



Full wwPDB EM Validation Report ⓘ

Jul 21, 2026 – 02:34 pm BST

PDB ID : 9S2F / pdb_00009s2f
EMDB ID : EMD-54494
Title : Human debranched intron spliceosome (DIS)
Authors : Boreikaite, V.; Vorlaender, M.K.; Plaschka, C.
Deposited on : 2025-07-21
Resolution : 3.14 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.dev133
Mogul : 1.8.4, CSD as541be (2020)
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) : 2.50

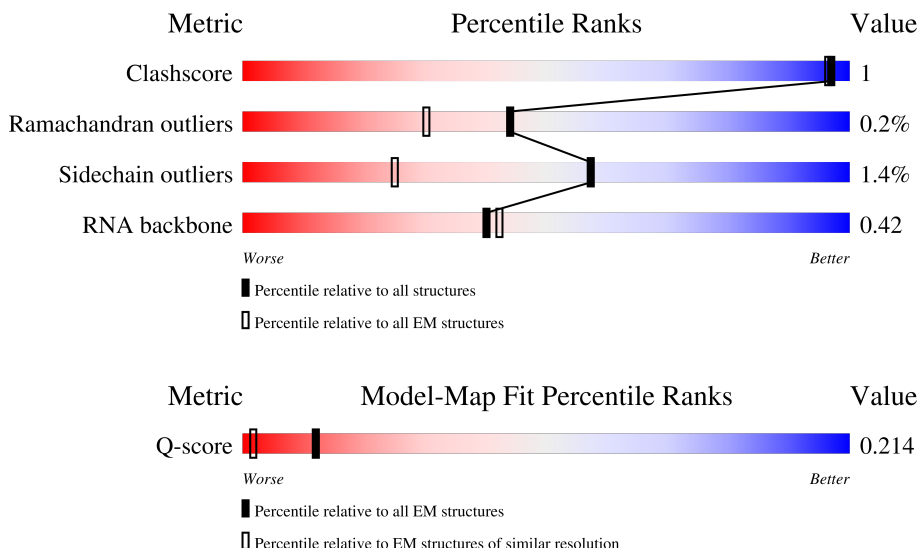
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

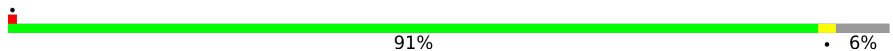
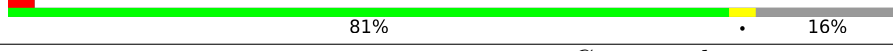
The reported resolution of this entry is 3.14 Å.

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	14483 (2.64 - 3.64)

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	35	703	 91% 6%
2	5	116	 61% 13% 5% 21%
3	A	2335	 81% 16%

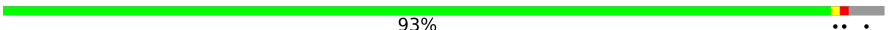
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Mol	Chain	Length	Quality of chain
4	B	2136	
5	C	972	
6	E	357	
7	GP	931	
8	I	855	
9	J	848	
10	K	225	
11	L	802	
12	M	243	
13	N	144	
14	O	420	
15	P	229	
16	Q	1485	
17	R	536	
18	S	166	
19	T	514	
20	W	579	
21	WD	315	
22	Z	166	
23	a	126	
24	b	240	
25	c	119	
26	d	118	
27	e	92	
28	f	86	

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Mol	Chain	Length	Quality of chain
29	g	76	 93% ..
30	q	504	 20% 80%
30	r	504	 24% 76%
30	s	504	 26% 74%
30	t	504	 20% 80%
31	y	301	 12% 27% 72%
32	D	285	 18% 82%
33	IN	10	 70% 30%
34	6	106	 10% 21% 11% 67%

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 77158 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 Probable ATP-dependent RNA helicase DHX35.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	35	658	Total	C	N	O	S	0	0
			5214	3323	916	946	29		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	92	Total	C	N	O	P	0	0
			1936	867	322	655	92		

- Molecule 3 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1961	Total	C	N	O	S	0	0
			16319	10523	2860	2865	71		

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	19	Total	C	N	O	S	0	0
			140	86	25	28	1		

- Molecule 5 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	890	Total	C	N	O	S	0	0
			7040	4503	1174	1329	34		

- Molecule 6 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	299	Total	C	N	O	S	0	0
			2341	1470	411	447	13		

- Molecule 7 is a protein called G patch domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	GP	331	Total	C	N	O	S	0	0
			2447	1550	420	475	2		

- Molecule 8 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	719	Total	C	N	O		0	0
			3620	2182	719	719			

- Molecule 9 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	561	Total	C	N	O	S	0	0
			3360	2067	645	643	5		

- Molecule 10 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	209	Total	C	N	O		0	0
			1052	634	209	209			

- Molecule 11 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	485	Total	C	N	O	S	0	0
			3057	1882	576	592	7		

- Molecule 12 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	113	Total	C	N	O		0	0
			569	343	113	113			

- Molecule 13 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	142	Total	C	N	O	S	0	0
			1178	743	216	207	12		

- Molecule 14 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	245	Total	C	N	O	0	0
			1242	752	245	245		

- Molecule 15 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	85	Total	C	N	O	S	0	0
			738	452	145	139	2		

- Molecule 16 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	1296	Total	C	N	O	0	0
			6558	3966	1296	1296		

- Molecule 17 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	R	250	Total	C	N	O	P	S	0	0
			2000	1256	353	377	2	12		

- Molecule 18 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	159	Total	C	N	O	S	0	0
			1236	787	215	227	7		

- Molecule 19 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	360	Total	C	N	O	S	0	0
			2714	1706	496	504	8		

- Molecule 20 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	485	Total	C	N	O	S	0	0
			3925	2505	678	718	24		

- Molecule 21 is a protein called WD repeat domain-containing protein 83.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	WD	292	Total	C	N	O	0	0
			1446	862	292	292		

- Molecule 22 is a protein called Coiled-coil domain-containing protein 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	Z	92	Total	C	N	O	0	0
			473	289	92	92		

- Molecule 23 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	83	Total	C	N	O	S	0	0
			651	408	114	122	7		

- Molecule 24 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	95	Total	C	N	O	S	0	0
			725	455	136	127	7		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	c	81	Total	C	N	O	S	0	0
			641	409	112	116	4		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	97	Total	C	N	O	S	0	0
			784	490	148	141	5		

- Molecule 27 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	79	Total	C	N	O	S	0	0
			653	412	116	120	5		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	f	76	Total	C	N	O	S	0	0
			593	383	97	107	6		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein G.

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

- Molecule 30 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	q	103	Total	C	N	O		0	0
			524	318	103	103			
30	r	119	Total	C	N	O		0	0
			606	368	119	119			
30	s	132	Total	C	N	O		0	0
			679	415	132	132			
30	t	103	Total	C	N	O		0	0
			524	318	103	103			

- Molecule 31 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	y	83	Total	C	N	O		0	0
			414	248	83	83			

- Molecule 32 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	D	51	Total	C	N	O		0	0
			255	153	51	51			

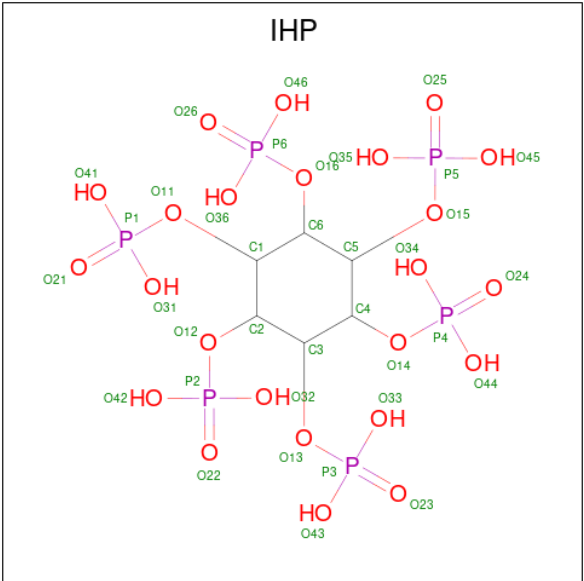
- Molecule 33 is a RNA chain called Intron.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	IN	10	Total	C	O	P		0	0
			120	50	60	10			

- Molecule 34 is a RNA chain called U6 snRNA.

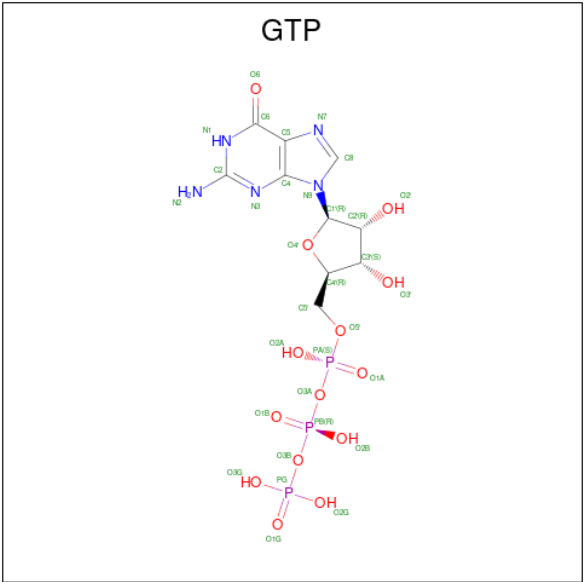
Mol	Chain	Residues	Atoms					AltConf	Trace
34	6	35	Total	C	N	O	P	0	0
			744	333	132	244	35		

- Molecule 35 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 36 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	C	1	Total	Mg	0
			1	1	

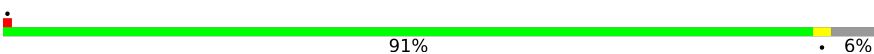
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

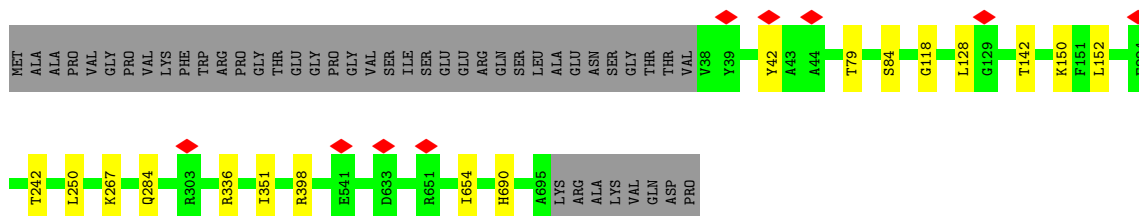
Mol	Chain	Residues	Atoms		AltConf
38	N	3	Total	Zn	0
			3	3	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

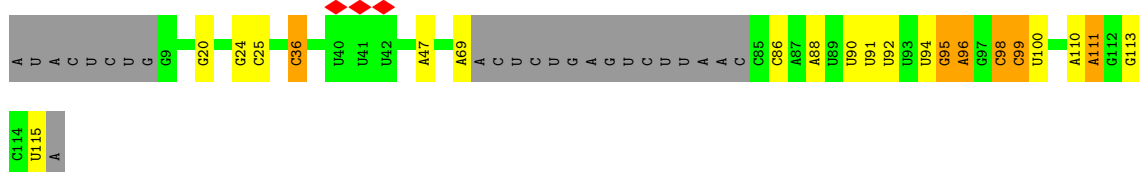
- Molecule 1: Probable ATP-dependent RNA helicase DHX35

Chain 35: 



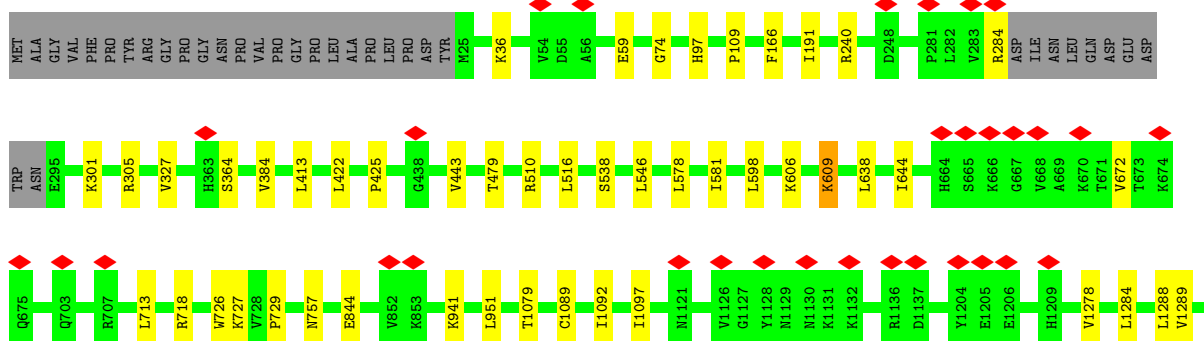
- Molecule 2: U5 snRNA

Chain 5: 



- Molecule 3: Pre-mRNA-processing-splicing factor 8

Chain A: 

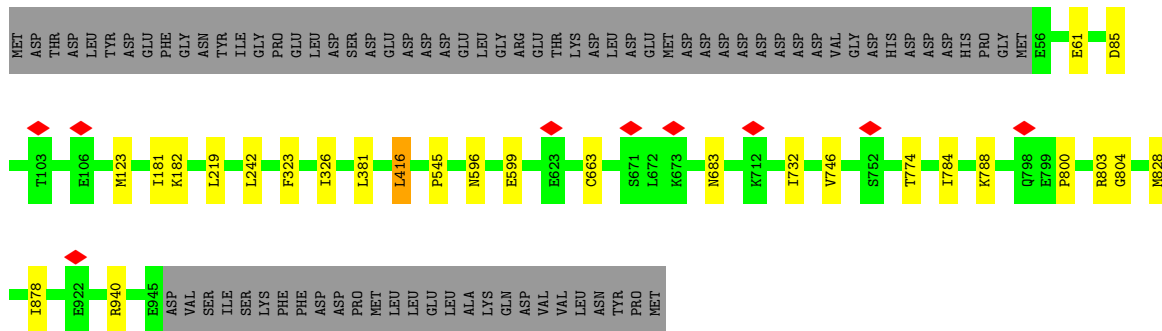




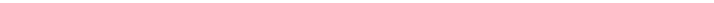
[illegible]

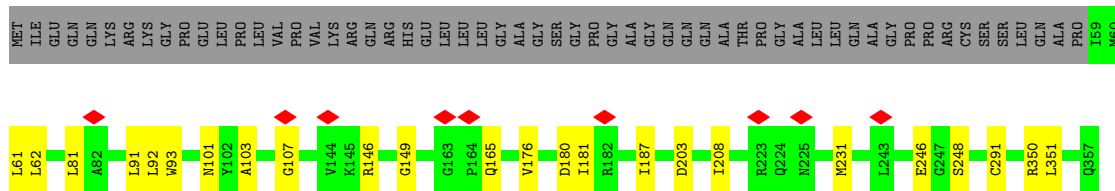
- Molecule 5: 116 kDa U5 small nuclear ribonucleoprotein component

Chain C: 89% 8%

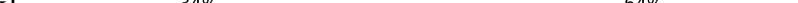


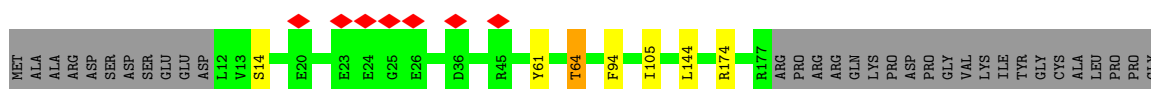
- Molecule 6: U5 small nuclear ribonucleoprotein 40 kDa protein.

Chain E:  77% 7% 16%

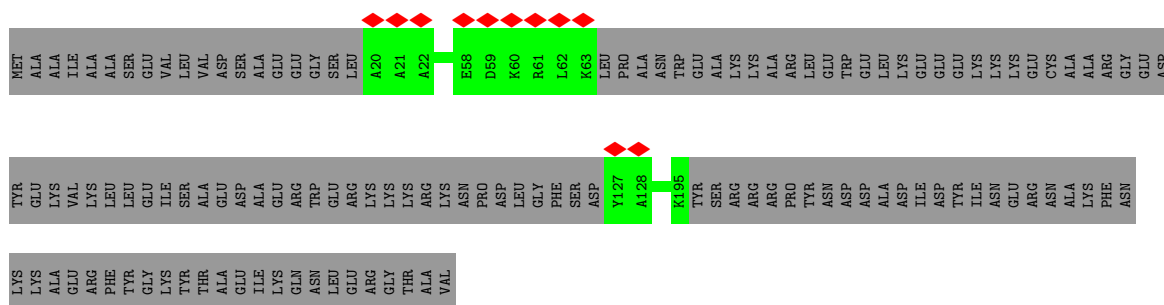


- Molecule 7: G patch domain-containing protein 1

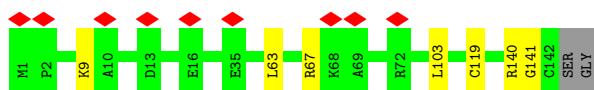
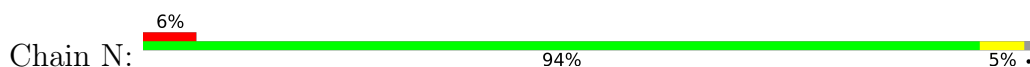
Chain GP: 



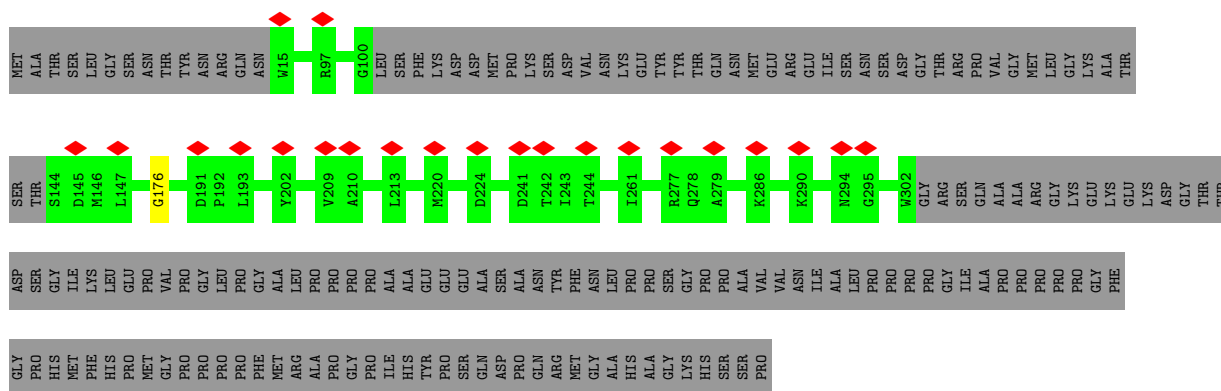
- Molecule 12: Pre-mRNA-splicing factor SYF2



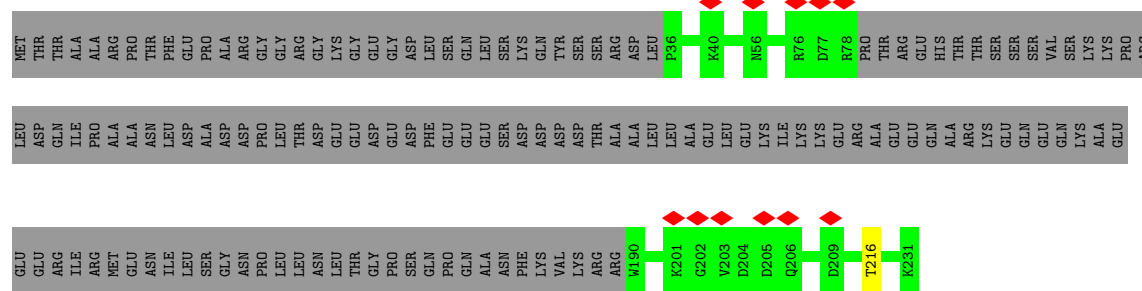
- Molecule 13: Protein BUD31 homolog



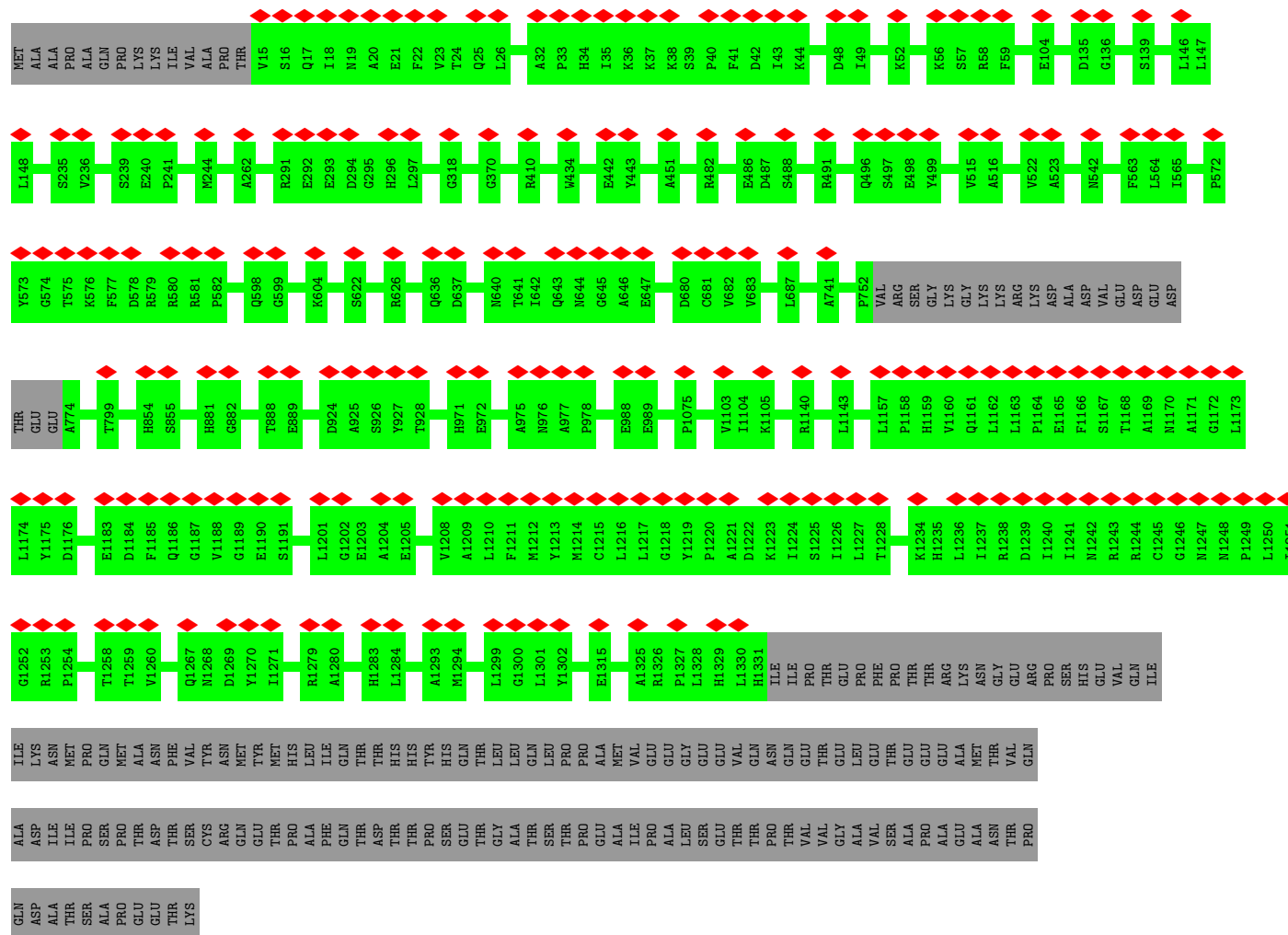
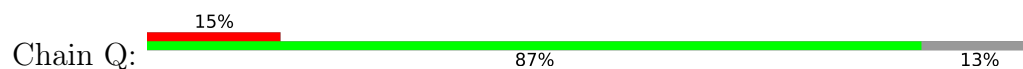
- Molecule 14: Pre-mRNA-splicing factor RBM22



- Molecule 15: Spliceosome-associated protein CWC15 homolog

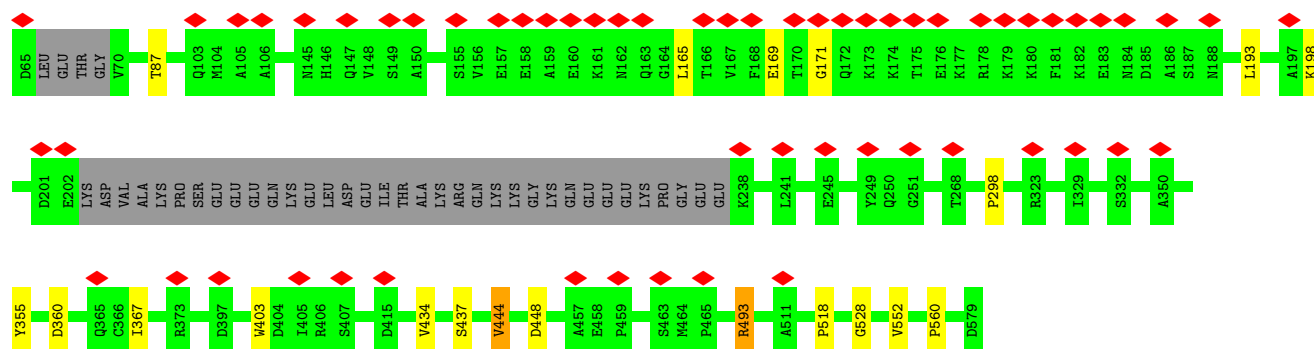


• Molecule 16: Intron-binding protein aquarius

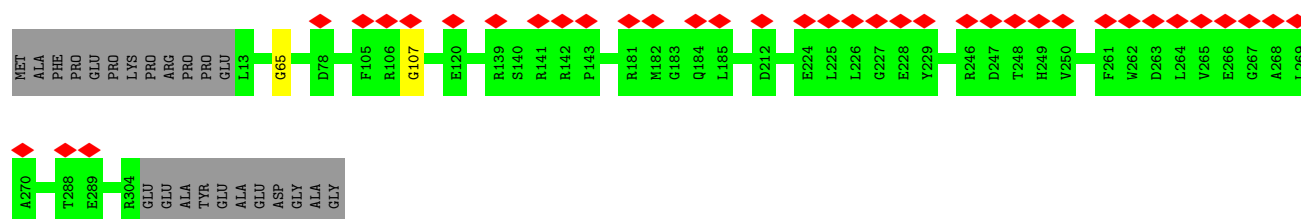


• Molecule 17: SNW domain-containing protein 1

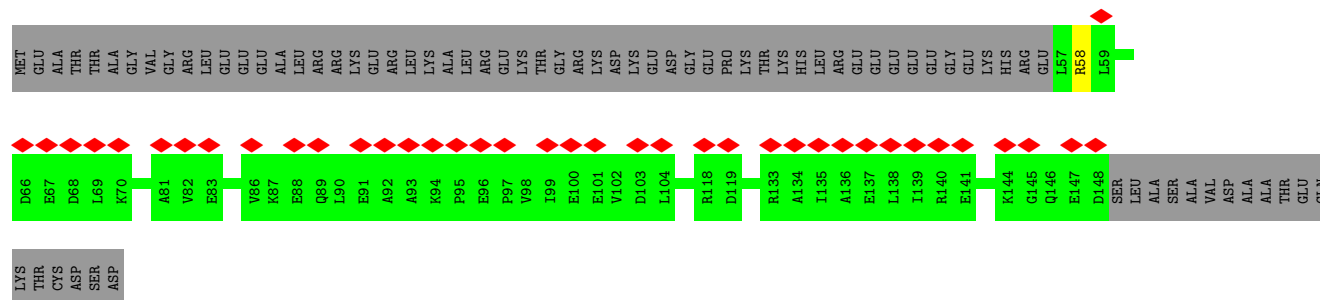




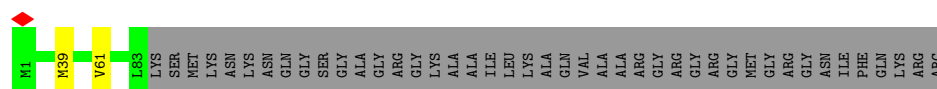
- Molecule 21: WD repeat domain-containing protein 83



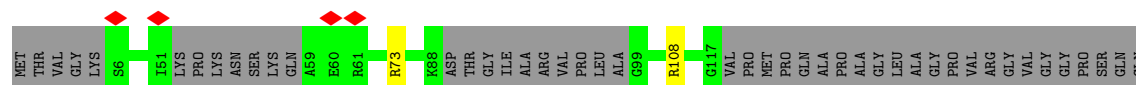
- Molecule 22: Coiled-coil domain-containing protein 12



- Molecule 23: Small nuclear ribonucleoprotein Sm D3



- Molecule 24: Small nuclear ribonucleoprotein-associated proteins B and B'



VAL MET THR PRO GLN ARG GLY THR VAL ALA ALA ALA ALA ALA ALA ALA THR THR ALA ILE SER ALA GLY PRO ALA ALA THR GLY MET GLN ARG TYR PRO PRO GLY ARG PRO GLY ARG PRO MET GLY ARG PRO

PRO PRO MET GLY ILE PRO GLY ARG THR PRO MET GLY MET PRO ALA ALA THR GLY MET ARG PRO PRO GLY MET GLN ARG TYR PRO PRO GLY ARG PRO GLY ARG PRO ARG PRO

• Molecule 25: Small nuclear ribonucleoprotein Sm D1

Chain c:  67% 32%

H1 N64 N81 VAL ASP VAL GLU PRO LYS VAL LYS SER LYS LYS ARG ALA VAL ALA GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG

• Molecule 26: Small nuclear ribonucleoprotein Sm D2

Chain d:  10% 78% 18%

MET SER LEU LEU ASN LYS PRO LYS SER LYS MET THR PRO THR GLU LEU Q17 E20 R47 P78 K79 S80 G81 K82 G83 K84 K85 K86 S87 K88 I107 V108 F113 LEU ILE ALA GLY LYS

• Molecule 27: Small nuclear ribonucleoprotein E

Chain e:  82% 14%

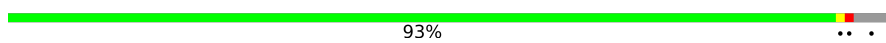
MET ALA TYR ARG GLN GLN LYS VAL GLN LYS VAL M14 Q38 I77 D82 S91 N92

• Molecule 28: Small nuclear ribonucleoprotein F

Chain f:  80% 8% 12%

M1 S2 L3 P4 L5 L23 M27 Y39 V62 E76 GLU GLU GLU GLU ASP GLY GLU MET ARG GLU

• Molecule 29: Small nuclear ribonucleoprotein G

Chain g:  93%

MET SER LYS A4 L17 L70 V76

• Molecule 30: Pre-mRNA-processing factor 19

Chain q:  20% 80%

MET SER LEU ILE CYS SER ILE SER ASN GLU VAL PRO E13 H14 S21 N22 L29 E36 P41 I42 N43 N44 Q51 LEU ILE ASP ILE ILE LYS VAL VAL ALA HIS PRO PRO ARG ARG PRO PRO LYS PRO PRO SER SER ALA THR SER I71 L134 LYS PRO PRO GLN ALA ALA GLY LEU ILE VAL PRO GLN

GLY	HIS	LEU	ILE	ALA
HIS	ASN	LYS	PHE	HIS
ALA	PHE	ASN	GLY	GLY
PHE	THR	THR	THR	SER
ILE	LEU	LEU	MET	VAL
ALA	GLN	ASP	ASP	GLY
SER	LEU	SER	SER	LEU
THR	ASP	GLN	ILE	SER
GLY	ASN	ILE	LYS	LEU
MET	ASN	ILE	LYS	HIS
ASP	PHE	ILE	ILE	ALA
ARG	GLU	TRP	TRP	THR
SER	VAL	ASP	ASP	GLY
LEU	LYS	LYS	LEU	ASP
LYS	SER	SER	LYS	TVR
PHE	LEU	ILE	GLU	LEU
TYR	ILE	PHE	ARG	LEU
SER	ASP	THR	THR	SER
LEU	GLN	VAL	ASN	SER
	SER	ALA	ALA	ASP
	GLY	ASN	ASN	ASP
	THR	PHE	PHE	GLN
	TYR	TYR	PRO	TYR
	LEU	LEU	GLY	TRP
	ALA	ALA	HIS	ALA
	LEU	SER	SER	PHE
	GLY	GLY	GLY	SER
	GLY	PRO	PRO	ASP
	THR	ILE	ILE	ILE
	ASP	THR	THR	GLN
	VAL	SER	SER	THR
	GLN	ILE	ILE	GLY
	ILE	ALA	ALA	ARG
	TYR	PHE	PHE	VAL
	ILE	SER	SER	VAL
	CYS	GLU	GLU	THR
	LYS	ASN	ASN	LYS
	GLN	GLY	GLY	VAL
	TRP	TYR	TYR	THR
	THR	THR	THR	ASP
	GLU	LEU	LEU	GLU
	ILE	ALA	ALA	THR
	LEU	THR	THR	SER
	HIS	ALA	ALA	GLY
	PHE	ALA	ALA	CYS
	THR	ASP	ASP	SER
	GLU	ASP	ASP	CYS
	HIS	SER	SER	THR
	SER	SER	SER	CYS
	GLY	VAL	VAL	ALA
	LEU	LYS	LYS	GLN
	THR	THR	THR	GLN
	THR	THR	THR	PHE
	GLY	ASP	ASP	HIS
	VAL	LEU	LEU	PRO
	ALA	ASP	ASP	ASP
	PHE	LYS	LYS	GLY
	THR	THR	THR	THR

- Molecule 30: Pre-mRNA-processing factor 19



TYR	ILE	ARG	LEU	GLY	GLU	VAL	MET
SER	PHE	THR	SER	HIS	GLU	PRO	SER
LEU	GLN	ASN	SER	THR	LEU	GLN	LEU
		VAL	SER	LYS	SER	ALA	ILE
		ALA	ASP	LYS	VAL	VAL	CYS
		ASN	ASP	VAL	TYR	PRO	SER
		PHE	GLN	THR	ARG	SER	ILE
		PRO	TYR	SER	GLN	SER	SER
		THR	VAL	VAL	VAL	GLN	ASN
		ALA	HIS	VAL	ALA	PRO	GLU
		SER	PHE	PHE	SER	SER	VAL
		GLY	SER	HIS	HIS	VAL	PRO
		PRO	ASP	PRO	VAL	VAL	E13
		ILE	ILE	SER	GLY	GLY	H14
		THR	GLN	GLN	LEU	ALA	P15
		ASP	SER	ASP	HIS	GLY	
		VAL	THR	THR	SER	GLU	
		GLN	ILE	LEU	ALA	PRO	
		ILE	ALA	VAL	ALA	PRO	
		PHE	VAL	PHE	SER	MET	
		GLU	THR	SER	ILE	ASP	
		CYS	GLU	ALA	PRO	LEU	
		LYS	ASN	SER	GLY	GLY	
		GLN	GLY	PRO	ILE	GLU	
		TRP	THR	ASP	LEU	LEU	
		THR	TYR	THR	ALA	VAL	
		GLU	LEU	THR	GLU	VAL	
		ILE	ALA	ILE	ASP	MET	
		ALA	THR	ARG	LEU	THR	
		HIS	ALA	ILE	CYS	PRO	
		PHE	ALA	TRP	PRO	GLU	
		THR	ASP	SER	ILE	ILE	
		GLU	ASP	VAL	ASP	ARG	
		HIS	THR	PRO	GLN	SER	
		SER	SER	ASN	LYS	PRO	
		SER	CYS	ASN	LYS	PRO	
		VAL	ALA	ALA	LEU	PRO	
		LYS	GLN	SER	ILE	GLN	
		LEU	PHE	CYS	LEU	ASP	
		THR	THR	VAL	THR	LYS	
		GLY	ASP	GLN	GLY	ALA	
		VAL	LEU	VAL	GLY	THR	
		ALA	ARG	VAL	ALA	VAL	
		PHE	LYS	ARG	ASP	LEU	
		GLY	ILE	ALA	THR	THR	
		HIS	LYS	HIS	ASN	THR	
		HIS	ASN	GLU	VAL	GLU	
		ALA	PHE	SER	VAL	ARG	
		LYS	GLY	ALA	VAL	LYS	
		ALA	THR	THR	VAL	THR	
		PHE	THR	VAL	PHE	VAL	
		ILE	LEU	THR	ASP	ARG	
		ALA	GLN	LEU	LYS	GLY	
		SER	LEU	SER	LYS	LYS	
		THR	ASN	SER	THR	THR	
		GLY	ILE	LEU	GLU	VAL	
		MET	LYS	HIS	GLN	PRO	
		ASP	PHE	ALA	ILE	GLU	
		ARG	GLU	THR	LEU	GLU	
		SER	VAL	GLY	ALA	LEU	
		LEU	ASP	ASP	THR	VAL	
		LYS	LYS	TYR	LEU	LYS	
		PHE	LEU	LEU	LYS	PRO	
						GLN	
						ALA	
						GLY	
						LEU	
						THR	
						VAL	
						ASP	
						THR	
						GLY	
						LEU	
						THR	
						VAL	
						PRO	
						GLY	

- Molecule 31: Peptidyl-prolyl cis-trans isomerase E



M1	A2	T3	T4	K5	R6	V7	L8	Y9	G12	L13	A14	E15	E16	P28	T33	D34	I35	Q36	I37	P38	L39	D40	Y41	E42	T43	E44	K45	H46	R47	G48	F49	A50	E55	L56	A61	N80	L81	A82	K83	P80	MET	ARG	L1E	LYS	GLU	GLY	SER	SER	ARG	PRO	VAL	TRP	SER		
ASP	ASP	ASP	TRP	LEU	LVS	LVS	PHE	GLY	LVS	LEU	GLU	GLU	GLU	GLY	GLY	PRO	ASN	LVS	ALA	THR	GLN	GLU	GLY	GLY	PRO	ILE	ALA	LYS	LYS	ALA	ARG	ASN	PRO	GLN	VAL	TYR	MET	ASP	ILE	LVS	ILE	GLY	ASN	THR	GLY	GLY	LVS	PRO	LYS	ALA	GLY	ARG	ILE	GLN	
MET	LEU	ASP	ARG	ASP	VAL	VAL	PRO	MET	THR	ALA	GLU	ASN	PHE	THR	GLY	LYS	GLY	PHE	ASN	THR	SER	SER	PHE	PHE	HIS	ILE	ILE	PRO	GLM	PHE	MET	CYS	GLM	GLY	GLY	ASP	PHE	THR	VAL	VAL	PHE	ASN	HIS	GLY	GLY	VAL	VAL	THR	GLY	GLY	LEU	VAL	LEU	ARG	GLM
LYS	PHE	ASP	ASP	ASN	PHE	ILE	LYS	HIS	THR	THR	GLY	PRO	GLY	GLY	ASN	PRO	ASN	THR	GLY	GLM	PHE	PHE	LEU	CYS	THR	ASP	LYS	THR	TRP	LEU	ASP	GLY	LYS	HIS	VAL	VAL	THR	GLY	GLY	GLY	LEU	VAL	LEU	ARG	GLM										

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	153470	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	2250	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	13.703	Depositor
Minimum map value	0.000	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.117	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	532.5376, 532.5376, 532.5376	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1887, 1.1887, 1.1887	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	35	0.36	0/5319	0.61	0/7204
2	5	0.46	0/2157	0.81	4/3351 (0.1%)
3	A	0.47	0/16762	0.71	5/22721 (0.0%)
4	B	0.33	0/139	0.71	0/183
5	C	0.34	0/7199	0.61	0/9782
6	E	0.26	0/2394	0.60	0/3243
7	GP	0.35	0/2504	0.64	0/3400
8	I	0.20	0/3644	0.73	0/5105
9	J	0.24	0/3403	0.66	0/4702
10	K	0.18	0/1058	0.64	0/1481
11	L	0.28	0/3094	0.62	0/4240
12	M	0.15	0/570	0.54	0/796
13	N	0.24	0/1204	0.61	0/1614
14	O	0.23	0/1255	0.68	0/1758
15	P	0.36	0/749	0.71	0/992
16	Q	0.20	0/6624	0.62	0/9290
17	R	0.31	0/2017	0.62	0/2707
18	S	0.25	0/1268	0.56	0/1714
19	T	0.48	0/2781	0.75	0/3798
20	W	0.22	0/4030	0.59	0/5449
21	WD	0.12	0/1453	0.38	0/2021
22	Z	0.18	0/479	0.57	0/674
23	a	0.79	0/659	0.80	0/888
24	b	0.60	0/734	0.75	0/977
25	c	0.68	0/649	0.84	0/877
26	d	0.61	0/794	0.92	0/1061
27	e	0.73	0/661	0.88	0/886
28	f	0.66	0/605	0.91	1/817 (0.1%)
29	g	0.85	0/575	0.99	1/768 (0.1%)
30	q	0.22	0/527	0.69	0/738
30	r	0.21	0/610	0.63	0/855
30	s	0.25	0/688	0.70	1/969 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	t	0.22	0/527	0.60	0/738
31	y	0.17	0/415	0.44	0/578
32	D	0.27	0/255	0.70	0/355
33	IN	0.26	0/129	0.66	0/196
34	6	0.23	0/831	0.68	1/1292 (0.1%)
All	All	0.37	0/78762	0.67	13/108220 (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
1	35	0	2
3	A	0	2
6	E	0	1
10	K	0	1
20	W	0	1
All	All	0	7

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	609	LYS	CB-CG-CD	-10.85	86.34	111.30
3	A	609	LYS	CA-CB-CG	7.96	130.03	114.10
3	A	941	LYS	N-CA-C	7.87	127.19	109.81
28	f	39	TYR	CA-CB-CG	7.06	126.61	113.90
2	5	98	C	O3'-P-O5'	6.46	113.70	104.00
29	g	70	LEU	CA-CB-CG	6.33	138.44	116.30
2	5	98	C	C4'-C3'-O3'	5.61	121.41	113.00
30	s	65	PRO	N-CA-C	5.49	117.40	110.70
34	6	33	G	C2'-C3'-O3'	5.46	121.89	113.70
2	5	99	C	O5'-C5'-C4'	5.36	119.54	111.50
3	A	1601	LEU	CA-CB-CG	5.14	134.30	116.30
3	A	1342	TRP	CA-CB-CG	5.11	123.31	113.60
2	5	95	G	C4'-C3'-O3'	5.01	116.91	109.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	35	336	ARG	Sidechain
1	35	398	ARG	Sidechain
3	A	1370	ARG	Sidechain
3	A	1384	ARG	Sidechain
6	E	146	ARG	Sidechain
10	K	27	GLY	Peptide
20	W	493	ARG	Sidechain

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	35	5214	0	5301	4	0
2	5	1936	0	982	4	0
3	A	16319	0	16319	25	0
4	B	140	0	148	1	0
5	C	7040	0	7057	13	0
6	E	2341	0	2275	10	0
7	GP	2447	0	2282	6	0
8	I	3620	0	1770	2	0
9	J	3360	0	2194	0	0
10	K	1052	0	516	1	0
11	L	3057	0	2289	7	0
12	M	569	0	271	0	0
13	N	1178	0	1184	4	0
14	O	1242	0	615	0	0
15	P	738	0	723	0	0
16	Q	6558	0	3186	0	0
17	R	2000	0	2018	4	0
18	S	1236	0	1210	5	0
19	T	2714	0	2548	11	0
20	W	3925	0	3826	8	0
21	WD	1446	0	698	0	0
22	Z	473	0	246	1	0
23	a	651	0	669	1	0
24	b	725	0	747	2	0
25	c	641	0	689	0	0
26	d	784	0	826	4	0
27	e	653	0	668	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	f	593	0	607	3	0
29	g	568	0	590	1	0
30	q	524	0	266	0	0
30	r	606	0	306	0	0
30	s	679	0	359	0	0
30	t	524	0	266	0	0
31	y	414	0	216	1	0
32	D	255	0	126	0	0
33	IN	120	0	61	0	0
34	6	744	0	377	0	0
35	A	36	0	6	0	0
36	C	32	0	12	0	0
37	C	1	0	0	0	0
38	N	3	0	0	0	0
All	All	77158	0	64449	99	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 1.

All (99) 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)
3:A:672:VAL:HG23	19:T:268:LYS:HE3	1.78	0.66
20:W:165:LEU:HD11	20:W:171:GLY:HA2	1.77	0.65
7:GP:368:PRO:HG2	7:GP:371:TYR:HB2	1.82	0.61
3:A:606:LYS:HD3	3:A:609:LYS:HE2	1.81	0.61
11:L:25:LYS:HD2	11:L:159:LEU:HD12	1.82	0.61
19:T:354:ILE:HD12	19:T:398:TRP:HZ3	1.66	0.61
2:5:100:U:H3	2:5:111:A:H61	1.50	0.60
28:f:1:MET:HE2	28:f:3:LEU:HB2	1.84	0.59
18:S:55:ARG:HB3	18:S:63:GLN:HB3	1.87	0.57
3:A:1289:VAL:HG21	4:B:42:SER:HA	1.85	0.57
23:a:39:MET:HE2	24:b:73:ARG:HH11	1.69	0.56
20:W:528:GLY:HA2	20:W:552:VAL:HG13	1.87	0.56
13:N:119:CYS:HB2	13:N:141:GLY:HA2	1.88	0.55
19:T:418:THR:HG21	19:T:467:ALA:HA	1.89	0.55
26:d:107:ILE:HG22	26:d:108:VAL:HG23	1.89	0.55
8:I:68:TYR:H	31:y:28:PRO:HB3	1.71	0.55
6:E:61:LEU:HD23	24:b:108:ARG:HE	1.72	0.55
28:f:23:LEU:HD12	28:f:27:MET:HE3	1.90	0.54
17:R:3:LEU:HA	17:R:6:PHE:HD2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:35:142:THR:HG21	1:35:150:LYS:HE3	1.90	0.53
3:A:1817:LEU:HD23	3:A:1917:PHE:HB2	1.91	0.53
10:K:17:PRO:HB2	20:W:57:ALA:HB2	1.90	0.53
8:I:496:SER:HA	22:Z:58:ARG:H	1.74	0.52
5:C:323:PHE:HA	5:C:326:ILE:HD12	1.91	0.52
5:C:663:CYS:HB2	5:C:828:MET:HB2	1.91	0.52
3:A:727:LYS:HE3	3:A:729:PRO:HA	1.92	0.52
3:A:1930:TYR:HE1	7:GP:144:LEU:HB2	1.75	0.52
2:5:98:C:H42	2:5:113:G:H1	1.57	0.51
5:C:596:ASN:HB2	5:C:599:GLU:HG3	1.92	0.51
13:N:140:ARG:HH21	20:W:198:LYS:HE2	1.75	0.51
19:T:314:ILE:HD12	19:T:324:HIS:HB2	1.93	0.51
3:A:36:LYS:HA	20:W:169:GLU:HG2	1.92	0.50
18:S:94:GLY:HA2	18:S:118:PRO:HG3	1.94	0.50
29:g:17:LEU:HD13	29:g:70:LEU:HG	1.93	0.50
13:N:63:LEU:HD23	13:N:67:ARG:HD2	1.94	0.49
6:E:91:LEU:HB3	6:E:101:ASN:HD21	1.77	0.48
19:T:254:VAL:HG22	19:T:261:LEU:HD23	1.95	0.48
5:C:774:THR:HA	5:C:784:ILE:HD12	1.94	0.48
3:A:301:LYS:HE3	5:C:940:ARG:HA	1.95	0.48
6:E:81:LEU:HD23	6:E:93:TRP:HB2	1.96	0.48
7:GP:174:ARG:HB3	7:GP:216:THR:HB	1.96	0.48
1:35:267:LYS:HB3	7:GP:346:LEU:HD22	1.95	0.48
19:T:213:GLU:HG3	19:T:218:TRP:CE2	2.50	0.47
26:d:108:VAL:HG13	28:f:62:VAL:HG13	1.96	0.47
5:C:732:ILE:HG12	5:C:746:VAL:HG22	1.95	0.47
2:5:36:C:H4'	3:A:284:ARG:HH21	1.79	0.47
5:C:800:PRO:HA	5:C:803:ARG:HG2	1.97	0.47
20:W:434:VAL:HG22	20:W:444:VAL:HG13	1.98	0.46
2:5:96:A:H1'	26:d:47:ARG:HE	1.81	0.46
1:35:118:GLY:HA2	1:35:128:LEU:HD13	1.99	0.45
11:L:104:LEU:HD22	11:L:370:MET:HG3	1.98	0.45
6:E:62:LEU:HB2	6:E:351:LEU:HB2	1.99	0.45
3:A:1278:VAL:HG13	3:A:1284:LEU:HD12	1.98	0.45
11:L:222:LEU:H	17:R:104:GLN:HE22	1.65	0.45
17:R:66:GLU:HG2	17:R:67:ILE:HG13	1.99	0.44
3:A:1345:GLN:HG2	3:A:1350:ILE:HG12	1.99	0.44
7:GP:61:TYR:HB3	7:GP:64:THR:HG23	1.98	0.44
19:T:450:VAL:HG11	19:T:489:TYR:HE2	1.82	0.44
26:d:78:PRO:HG2	26:d:85:LYS:HG2	1.99	0.44
3:A:1876:LEU:HD12	3:A:1884:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:165:GLN:HB3	6:E:181:ILE:HD12	2.00	0.44
11:L:192:ARG:HA	11:L:192:ARG:HD3	1.78	0.44
5:C:381:LEU:HG	5:C:416:LEU:HD21	2.00	0.44
3:A:516:LEU:HD11	3:A:538:SER:HB2	2.00	0.43
3:A:1562:MET:HE3	3:A:1562:MET:HB3	1.89	0.43
19:T:354:ILE:HD12	19:T:398:TRP:CZ3	2.51	0.43
18:S:20:MET:HG3	18:S:142:VAL:HG22	2.01	0.43
3:A:109:PRO:HB3	3:A:191:ILE:HD12	2.00	0.43
18:S:56:ILE:HG23	18:S:62:ILE:HG22	2.01	0.43
5:C:181:ILE:HG13	5:C:182:LYS:HG2	1.99	0.43
5:C:746:VAL:HG21	5:C:788:LYS:HE3	2.01	0.43
6:E:180:ASP:HB2	6:E:187:ILE:HD11	2.00	0.43
11:L:107:ALA:HB1	11:L:367:GLN:HG3	2.01	0.43
6:E:246:GLU:HG3	6:E:248:SER:H	1.84	0.42
19:T:398:TRP:CD1	19:T:405:PHE:HA	2.54	0.42
20:W:518:PRO:HG3	20:W:560:PRO:HA	2.00	0.42
20:W:360:ASP:HB2	20:W:367:ILE:HD11	2.00	0.42
3:A:1742:VAL:HG21	7:GP:94:PHE:HB2	2.02	0.42
3:A:305:ARG:HG2	5:C:878:ILE:HG12	2.01	0.42
6:E:92:LEU:HB2	6:E:103:ALA:HB3	2.01	0.42
3:A:422:LEU:HD21	3:A:638:LEU:HD12	2.02	0.42
18:S:25:LEU:HD13	18:S:98:LEU:HD22	2.00	0.42
3:A:1311:PHE:HD1	3:A:1311:PHE:HA	1.65	0.42
5:C:123:MET:HE2	5:C:545:PRO:HD2	2.01	0.42
19:T:398:TRP:HD1	19:T:405:PHE:HA	1.85	0.42
6:E:61:LEU:HD11	6:E:350:ARG:HB3	2.02	0.42
3:A:1342:TRP:HB2	3:A:1353:PHE:HB2	2.02	0.41
11:L:54:LEU:HD23	11:L:54:LEU:HA	1.91	0.41
19:T:354:ILE:HD11	19:T:375:VAL:HG11	2.03	0.41
3:A:1577:PHE:CE1	3:A:1582:TRP:HD1	2.38	0.41
3:A:59:GLU:HB2	13:N:103:LEU:HD13	2.03	0.41
3:A:578:LEU:HA	3:A:581:ILE:HD12	2.02	0.41
17:R:91:ASP:HB3	17:R:97:LYS:HE3	2.02	0.41
11:L:63:TRP:HH2	11:L:95:GLN:HB3	1.86	0.40
3:A:1288:LEU:HD13	3:A:1330:MET:HG2	2.03	0.40
3:A:1312:PRO:HB2	3:A:1314:VAL:HG12	2.02	0.40
5:C:242:LEU:HD23	5:C:242:LEU:HA	1.93	0.40
1:35:250:LEU:HD23	1:35:250:LEU:HA	1.86	0.40
6:E:176:VAL:HG11	6:E:208:ILE:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	35	656/703 (93%)	644 (98%)	12 (2%)	0	100	100
3	A	1955/2335 (84%)	1896 (97%)	55 (3%)	4 (0%)	43	70
4	B	17/2136 (1%)	17 (100%)	0	0	100	100
5	C	888/972 (91%)	865 (97%)	22 (2%)	1 (0%)	48	76
6	E	297/357 (83%)	281 (95%)	14 (5%)	2 (1%)	18	47
7	GP	321/931 (34%)	302 (94%)	19 (6%)	0	100	100
8	I	717/855 (84%)	703 (98%)	14 (2%)	0	100	100
9	J	559/848 (66%)	549 (98%)	10 (2%)	0	100	100
10	K	207/225 (92%)	192 (93%)	14 (7%)	1 (0%)	24	54
11	L	471/802 (59%)	464 (98%)	5 (1%)	2 (0%)	30	59
12	M	109/243 (45%)	108 (99%)	1 (1%)	0	100	100
13	N	140/144 (97%)	139 (99%)	1 (1%)	0	100	100
14	O	241/420 (57%)	225 (93%)	15 (6%)	1 (0%)	30	59
15	P	81/229 (35%)	76 (94%)	5 (6%)	0	100	100
16	Q	1292/1485 (87%)	1264 (98%)	28 (2%)	0	100	100
17	R	238/536 (44%)	226 (95%)	11 (5%)	1 (0%)	30	59
18	S	157/166 (95%)	152 (97%)	5 (3%)	0	100	100
19	T	356/514 (69%)	336 (94%)	19 (5%)	1 (0%)	36	64
20	W	479/579 (83%)	450 (94%)	27 (6%)	2 (0%)	30	59
21	WD	290/315 (92%)	286 (99%)	2 (1%)	2 (1%)	18	47
22	Z	90/166 (54%)	85 (94%)	5 (6%)	0	100	100
23	a	81/126 (64%)	81 (100%)	0	0	100	100
24	b	89/240 (37%)	87 (98%)	2 (2%)	0	100	100
25	c	79/119 (66%)	75 (95%)	4 (5%)	0	100	100
26	d	95/118 (80%)	92 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	e	77/92 (84%)	72 (94%)	5 (6%)	0	100	100
28	f	74/86 (86%)	71 (96%)	3 (4%)	0	100	100
29	g	71/76 (93%)	70 (99%)	1 (1%)	0	100	100
30	q	99/504 (20%)	97 (98%)	2 (2%)	0	100	100
30	r	115/504 (23%)	113 (98%)	2 (2%)	0	100	100
30	s	130/504 (26%)	127 (98%)	2 (2%)	1 (1%)	16	44
30	t	99/504 (20%)	98 (99%)	0	1 (1%)	12	38
31	y	81/301 (27%)	81 (100%)	0	0	100	100
32	D	49/285 (17%)	49 (100%)	0	0	100	100
All	All	10700/18420 (58%)	10373 (97%)	308 (3%)	19 (0%)	44	70

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	O	176	GLY
17	R	135	PRO
30	s	65	PRO
3	A	1092	ILE
20	W	298	PRO
21	WD	65	GLY
21	WD	107	GLY
11	L	63	TRP
5	C	804	GLY
6	E	149	GLY
20	W	58	PRO
3	A	74	GLY
3	A	425	PRO
6	E	107	GLY
10	K	45	PRO
19	T	286	GLY
3	A	1834	GLY
11	L	596	GLY
30	t	15	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	35	567/603 (94%)	558 (98%)	9 (2%)	55	71
3	A	1773/2108 (84%)	1740 (98%)	33 (2%)	50	69
4	B	15/1908 (1%)	15 (100%)	0	100	100
5	C	790/866 (91%)	785 (99%)	5 (1%)	78	80
6	E	256/300 (85%)	253 (99%)	3 (1%)	63	74
7	GP	239/795 (30%)	235 (98%)	4 (2%)	53	70
8	I	25/749 (3%)	25 (100%)	0	100	100
9	J	139/751 (18%)	138 (99%)	1 (1%)	76	79
10	K	7/196 (4%)	7 (100%)	0	100	100
11	L	180/709 (25%)	179 (99%)	1 (1%)	78	80
12	M	3/209 (1%)	3 (100%)	0	100	100
13	N	129/130 (99%)	128 (99%)	1 (1%)	73	78
14	O	15/361 (4%)	15 (100%)	0	100	100
15	P	79/203 (39%)	78 (99%)	1 (1%)	61	73
16	Q	68/1336 (5%)	68 (100%)	0	100	100
17	R	214/457 (47%)	211 (99%)	3 (1%)	59	72
18	S	129/134 (96%)	126 (98%)	3 (2%)	44	66
19	T	275/441 (62%)	271 (98%)	4 (2%)	57	71
20	W	425/502 (85%)	417 (98%)	8 (2%)	50	69
21	WD	8/264 (3%)	8 (100%)	0	100	100
22	Z	7/143 (5%)	7 (100%)	0	100	100
23	a	73/101 (72%)	72 (99%)	1 (1%)	59	72
24	b	75/177 (42%)	75 (100%)	0	100	100
25	c	76/101 (75%)	75 (99%)	1 (1%)	61	73
26	d	91/110 (83%)	91 (100%)	0	100	100
27	e	74/84 (88%)	70 (95%)	4 (5%)	20	46
28	f	65/74 (88%)	64 (98%)	1 (2%)	57	71
29	g	63/66 (96%)	62 (98%)	1 (2%)	55	71
30	q	5/435 (1%)	5 (100%)	0	100	100
30	r	6/435 (1%)	6 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	s	10/435 (2%)	9 (90%)	1 (10%)	7	25
30	t	5/435 (1%)	5 (100%)	0	100	100
31	y	2/252 (1%)	2 (100%)	0	100	100
32	D	1/240 (0%)	1 (100%)	0	100	100
All	All	5889/16110 (37%)	5804 (99%)	85 (1%)	57	72

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	35	42	TYR
1	35	79	THR
1	35	84	SER
1	35	152	LEU
1	35	242	THR
1	35	284	GLN
1	35	351	ILE
1	35	654	ILE
1	35	690	HIS
3	A	97	HIS
3	A	166	PHE
3	A	240	ARG
3	A	327	VAL
3	A	364	SER
3	A	384	VAL
3	A	413	LEU
3	A	443	VAL
3	A	479	THR
3	A	510	ARG
3	A	546	LEU
3	A	598	LEU
3	A	644	ILE
3	A	713	LEU
3	A	718	ARG
3	A	726	TRP
3	A	757	ASN
3	A	844	GLU
3	A	951	LEU
3	A	1079	THR
3	A	1089	CYS
3	A	1097	ILE
3	A	1311	PHE

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Mol	Chain	Res	Type
3	A	1342	TRP
3	A	1369	TYR
3	A	1438	VAL
3	A	1504	GLU
3	A	1582	TRP
3	A	1601	LEU
3	A	1613	THR
3	A	1692	MET
3	A	1702	LEU
3	A	1898	LYS
5	C	61	GLU
5	C	85	ASP
5	C	219	LEU
5	C	416	LEU
5	C	683	ASN
6	E	203	ASP
6	E	231	MET
6	E	291	CYS
7	GP	14	SER
7	GP	64	THR
7	GP	105	ILE
7	GP	247	LEU
9	J	300	ASP
11	L	149	LEU
13	N	9	LYS
15	P	216	THR
17	R	111	VAL
17	R	280	ILE
17	R	293	ILE
18	S	20	MET
18	S	62	ILE
18	S	152	ARG
19	T	216	ASN
19	T	416	ILE
19	T	432	ASP
19	T	489	TYR
20	W	87	THR
20	W	193	LEU
20	W	355	TYR
20	W	403	TRP
20	W	437	SER
20	W	444	VAL

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Mol	Chain	Res	Type
20	W	448	ASP
20	W	493	ARG
23	a	61	VAL
25	c	64	ASN
27	e	14	MET
27	e	38	GLN
27	e	77	ILE
27	e	82	ASP
28	f	5	LEU
29	g	70	LEU
30	s	65	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	35	40	ASN
1	35	527	GLN
1	35	558	HIS
3	A	680	HIS
3	A	757	ASN
3	A	834	HIS
3	A	1018	ASN
3	A	1023	ASN
3	A	1069	ASN
3	A	1169	GLN
3	A	1446	GLN
3	A	1466	ASN
3	A	1468	ASN
3	A	1469	ASN
3	A	1586	HIS
3	A	2004	GLN
5	C	201	ASN
5	C	768	GLN
5	C	859	GLN
6	E	207	GLN
6	E	215	ASN
7	GP	37	GLN
7	GP	50	HIS
9	J	291	GLN
11	L	30	GLN
17	R	104	GLN
17	R	231	HIS

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Mol	Chain	Res	Type
17	R	307	GLN
18	S	13	ASN
19	T	283	HIS
19	T	417	ASN
19	T	437	HIS
20	W	484	GLN
24	b	12	HIS
27	e	83	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	5	90/116 (77%)	15 (16%)	6 (6%)
33	IN	9/10 (90%)	3 (33%)	0
34	6	34/106 (32%)	13 (38%)	3 (8%)
All	All	133/232 (57%)	31 (23%)	9 (6%)

All (31) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	5	20	G
2	5	25	C
2	5	36	C
2	5	69	A
2	5	86	C
2	5	88	A
2	5	90	U
2	5	92	U
2	5	94	U
2	5	95	G
2	5	96	A
2	5	99	C
2	5	110	A
2	5	111	A
2	5	115	U
33	IN	12	U
33	IN	17	U
33	IN	20	U
34	6	5	U
34	6	6	C
34	6	7	G

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Mol	Chain	Res	Type
34	6	9	U
34	6	10	U
34	6	12	G
34	6	26	U
34	6	27	A
34	6	28	A
34	6	29	A
34	6	33	G
34	6	34	G
34	6	35	A

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	5	20	G
2	5	24	G
2	5	47	A
2	5	90	U
2	5	91	U
2	5	95	G
34	6	5	U
34	6	27	A
34	6	33	G

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
17	SEP	R	224	17	8,9,10	1.47	1 (12%)	8,12,14	1.20	1 (12%)
17	SEP	R	232	17	8,9,10	1.44	1 (12%)	8,12,14	1.78	2 (25%)

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
17	SEP	R	224	17	-	0/5/8/10	-
17	SEP	R	232	17	-	0/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	R	224	SEP	P-O1P	3.25	1.61	1.50
17	R	232	SEP	P-O1P	3.08	1.60	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	R	232	SEP	P-OG-CB	-3.59	108.40	118.30
17	R	232	SEP	OG-CB-CA	2.85	110.91	108.14
17	R	224	SEP	P-OG-CB	-2.53	111.32	118.30

There are no chirality outliers.

There are no torsion outliers.

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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	GTP	C	1500	37	30,34,34	0.97	1 (3%)	46,54,54	1.88	11 (23%)
35	IHP	A	3000	-	36,36,36	2.33	10 (27%)	54,60,60	1.66	9 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	GTP	C	1500	37	-	0/22/38/38	0/3/3/3
35	IHP	A	3000	-	-	8/30/54/54	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	3000	IHP	P2-O12	6.40	1.71	1.59
35	A	3000	IHP	P6-O16	4.70	1.68	1.59
35	A	3000	IHP	P3-O13	4.50	1.67	1.59
35	A	3000	IHP	C3-C2	-4.35	1.43	1.52
35	A	3000	IHP	P1-O11	4.29	1.67	1.59
35	A	3000	IHP	P5-O15	4.27	1.67	1.59
35	A	3000	IHP	P4-O14	4.26	1.67	1.59
35	A	3000	IHP	O13-C3	-2.73	1.34	1.44
36	C	1500	GTP	C5-N7	-2.38	1.34	1.39
35	A	3000	IHP	O12-C2	-2.12	1.36	1.44
35	A	3000	IHP	P1-O21	2.07	1.57	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	3000	IHP	O12-C2-C1	7.09	125.41	108.69
36	C	1500	GTP	PB-O3B-PG	-4.96	115.81	132.83
36	C	1500	GTP	C5-C4-N3	-4.94	120.45	128.46
36	C	1500	GTP	C2-N3-C4	4.33	120.01	112.30
35	A	3000	IHP	O11-C1-C2	3.69	117.38	108.69
36	C	1500	GTP	PA-O3A-PB	-3.56	120.61	132.83
35	A	3000	IHP	O15-C5-C6	3.53	117.01	108.69
36	C	1500	GTP	N9-C4-N3	3.30	132.57	125.94
36	C	1500	GTP	C2-N1-C6	-3.14	119.37	125.10
36	C	1500	GTP	N9-C8-N7	-3.07	107.62	113.39
35	A	3000	IHP	O11-P1-O21	2.92	120.68	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	3000	IHP	O11-C1-C6	-2.79	102.12	108.69
36	C	1500	GTP	C5-C6-N1	2.77	120.22	113.19
36	C	1500	GTP	C8-N7-C5	2.72	109.17	104.24
35	A	3000	IHP	C4-C3-C2	2.38	115.61	110.41
36	C	1500	GTP	O6-C6-C5	-2.33	120.41	126.60
35	A	3000	IHP	O35-P5-O25	2.27	119.55	110.68
35	A	3000	IHP	O15-C5-C4	-2.23	103.42	108.69
35	A	3000	IHP	O41-P1-O11	-2.21	96.09	105.99
36	C	1500	GTP	O5'-C5'-C4'	2.15	116.37	108.99

There are no chirality outliers.

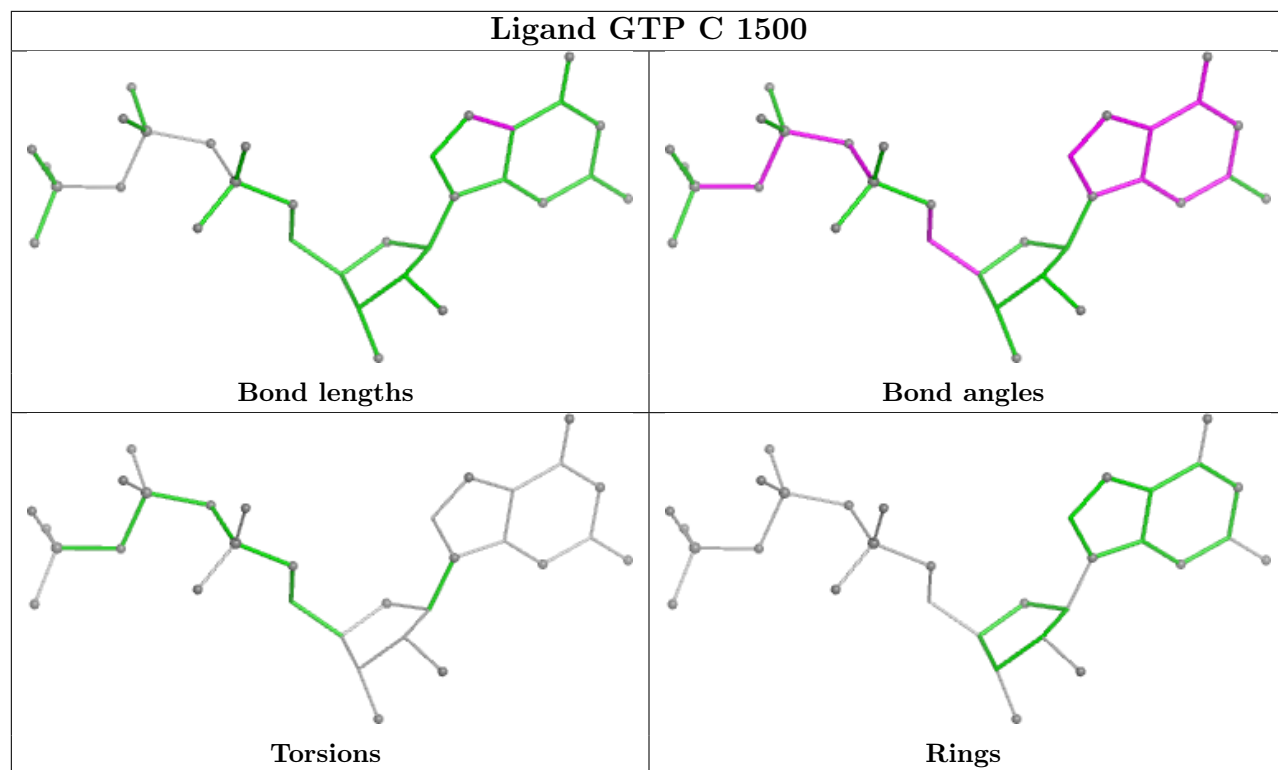
All (8) torsion outliers are listed below:

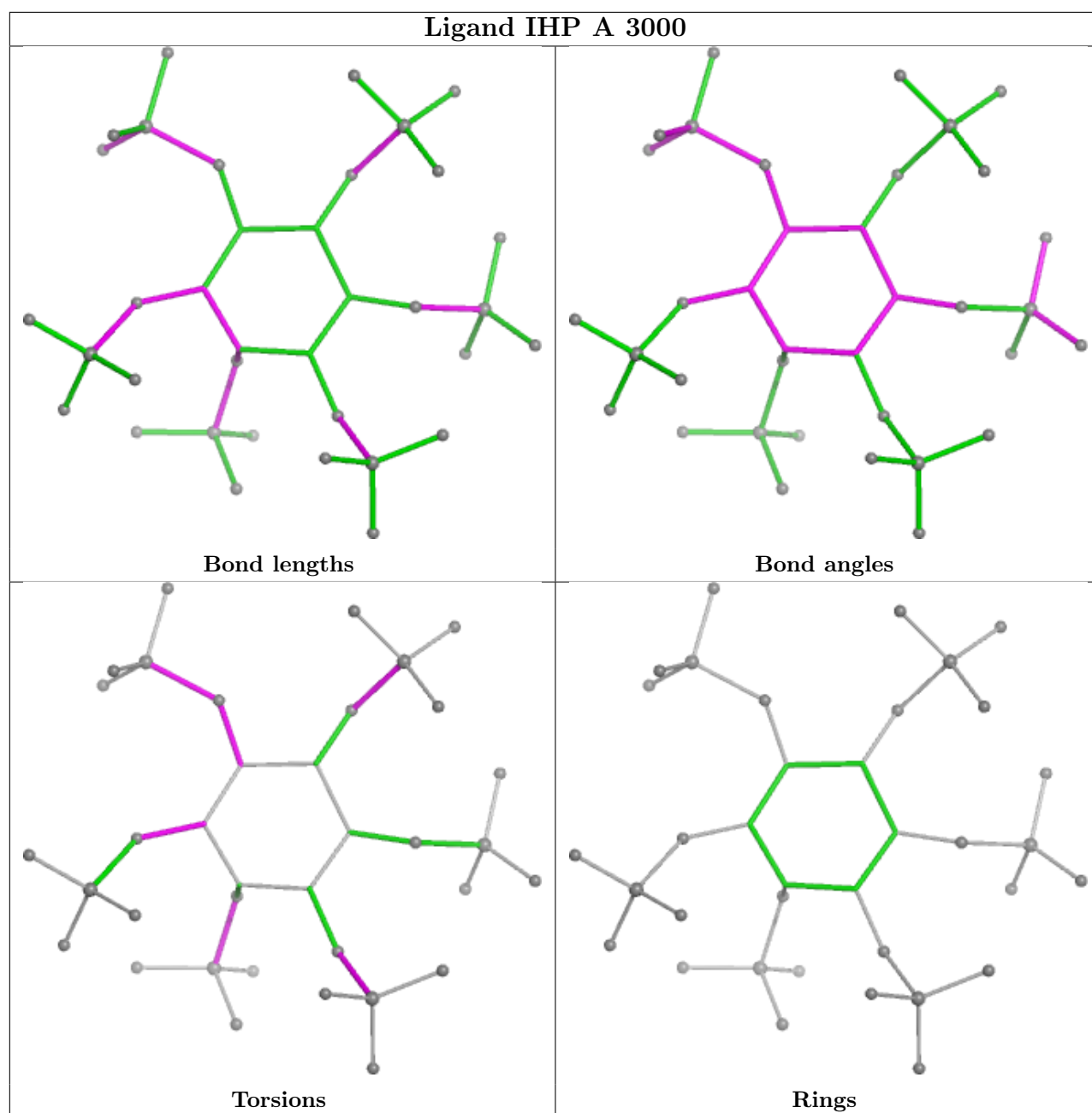
Mol	Chain	Res	Type	Atoms
35	A	3000	IHP	C2-C1-O11-P1
35	A	3000	IHP	C6-C1-O11-P1
35	A	3000	IHP	C4-O14-P4-O44
35	A	3000	IHP	C6-O16-P6-O26
35	A	3000	IHP	C3-C2-O12-P2
35	A	3000	IHP	C6-O16-P6-O36
35	A	3000	IHP	C1-O11-P1-O31
35	A	3000	IHP	C3-O13-P3-O33

There are no ring outliers.

No monomer is involved in short contacts.

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.

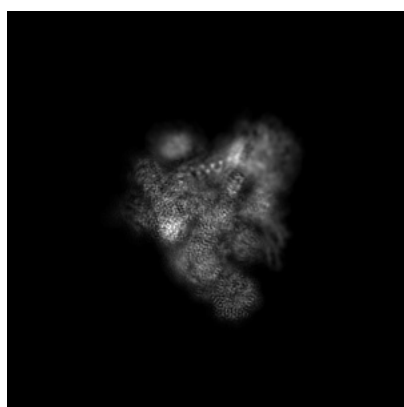
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54494. These allow visual inspection of the internal detail of the map and identification of artifacts.

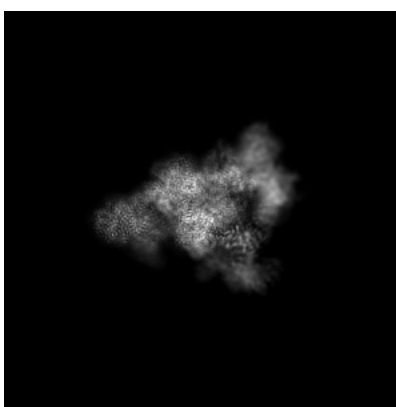
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

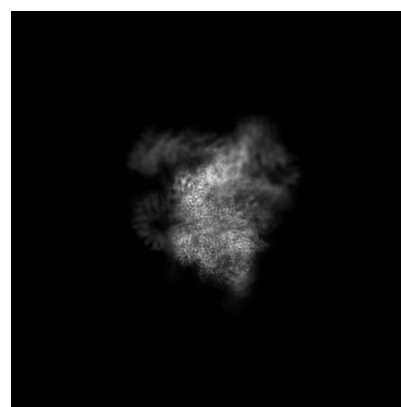
6.1.1 Primary map



X



Y

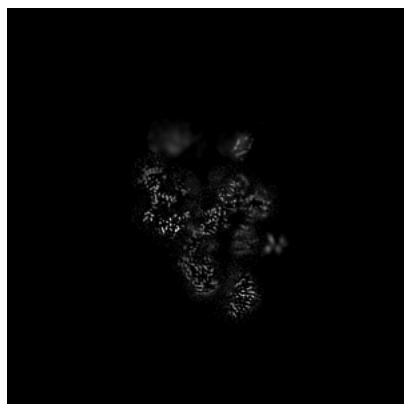


Z

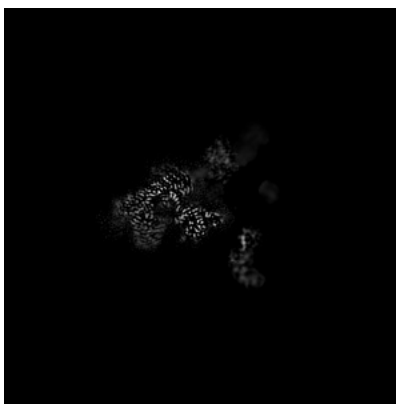
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 224



Y Index: 224



Z Index: 224

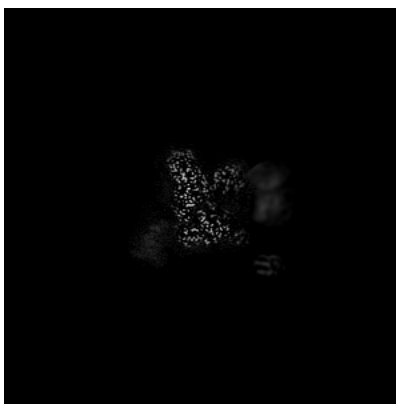
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

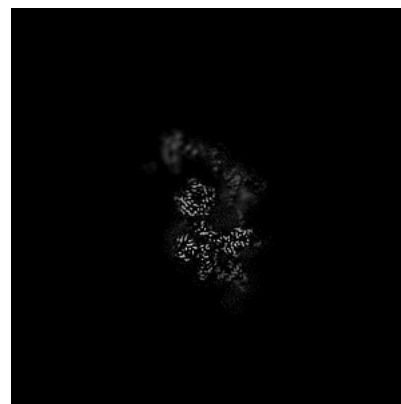
6.3.1 Primary map



X Index: 214



Y Index: 186

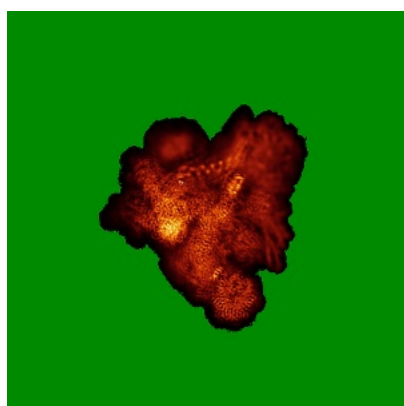


Z Index: 213

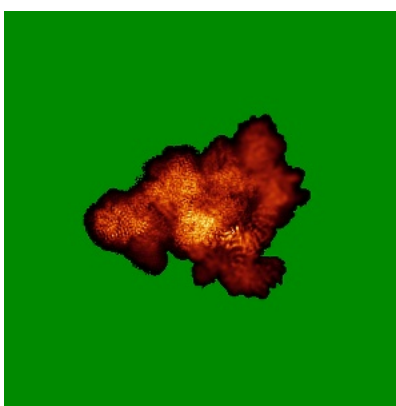
The images above show the largest variance slices of the map in three orthogonal directions.

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.

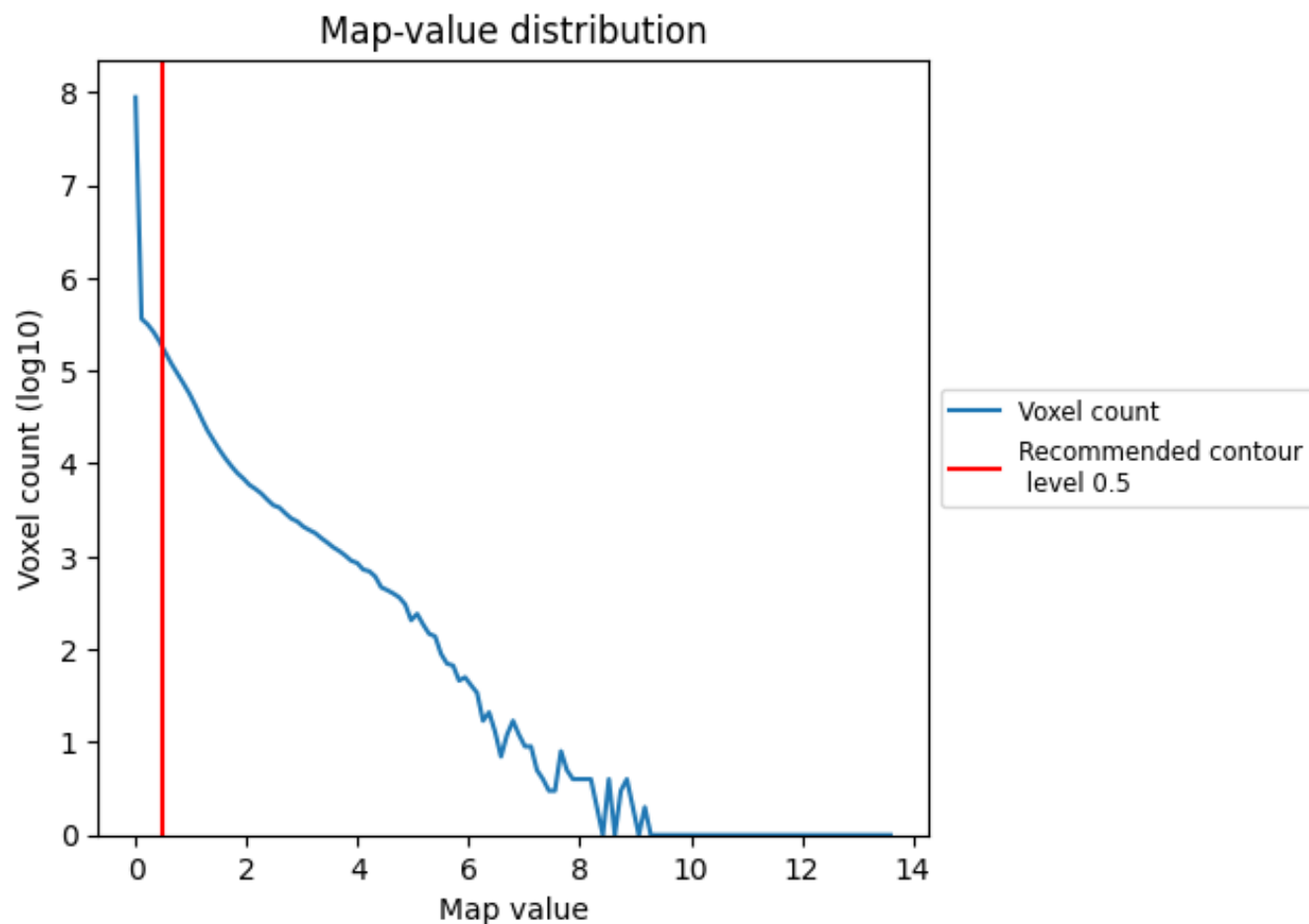
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

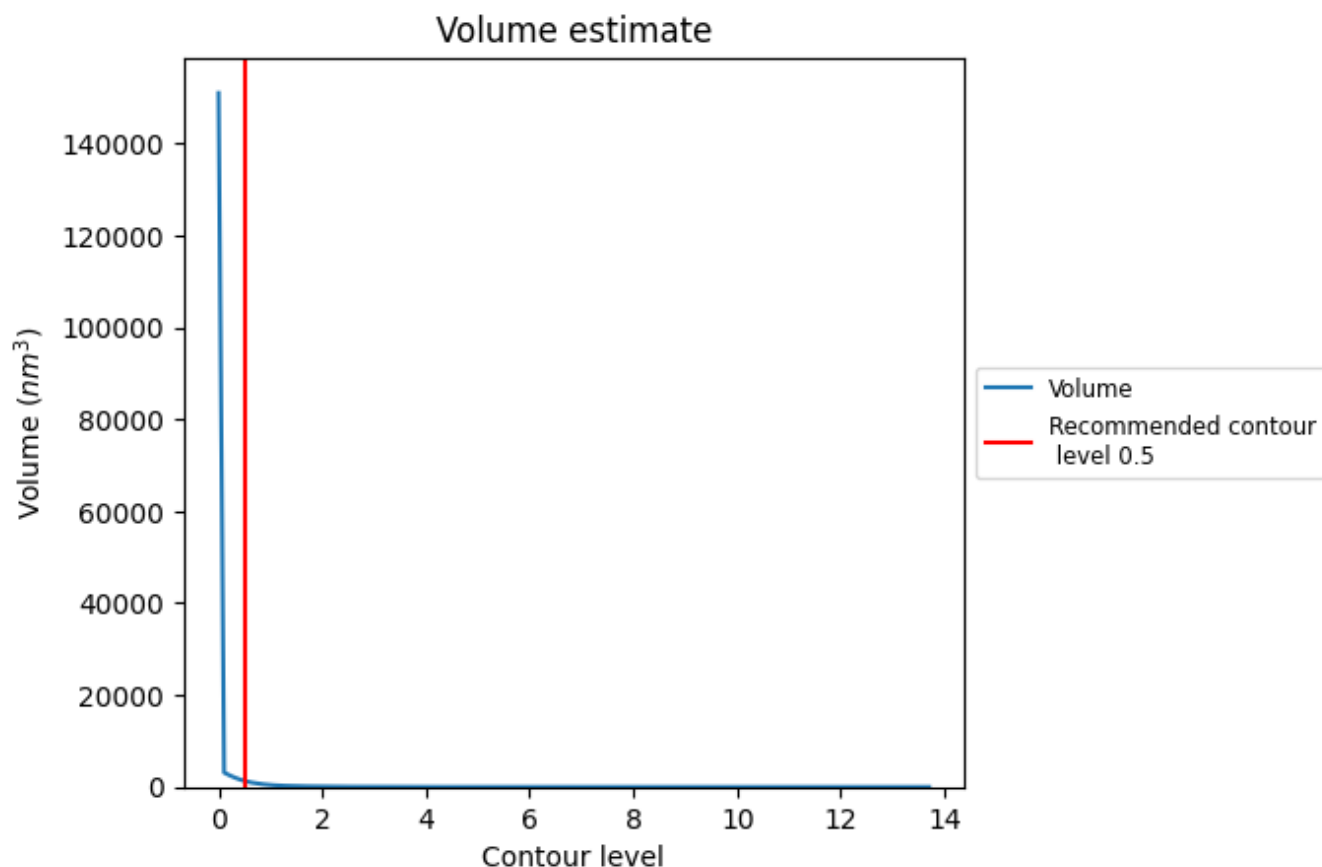
This section contains the results of statistical analysis of the map.

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.

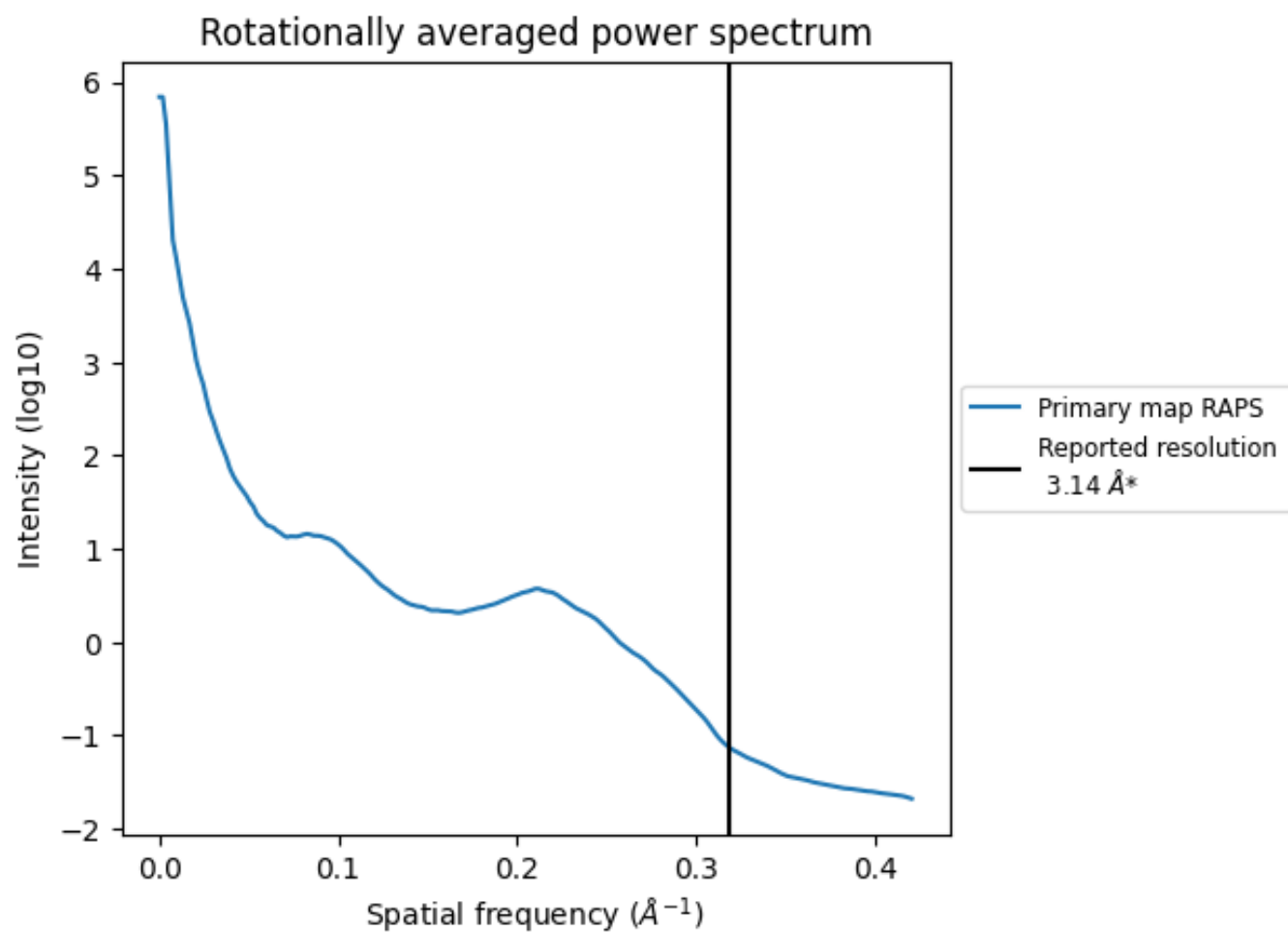
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1327 nm^3 ; this corresponds to an approximate mass of 1199 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 0.318 $\text{\AA}^{-1}$

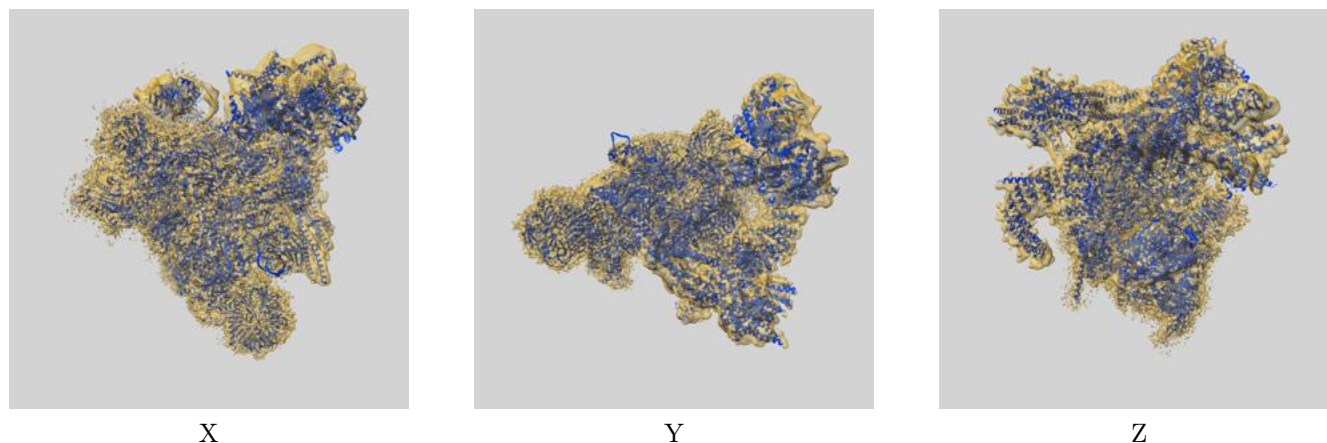
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

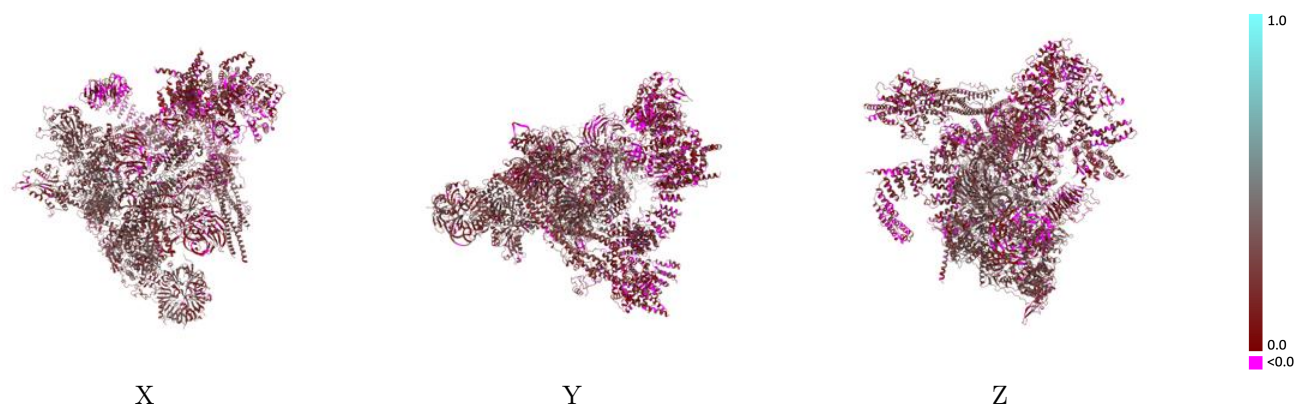
This section contains information regarding the fit between EMDB map EMD-54494 and PDB model 9S2F. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



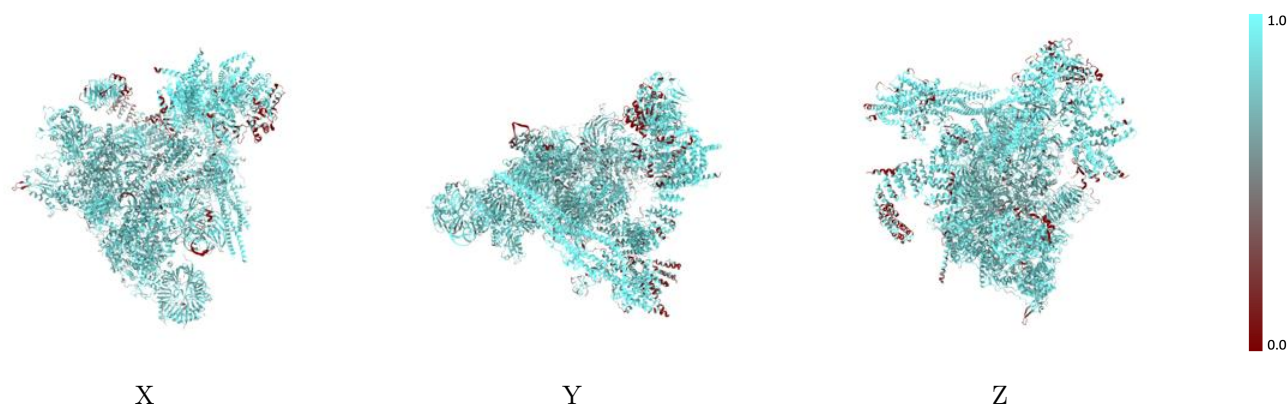
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



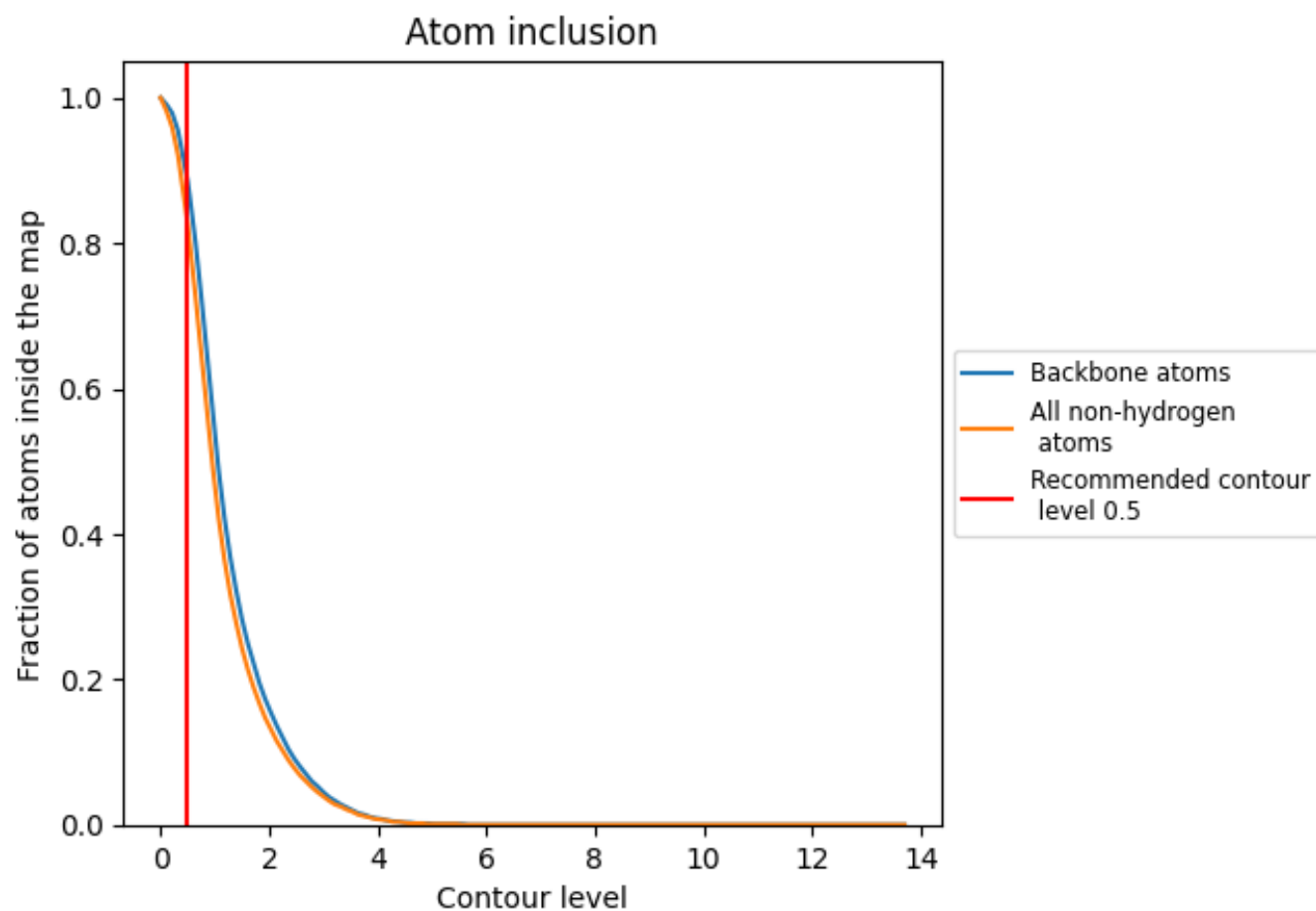
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 88% of all backbone atoms, 83% 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	 0.8260	 0.2140
35	 0.8180	 0.2690
5	 0.8840	 0.2420
6	 0.6090	 0.0970
A	 0.8430	 0.2780
B	 0.7100	 0.2670
C	 0.8620	 0.2550
D	 0.9250	 0.1580
E	 0.8460	 0.1650
GP	 0.7690	 0.2570
I	 0.9060	 0.1610
IN	 0.9080	 0.1730
J	 0.7700	 0.1650
K	 0.9150	 0.1990
L	 0.7930	 0.2040
M	 0.8770	 0.2030
N	 0.7500	 0.2100
O	 0.8410	 0.2250
P	 0.7080	 0.2290
Q	 0.8100	 0.1080
R	 0.7980	 0.2090
S	 0.8650	 0.1770
T	 0.8800	 0.3010
W	 0.7450	 0.1210
WD	 0.8620	 0.0440
Z	 0.5880	 0.0700
a	 0.8540	 0.2430
b	 0.8000	 0.2610
c	 0.8370	 0.2380
d	 0.7020	 0.1770
e	 0.8370	 0.2780
f	 0.8320	 0.2870
g	 0.8540	 0.2420
q	 0.8630	 0.2020
r	 0.8730	 0.1630



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Chain	Atom inclusion	Q-score
s	 0.9400	 0.1890
t	 0.8760	 0.1560
y	 0.5480	 0.0870