALA:HB3	18:O:165:PRO:HD3	1.93	0.51
22:R:140:PRO:HG3	24:T:321:VAL:HG21	1.91	0.51
4:A:545:LEU:HD13	4:A:577:VAL:HG21	1.93	0.51
4:A:585:ARG:NH2	15:L2:197:ASP:OD1	2.42	0.51
7:DX:488:ASN:OD1	25:TF:153:ASN:ND2	2.42	0.51
4:A:1450:HIS:O	4:A:1452:ARG:N	2.43	0.51
13:L:24:MET:O	22:R:270:ARG:NH2	2.43	0.51
7:DX:330:ILE:HD12	7:DX:360:LYS:HD2	1.93	0.51
7:DX:397:VAL:HG22	7:DX:683:PHE:CE1	2.45	0.51
4:A:95:ASN:O	4:A:104:ARG:NH2	2.44	0.51
7:DX:443:TYR:OH	25:TF:204:THR:N	2.39	0.51
1:2:30:A:OP2	4:A:853:ARG:NH1	2.43	0.51
25:TF:161:MET:O	25:TF:166:TYR:N	2.43	0.51
4:A:1519:LEU:O	4:A:1521:GLN:N	2.43	0.51
4:A:1715:MET:HE3	4:A:1715:MET:HA	1.92	0.51
5:C:669:THR:OG1	5:C:832:MET:SD	2.54	0.51
7:DX:215:ILE:HD11	7:DX:454:VAL:HG13	1.92	0.51
16:M:214:ASP:OD1	22:R:269:LYS:NZ	2.40	0.50
4:A:142:ARG:NH2	4:A:608:PHE:O	2.44	0.50
4:A:801:ILE:HD11	4:A:984:LEU:HD21	1.93	0.50
26:W:441:LYS:NZ	26:W:480:ASP:OD2	2.35	0.50
5:C:431:PHE:O	5:C:434:PHE:N	2.42	0.50
4:A:1497:GLU:O	4:A:1526:ARG:NH2	2.44	0.50
11:J:82:ASN:O	11:J:84:MET:N	2.45	0.50
26:W:445:ASN:ND2	26:W:483:ARG:O	2.42	0.50
9:I:484:VAL:O	9:I:487:SER:OG	2.26	0.50
5:C:146:THR:OG1	42:C:1101:GTP:O2B	2.29	0.50
4:A:1885:PRO:O	4:A:1888:ALA:N	2.45	0.50
11:J:186:PRO:O	11:J:217:HIS:NE2	2.45	0.50
5:C:600:ASN:ND2	5:C:603:GLU:OE1	2.42	0.49
13:L:497:GLU:O	13:L:500:SER:N	2.44	0.49
14:L1:197:ARG:NH2	14:L1:199:PRO:O	2.45	0.49
19:P:67:GLU:OE1	24:T:456:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:743:THR:HG22	4:A:774:LEU:HD21	1.94	0.49
4:A:240:ASP:OD1	4:A:240:ASP:N	2.41	0.49
30:b:38:MET:SD	31:c:61:ARG:NH2	2.86	0.49
4:A:1628:TYR:N	4:A:1651:GLN:OE1	2.45	0.49
24:T:190:VAL:HG22	24:T:447:ALA:HB1	1.95	0.49
4:A:1611:LYS:NZ	4:A:1621:ASP:OD2	2.42	0.49
4:A:989:LEU:O	4:A:993:VAL:HG12	2.13	0.48
21:Q:567:LEU:HB3	21:Q:609:VAL:HG11	1.95	0.48
24:T:447:ALA:HB3	24:T:460:ALA:HB3	1.95	0.48
18:O:262:TYR:O	18:O:289:ARG:NH1	2.41	0.48
2:5:3:A:N6	2:5:81:G:N3	2.61	0.48
7:DX:540:VAL:HG21	7:DX:601:ALA:HB2	1.95	0.48
16:M:213:LEU:HD11	22:R:265:VAL:HG13	1.96	0.48
19:P:89:ARG:NH2	19:P:93:ASP:OD2	2.46	0.48
4:A:915:ASP:OD2	4:A:1432:ARG:NE	2.47	0.48
4:A:1551:THR:HG22	4:A:1553:ILE:H	1.78	0.48
9:I:418:ASP:OD1	9:I:419:ALA:N	2.46	0.48
8:E:187:ASN:O	8:E:210:ILE:HD11	2.14	0.48
9:I:688:ALA:HA	9:I:691:ILE:HD12	1.94	0.48
16:M:213:LEU:CD1	22:R:265:VAL:HG13	2.44	0.48
4:A:663:THR:O	4:A:668:ARG:NH2	2.40	0.48
14:L1:156:ASP:OD1	14:L1:156:ASP:N	2.47	0.48
30:i:81:THR:OG1	31:j:57:THR:O	2.29	0.48
4:A:1939:ASN:O	4:A:1942:LYS:N	2.47	0.48
11:J:202:GLU:O	11:J:204:ASP:N	2.47	0.48
11:J:257:ASN:O	11:J:259:THR:N	2.47	0.48
4:A:1337:GLN:NE2	4:A:1705:TYR:O	2.46	0.48
7:DX:698:ARG:NH1	27:X:253:GLU:OE1	2.45	0.48
14:L1:97:LYS:NZ	14:L1:131:GLU:OE1	2.47	0.48
20:PX:706:ILE:HD13	20:PX:709:ILE:HD12	1.94	0.48
5:C:243:GLU:OE2	5:C:247:ARG:NH1	2.46	0.48
9:I:232:CYS:HA	9:I:235:ILE:HG22	1.95	0.48
4:A:760:ASP:O	4:A:763:VAL:N	2.47	0.47
4:A:1327:ILE:HD11	4:A:1358:ILE:HG23	1.96	0.47
9:I:388:VAL:HG21	9:I:404:TRP:CZ2	2.48	0.47
5:C:212:VAL:HG23	5:C:902:MET:SD	2.55	0.47
5:C:730:LEU:HA	5:C:733:ALA:HB3	1.95	0.47
41:J:3000:IHP:O14	13:L:307:LYS:NZ	2.38	0.47
4:A:1486:THR:O	4:A:1488:PHE:N	2.43	0.47
22:R:265:VAL:HG12	22:R:265:VAL:O	2.14	0.47
4:A:790:GLY:O	4:A:792:TYR:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:203:ASN:OD1	16:M:204:GLU:N	2.48	0.47
18:O:168:CYS:O	18:O:171:PHE:N	2.41	0.47
13:L:66:GLU:N	13:L:66:GLU:OE1	2.47	0.47
2:5:4:C:O2	2:5:81:G:N2	2.28	0.47
5:C:264:ASP:OD1	5:C:314:SER:OG	2.26	0.47
13:L:146:ASP:OD1	13:L:147:ASP:N	2.48	0.47
18:O:238:TYR:N	18:O:308:ARG:O	2.47	0.47
25:TF:626:LEU:HD22	25:TF:660:ILE:HG22	1.95	0.47
26:W:433:GLU:HG3	26:W:440:THR:HG21	1.97	0.47
4:A:1313:GLU:OE2	4:A:1464:ARG:NH2	2.47	0.47
4:A:936:ASP:OD1	4:A:936:ASP:N	2.48	0.47
16:M:77:ALA:O	16:M:81:GLY:N	2.44	0.47
26:W:419:ARG:HH21	26:W:431:ILE:HG21	1.80	0.47
36:o:4:LEU:HD23	36:o:35:GLU:H	1.80	0.47
36:o:25:ASN:ND2	37:p:37:GLU:OE2	2.46	0.47
35:n:42:ILE:O	35:n:60:THR:N	2.43	0.46
36:o:92:THR:HG23	36:o:117:TYR:HB2	1.97	0.46
3:6:94:C:O2'	3:6:95:A:OP1	2.24	0.46
5:C:850:VAL:HG22	5:C:891:LEU:HD11	1.97	0.46
14:L1:441:THR:O	15:L2:435:LYS:NZ	2.47	0.46
13:L:524:VAL:HG21	38:q:109:TYR:CE2	2.50	0.46
3:6:56:C:OP1	4:A:658:LYS:NZ	2.40	0.46
4:A:1312:LYS:NZ	15:L2:361:MET:O	2.42	0.46
26:W:220:GLN:NE2	26:W:317:GLY:O	2.44	0.46
4:A:1858:ARG:O	4:A:1860:ALA:N	2.48	0.46
2:5:56:U:OP1	19:P:39:THR:OG1	2.30	0.46
4:A:1773:VAL:HG22	4:A:1856:VAL:HG22	1.98	0.46
2:5:60:G:H2'	2:5:61:U:H5'	1.98	0.46
5:C:267:LEU:HD13	5:C:267:LEU:H	1.80	0.46
5:C:600:ASN:OD1	5:C:600:ASN:N	2.48	0.46
25:TF:786:ARG:NE	25:TF:798:LEU:O	2.45	0.46
33:l:77:GLY:HA2	33:l:80:ILE:HD12	1.98	0.46
4:A:1007:VAL:HG22	4:A:1008:LEU:H	1.80	0.45
6:D:225:GLU:OE2	6:D:239:ARG:NE	2.48	0.45
32:k:110:VAL:HG13	34:m:64:ILE:HG22	1.97	0.45
2:5:9:G:H3'	2:5:10:U:H5''	1.98	0.45
22:R:274:ASP:OD2	22:R:276:ARG:NE	2.44	0.45
25:TF:614:ILE:HG21	25:TF:652:THR:HG22	1.98	0.45
34:m:67:ARG:O	34:m:70:ASN:ND2	2.49	0.45
4:A:1369:GLU:O	4:A:1373:VAL:HG22	2.16	0.45
21:Q:716:LEU:O	21:Q:768:ARG:NH1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:S:66:THR:HG21	26:W:55:VAL:HG22	1.98	0.45
29:h:19:VAL:HG12	29:h:75:PRO:HD3	1.98	0.45
7:DX:369:GLU:O	7:DX:416:ARG:NH1	2.49	0.45
6:D:113:ARG:NH2	9:I:216:ASN:OD1	2.47	0.45
7:DX:187:ARG:NH1	7:DX:508:GLU:O	2.48	0.45
7:DX:645:VAL:O	7:DX:657:VAL:HG23	2.16	0.45
13:L:467:LYS:NZ	13:L:469:ASP:OD1	2.43	0.45
2:5:5:U:O2'	2:5:6:C:O5'	2.28	0.45
4:A:1512:THR:O	4:A:1514:ALA:N	2.50	0.45
9:I:576:LYS:NZ	11:J:314:GLU:OE1	2.46	0.45
14:L1:201:ARG:NH1	14:L1:254:ALA:O	2.49	0.45
4:A:373:PRO:O	5:C:358:ARG:NH2	2.50	0.45
11:J:85:GLN:O	11:J:87:ALA:N	2.50	0.45
24:T:389:LEU:HD22	24:T:424:GLY:HA2	1.98	0.45
26:W:414:PHE:HA	26:W:477:LEU:HD23	1.98	0.45
26:W:507:ASP:O	26:W:509:SER:N	2.50	0.45
16:M:83:ASP:O	16:M:85:GLU:N	2.50	0.45
21:Q:852:ARG:NH1	21:Q:1030:LEU:O	2.46	0.45
25:TF:794:LEU:HD23	25:TF:805:VAL:HG21	1.98	0.45
4:A:181:ILE:HG13	4:A:563:ALA:HB1	1.99	0.45
7:DX:395:ILE:HD12	7:DX:397:VAL:HG21	1.98	0.45
9:I:703:VAL:HG23	9:I:704:HIS:CD2	2.51	0.44
11:J:169:ASN:O	11:J:172:GLY:N	2.48	0.44
14:L1:111:LEU:HD23	14:L1:175:LEU:HD21	1.98	0.44
17:N:88:ASP:O	17:N:90:ALA:N	2.50	0.44
20:PX:410:LYS:NZ	20:PX:520:ASP:OD1	2.50	0.44
26:W:290:LEU:HD21	26:W:302:LEU:HD13	1.98	0.44
9:I:547:LYS:HB2	11:J:306:LYS:HE3	1.99	0.44
9:I:416:ASP:O	9:I:420:ALA:N	2.48	0.44
14:L1:66:THR:N	14:L1:90:ASN:O	2.46	0.44
20:PX:407:LEU:O	20:PX:411:VAL:HG23	2.18	0.44
23:S:44:ASN:OD1	23:S:47:ASN:ND2	2.50	0.44
4:A:1988:ASN:O	4:A:1990:VAL:N	2.51	0.44
14:L1:338:ALA:O	14:L1:345:ALA:N	2.41	0.44
2:5:26:C:N4	4:A:457:LYS:O	2.49	0.44
4:A:994:ASP:O	4:A:996:ASN:N	2.50	0.44
2:5:75:C:O2'	2:5:76:A:O5'	2.35	0.44
3:6:50:C:OP2	3:6:69:U:O2'	2.32	0.44
5:C:817:ARG:NE	5:C:821:TYR:OH	2.51	0.44
21:Q:467:LEU:O	21:Q:1124:ARG:NH2	2.48	0.44
33:l:61:ASN:O	33:l:65:LYS:N	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L1:527:THR:O	15:L2:87:LYS:NZ	2.50	0.44
32:d:47:ARG:HH21	32:d:107:ILE:HD11	1.83	0.44
9:I:562:ASN:O	9:I:566:VAL:HG22	2.18	0.43
11:J:364:ILE:HG23	11:J:383:TRP:CZ2	2.53	0.43
25:TF:619:VAL:HG13	25:TF:660:ILE:HD11	2.00	0.43
29:h:53:ASP:OD1	29:h:54:GLY:N	2.49	0.43
4:A:388:ASP:OD1	4:A:388:ASP:N	2.50	0.43
5:C:600:ASN:O	5:C:602:SER:N	2.51	0.43
24:T:274:LEU:HB2	24:T:285:THR:HG22	2.00	0.43
38:s:123:LYS:NZ	38:s:334:GLU:OE2	2.44	0.43
30:i:3:ILE:O	30:i:5:LYS:N	2.47	0.43
5:C:262:LYS:HG2	42:C:1101:GTP:C5	2.53	0.43
9:I:290:ILE:HG21	9:I:350:LEU:HD13	1.99	0.43
10:IN:10:N:H2'	10:IN:11:N:H4'	2.00	0.43
21:Q:433:GLU:OE1	21:Q:649:ARG:NH1	2.51	0.43
38:s:177:ARG:NE	38:s:390:GLU:O	2.52	0.43
7:DX:607:GLN:O	7:DX:611:VAL:HG23	2.19	0.43
21:Q:168:VAL:HG22	21:Q:217:LEU:HD11	2.01	0.43
18:O:245:SER:OG	18:O:272:THR:O	2.35	0.43
32:k:55:ARG:O	32:k:68:GLU:N	2.41	0.43
2:5:83:A:N7	30:b:5:LYS:NZ	2.60	0.43
3:6:101:U:H2'	7:DX:510:PRO:HB3	2.00	0.43
4:A:1654:TRP:NE1	4:A:1690:SER:O	2.48	0.43
32:k:49:ASN:ND2	32:k:75:THR:O	2.44	0.43
4:A:65:ASP:OD1	4:A:67:THR:N	2.50	0.43
26:W:524:ASP:OD2	26:W:527:THR:N	2.46	0.43
5:C:640:TYR:O	5:C:644:VAL:HG23	2.18	0.43
11:J:462:GLU:OE2	11:J:470:ARG:NH2	2.49	0.43
26:W:445:ASN:OD1	26:W:446:VAL:N	2.51	0.43
4:A:428:PRO:HD2	4:A:431:MET:HE3	2.01	0.42
4:A:1482:LEU:O	4:A:1485:GLY:N	2.51	0.42
5:C:846:CYS:O	5:C:850:VAL:HG23	2.18	0.42
20:PX:459:ALA:O	20:PX:463:ALA:N	2.45	0.42
21:Q:581:ARG:NE	21:Q:596:SER:O	2.45	0.42
4:A:756:GLY:O	4:A:758:THR:N	2.52	0.42
11:J:309:GLU:HA	11:J:313:ILE:HD12	2.02	0.42
17:N:18:TRP:NE1	17:N:22:GLU:OE2	2.49	0.42
29:a:22:GLU:OE2	30:b:25:ARG:NH2	2.51	0.42
5:C:116:VAL:HG23	5:C:156:THR:O	2.19	0.42
5:C:212:VAL:HG22	5:C:241:ASN:OD1	2.19	0.42
25:TF:176:GLY:O	25:TF:178:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:148:ARG:NH1	4:A:562:ASP:OD2	2.47	0.42
4:A:443:LEU:O	4:A:447:VAL:HG23	2.20	0.42
4:A:1518:GLY:O	15:L2:194:ARG:NH1	2.50	0.42
4:A:1893:GLU:O	4:A:1897:ASP:N	2.53	0.42
14:L1:389:MET:HE1	14:L1:517:LEU:HD23	2.01	0.42
4:A:1926:PHE:O	4:A:1930:VAL:HG23	2.20	0.42
7:DX:198:TYR:O	7:DX:227:ARG:NH1	2.52	0.42
30:b:2:THR:OG1	30:b:3:ILE:N	2.52	0.42
4:A:550:VAL:O	4:A:554:VAL:HG23	2.19	0.42
4:A:1046:GLY:HA2	4:A:1050:ALA:HB3	2.01	0.42
5:C:859:GLY:O	25:TF:532:GLN:NE2	2.45	0.42
17:N:120:CYS:SG	17:N:121:ILE:N	2.92	0.42
30:i:83:ASP:OD1	30:i:83:ASP:N	2.52	0.42
38:s:20:VAL:HG22	38:s:47:LEU:HD13	2.01	0.42
4:A:1224:VAL:HB	4:A:1273:THR:HG21	2.01	0.42
16:M:75:LYS:O	16:M:79:ASP:N	2.46	0.42
3:6:90:G:H3'	3:6:91:U:H5''	2.02	0.42
4:A:875:ARG:NH2	13:L:128:GLU:OE2	2.53	0.42
21:Q:315:GLU:OE2	21:Q:424:ARG:NH2	2.50	0.42
8:E:97:VAL:HG12	8:E:129:VAL:HG21	2.00	0.42
13:L:9:GLY:O	13:L:41:LYS:NZ	2.53	0.42
20:PX:742:ARG:O	20:PX:746:LYS:NZ	2.41	0.42
22:R:3:MET:SD	22:R:4:LYS:N	2.93	0.42
25:TF:155:ASN:OD1	25:TF:155:ASN:N	2.52	0.42
11:J:325:TYR:OH	11:J:341:ASP:OD2	2.38	0.41
4:A:1310:THR:HG22	4:A:1310:THR:O	2.20	0.41
4:A:1392:GLN:OE1	4:A:1394:ARG:NH2	2.46	0.41
14:L1:102:THR:OG1	14:L1:104:SER:OG	2.36	0.41
15:L2:76:ASP:OD1	15:L2:76:ASP:N	2.53	0.41
23:S:82:ASP:OD1	23:S:106:ASN:ND2	2.46	0.41
25:TF:626:LEU:HD23	25:TF:665:PHE:HB2	2.02	0.41
4:A:670:GLU:OE2	4:A:770:ARG:NH1	2.53	0.41
7:DX:272:GLU:OE2	7:DX:281:ARG:NH1	2.48	0.41
10:IN:27:N:H5''	18:O:162:ARG:CG	2.51	0.41
4:A:286:ASP:O	4:A:287:ILE:HG22	2.20	0.41
34:m:39:ASP:OD2	34:m:43:ASN:ND2	2.47	0.41
37:p:27:SER:O	37:p:31:VAL:HG23	2.21	0.41
7:DX:317:ILE:HD13	7:DX:320:LEU:HD12	2.02	0.41
15:L2:152:ARG:NH1	15:L2:214:ASP:OD1	2.49	0.41
20:PX:614:GLU:HA	20:PX:618:ILE:HD12	2.02	0.41
27:X:254:GLU:O	27:X:257:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:454:ARG:O	9:I:457:ALA:N	2.48	0.41
24:T:322:ASP:N	24:T:322:ASP:OD1	2.53	0.41
13:L:438:GLN:OE1	13:L:439:MET:N	2.49	0.41
20:PX:435:ARG:NH1	20:PX:494:GLU:O	2.49	0.41
21:Q:1071:GLU:OE2	21:Q:1124:ARG:NE	2.50	0.41
5:C:445:PRO:O	5:C:449:ALA:N	2.50	0.41
11:J:89:TRP:CD1	11:J:112:ALA:HB2	2.56	0.41
25:TF:387:GLY:O	25:TF:390:SER:OG	2.34	0.41
25:TF:569:ILE:O	25:TF:572:VAL:HG22	2.21	0.41
26:W:194:GLN:O	26:W:198:ASP:N	2.49	0.41
32:d:39:ASN:ND2	32:d:118:GLU:OE1	2.54	0.41
33:e:61:ASN:O	33:e:65:LYS:N	2.53	0.41
34:m:69:ASN:OD1	34:m:70:ASN:N	2.53	0.41
11:J:253:GLU:OE2	22:R:4:LYS:NZ	2.45	0.41
14:L1:14:VAL:HA	14:L1:222:ILE:HD12	2.01	0.41
20:PX:339:ASP:N	20:PX:339:ASP:OD1	2.54	0.41
32:k:42:VAL:HG12	32:k:111:LYS:HA	2.03	0.41
39:y:13:LEU:HD21	39:y:65:ALA:HB1	2.02	0.41
4:A:933:LYS:HA	4:A:933:LYS:HE2	2.03	0.40
14:L1:106:LEU:HD23	14:L1:238:PRO:HB3	2.03	0.40
20:PX:401:ARG:NH1	25:TF:330:ASN:OD1	2.46	0.40
1:2:9:U:O2'	1:2:10:U:O4'	2.39	0.40
3:6:81:U:O2'	3:6:82:C:OP1	2.36	0.40
4:A:468:PHE:O	4:A:471:THR:HG22	2.21	0.40
4:A:1325:VAL:HB	4:A:1358:ILE:HD11	2.03	0.40
5:C:522:ASP:O	5:C:524:GLU:N	2.54	0.40
9:I:543:GLN:HB2	11:J:306:LYS:HA	2.04	0.40
29:a:41:ASN:OD1	29:a:66:GLY:N	2.47	0.40
34:m:31:TYR:OH	34:m:51:GLU:OE2	2.35	0.40
5:C:156:THR:OG1	5:C:157:HIS:ND1	2.55	0.40
18:O:40:ASP:O	18:O:54:THR:HG23	2.21	0.40
4:A:1652:LYS:O	4:A:1692:THR:OG1	2.39	0.40
5:C:400:MET:HA	5:C:400:MET:HE2	2.04	0.40
14:L1:399:THR:HG22	14:L1:413:MET:HG2	2.03	0.40
18:O:98:ARG:NH1	18:O:99:ASP:OD1	2.51	0.40
20:PX:469:ARG:NH2	20:PX:487:GLU:OE1	2.54	0.40
21:Q:91:MET:O	21:Q:95:VAL:HG23	2.22	0.40
33:e:39:LEU:HD12	33:e:75:LEU:HD22	2.04	0.40
34:m:36:VAL:O	34:m:45:GLN:NE2	2.47	0.40
4:A:880:GLN:O	4:A:882:ALA:N	2.55	0.40
4:A:1590:PHE:CE1	4:A:1715:MET:HE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1641:SER:OG	20:PX:367:GLN:NE2	2.55	0.40
4:A:1863:ASP:OD2	15:L2:132:ASN:ND2	2.55	0.40
8:E:64:PHE:O	8:E:73:ASN:ND2	2.49	0.40
9:I:41:ASN:OD1	9:I:45:ARG:NH2	2.54	0.40
9:I:215:GLN:NE2	9:I:217:VAL:O	2.55	0.40
16:M:93:SER:O	16:M:97:THR:OG1	2.38	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	
4	A	1976/2329 (85%)	1789 (90%)	101 (5%)	86 (4%)	2	12
5	C	896/974 (92%)	800 (89%)	66 (7%)	30 (3%)	3	17
6	D	192/267 (72%)	185 (96%)	7 (4%)	0	100	100
7	DX	680/739 (92%)	634 (93%)	36 (5%)	10 (2%)	8	35
8	E	310/331 (94%)	295 (95%)	13 (4%)	2 (1%)	21	56
9	I	743/855 (87%)	702 (94%)	37 (5%)	4 (0%)	24	60
11	J	570/744 (77%)	531 (93%)	22 (4%)	17 (3%)	3	19
12	K	201/238 (84%)	196 (98%)	4 (2%)	1 (0%)	24	60
13	L	611/755 (81%)	570 (93%)	28 (5%)	13 (2%)	5	27
14	L1	468/533 (88%)	435 (93%)	26 (6%)	7 (2%)	8	35
15	L2	358/460 (78%)	336 (94%)	16 (4%)	6 (2%)	7	32
16	M	190/234 (81%)	179 (94%)	6 (3%)	5 (3%)	4	23
17	N	140/147 (95%)	123 (88%)	10 (7%)	7 (5%)	1	10
18	O	334/408 (82%)	302 (90%)	23 (7%)	9 (3%)	4	22
19	P	146/230 (64%)	130 (89%)	10 (7%)	6 (4%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	PX	470/809 (58%)	468 (100%)	2 (0%)	0	100	100
21	Q	1376/1467 (94%)	1336 (97%)	39 (3%)	1 (0%)	48	80
22	R	274/535 (51%)	243 (89%)	26 (10%)	5 (2%)	6	31
23	S	167/169 (99%)	158 (95%)	9 (5%)	0	100	100
24	T	385/494 (78%)	342 (89%)	35 (9%)	8 (2%)	5	27
25	TF	551/830 (66%)	507 (92%)	35 (6%)	9 (2%)	7	34
26	W	490/567 (86%)	435 (89%)	40 (8%)	15 (3%)	3	19
27	X	78/500 (16%)	75 (96%)	2 (3%)	1 (1%)	9	38
28	Z	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
29	a	79/136 (58%)	78 (99%)	1 (1%)	0	100	100
29	h	79/136 (58%)	69 (87%)	8 (10%)	2 (2%)	4	23
30	b	92/160 (58%)	87 (95%)	5 (5%)	0	100	100
30	i	75/160 (47%)	69 (92%)	5 (7%)	1 (1%)	9	38
31	c	78/127 (61%)	76 (97%)	2 (3%)	0	100	100
31	j	78/127 (61%)	72 (92%)	6 (8%)	0	100	100
32	d	90/118 (76%)	86 (96%)	4 (4%)	0	100	100
32	k	75/118 (64%)	72 (96%)	3 (4%)	0	100	100
33	e	78/90 (87%)	74 (95%)	1 (1%)	3 (4%)	2	15
33	l	78/90 (87%)	73 (94%)	3 (4%)	2 (3%)	4	23
34	f	70/85 (82%)	68 (97%)	2 (3%)	0	100	100
34	m	70/85 (82%)	66 (94%)	3 (4%)	1 (1%)	9	36
35	g	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
35	n	75/77 (97%)	68 (91%)	5 (7%)	2 (3%)	4	22
36	o	160/253 (63%)	154 (96%)	5 (3%)	1 (1%)	21	56
37	p	74/217 (34%)	70 (95%)	4 (5%)	0	100	100
38	q	117/492 (24%)	115 (98%)	2 (2%)	0	100	100
38	r	129/492 (26%)	127 (98%)	1 (1%)	1 (1%)	16	50
38	s	465/492 (94%)	450 (97%)	14 (3%)	1 (0%)	43	76
38	t	124/492 (25%)	121 (98%)	3 (2%)	0	100	100
39	y	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
All	All	13911/18787 (74%)	12978 (93%)	677 (5%)	256 (2%)	9	31

All (256) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	68	SER
4	A	69	ARG
4	A	167	ASP
4	A	287	ILE
4	A	305	PRO
4	A	588	TYR
4	A	690	PRO
4	A	694	LYS
4	A	695	GLN
4	A	757	ALA
4	A	934	PRO
4	A	980	MET
4	A	995	HIS
4	A	1067	GLN
4	A	1135	MET
4	A	1310	THR
4	A	1311	PRO
4	A	1393	ASN
4	A	1394	ARG
4	A	1451	GLN
4	A	1455	GLY
4	A	1456	LYS
4	A	1487	TYR
4	A	1489	PRO
4	A	1513	ASN
4	A	1520	ASN
4	A	1730	ASN
4	A	1745	GLN
4	A	1846	PRO
4	A	1858	ARG
4	A	1873	PRO
4	A	1990	VAL
5	C	158	PRO
5	C	181	GLY
5	C	308	GLY
5	C	309	ASN
5	C	392	VAL
5	C	404	GLY
5	C	405	ILE
5	C	444	SER
5	C	539	ALA
5	C	619	PRO

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Mol	Chain	Res	Type
5	C	636	THR
5	C	737	TRP
5	C	782	PRO
5	C	843	PRO
7	DX	225	ARG
7	DX	226	ASN
7	DX	241	ALA
8	E	128	ALA
9	I	414	ASN
13	L	79	PRO
13	L	81	GLN
13	L	90	GLY
13	L	137	PRO
13	L	228	ASN
13	L	349	MET
14	L1	227	LYS
14	L1	228	GLN
15	L2	327	ASN
16	M	54	PRO
16	M	83	ASP
17	N	124	VAL
17	N	125	PRO
17	N	126	LYS
18	O	130	ASP
18	O	135	ILE
18	O	165	PRO
18	O	183	PRO
18	O	194	ASP
19	P	36	PRO
22	R	10	PRO
25	TF	151	ASP
25	TF	168	PRO
25	TF	546	ASP
26	W	105	GLU
26	W	176	PRO
26	W	190	THR
26	W	191	PRO
26	W	508	GLN
27	X	219	LYS
4	A	36	SER
4	A	432	PRO
4	A	453	HIS

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Mol	Chain	Res	Type
4	A	581	THR
4	A	725	THR
4	A	881	ARG
4	A	982	LEU
4	A	1007	VAL
4	A	1084	ILE
4	A	1094	SER
4	A	1225	ASP
4	A	1328	PRO
4	A	1329	GLN
4	A	1571	ARG
4	A	1859	LYS
4	A	1965	SER
4	A	1989	ASN
5	C	97	VAL
5	C	371	ARG
5	C	415	ASN
5	C	431	PHE
5	C	600	ASN
5	C	729	ASP
5	C	929	PRO
7	DX	242	GLY
7	DX	247	TYR
9	I	415	GLY
11	J	83	ARG
11	J	85	GLN
11	J	101	GLU
11	J	102	ILE
11	J	169	ASN
11	J	186	PRO
11	J	203	ILE
11	J	258	GLU
11	J	273	GLU
13	L	39	HIS
13	L	92	THR
13	L	268	LYS
14	L1	151	SER
16	M	163	HIS
17	N	88	ASP
17	N	89	ALA
17	N	104	CYS
18	O	111	GLN

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Mol	Chain	Res	Type
19	P	206	LYS
22	R	16	ASP
24	T	481	PRO
25	TF	148	MET
25	TF	180	VAL
26	W	84	SER
33	e	32	TYR
33	l	72	ARG
4	A	248	ASP
4	A	454	ARG
4	A	464	LEU
4	A	523	THR
4	A	559	ASN
4	A	562	ASP
4	A	724	PRO
4	A	794	SER
4	A	849	ASN
4	A	865	ASN
4	A	994	ASP
4	A	1012	LYS
4	A	1068	ASP
4	A	1273	THR
4	A	1450	HIS
4	A	1481	THR
4	A	1767	ASN
5	C	239	MET
5	C	730	LEU
7	DX	258	GLY
11	J	34	THR
11	J	86	LEU
11	J	99	ILE
11	J	202	GLU
11	J	257	ASN
13	L	42	SER
15	L2	268	ASP
16	M	84	TYR
17	N	74	SER
18	O	169	SER
19	P	48	GLN
19	P	49	GLU
21	Q	349	ASN
22	R	21	GLN

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Mol	Chain	Res	Type
24	T	248	LYS
26	W	68	PHE
29	h	46	GLU
38	r	22	GLY
4	A	232	ASN
4	A	297	ARG
4	A	1247	THR
4	A	1274	GLN
5	C	443	LYS
7	DX	240	ASP
7	DX	658	LYS
12	K	71	PHE
13	L	146	ASP
13	L	440	ARG
14	L1	191	LEU
14	L1	206	LEU
14	L1	229	LYS
15	L2	160	SER
15	L2	199	SER
15	L2	210	LYS
18	O	168	CYS
18	O	182	CYS
22	R	113	VAL
24	T	444	GLY
24	T	483	VAL
25	TF	176	GLY
26	W	67	LYS
26	W	360	GLY
33	e	13	PRO
30	i	4	SER
35	n	59	MET
4	A	426	HIS
4	A	665	THR
4	A	939	PRO
4	A	940	PRO
4	A	993	VAL
4	A	1136	LYS
4	A	1668	ASP
5	C	65	ASP
5	C	273	PRO
7	DX	168	GLU
7	DX	239	LEU

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Mol	Chain	Res	Type
13	L	229	PRO
14	L1	2	ALA
15	L2	209	GLY
16	M	152	TYR
19	P	30	TYR
24	T	438	SER
25	TF	154	SER
26	W	136	ASP
26	W	317	GLY
26	W	406	GLN
26	W	484	PHE
26	W	537	HIS
33	e	12	GLN
29	h	54	GLY
38	s	56	LYS
4	A	981	ASP
4	A	1296	ASN
4	A	1939	ASN
11	J	218	GLY
11	J	288	LEU
19	P	22	ASP
25	TF	196	ALA
4	A	296	ILE
4	A	759	VAL
5	C	601	PRO
5	C	803	GLU
11	J	100	GLY
24	T	167	LYS
34	m	74	VAL
35	n	68	VAL
4	A	1318	GLY
5	C	828	THR
5	C	866	PRO
8	E	205	GLY
22	R	12	PRO
26	W	531	VAL
24	T	182	GLY
4	A	417	PRO
4	A	1190	PRO
36	o	32	PRO
4	A	659	GLY
9	I	360	PRO

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Mol	Chain	Res	Type
9	I	799	GLY
24	T	261	ILE
25	TF	195	GLY
33	l	44	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1790/2100 (85%)	1733 (97%)	57 (3%)	34	67
5	C	793/861 (92%)	772 (97%)	21 (3%)	40	72
6	D	173/230 (75%)	171 (99%)	2 (1%)	63	82
7	DX	604/652 (93%)	597 (99%)	7 (1%)	63	82
8	E	275/291 (94%)	268 (98%)	7 (2%)	42	72
9	I	660/754 (88%)	638 (97%)	22 (3%)	33	67
11	J	508/650 (78%)	501 (99%)	7 (1%)	59	80
12	K	183/214 (86%)	182 (100%)	1 (0%)	81	89
13	L	543/645 (84%)	528 (97%)	15 (3%)	38	70
14	L1	406/452 (90%)	391 (96%)	15 (4%)	30	64
15	L2	331/417 (79%)	330 (100%)	1 (0%)	86	91
16	M	178/212 (84%)	174 (98%)	4 (2%)	45	74
17	N	125/129 (97%)	121 (97%)	4 (3%)	34	67
18	O	295/351 (84%)	290 (98%)	5 (2%)	53	78
19	P	129/197 (66%)	124 (96%)	5 (4%)	28	62
20	PX	423/724 (58%)	420 (99%)	3 (1%)	76	86
21	Q	1235/1311 (94%)	1232 (100%)	3 (0%)	87	92
22	R	235/447 (53%)	223 (95%)	12 (5%)	21	55
23	S	137/137 (100%)	135 (98%)	2 (2%)	57	80
24	T	335/421 (80%)	320 (96%)	15 (4%)	24	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	TF	493/718 (69%)	480 (97%)	13 (3%)	40	72
26	W	444/502 (88%)	426 (96%)	18 (4%)	27	61
27	X	69/443 (16%)	66 (96%)	3 (4%)	26	60
28	Z	63/63 (100%)	63 (100%)	0	100	100
29	a	71/106 (67%)	70 (99%)	1 (1%)	59	80
29	h	71/106 (67%)	70 (99%)	1 (1%)	59	80
30	b	79/116 (68%)	78 (99%)	1 (1%)	61	81
30	i	70/116 (60%)	68 (97%)	2 (3%)	37	70
31	c	73/98 (74%)	73 (100%)	0	100	100
31	j	73/98 (74%)	73 (100%)	0	100	100
32	d	84/103 (82%)	83 (99%)	1 (1%)	63	82
32	k	72/103 (70%)	72 (100%)	0	100	100
33	e	71/81 (88%)	71 (100%)	0	100	100
33	l	71/81 (88%)	70 (99%)	1 (1%)	59	80
34	f	61/71 (86%)	61 (100%)	0	100	100
34	m	61/71 (86%)	59 (97%)	2 (3%)	33	67
35	g	69/69 (100%)	68 (99%)	1 (1%)	59	80
35	n	69/69 (100%)	68 (99%)	1 (1%)	59	80
36	o	151/225 (67%)	150 (99%)	1 (1%)	76	86
37	p	68/192 (35%)	67 (98%)	1 (2%)	57	80
38	q	108/417 (26%)	107 (99%)	1 (1%)	70	85
38	r	114/417 (27%)	112 (98%)	2 (2%)	51	77
38	s	396/417 (95%)	392 (99%)	4 (1%)	68	84
38	t	115/417 (28%)	115 (100%)	0	100	100
39	y	64/64 (100%)	63 (98%)	1 (2%)	55	79
All	All	12438/16358 (76%)	12175 (98%)	263 (2%)	46	75

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	21	GLU
4	A	68	SER
4	A	70	LYS

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Mol	Chain	Res	Type
4	A	79	LEU
4	A	87	HIS
4	A	103	ILE
4	A	120	ASN
4	A	129	VAL
4	A	209	VAL
4	A	213	THR
4	A	227	LEU
4	A	240	ASP
4	A	246	LEU
4	A	298	THR
4	A	305	PRO
4	A	327	VAL
4	A	532	PHE
4	A	560	ASN
4	A	577	VAL
4	A	587	LYS
4	A	603	LEU
4	A	669	VAL
4	A	690	PRO
4	A	801	ILE
4	A	836	GLU
4	A	840	GLU
4	A	876	HIS
4	A	885	GLU
4	A	891	MET
4	A	934	PRO
4	A	961	SER
4	A	969	MET
4	A	1020	PHE
4	A	1097	GLU
4	A	1177	MET
4	A	1267	ARG
4	A	1312	LYS
4	A	1329	GLN
4	A	1358	ILE
4	A	1480	HIS
4	A	1487	TYR
4	A	1489	PRO
4	A	1497	GLU
4	A	1512	THR
4	A	1551	THR

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Mol	Chain	Res	Type
4	A	1630	TRP
4	A	1651	GLN
4	A	1667	HIS
4	A	1694	VAL
4	A	1715	MET
4	A	1846	PRO
4	A	1873	PRO
4	A	1877	ILE
4	A	1893	GLU
4	A	1899	ILE
4	A	1920	ILE
4	A	1924	THR
5	C	76	TYR
5	C	92	LEU
5	C	145	LYS
5	C	233	ASP
5	C	235	HIS
5	C	258	LEU
5	C	267	LEU
5	C	326	PHE
5	C	380	PRO
5	C	381	MET
5	C	392	VAL
5	C	501	MET
5	C	619	PRO
5	C	698	LYS
5	C	718	LEU
5	C	728	TRP
5	C	737	TRP
5	C	760	LYS
5	C	796	LEU
5	C	807	ARG
5	C	930	THR
6	D	155	ARG
6	D	243	LEU
7	DX	66	TYR
7	DX	213	THR
7	DX	243	LYS
7	DX	260	THR
7	DX	367	ILE
7	DX	681	ASN
7	DX	708	GLN

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Mol	Chain	Res	Type
8	E	127	ASN
8	E	186	ASP
8	E	187	ASN
8	E	255	ASN
8	E	293	TYR
8	E	295	LEU
8	E	314	MET
9	I	34	ILE
9	I	176	TYR
9	I	215	GLN
9	I	250	ILE
9	I	295	THR
9	I	351	MET
9	I	372	ILE
9	I	395	ILE
9	I	399	LYS
9	I	417	LEU
9	I	438	LEU
9	I	487	SER
9	I	515	ILE
9	I	551	LEU
9	I	569	ILE
9	I	578	GLU
9	I	628	ASP
9	I	663	LEU
9	I	735	GLU
9	I	791	LYS
9	I	798	ARG
9	I	802	LYS
11	J	89	TRP
11	J	97	GLU
11	J	117	HIS
11	J	119	SER
11	J	147	ILE
11	J	309	GLU
11	J	603	CYS
12	K	79	GLU
13	L	13	ASN
13	L	89	VAL
13	L	132	THR
13	L	137	PRO
13	L	162	ASN

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Mol	Chain	Res	Type
13	L	316	ARG
13	L	318	TYR
13	L	347	THR
13	L	355	GLN
13	L	361	LEU
13	L	365	GLN
13	L	366	ASN
13	L	438	GLN
13	L	452	GLN
13	L	467	LYS
14	L1	3	THR
14	L1	32	ASN
14	L1	37	SER
14	L1	62	PHE
14	L1	118	SER
14	L1	121	LEU
14	L1	134	ILE
14	L1	156	ASP
14	L1	157	ILE
14	L1	176	SER
14	L1	193	VAL
14	L1	226	GLU
14	L1	235	ASN
14	L1	449	LEU
14	L1	532	SER
15	L2	184	ARG
16	M	54	PRO
16	M	63	ARG
16	M	83	ASP
16	M	151	PHE
17	N	111	THR
17	N	125	PRO
17	N	126	LYS
17	N	135	ILE
18	O	40	ASP
18	O	42	TYR
18	O	115	ARG
18	O	163	ASN
18	O	199	GLN
19	P	3	THR
19	P	54	LEU
19	P	59	LEU

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Mol	Chain	Res	Type
19	P	90	GLN
19	P	216	ILE
20	PX	344	LEU
20	PX	440	MET
20	PX	443	GLN
21	Q	318	ASP
21	Q	825	VAL
21	Q	1118	GLU
22	R	3	MET
22	R	4	LYS
22	R	21	GLN
22	R	53	PHE
22	R	91	THR
22	R	107	ILE
22	R	156	LEU
22	R	160	VAL
22	R	200	ILE
22	R	204	GLU
22	R	241	THR
22	R	290	LEU
23	S	100	ASN
23	S	147	ASN
24	T	92	MET
24	T	93	LEU
24	T	261	ILE
24	T	272	GLN
24	T	289	ASP
24	T	344	SER
24	T	345	MET
24	T	346	CYS
24	T	387	GLN
24	T	388	ASN
24	T	389	LEU
24	T	435	GLN
24	T	436	PRO
24	T	446	TYR
24	T	451	ASP
25	TF	153	ASN
25	TF	155	ASN
25	TF	194	VAL
25	TF	200	GLU
25	TF	202	THR

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Mol	Chain	Res	Type
25	TF	368	LEU
25	TF	392	ARG
25	TF	451	ILE
25	TF	536	PRO
25	TF	590	MET
25	TF	682	VAL
25	TF	777	PRO
25	TF	829	GLN
26	W	58	LYS
26	W	69	ASP
26	W	133	PHE
26	W	282	GLN
26	W	294	CYS
26	W	299	LYS
26	W	305	VAL
26	W	312	VAL
26	W	343	VAL
26	W	354	LYS
26	W	369	HIS
26	W	385	LYS
26	W	410	SER
26	W	417	ASN
26	W	434	TRP
26	W	454	MET
26	W	481	LYS
26	W	504	PHE
27	X	246	GLN
27	X	247	ASP
27	X	257	ASN
29	a	47	THR
30	b	38	MET
32	d	48	ASN
35	g	22	ASN
29	h	77	MET
30	i	35	ASP
30	i	89	ASP
33	l	44	ILE
34	m	72	LEU
34	m	73	TYR
35	n	32	ARG
36	o	106	ILE
37	p	34	GLN

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Mol	Chain	Res	Type
38	q	16	VAL
38	r	104	LEU
38	r	115	CYS
38	s	24	ILE
38	s	211	THR
38	s	390	GLU
38	s	432	ASP
39	y	33	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	63	HIS
4	A	285	ASN
4	A	323	HIS
4	A	449	ASN
4	A	553	HIS
4	A	646	ASN
4	A	651	GLN
4	A	849	ASN
4	A	986	ASN
4	A	1005	ASN
4	A	1137	HIS
4	A	1140	ASN
4	A	1174	ASN
4	A	1207	ASN
4	A	1219	GLN
4	A	1234	ASN
4	A	1324	HIS
4	A	1336	GLN
4	A	1443	GLN
4	A	1524	ASN
5	C	142	HIS
5	C	235	HIS
5	C	287	GLN
5	C	333	GLN
5	C	387	GLN
5	C	906	HIS
5	C	954	ASN
6	D	39	ASN
7	DX	412	GLN
7	DX	514	GLN

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Mol	Chain	Res	Type
7	DX	576	HIS
7	DX	644	GLN
8	E	179	GLN
8	E	252	HIS
8	E	254	HIS
8	E	255	ASN
9	I	166	HIS
9	I	392	ASN
9	I	440	ASN
9	I	615	HIS
9	I	704	HIS
9	I	718	HIS
9	I	806	GLN
12	K	123	GLN
12	K	219	GLN
13	L	73	HIS
13	L	209	GLN
13	L	221	HIS
13	L	452	GLN
13	L	565	ASN
14	L1	52	ASN
15	L2	207	GLN
15	L2	288	GLN
15	L2	434	GLN
16	M	160	HIS
17	N	58	GLN
17	N	139	HIS
18	O	249	GLN
19	P	5	HIS
19	P	94	GLN
19	P	221	HIS
20	PX	566	GLN
20	PX	586	HIS
20	PX	600	GLN
21	Q	161	HIS
21	Q	507	HIS
21	Q	527	HIS
21	Q	615	GLN
21	Q	682	GLN
21	Q	989	ASN
21	Q	1068	GLN
21	Q	1154	ASN

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Mol	Chain	Res	Type
21	Q	1268	GLN
22	R	234	HIS
22	R	246	ASN
23	S	100	ASN
23	S	124	HIS
23	S	147	ASN
24	T	302	GLN
24	T	330	HIS
25	TF	376	GLN
25	TF	471	HIS
25	TF	771	ASN
25	TF	776	HIS
26	W	102	HIS
26	W	251	ASN
26	W	279	ASN
26	W	329	ASN
31	c	16	ASN
31	c	21	ASN
32	d	34	ASN
32	d	38	ASN
33	e	37	HIS
32	k	112	ASN
35	n	22	ASN
36	o	127	HIS
37	p	54	HIS
38	s	183	ASN
38	s	245	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	38/228 (16%)	18 (47%)	4 (10%)
10	IN	1/51 (1%)	1 (100%)	0
2	5	110/112 (98%)	33 (30%)	12 (10%)
3	6	100/101 (99%)	48 (48%)	13 (13%)
All	All	249/492 (50%)	100 (40%)	29 (11%)

All (100) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	U

Continued on next page...

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Mol	Chain	Res	Type
1	2	19	U
1	2	21	G
1	2	25	A
1	2	26	G
1	2	30	A
1	2	31	A
1	2	32	A
1	2	33	G
1	2	34	U
1	2	35	G
1	2	36	U
1	2	37	A
1	2	38	G
1	2	39	U
1	2	40	A
1	2	41	U
1	2	42	C
2	5	4	C
2	5	6	C
2	5	8	G
2	5	9	G
2	5	10	U
2	5	20	U
2	5	23	A
2	5	24	A
2	5	25	C
2	5	26	C
2	5	28	U
2	5	43	U
2	5	60	G
2	5	73	U
2	5	74	A
2	5	76	A
2	5	77	U
2	5	79	G
2	5	80	A
2	5	81	G
2	5	82	U
2	5	83	A
2	5	94	U
2	5	96	U
2	5	100	G

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Mol	Chain	Res	Type
2	5	101	A
2	5	105	C
2	5	110	G
2	5	112	G
2	5	113	A
2	5	114	G
2	5	115	A
2	5	117	C
3	6	4	C
3	6	5	U
3	6	6	U
3	6	7	C
3	6	8	C
3	6	9	G
3	6	10	A
3	6	20	C
3	6	21	U
3	6	22	A
3	6	23	A
3	6	24	A
3	6	29	G
3	6	32	C
3	6	33	A
3	6	34	A
3	6	37	C
3	6	38	A
3	6	39	G
3	6	40	A
3	6	41	G
3	6	43	A
3	6	44	G
3	6	46	U
3	6	48	A
3	6	49	G
3	6	54	G
3	6	56	C
3	6	62	G
3	6	64	A
3	6	69	U
3	6	74	C
3	6	77	A
3	6	79	A

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Mol	Chain	Res	Type
3	6	81	U
3	6	82	C
3	6	84	U
3	6	85	G
3	6	86	A
3	6	89	C
3	6	90	G
3	6	91	U
3	6	92	U
3	6	93	C
3	6	95	A
3	6	96	A
3	6	97	A
3	6	101	U
10	IN	2	U

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	18	U
1	2	25	A
1	2	29	C
1	2	34	U
2	5	3	A
2	5	5	U
2	5	9	G
2	5	19	A
2	5	25	C
2	5	27	G
2	5	79	G
2	5	82	U
2	5	109	C
2	5	111	A
2	5	112	G
2	5	114	G
3	6	23	A
3	6	28	G
3	6	32	C
3	6	38	A
3	6	39	G
3	6	41	G
3	6	43	A

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Mol	Chain	Res	Type
3	6	45	A
3	6	48	A
3	6	53	G
3	6	81	U
3	6	85	G
3	6	90	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 14 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
41	IHP	A	3000	-	36,36,36	2.12	7 (19%)	60,60,60	1.36	9 (15%)
41	IHP	J	3000	-	36,36,36	2.37	10 (27%)	60,60,60	0.99	4 (6%)
42	GTP	C	1101	40	33,34,34	1.17	1 (3%)	50,54,54	1.99	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
41	IHP	A	3000	-	-	2/30/54/54	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	IHP	J	3000	-	-	4/30/54/54	0/1/1/1
42	GTP	C	1101	40	-	0/22/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	J	3000	IHP	C3-C2	-5.55	1.40	1.52
41	A	3000	IHP	P5-O15	5.30	1.68	1.59
41	A	3000	IHP	P4-O14	5.07	1.68	1.59
41	A	3000	IHP	P6-O16	5.00	1.68	1.59
41	J	3000	IHP	P3-O13	4.97	1.68	1.59
41	A	3000	IHP	P2-O12	4.92	1.68	1.59
41	J	3000	IHP	P2-O12	4.74	1.67	1.59
41	J	3000	IHP	P4-O14	4.63	1.67	1.59
41	J	3000	IHP	P1-O11	4.52	1.67	1.59
41	J	3000	IHP	P5-O15	4.36	1.67	1.59
41	A	3000	IHP	P3-O13	4.23	1.66	1.59
41	J	3000	IHP	P6-O16	4.05	1.66	1.59
41	A	3000	IHP	P1-O11	3.68	1.66	1.59
41	J	3000	IHP	O12-C2	-3.45	1.32	1.44
41	J	3000	IHP	O13-C3	-2.81	1.34	1.44
41	J	3000	IHP	C2-C1	-2.69	1.46	1.52
42	C	1101	GTP	C5-N7	-2.35	1.34	1.39
41	A	3000	IHP	C6-C5	2.00	1.56	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	C	1101	GTP	C5-C4-N3	-5.79	119.17	128.39
42	C	1101	GTP	C2-N3-C4	5.44	121.67	112.30
42	C	1101	GTP	C2-N1-C6	-4.95	116.14	125.11
42	C	1101	GTP	C5-C6-N1	3.88	123.14	113.25
42	C	1101	GTP	O6-C6-C5	-3.57	117.10	126.53
42	C	1101	GTP	O3G-PG-O3B	3.35	115.87	104.64
42	C	1101	GTP	O4'-C1'-N9	3.30	115.83	108.36
41	A	3000	IHP	O16-C6-C5	-3.28	101.79	108.76
41	A	3000	IHP	C5-C6-C1	3.18	117.41	110.43
41	A	3000	IHP	O11-C1-C2	-3.11	102.14	108.76
41	A	3000	IHP	P5-O15-C5	-3.03	115.35	123.43
41	A	3000	IHP	P6-O16-C6	-3.00	115.42	123.43
41	J	3000	IHP	C4-C3-C2	2.87	116.73	110.43
42	C	1101	GTP	N9-C4-N3	2.59	131.12	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	A	3000	IHP	C6-C1-C2	2.58	116.09	110.43
41	J	3000	IHP	C3-C2-C1	2.42	115.74	110.43
41	A	3000	IHP	C6-C5-C4	2.41	115.71	110.43
41	A	3000	IHP	O11-P1-O21	-2.23	101.38	109.33
41	A	3000	IHP	O11-C1-C6	2.20	113.44	108.76
42	C	1101	GTP	C5-C4-N9	2.18	109.55	105.66
42	C	1101	GTP	N9-C8-N7	-2.10	109.51	113.40
41	J	3000	IHP	O46-P6-O36	2.05	115.49	107.80
41	J	3000	IHP	O12-C2-C1	-2.03	104.44	108.76

There are no chirality outliers.

All (6) torsion outliers are listed below:

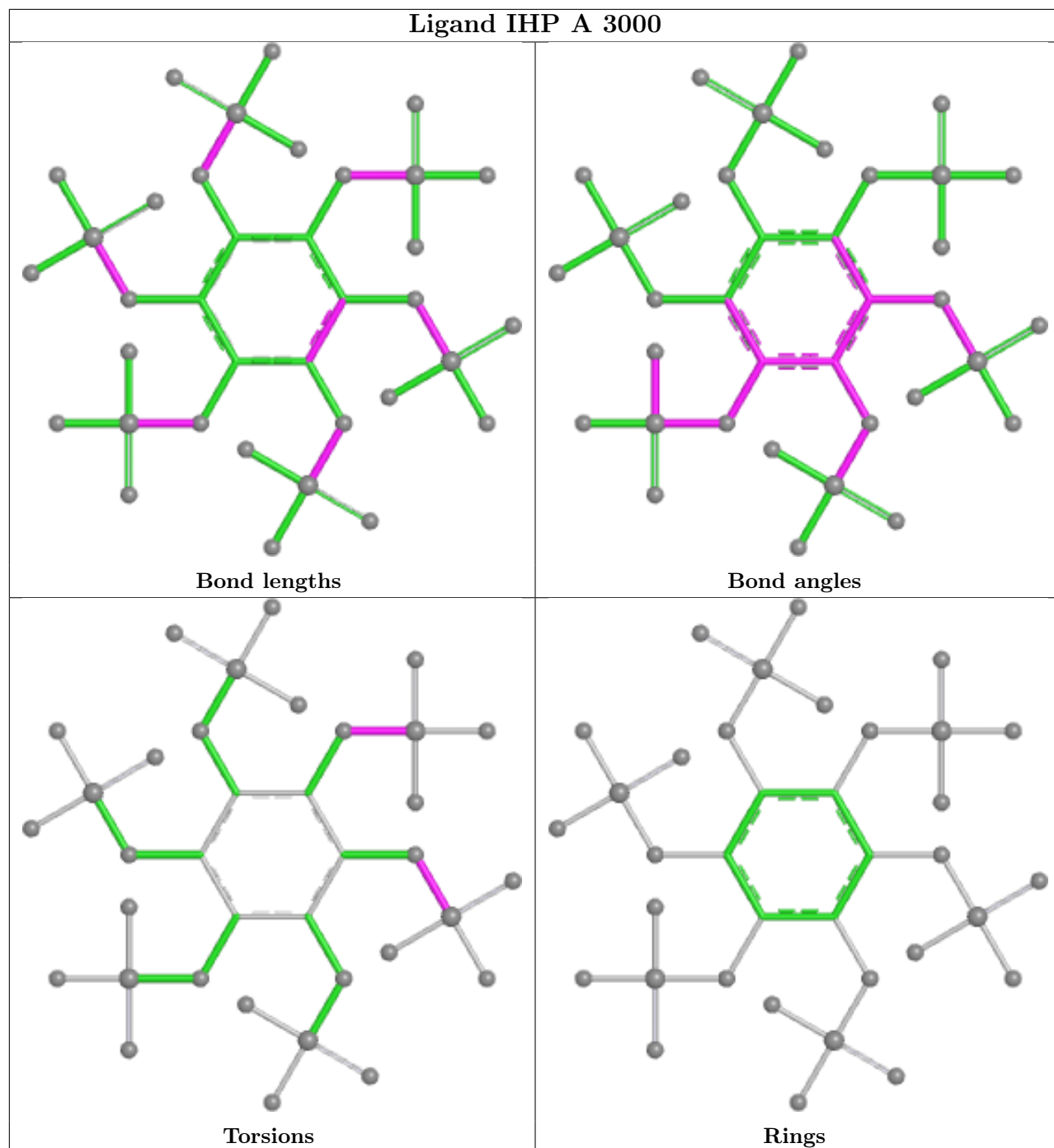
Mol	Chain	Res	Type	Atoms
41	J	3000	IHP	C4-O14-P4-O24
41	J	3000	IHP	C5-O15-P5-O25
41	A	3000	IHP	C4-O14-P4-O44
41	J	3000	IHP	C5-O15-P5-O35
41	J	3000	IHP	C5-O15-P5-O45
41	A	3000	IHP	C5-O15-P5-O25

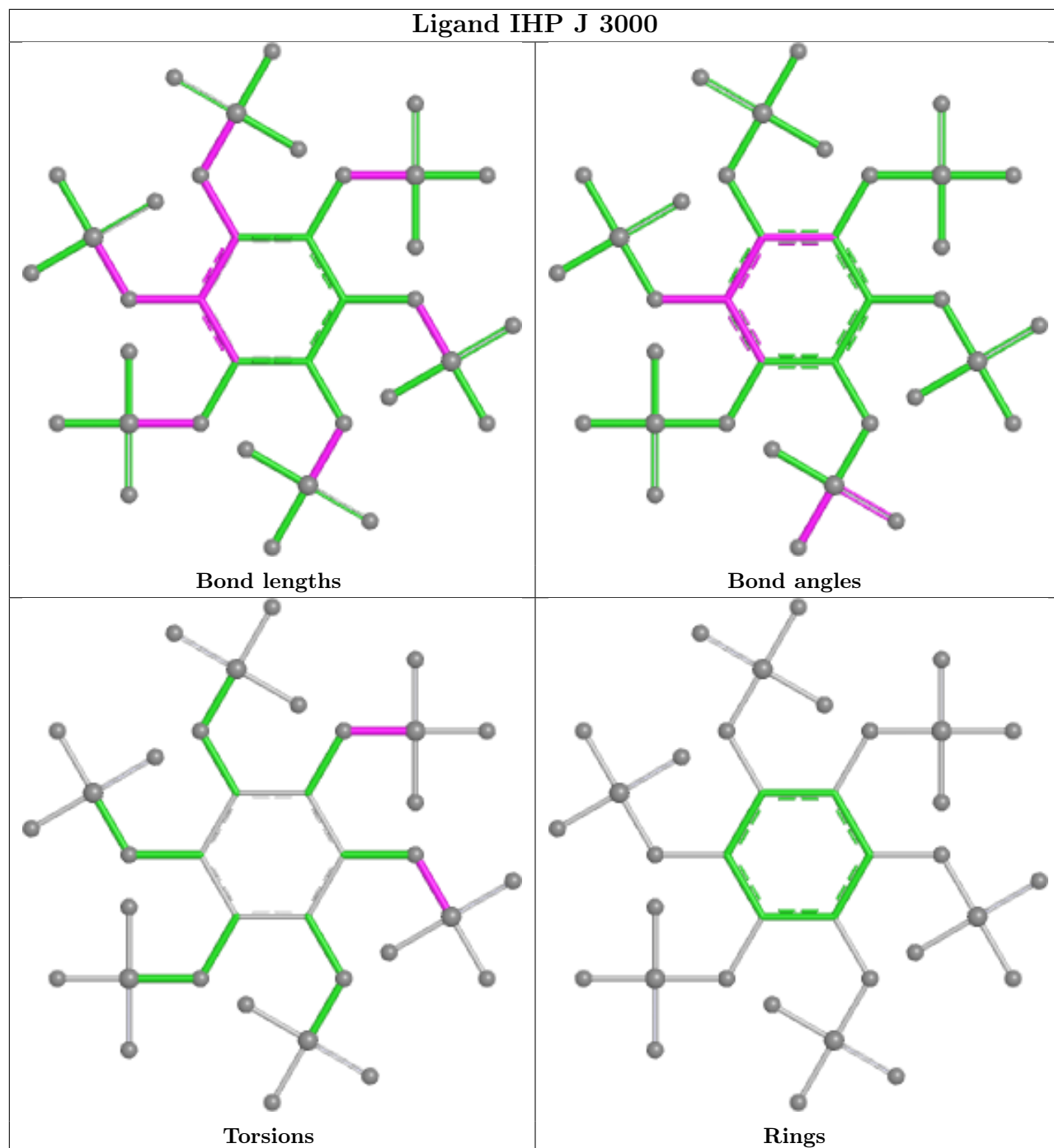
There are no ring outliers.

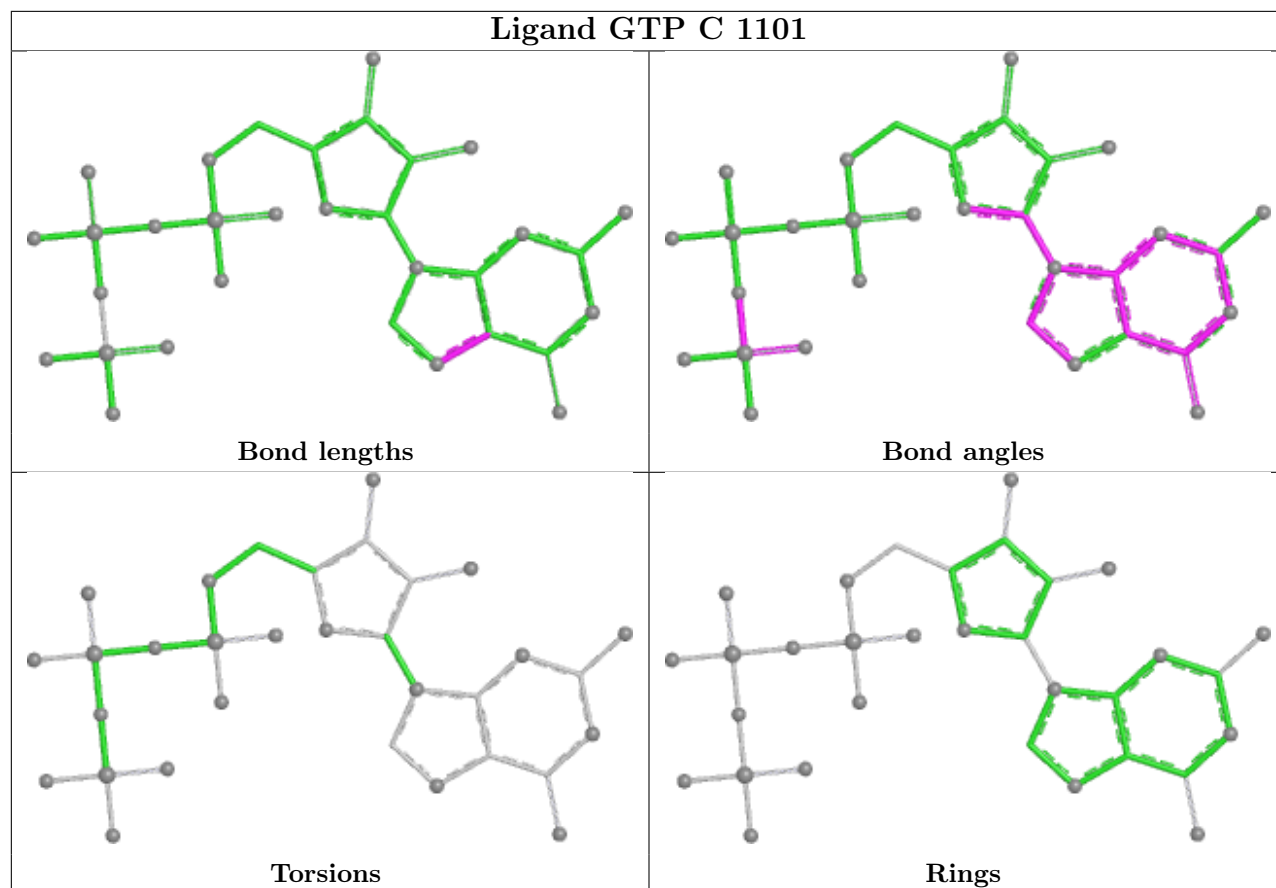
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	J	3000	IHP	2	0
42	C	1101	GTP	6	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

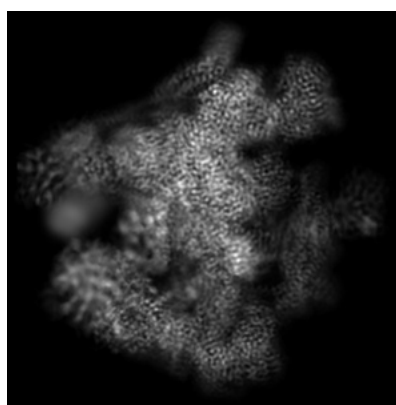
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19398. These allow visual inspection of the internal detail of the map and identification of artifacts.

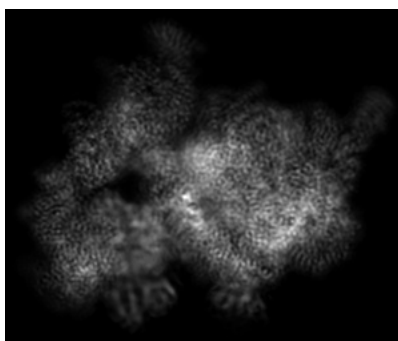
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

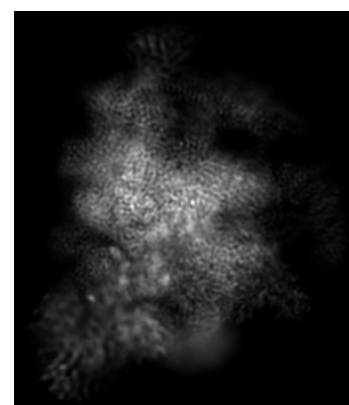
6.1.1 Primary map



X



Y

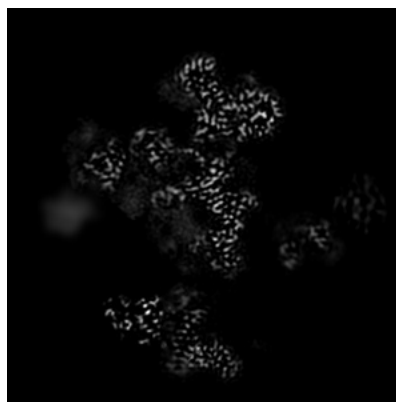


Z

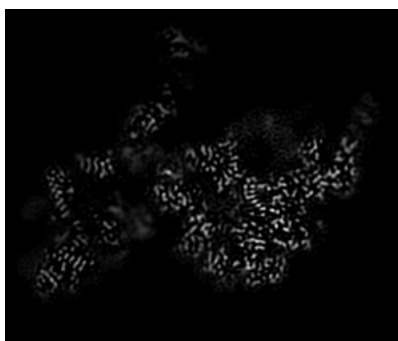
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

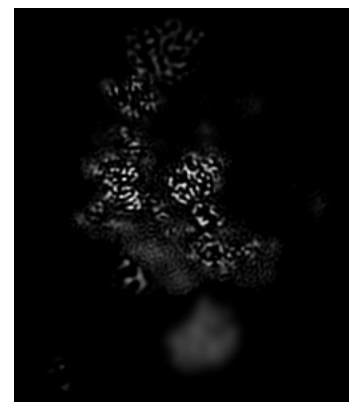
6.2.1 Primary map



X Index: 99



Y Index: 115

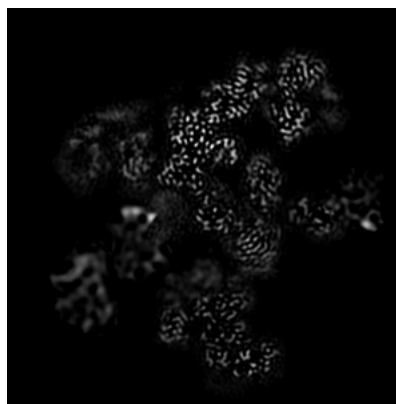


Z Index: 118

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: 73



Y Index: 122

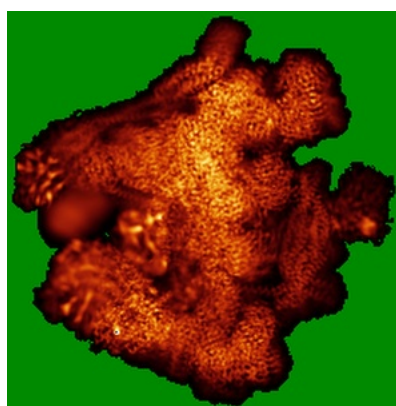


Z Index: 132

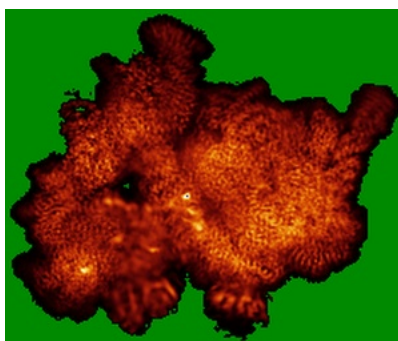
The images above show the largest variance slices of the map in three orthogonal directions.

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

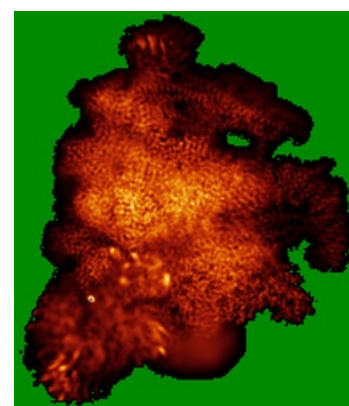
6.4.1 Primary map



X



Y

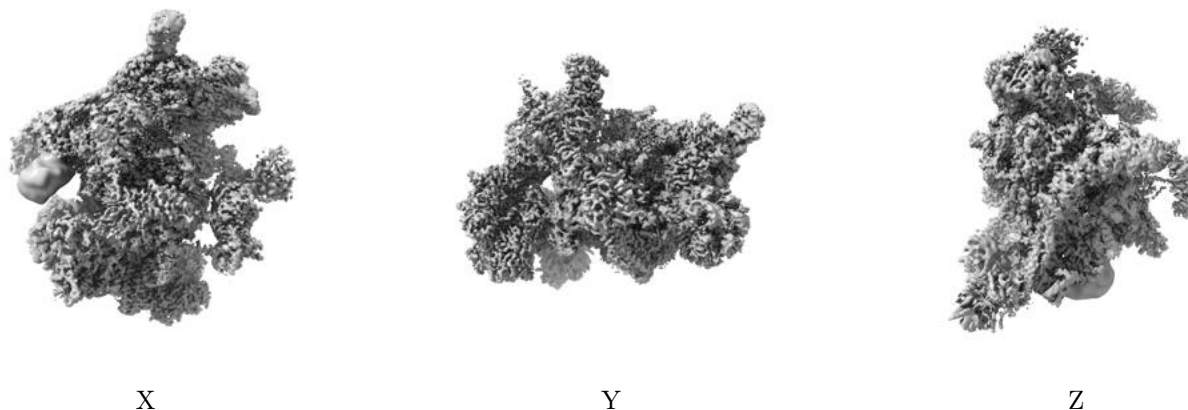


Z

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

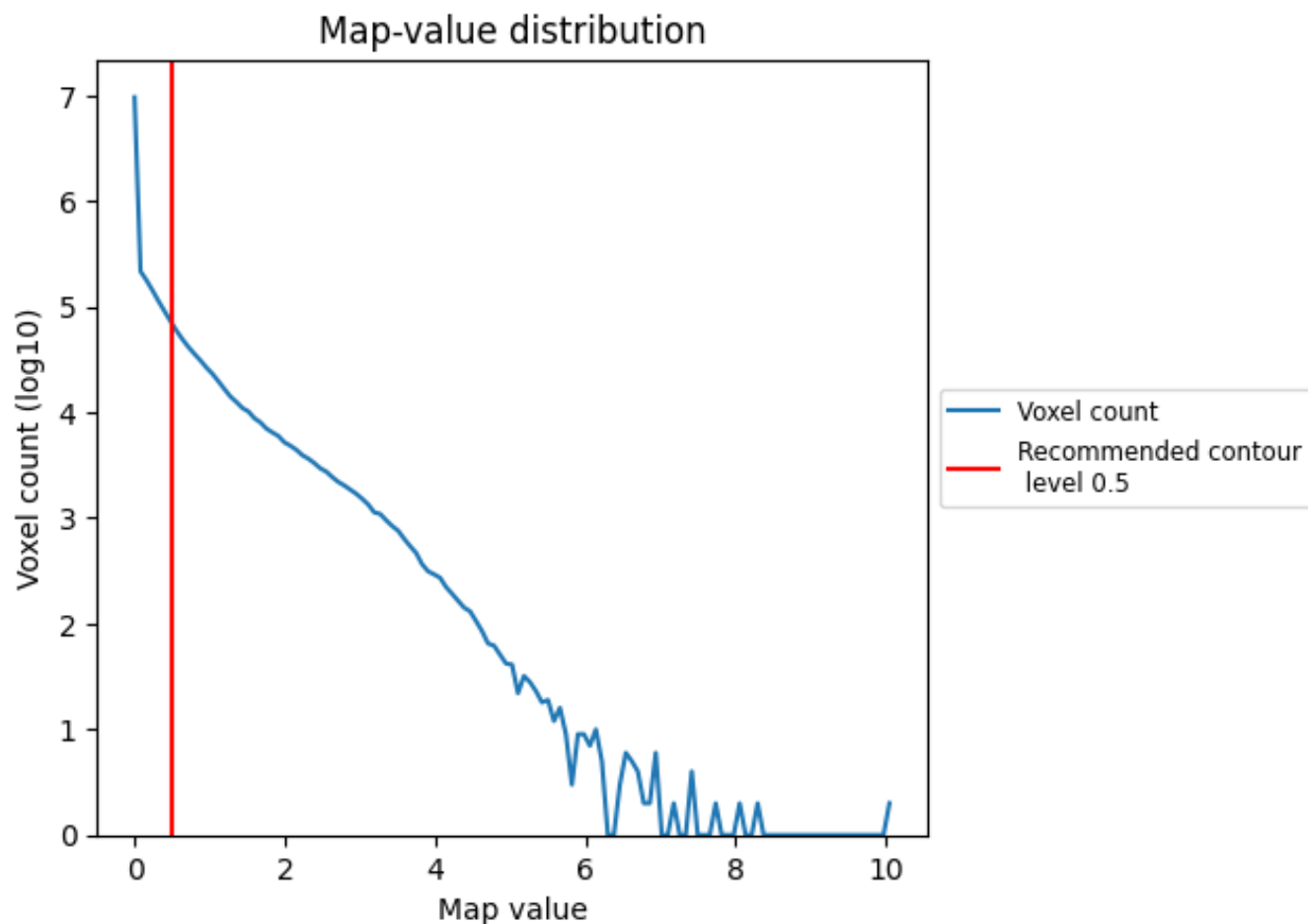
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

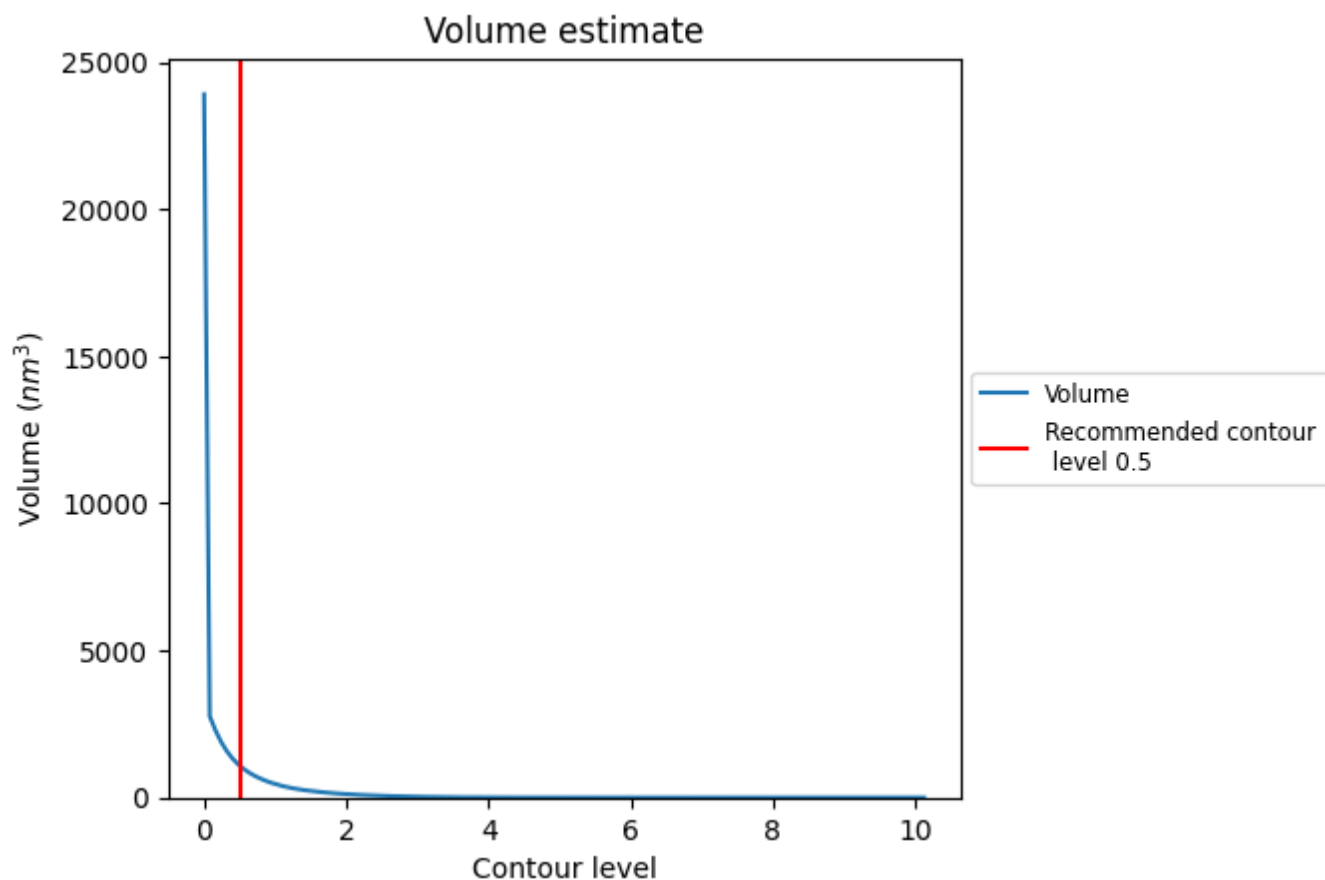
This section contains the results of statistical analysis of the map.

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 1088 nm³; this corresponds to an approximate mass of 983 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

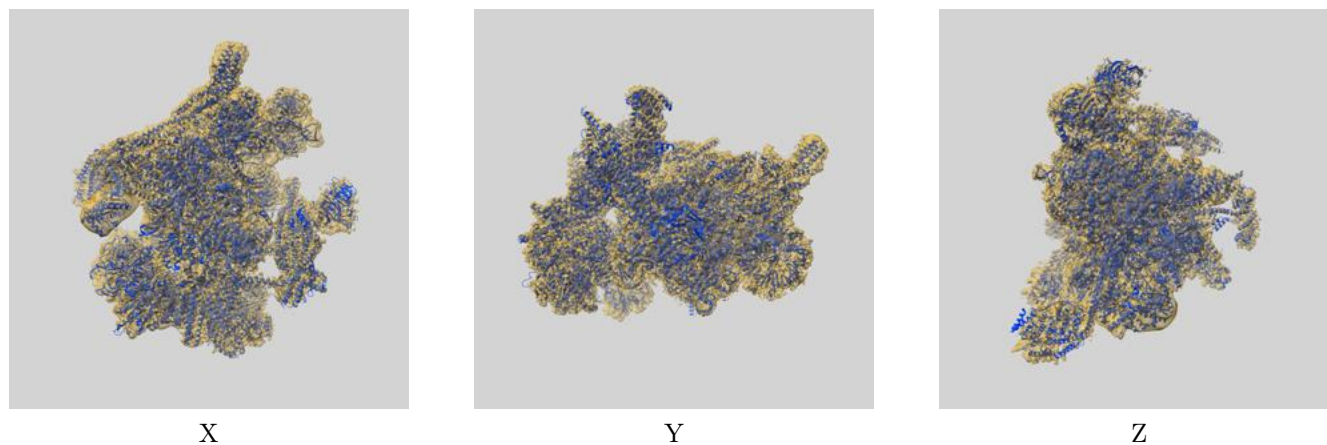
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

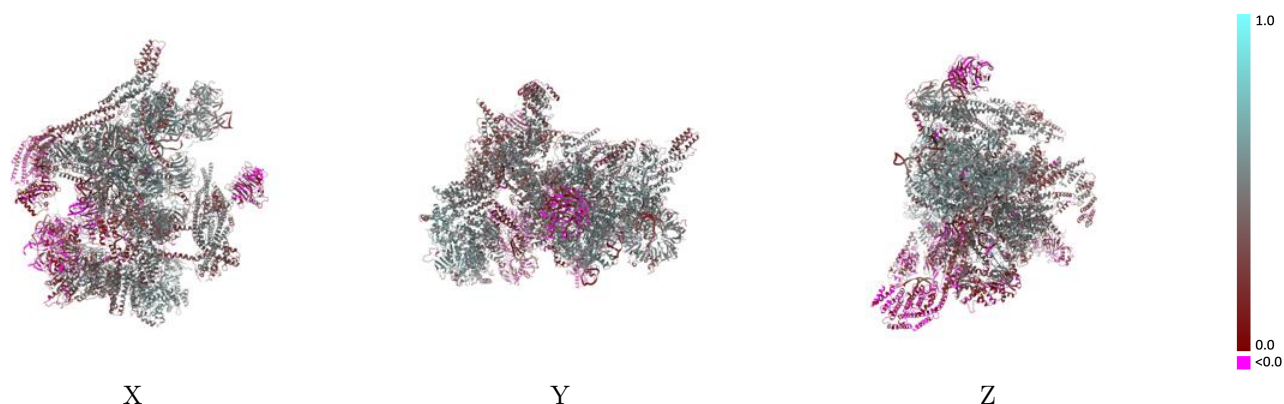
This section contains information regarding the fit between EMDB map EMD-19398 and PDB model 8RO1. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



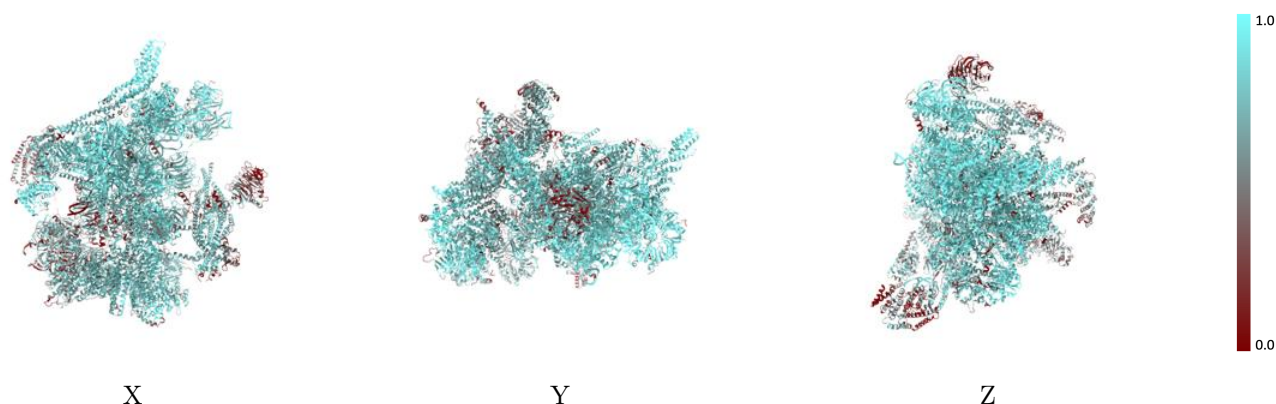
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



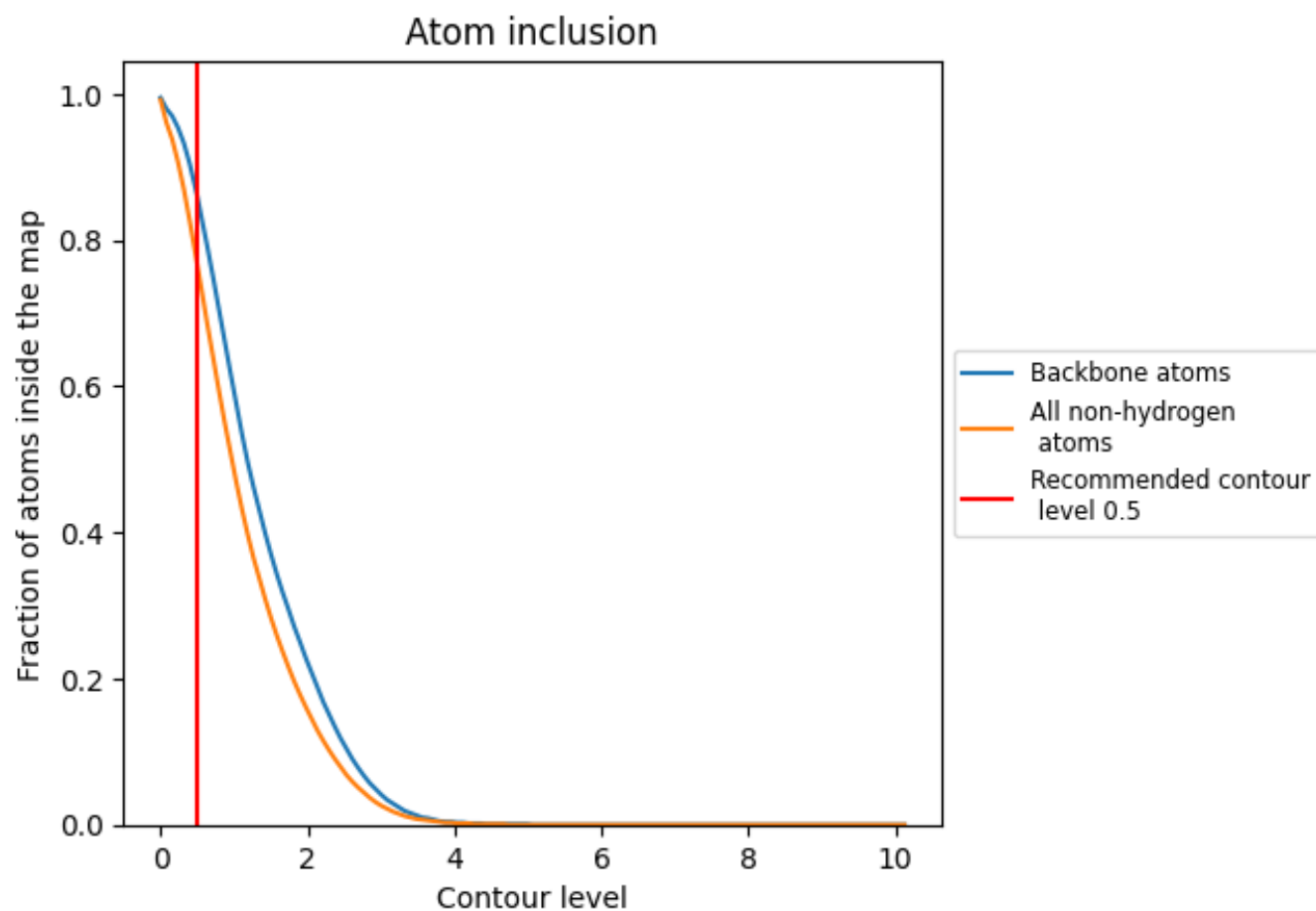
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 77% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7670	 0.3730
2	 0.7910	 0.1990
5	 0.9250	 0.3860
6	 0.9140	 0.3690
A	 0.8850	 0.4550
C	 0.9180	 0.5080
D	 0.5890	 0.2280
DX	 0.6750	 0.3620
E	 0.8960	 0.5150
I	 0.8270	 0.4520
IN	 0.6210	 0.1200
J	 0.7830	 0.4420
K	 0.6830	 0.4120
L	 0.6470	 0.3620
L1	 0.6700	 0.1440
L2	 0.8300	 0.3910
M	 0.7920	 0.3580
N	 0.9560	 0.5340
O	 0.8550	 0.4330
P	 0.5210	 0.2890
PX	 0.4250	 0.0570
Q	 0.8260	 0.5110
R	 0.8360	 0.4130
S	 0.7870	 0.4330
T	 0.9160	 0.5250
TF	 0.8020	 0.3470
W	 0.6480	 0.1480
X	 0.6800	 0.3030
Z	 0.5270	 0.3770
a	 0.9090	 0.4940
b	 0.8700	 0.4320
c	 0.9090	 0.4700
d	 0.7610	 0.3600
e	 0.8350	 0.4480
f	 0.8730	 0.4600



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Chain	Atom inclusion	Q-score
g	 0.7800	 0.4020
h	 0.7000	 0.0770
i	 0.6120	 0.0830
j	 0.5460	 0.0620
k	 0.5100	 0.0410
l	 0.5990	 0.0350
m	 0.6370	 0.0790
n	 0.6310	 0.0690
o	 0.6180	 0.0970
p	 0.6400	 0.0810
q	 0.7330	 0.4560
r	 0.4840	 0.3560
s	 0.4260	 0.1830
t	 0.5390	 0.3670
y	 0.6720	 0.4330