



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:11 AM UTC

PDB ID : 6ZYM / pdb_00006zym
EMDB ID : EMD-11569
Title : Human C Complex Spliceosome - High-resolution CORE
Authors : Bertram, K.; Kastner, B.
Deposited on : 2020-08-02
Resolution : 3.40 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:

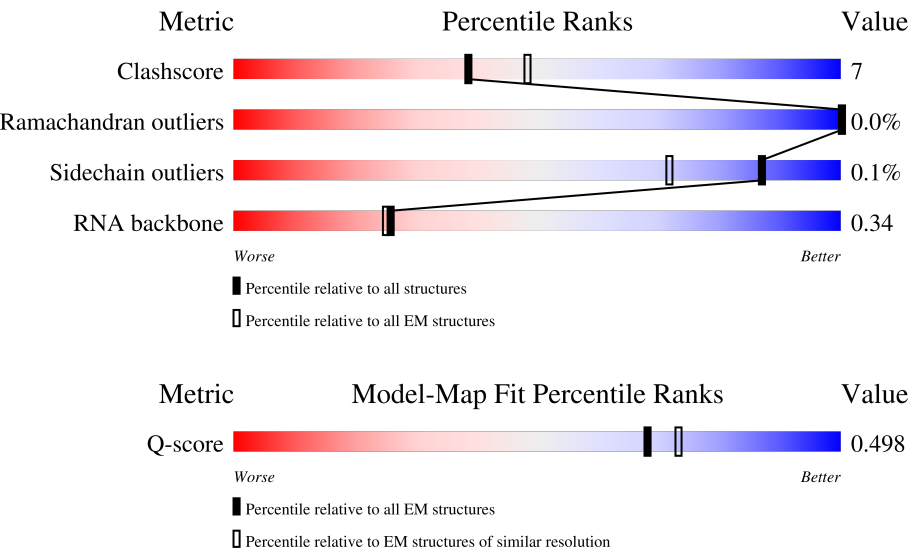
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 3.40 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.



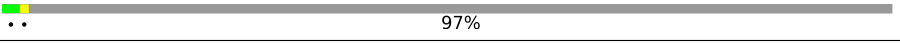
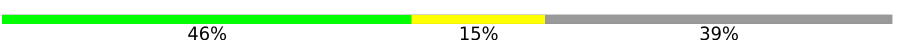
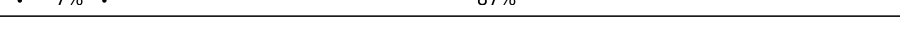
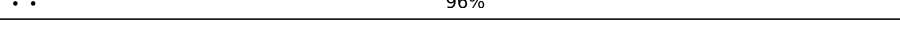
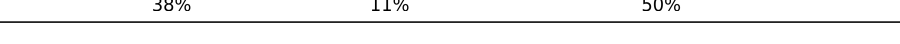
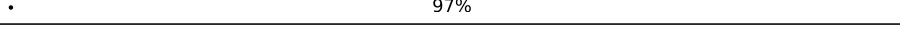
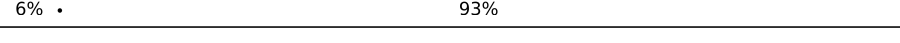
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	188	5% 6% . 86%
2	5	116	51% 13% 36%
3	6	79	56% 39% 5%

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Mol	Chain	Length	Quality of chain
4	9	450	 97%
5	A	1755	 80% 18%
6	B	952	 75% 19% 6%
7	C	536	 36% 5% 58%
8	D	514	 46% 15% 39%
9	E	579	 11% 87%
10	F	357	 61% 22% 16%
11	L	802	 23% 75%
12	O	848	 25% 70%
13	P	218	 72% 17% 11%
14	Q	144	 85% 10%
15	R	229	 32% 6% 62%
16	S	2752	 99%
17	T	908	 19% 78%
18	V	166	 81% 17%
19	Y	324	 7% 87%
19	Z	324	 96%
20	p	654	 38% 11% 50%
21	r	1227	 97%
22	s	285	 6% 93%
23	t	425	 11% 87%
24	u	178	 70% 16% 12%
25	x	258	 10% 88%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	ZN	u	1001	-	-	X	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 48271 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	27	Total	C	N	O	P	0	0
			575	257	99	192	27		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	74	Total	C	N	O	P	0	0
			1548	693	256	525	74		

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	79	Total	C	N	O	P	0	0
			1690	756	312	543	79		

- Molecule 4 is a protein called Corepressor interacting with RBPJ 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	9	14	Total	C	N	O	S	0	0
			112	68	21	22	1		

- Molecule 5 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	1722	Total	C	N	O	S	0	0
			14270	9190	2521	2494	65		

- Molecule 6 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	895	Total	C	N	O	S	0	0
			6953	4447	1163	1309	34		

- Molecule 7 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	224	Total	C	N	O	S	0	0
			1703	1074	308	312	9		

- Molecule 8 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	315	Total	C	N	O	S	0	0
			2481	1565	451	458	7		

- Molecule 9 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	78	Total	C	N	O	S	0	0
			629	400	107	118	4		

- Molecule 10 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	299	Total	C	N	O	S	0	0
			2230	1407	381	430	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	202	Total	C	N	O	S	0	0
			1611	1012	297	296	6		

- Molecule 12 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	252	Total	C	N	O	S	0	0
			2108	1345	381	377	5		

- Molecule 13 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	195	Total	C	N	O	S	0	0
			1577	991	279	290	17		

- Molecule 14 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	142	Total	C	N	O	S	0	0
			1162	733	216	202	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	87	Total	C	N	O	S	0	0
			681	421	134	125	1		

- Molecule 16 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	30	Total	C	N	O	S	0	0
			230	140	49	40	1		

- Molecule 17 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	203	Total	C	N	O	S	0	0
			1669	1071	278	307	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	163	Total	C	N	O	S	0	0
			1081	677	200	199	5		

- Molecule 19 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Y	41	Total	C	N	O	P	0	0
			873	391	155	286	41		
19	Z	13	Total	C	N	O	P	0	0
			276	123	50	90	13		

- Molecule 20 is a protein called WD repeat-containing protein 70.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	p	325	Total	C	N	O	S	0	0
			2372	1493	421	442	16		

- Molecule 21 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase

PRP16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	r	35	Total	C	N	O	S	0	0
			259	157	50	51	1		

- Molecule 22 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	s	20	Total	C	N	O	S	0	0
			158	96	33	28	1		

- Molecule 23 is a protein called Pre-mRNA-splicing factor CWC25 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	t	56	Total	C	N	O		0	0
			418	259	80	79			

- Molecule 24 is a protein called Splicing factor YJU2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	u	157	Total	C	N	O	S	0	0
			1286	819	226	231	10		

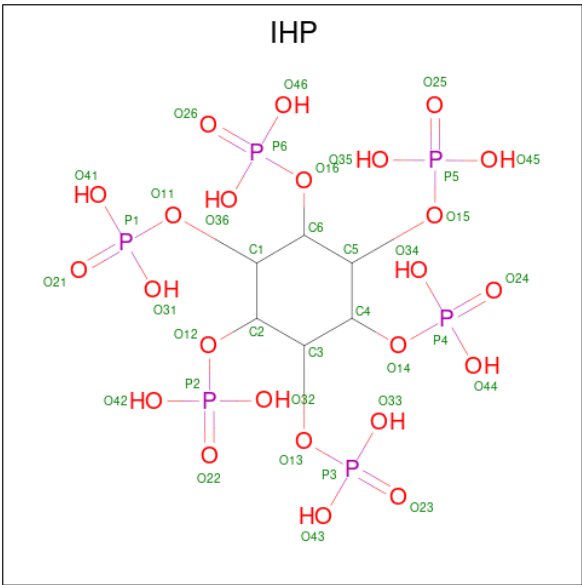
- Molecule 25 is a protein called Protein FRG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	x	30	Total	C	N	O	S	0	0
			239	149	49	40	1		

- Molecule 26 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

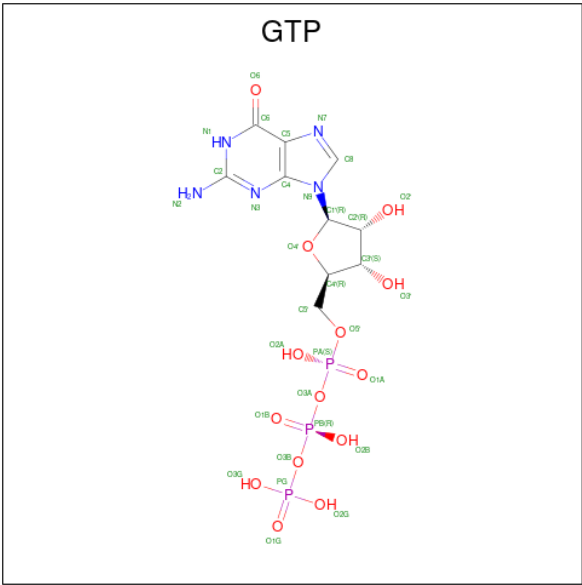
Mol	Chain	Residues	Atoms		AltConf
26	6	5	Total	Mg	0
			5	5	

- Molecule 27 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



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

- Molecule 28 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



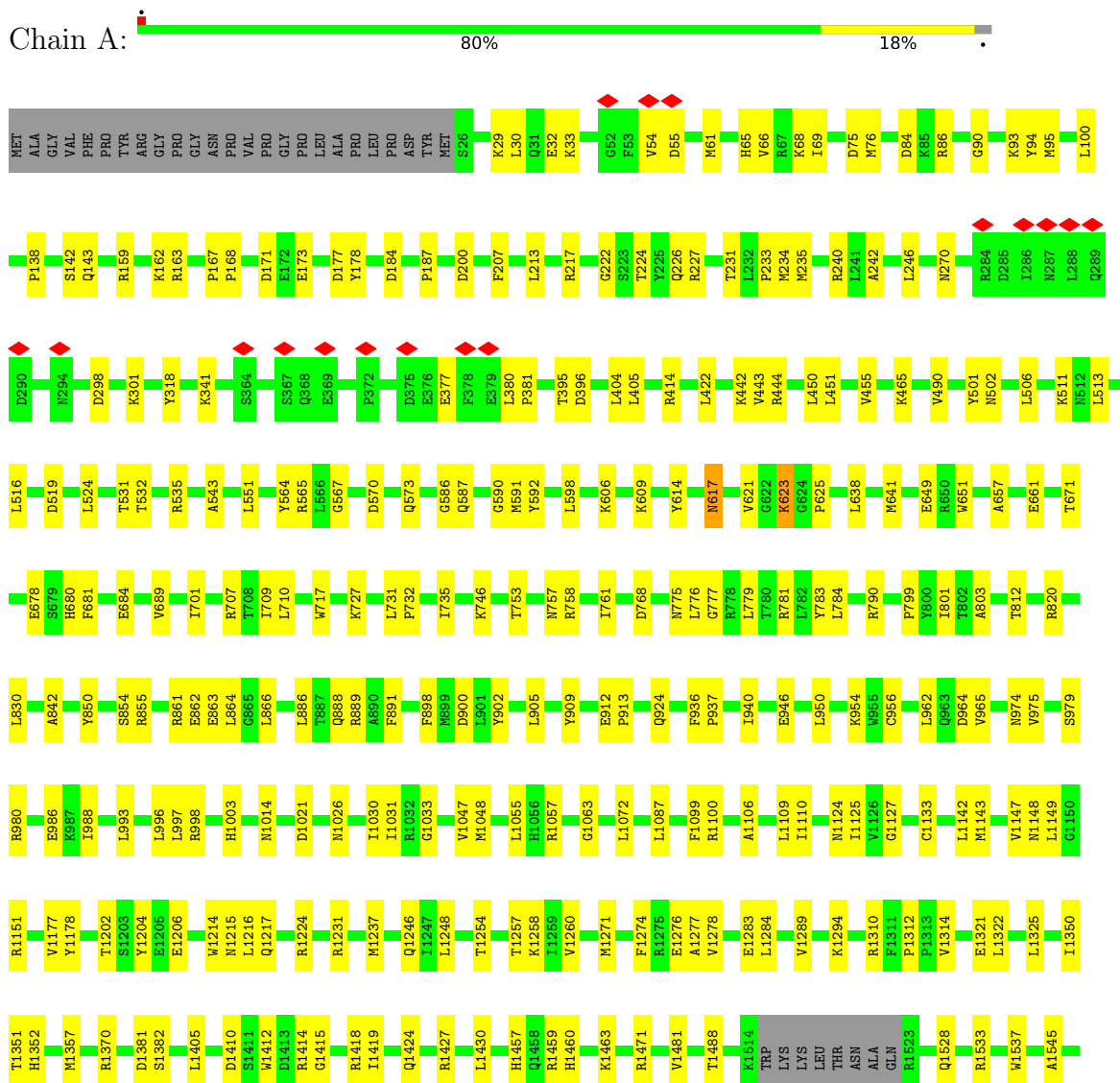
Mol	Chain	Residues	Atoms					AltConf
28	B	1	Total	C	N	O	P	0
			32	10	5	14	3	

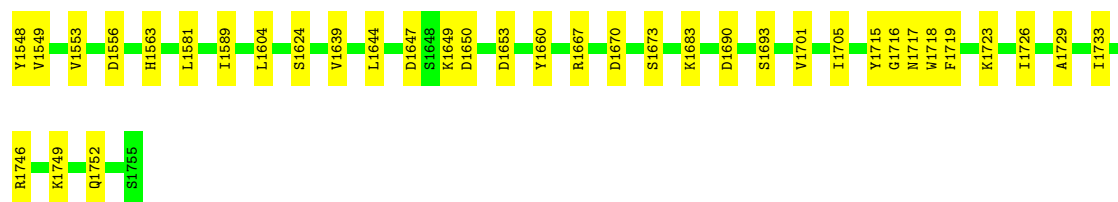
- Molecule 29 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
29	P	3	Total 3	Zn 3	0
29	Q	3	Total 3	Zn 3	0
29	u	1	Total 1	Zn 1	0

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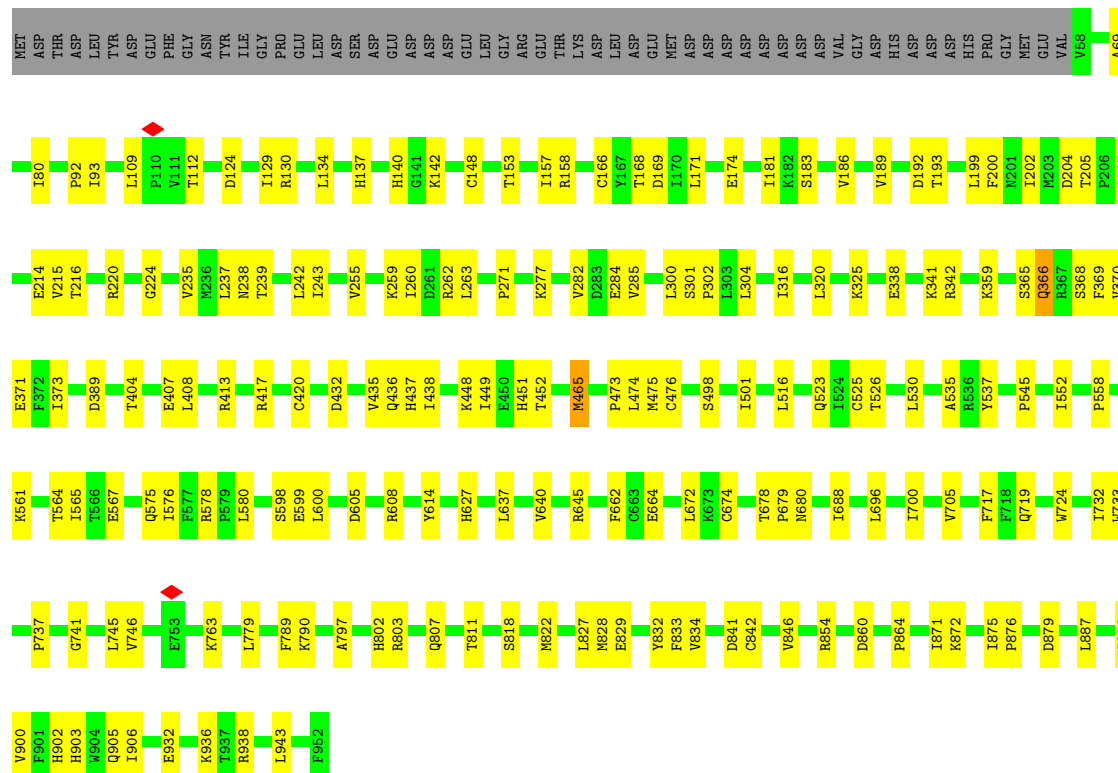
- Molecule 5: Pre-mRNA-processing-splicing factor 8





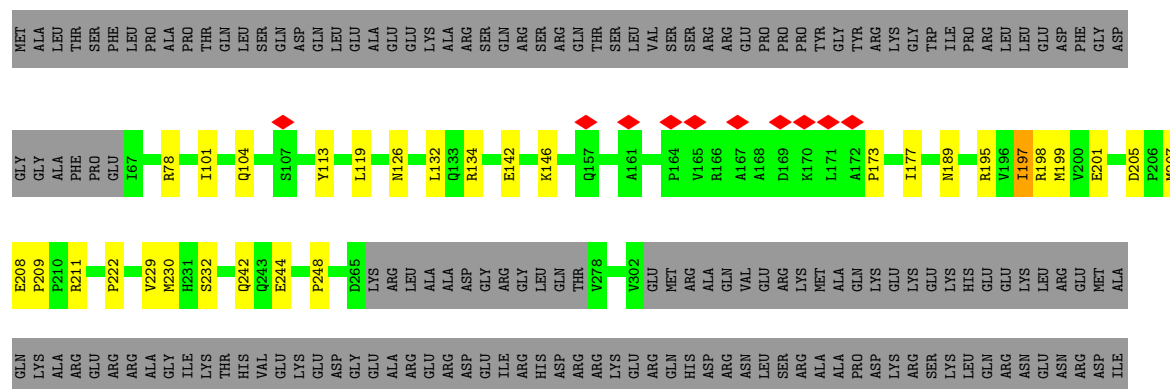
- Molecule 6: 116 kDa U5 small nuclear ribonucleoprotein component

Chain B: 75% 19% 6%



- Molecule 7: SNW domain-containing protein 1

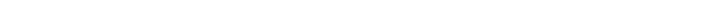
Chain C: 36% 5% 58%



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

- Molecule 8: Pleiotropic regulator 1

Chain D:  46% 15% 39%

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

SER	ALA	ALA	GLN	SER	LEU	ALA	VAL	ALA	ALA	LEU	PRO	LEU	GLN	THR	LYS	ALA	ASP	ASN	ARG	THR	ALA	PRO	SER	GLY	SER	GLU	TYR	ARG	HIS	PRO	GLY	ALA	ASP	ARG	PRO	GLN	THR	MET	THR	GLY	ASN	THR	LYS	ASN	SER	ALA	LEU	MET	ALA	LYS
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LYS	P186	L196	I200	E213	P214	W218	F219	V220	L240	I246	V249	V254	S255	T256	R257	Y260	L261	F262	C263	C264	G265	E266	D267	C272	W273	D274	L275	E276	R282	H287	A290	V291	L294	D301	C306	S307	R308	D309
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R313	L314	H324	V333	A334	H350	D351	F352	T353	I354	D358	R365	T369	K372	V375	H381	F382	R383	K389	F400	F401	D402	L409	L419	D424	G425	V426	L427	M436	V439	R442	T443	G444	K455	P456	G457	S458	E462	S473	F474	F475
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L478	T479	A480	E481	T485	I486	K487	V488	D492	T496	E497	E498	L499	H500	PRO	VAL	SER	TRP	LYS	PRO	GLU	ILE	ILE	LYS	ARG	LYS	ARG	PHE
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- Molecule 9: Pre-mRNA-processing factor 17

Chain E: 11% . 87%

MET	SER	ALA	ALA	ILE	ALA	ALA	LEU	ALA	ALA	SER	TYR	GLY	SER	GLY	SER	GLY	SER	GLU	SER	ASP	ASP	ASP	CYS	PRO	LEU	PRO	ALA	ALA	ALA	ASP	SER	SER	MET	HIS	THR	LEU	LYS	PRO	SER	SER	SER	SER	LYS	PRO	PRO	SER	LEU	VAL	VAL	VAL	ASP	SER	ALA	ALA	PRO	PRO	GLU	PAY
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ALA	VAL	LYS	GLU	ASP	LEU	GLU	THR	GLY	V73	A90	P91	E92		N97	P98		T101	M104	R108	L111	I120	M124	Q128	L139	M145	H146	VAL	SER	ALA	ALA	LYS	THR	ILE	GLY	SER	VAL	GLU	GLU	ALA	GLU	LYS	ASN	GLN	GLY	LEU	THR	VAL	PHE	PHE	GLU	THR
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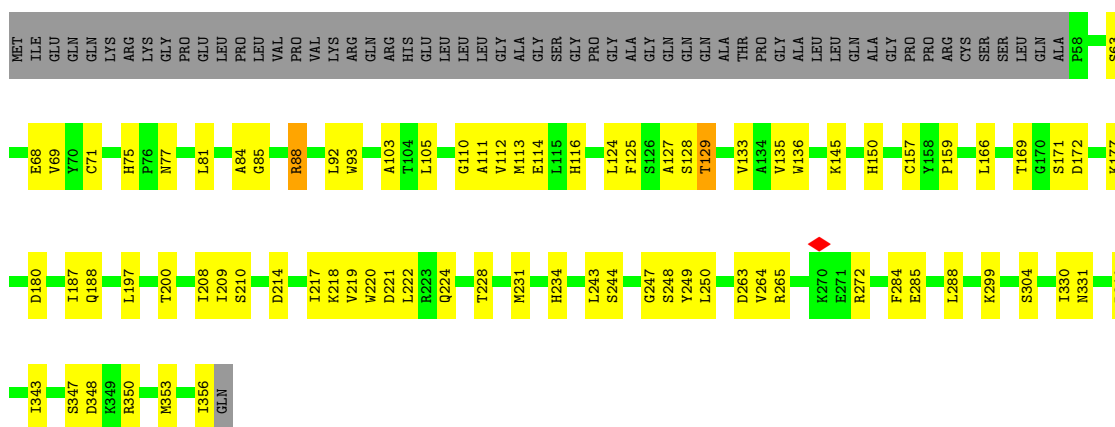
GLU GLY LYS LYS GLU GLU GLY LYS THR ILE LEU HIS VAL LYS GLY LYS MET MET TYR ASP TYR GLN GLY ARG SER SER LEU HIS ILE LEU PRO PRO GLN ASP VAL GLY VAL ASN ASN LEU LEU ARG SER SER THR MET MET PRO PRO GLU GLY LYS TYR TYR LEU LEU PRO PRO LYS LYS GLN ILE ILE HIS HIS VAL VAL TRP SER GLY HIS THR HIS LYS LYS

VAL	SER	ALA	ALA	VAL	ARG	LEU	PHE	PRO	LEU	SER	GLY	HIS	LEU	LEU	LEU	SER	CYS	SER	MET	ASP	CYS	LYS	ILE	LYS	LEU	TRP	GLU	VAL	TYR	GLY	GLU	ARG	ARG	CYS	LEU	ARG	THR	PHE	ILE	GLY	GLY	SER	LYS	ALA	VAL	ARG	ASP	ILE	CYS	PHE	ASN	THR	ALA	GLY	THR	GLN	PHE	LEU	SER	ALA
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ALA	TYR	ASP	ARG	TYR	LEU	LYS	LEU	TRP	ASP	THR	THR	GLU	GLY	THR	GLN	GLY	CYS	ILE	SER	ARG	ARG	PHE	THR	ASN	ARG	LYS	VAL	PRO	TYR	CYS	VAL	LYS	PHE	ASN	ASN	GLN	LYS	ASP	GLU	ASP	LYS	GLN	ASN	LEU	PHE	VAL	ALA	GLY	MET	SER	THR	ASP	LYS	LYS	ILE	VAL	GLN	TRP	ASP	ILE	ARG	SER	GLY	GLU	THR	TYR
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VAL	GLN	GLU	GLY	THR	TYR	ASP	ARG	HIS	LEU	GLY	ALA	VAL	VAL	ASP	GLU	ASN	THR	ILE	VAL	PHE	ARG	ARG	PHE	VAL	SER	THR	SER	ASP	LYS	SER	LEU	ARG	VAL	TRP	TRP	TRP	ASP	PHE	LYS	TYR	ILE	ALA	GLU	PRO	SER	MET	HIS	SER	MET	PRO	ALA	VAL	THR	LEU	ASP
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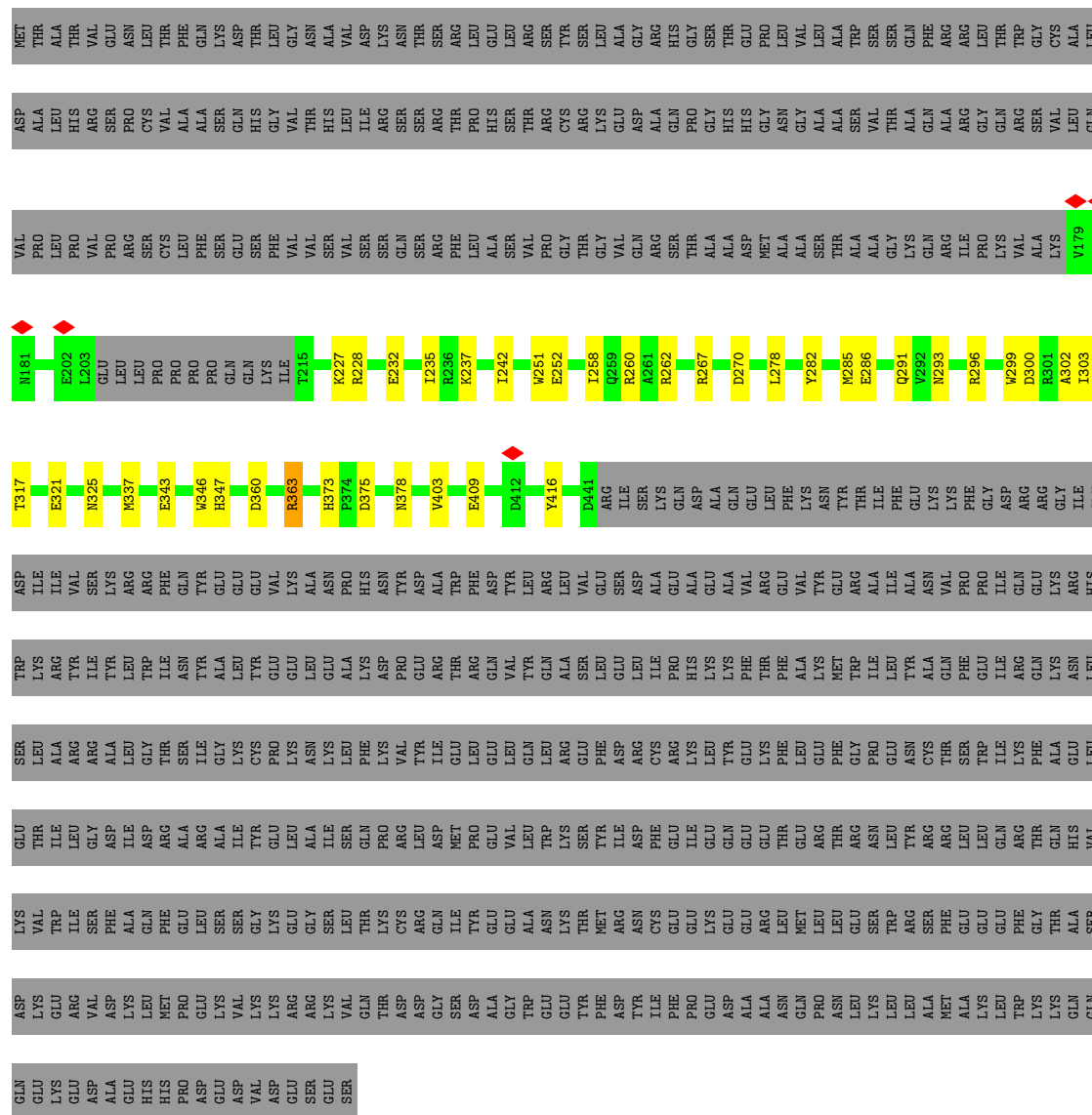
- Molecule 10: U5 small nuclear ribonucleoprotein 40 kDa protein



- Molecule 11: Cell division cycle 5-like protein



- Molecule 12: Crooked neck-like protein 1

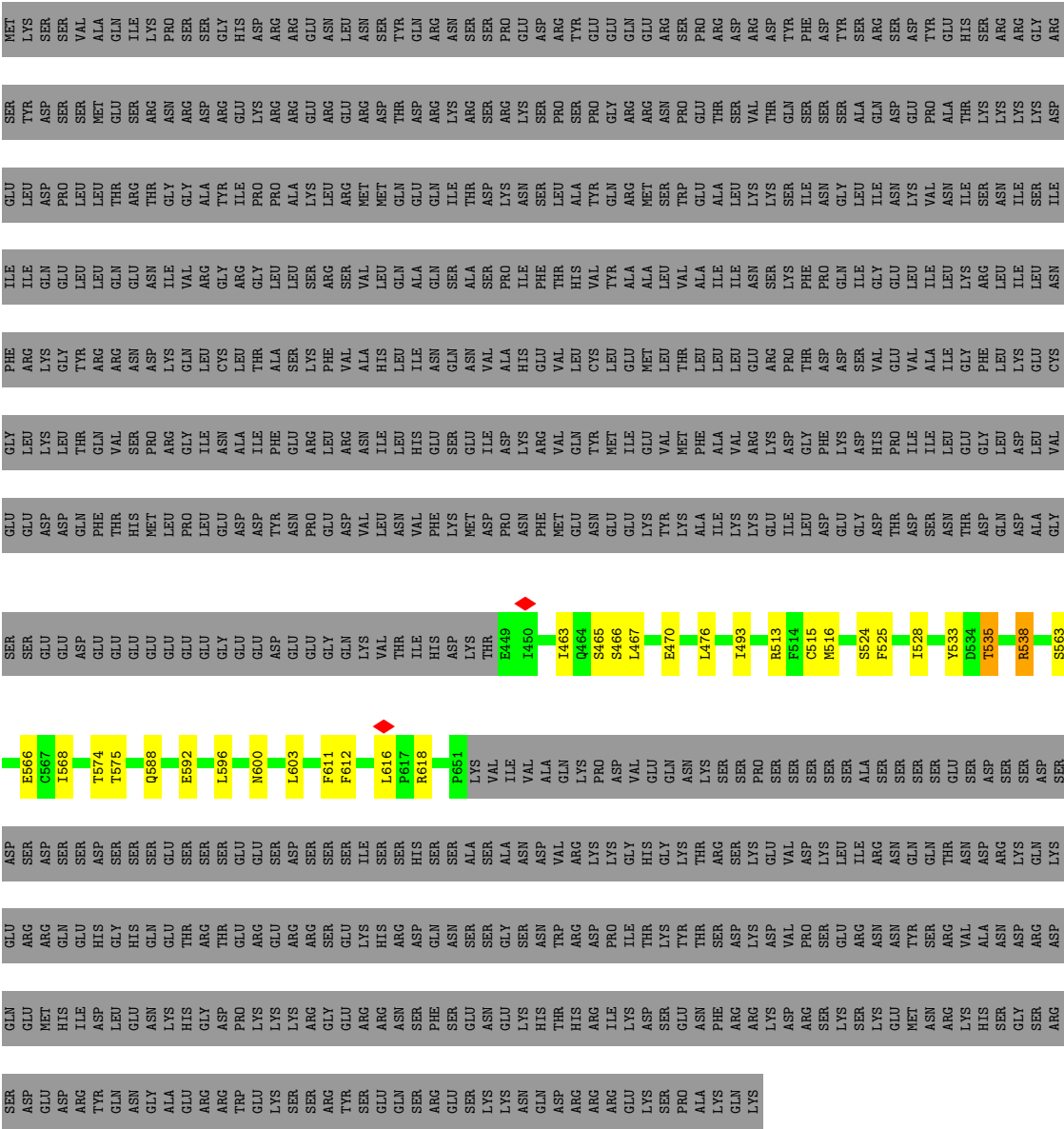


- Molecule 13: Pre-mRNA-splicing factor RBM22

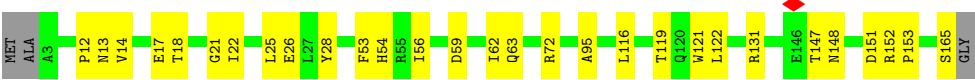
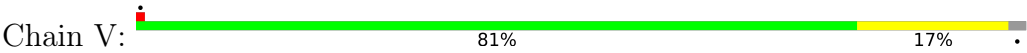




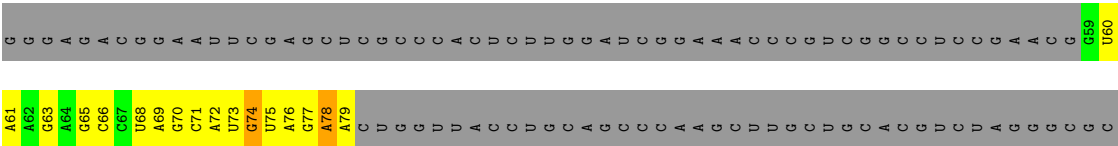




● Molecule 18: Peptidyl-prolyl cis-trans isomerase-like 1



● Molecule 19: pre-mRNA

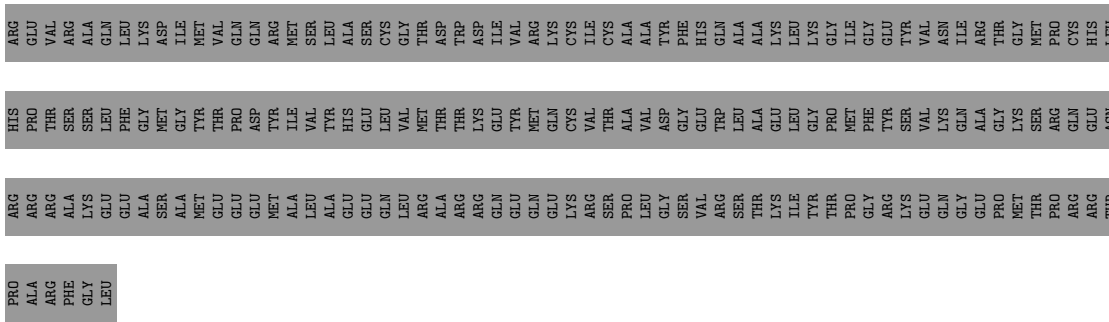




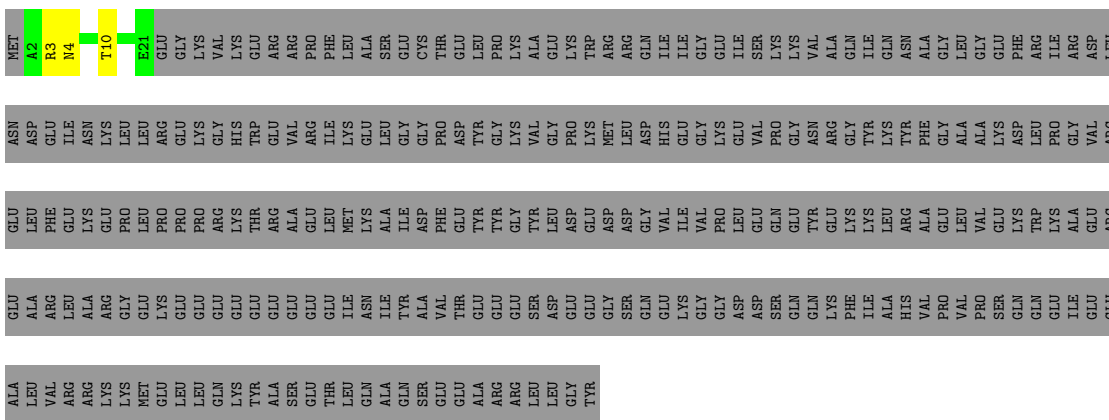
- Molecule 21: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16

97%

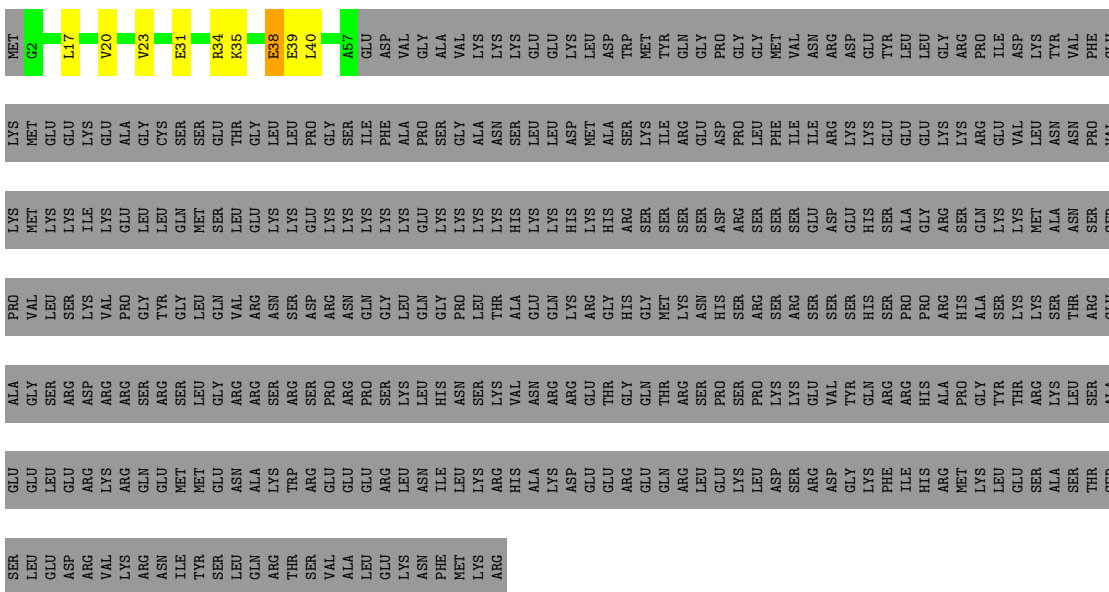




- Molecule 22: Pre-mRNA-splicing factor ISY1 homolog

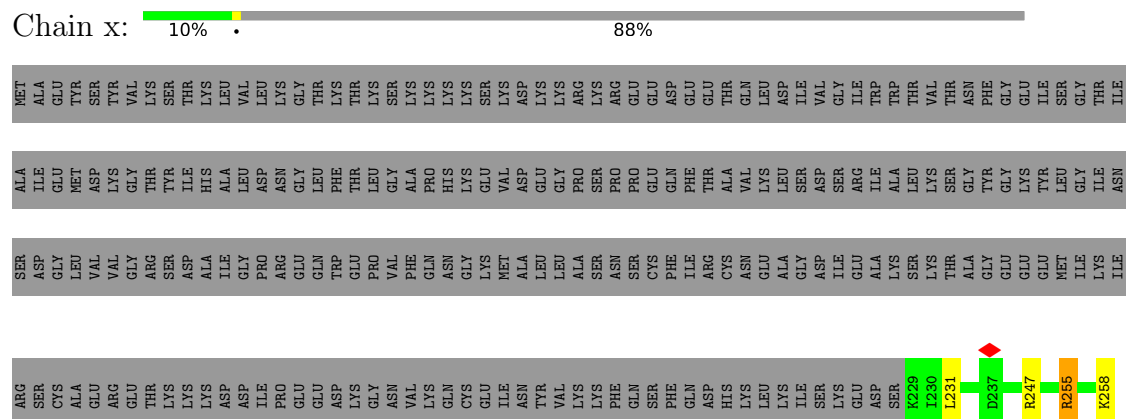


- Molecule 23: Pre-mRNA-splicing factor CWC25 homolog



- Molecule 24: Splicing factor YJU2

- Molecule 25: Protein FRG1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	411539	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 ($e^-/\text{\AA}^2$)	120	Depositor
Minimum defocus (nm)	-1	Depositor
Maximum defocus (nm)	-3	Depositor
Magnification	132000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.336	Depositor
Minimum map value	-0.185	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	466.39996, 466.39996, 466.39996	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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, 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	2	0.48	1/642 (0.2%)	0.58	0/998
2	5	0.39	0/1725	0.42	0/2681
3	6	0.42	0/1892	0.40	0/2947
4	9	0.14	0/113	0.44	0/148
5	A	0.48	0/14669	0.65	6/19894 (0.0%)
6	B	0.39	0/7112	0.63	1/9681 (0.0%)
7	C	0.44	1/1738 (0.1%)	0.69	0/2353
8	D	0.58	1/2547 (0.0%)	0.72	0/3471
9	E	0.35	0/650	0.63	0/886
10	F	0.41	1/2282 (0.0%)	0.67	1/3109 (0.0%)
11	L	0.40	0/1641	0.66	0/2208
12	O	0.37	0/2160	0.65	3/2920 (0.1%)
13	P	0.50	1/1613 (0.1%)	0.68	0/2174
14	Q	0.67	3/1187 (0.3%)	1.00	14/1591 (0.9%)
15	R	0.45	0/690	0.72	1/922 (0.1%)
16	S	0.49	0/233	0.68	0/312
17	T	0.53	3/1704 (0.2%)	0.85	4/2291 (0.2%)
18	V	0.26	0/1105	0.55	0/1511
19	Y	0.34	0/975	0.45	0/1514
19	Z	0.46	0/307	0.44	0/476
20	p	0.40	1/2424 (0.0%)	0.73	2/3295 (0.1%)
21	r	0.29	0/262	0.53	0/356
22	s	0.32	0/158	0.54	0/209
23	t	0.53	0/424	0.76	1/570 (0.2%)
24	u	0.69	4/1312 (0.3%)	0.97	9/1764 (0.5%)
25	x	0.30	0/240	0.60	1/317 (0.3%)
All	All	0.46	16/49805 (0.0%)	0.66	43/68598 (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
5	A	0	2
6	B	0	1
20	p	0	3
24	u	0	1
All	All	0	7

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	535	THR	CB-OG1	-11.46	1.25	1.43
24	u	136	VAL	CB-CG1	-9.78	1.20	1.52
7	C	197	ILE	CG1-CD1	-7.88	1.21	1.51
24	u	140	ARG	CZ-NH2	-6.69	1.24	1.33
24	u	136	VAL	CB-CG2	-6.23	1.31	1.52
14	Q	102	CYS	CA-C	6.05	1.60	1.53
14	Q	137	CYS	CB-SG	-5.98	1.61	1.81
8	D	478	LEU	CG-CD2	-5.65	1.33	1.52
14	Q	102	CYS	N-CA	-5.52	1.39	1.46
10	F	129	THR	CB-CG2	-5.50	1.34	1.52
1	2	38	A	C1'-N9	-5.45	1.39	1.48
13	P	30	GLU	CD-OE1	-5.45	1.15	1.25
24	u	46	CYS	CB-SG	5.41	1.99	1.81
17	T	535	THR	N-CA	-5.32	1.40	1.46
17	T	538	ARG	NE-CZ	-5.25	1.27	1.33
20	p	300	MET	SD-CE	-5.12	1.66	1.79

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	538	ARG	NE-CZ-NH2	-16.59	104.27	119.20
5	A	506	LEU	CB-CG-CD1	-14.05	68.54	110.70
17	T	535	THR	CA-CB-OG1	-13.02	90.07	109.60
24	u	136	VAL	CG1-CB-CG2	-12.51	83.29	110.80
14	Q	142	CYS	CA-CB-SG	-11.82	87.22	114.40
14	Q	101	CYS	CA-C-N	-11.14	102.68	122.84
14	Q	101	CYS	C-N-CA	-11.14	102.68	122.84
24	u	83	CYS	N-CA-C	-10.86	92.40	109.23
14	Q	102	CYS	N-CA-C	-9.77	94.64	107.73
17	T	538	ARG	NE-CZ-NH1	8.99	130.49	121.50
24	u	140	ARG	NE-CZ-NH2	-8.94	111.16	119.20
14	Q	139	CYS	CA-CB-SG	-8.30	95.31	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	u	80	CYS	CA-CB-SG	8.29	133.46	114.40
24	u	83	CYS	O-C-N	-8.10	113.88	123.27
6	B	465	MET	CG-SD-CE	-7.85	83.63	100.90
17	T	535	THR	N-CA-CB	-7.47	100.18	110.42
14	Q	101	CYS	CA-CB-SG	-7.01	98.27	114.40
24	u	46	CYS	CA-CB-SG	6.95	130.38	114.40
14	Q	117	CYS	CA-CB-SG	-6.76	98.86	114.40
12	O	363	ARG	CA-CB-CG	6.67	127.43	114.10
14	Q	101	CYS	O-C-N	6.42	129.50	122.11
20	p	426	MET	CG-SD-CE	6.33	114.83	100.90
14	Q	102	CYS	O-C-N	-6.28	115.47	122.75
14	Q	141	GLY	CA-C-N	6.24	133.22	121.81
14	Q	141	GLY	C-N-CA	6.24	133.22	121.81
14	Q	137	CYS	CA-CB-SG	-6.00	100.61	114.40
5	A	501	TYR	CA-C-N	-5.78	113.06	122.65
5	A	501	TYR	C-N-CA	-5.78	113.06	122.65
12	O	375	ASP	CA-C-N	5.76	128.65	120.53
12	O	375	ASP	C-N-CA	5.76	128.65	120.53
5	A	506	LEU	CB-CG-CD2	5.66	127.69	110.70
5	A	178	TYR	CA-CB-CG	5.63	124.04	113.90
23	t	38	GLU	CB-CG-CD	5.55	122.04	112.60
10	F	88	ARG	CA-CB-CG	5.49	125.09	114.10
14	Q	142	CYS	CB-CA-C	5.46	121.24	111.03
20	p	214	MET	CG-SD-CE	5.46	112.91	100.90
15	R	35	LEU	CD1-CG-CD2	-5.46	98.80	110.80
24	u	82	ARG	CA-C-N	-5.45	113.30	122.29
24	u	82	ARG	C-N-CA	-5.45	113.30	122.29
25	x	255	ARG	N-CA-C	5.39	117.23	111.36
24	u	140	ARG	NE-CZ-NH1	5.18	126.68	121.50
14	Q	105	CYS	CA-CB-SG	5.11	126.14	114.40
5	A	213	LEU	CA-CB-CG	5.07	134.04	116.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	1649	LYS	Peptide
5	A	380	LEU	Peptide
6	B	366	GLN	Peptide
20	p	227	CYS	Peptide
20	p	352	GLN	Peptide
20	p	431	PHE	Peptide

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Mol	Chain	Res	Type	Group
24	u	132	ASN	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	575	0	288	8	0
2	5	1548	0	785	3	0
3	6	1690	0	855	16	0
4	9	112	0	109	3	0
5	A	14270	0	14118	213	0
6	B	6953	0	6837	114	0
7	C	1703	0	1692	29	0
8	D	2481	0	2431	54	0
9	E	629	0	572	15	0
10	F	2230	0	2087	55	0
11	L	1611	0	1588	17	0
12	O	2108	0	1963	26	0
13	P	1577	0	1543	32	0
14	Q	1162	0	1163	14	0
15	R	681	0	635	9	0
16	S	230	0	238	3	0
17	T	1669	0	1662	20	0
18	V	1081	0	929	20	0
19	Y	873	0	440	10	0
19	Z	276	0	143	2	0
20	p	2372	0	2209	54	0
21	r	259	0	213	4	0
22	s	158	0	162	2	0
23	t	418	0	379	5	0
24	u	1286	0	1274	27	0
25	x	239	0	252	6	0
26	6	5	0	0	0	0
27	A	36	0	6	5	0
28	B	32	0	12	0	0
29	P	3	0	0	0	0
29	Q	3	0	0	0	0
29	u	1	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	48271	0	44585	669	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 7.

All (669) 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)
24:u:83:CYS:SG	29:u:1001:ZN:ZN	1.50	0.98
24:u:83:CYS:HG	29:u:1001:ZN:ZN	0.91	0.81
5:A:75:ASP:HA	5:A:502:ASN:HD22	1.45	0.80
13:P:96:VAL:HG21	13:P:213:LEU:HD23	1.65	0.79
5:A:591:MET:HG3	5:A:598:LEU:HD21	1.64	0.78
5:A:993:LEU:O	5:A:997:LEU:HB2	1.83	0.77
6:B:465:MET:HE1	6:B:475:MET:HG3	1.67	0.76
18:V:53:PHE:HB3	18:V:56:ILE:HD11	1.67	0.75
10:F:264:VAL:HA	10:F:272:ARG:HH22	1.51	0.74
5:A:902:TYR:HE2	5:A:1246:GLN:HB3	1.53	0.73
7:C:197:ILE:HD11	13:P:20:PHE:CE1	2.24	0.72
10:F:265:ARG:O	10:F:272:ARG:NH1	2.22	0.72
10:F:81:LEU:HD12	10:F:93:TRP:HB2	1.73	0.71
24:u:39:PHE:HB2	24:u:41:MET:HE2	1.71	0.71
5:A:623:LYS:NZ	5:A:623:LYS:HB3	2.05	0.71
20:p:396:ARG:NH2	20:p:440:THR:OG1	2.23	0.71
12:O:360:ASP:HA	12:O:363:ARG:HH12	1.54	0.70
5:A:761:ILE:HD12	5:A:775:ASN:HD22	1.57	0.70
11:L:53:TRP:HB3	11:L:54:LEU:HD12	1.73	0.69
7:C:113:TYR:OH	8:D:402:ASP:O	2.11	0.69
6:B:129:ILE:HG22	6:B:199:LEU:HB3	1.75	0.69
25:x:231:LEU:HD23	25:x:247:ARG:HH21	1.59	0.68
5:A:974:ASN:HB2	5:A:1178:TYR:HB3	1.76	0.68
6:B:860:ASP:HA	6:B:871:ILE:HG22	1.74	0.67
8:D:260:TYR:HB3	8:D:274:ASP:HA	1.76	0.67
7:C:197:ILE:HD11	13:P:20:PHE:HE1	1.60	0.67
6:B:137:HIS:HA	6:B:238:ASN:HB3	1.77	0.67
5:A:1214:TRP:NE1	5:A:1276:GLU:OE2	2.28	0.67
20:p:196:ARG:HH21	20:p:221:PHE:HE2	1.43	0.67
5:A:142:SER:HA	5:A:242:ALA:HB2	1.77	0.66
6:B:130:ARG:HH21	6:B:435:VAL:HG13	1.61	0.66
10:F:135:VAL:HB	10:F:145:LYS:HB2	1.77	0.66
6:B:171:LEU:HB2	6:B:174:GLU:HG3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:36:MET:HG2	13:P:57:TRP:HB3	1.78	0.66
5:A:231:THR:H	5:A:234:MET:HE3	1.61	0.66
5:A:30:LEU:HD11	10:F:214:ASP:HA	1.78	0.66
8:D:257:ARG:NH2	8:D:301:ASP:OD2	2.29	0.65
6:B:732:ILE:HG12	6:B:746:VAL:HG12	1.79	0.65
5:A:996:LEU:HD21	5:A:1047:VAL:HG21	1.78	0.65
2:5:20:G:H1'	5:A:465:LYS:HD3	1.80	0.64
6:B:148:CYS:SG	6:B:417:ARG:NH2	2.69	0.64
9:E:111:LEU:HD23	13:P:22:ILE:HD13	1.79	0.64
13:P:162:PRO:O	13:P:182:ARG:NH2	2.30	0.64
8:D:249:VAL:HA	8:D:265:GLY:HA2	1.80	0.64
5:A:1110:ILE:HD11	5:A:1149:LEU:HD13	1.80	0.64
6:B:282:VAL:HA	6:B:285:VAL:HG12	1.80	0.64
6:B:112:THR:OG1	6:B:153:THR:O	2.16	0.63
5:A:1321:GLU:OE2	5:A:1471:ARG:NH1	2.32	0.63
5:A:1660:TYR:OH	5:A:1717:ASN:O	2.15	0.63
6:B:404:THR:OG1	6:B:407:GLU:OE1	2.17	0.63
10:F:208:ILE:HB	10:F:220:TRP:HB2	1.81	0.62
18:V:119:THR:HG22	18:V:122:LEU:HD13	1.80	0.62
5:A:709:ILE:HD11	5:A:735:ILE:HD12	1.81	0.62
6:B:220:ARG:HE	6:B:580:LEU:HD23	1.64	0.62
10:F:208:ILE:HG12	10:F:222:LEU:HD11	1.81	0.62
6:B:69:ALA:HA	8:D:456:PRO:HG3	1.81	0.62
5:A:1424:GLN:HB2	5:A:1427:ARG:HB3	1.82	0.61
8:D:196:LEU:HD11	8:D:487:LYS:HD3	1.82	0.61
9:E:101:THR:OG1	13:P:89:GLU:OE2	2.15	0.61
5:A:587:GLN:NE2	25:x:255:ARG:NH2	2.48	0.61
5:A:1248:LEU:HD11	5:A:1294:LYS:HB3	1.82	0.61
20:p:302:CYS:HB3	20:p:338:CYS:SG	2.41	0.60
5:A:623:LYS:HB3	5:A:623:LYS:HZ3	1.67	0.60
13:P:66:LYS:NZ	19:Y:76:A:OP1	2.34	0.60
20:p:213:GLY:C	20:p:214:MET:HE2	2.27	0.60
5:A:783:TYR:HD2	5:A:784:LEU:HD12	1.67	0.60
7:C:195:ARG:NH1	13:P:29:GLY:O	2.35	0.60
9:E:124:MET:HG2	10:F:285:GLU:HA	1.84	0.60
19:Z:57:C:H3'	19:Z:58:G:H5''	1.83	0.60
5:A:1312:PRO:HB2	5:A:1314:VAL:HG12	1.82	0.59
10:F:264:VAL:HA	10:F:272:ARG:NH2	2.17	0.59
14:Q:14:GLY:HA2	14:Q:17:LEU:HD13	1.83	0.59
24:u:46:CYS:SG	24:u:83:CYS:HB3	2.42	0.59
24:u:74:PHE:H	24:u:91:THR:HG22	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:101:ILE:O	7:C:104:GLN:NE2	2.36	0.59
5:A:1014:ASN:ND2	5:A:1026:ASN:O	2.30	0.59
5:A:790:ARG:NH1	5:A:986:GLU:O	2.35	0.59
5:A:1125:ILE:HA	5:A:1147:VAL:HG11	1.84	0.59
8:D:306:CYS:HB2	8:D:333:VAL:HG13	1.85	0.59
5:A:217:ARG:HE	5:A:222:GLY:HA2	1.68	0.59
5:A:753:THR:O	5:A:757:ASN:ND2	2.35	0.58
11:L:19:LEU:HD22	11:L:54:LEU:HD22	1.83	0.58
11:L:218:LYS:NZ	12:O:270:ASP:OD2	2.37	0.58
20:p:209:TRP:CZ3	20:p:220:ALA:HA	2.38	0.58
12:O:296:ARG:HH22	12:O:325:ASN:HD22	1.52	0.58
10:F:197:LEU:HD22	10:F:288:LEU:HD11	1.85	0.58
15:R:30:TYR:CZ	15:R:35:LEU:HD23	2.39	0.58
20:p:490:THR:HG23	20:p:492:ASN:H	1.67	0.58
10:F:340:PRO:HB2	10:F:356:ILE:HB	1.84	0.58
4:9:102:ALA:H	4:9:107:TYR:HD2	1.52	0.58
5:A:235:MET:HB3	5:A:404:LEU:HD21	1.86	0.58
6:B:207:GLY:O	6:B:238:ASN:ND2	2.35	0.58
20:p:197:LEU:HB3	20:p:209:TRP:HB2	1.85	0.58
10:F:69:VAL:HA	10:F:85:GLY:HA3	1.86	0.57
14:Q:79:ILE:HG22	14:Q:84:ALA:HB3	1.85	0.57
8:D:307:SER:OG	8:D:309:ASP:OD1	2.21	0.57
6:B:224:GLY:HA3	6:B:438:ILE:HD12	1.86	0.57
6:B:846:VAL:HG13	6:B:887:LEU:HD11	1.87	0.57
7:C:126:ASN:HA	8:D:442:ARG:HD2	1.85	0.57
10:F:124:LEU:HB2	10:F:136:TRP:HB2	1.87	0.57
12:O:300:ASP:HA	12:O:303:ILE:HG12	1.84	0.57
20:p:346:LEU:HD12	20:p:358:ILE:HG22	1.86	0.57
5:A:850:TYR:HE2	5:A:864:LEU:HD21	1.70	0.57
7:C:78:ARG:HD3	18:V:95:ALA:HB3	1.87	0.57
6:B:449:ILE:HG13	6:B:465:MET:HB3	1.86	0.57
13:P:68:THR:HG23	13:P:82:GLN:HB3	1.87	0.57
5:A:909:TYR:HB2	5:A:1033:GLY:HA3	1.87	0.56
6:B:476:CYS:HB2	6:B:565:ILE:HB	1.86	0.56
1:2:24:A:H5"	5:A:781:ARG:HH21	1.70	0.56
5:A:964:ASP:O	5:A:1100:ARG:NH2	2.38	0.56
5:A:94:TYR:CD1	7:C:207:MET:HE1	2.40	0.56
5:A:200:ASP:OD1	5:A:240:ARG:NH1	2.35	0.56
5:A:1124:ASN:ND2	5:A:1148:ASN:OD1	2.39	0.56
5:A:1204:TYR:HE2	5:A:1206:GLU:HB3	1.70	0.56
7:C:222:PRO:O	13:P:123:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:240:ARG:NH2	5:A:240:ARG:HB3	2.20	0.56
5:A:891:PHE:O	11:L:83:ARG:NH2	2.34	0.56
5:A:184:ASP:HA	20:p:330:GLY:HA3	1.88	0.56
8:D:478:LEU:HD23	8:D:488:VAL:HG12	1.88	0.56
10:F:127:ALA:HB2	10:F:157:CYS:HB3	1.87	0.56
17:T:533:TYR:CZ	17:T:568:ILE:HG22	2.40	0.56
20:p:242:ASP:HB3	20:p:243:MET:HE2	1.88	0.56
5:A:414:ARG:NH2	6:B:408:LEU:O	2.39	0.56
15:R:214:THR:HG23	15:R:215:LEU:HG	1.88	0.56
6:B:216:THR:HG22	6:B:580:LEU:HD22	1.88	0.55
6:B:255:VAL:HG12	6:B:300:LEU:HD12	1.86	0.55
18:V:59:ASP:HA	18:V:116:LEU:HD22	1.88	0.55
6:B:525:CYS:SG	6:B:526:THR:N	2.80	0.55
13:P:145:ASP:HB3	13:P:147:LEU:HD23	1.89	0.55
10:F:133:VAL:HG21	10:F:169:THR:HG21	1.88	0.55
3:6:27:A:OP1	13:P:175:ARG:NH2	2.40	0.55
3:6:49:G:N7	11:L:33:ARG:NH2	2.55	0.55
10:F:69:VAL:O	10:F:331:ASN:ND2	2.40	0.55
10:F:166:LEU:HA	10:F:180:ASP:HA	1.88	0.55
5:A:988:ILE:HG21	5:A:1030:ILE:HG23	1.88	0.55
12:O:232:GLU:OE1	12:O:267:ARG:NH1	2.39	0.55
20:p:292:HIS:HE1	20:p:295:ILE:HD12	1.72	0.55
24:u:63:VAL:HB	24:u:73:ILE:HG13	1.87	0.55
5:A:586:GLY:HA3	5:A:1549:VAL:HG23	1.89	0.54
7:C:205:ASP:OD1	7:C:208:GLU:HB2	2.07	0.54
18:V:17:GLU:HA	18:V:22:ILE:HA	1.89	0.54
20:p:346:LEU:HD13	20:p:360:ASP:HA	1.89	0.54
6:B:834:VAL:HG21	6:B:875:ILE:HD12	1.88	0.54
5:A:758:ARG:NH2	5:A:900:ASP:OD1	2.33	0.54
5:A:1418:ARG:NH1	5:A:1463:LYS:O	2.40	0.54
5:A:442:LYS:NZ	27:A:3001:IHP:O43	2.39	0.54
14:Q:101:CYS:SG	14:Q:102:CYS:N	2.81	0.54
17:T:566:GLU:HB3	17:T:611:PHE:HB2	1.89	0.54
5:A:1217:GLN:HA	5:A:1224:ARG:HA	1.89	0.54
20:p:197:LEU:HD22	20:p:209:TRP:CD1	2.43	0.54
23:t:17:LEU:HA	23:t:20:VAL:HG12	1.90	0.54
5:A:1271:MET:HE1	5:A:1278:VAL:HG21	1.90	0.54
11:L:214:ILE:HG12	12:O:260:ARG:HG2	1.90	0.54
24:u:136:VAL:O	24:u:140:ARG:HG3	2.07	0.54
5:A:270:ASN:O	5:A:270:ASN:ND2	2.41	0.54
5:A:1624:SER:HB2	5:A:1693:SER:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:228:ARG:NH2	12:O:252:GLU:OE1	2.36	0.54
13:P:196:GLN:NE2	19:Y:76:A:N3	2.56	0.54
20:p:197:LEU:HD22	20:p:209:TRP:HD1	1.73	0.54
8:D:264:CYS:HB2	8:D:294:LEU:HD13	1.89	0.53
20:p:480:HIS:HD2	20:p:482:LYS:H	1.56	0.53
20:p:273:ILE:HD11	20:p:279:THR:HB	1.90	0.53
5:A:54:VAL:HG23	5:A:55:ASP:H	1.73	0.53
6:B:366:GLN:HB3	6:B:371:GLU:HB3	1.90	0.53
9:E:97:ASN:ND2	18:V:151:ASP:OD2	2.41	0.53
3:6:14:C:H2'	3:6:15:A:H8	1.74	0.53
12:O:337:MET:HE2	12:O:346:TRP:CD2	2.43	0.53
12:O:343:GLU:OE2	12:O:347:HIS:NE2	2.41	0.53
5:A:171:ASP:HB2	5:A:519:ASP:HB3	1.90	0.53
10:F:348:ASP:OD2	10:F:350:ARG:NH1	2.41	0.53
11:L:220:PRO:HG3	12:O:262:ARG:HD2	1.90	0.53
19:Y:152:C:O3'	22:s:3:ARG:NH1	2.42	0.53
6:B:523:GLN:HB3	6:B:558:PRO:HG3	1.90	0.53
18:V:148:ASN:ND2	18:V:152:ARG:O	2.42	0.53
6:B:215:VAL:HG11	6:B:242:LEU:HD22	1.90	0.53
7:C:142:GLU:HB3	7:C:146:LYS:HZ1	1.74	0.53
5:A:177:ASP:OD1	5:A:177:ASP:N	2.42	0.52
5:A:227:ARG:NH1	5:A:227:ARG:HB2	2.24	0.52
6:B:832:TYR:HD2	6:B:899:SER:HB3	1.73	0.52
15:R:57:ARG:NH2	15:R:62:GLU:OE1	2.42	0.52
5:A:86:ARG:HH22	7:C:211:ARG:HA	1.73	0.52
5:A:100:LEU:HD13	5:A:641:MET:HB2	1.92	0.52
5:A:1127:GLY:O	5:A:1151:ARG:NH2	2.39	0.52
5:A:1639:VAL:HG12	5:A:1719:PHE:HB3	1.90	0.52
13:P:46:LYS:HD2	19:Y:74:G:H21	1.74	0.52
17:T:524:SER:O	17:T:528:ILE:HG12	2.10	0.52
13:P:22:ILE:HG13	13:P:72:GLN:HE22	1.73	0.52
5:A:975:VAL:HB	5:A:1099:PHE:HB2	1.90	0.52
7:C:134:ARG:NH2	8:D:381:HIS:O	2.40	0.52
20:p:425:PRO:C	20:p:426:MET:HE2	2.35	0.52
23:t:35:LYS:O	23:t:38:GLU:HG3	2.09	0.52
1:2:18:U:H3'	5:A:707:ARG:HH22	1.73	0.52
6:B:854:ARG:NH1	6:B:879:ASP:OD2	2.43	0.52
6:B:876:PRO:HG2	6:B:879:ASP:HB2	1.91	0.52
13:P:92:LEU:HA	19:Y:78:A:H61	1.75	0.52
5:A:443:VAL:HG21	5:A:614:TYR:CD1	2.45	0.52
15:R:213:ASP:OD2	15:R:216:ARG:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:5:ILE:HD12	16:S:19:VAL:HG11	1.91	0.52
21:r:379:THR:O	21:r:383:LEU:HG	2.10	0.52
1:2:24:A:OP1	5:A:781:ARG:NE	2.41	0.52
5:A:298:ASP:OD2	5:A:301:LYS:HE2	2.09	0.52
6:B:260:ILE:HD12	6:B:263:LEU:HD21	1.90	0.52
5:A:143:GLN:NE2	5:A:207:PHE:O	2.39	0.52
5:A:617:ASN:HA	5:A:621:VAL:HG23	1.92	0.52
1:2:29:A:H2'	1:2:30:A:C8	2.44	0.51
4:9:104:ARG:O	4:9:104:ARG:NH1	2.44	0.51
6:B:134:LEU:HB2	6:B:204:ASP:HA	1.92	0.51
6:B:316:ILE:HG22	6:B:420:CYS:HB3	1.92	0.51
10:F:265:ARG:H	10:F:272:ARG:HH12	1.59	0.51
20:p:472:ALA:O	20:p:490:THR:OG1	2.28	0.51
8:D:272:CYS:HB3	8:D:282:ARG:HB2	1.91	0.51
9:E:92:GLU:HG2	18:V:72:ARG:HG2	1.92	0.51
10:F:63:SER:HB2	10:F:350:ARG:HB3	1.90	0.51
10:F:248:SER:O	10:F:264:VAL:N	2.44	0.51
5:A:1382:SER:HA	5:A:1415:GLY:HA2	1.93	0.51
6:B:779:LEU:O	6:B:938:ARG:NH1	2.42	0.51
5:A:1545:ALA:O	25:x:255:ARG:NE	2.44	0.51
9:E:108:ARG:NH2	13:P:131:THR:O	2.44	0.51
13:P:146:MET:HE1	13:P:150:LEU:HD22	1.92	0.51
6:B:501:ILE:HG23	6:B:530:LEU:HD21	1.92	0.51
11:L:154:GLU:HG2	24:u:49:TYR:CE2	2.46	0.51
8:D:358:ASP:HB3	8:D:365:ARG:NH1	2.25	0.51
1:2:22:U:H4'	5:A:678:GLU:OE2	2.11	0.51
27:A:3001:IHP:O35	25:x:255:ARG:NH1	2.44	0.51
20:p:187:ALA:C	20:p:188:LEU:HD12	2.36	0.51
6:B:183:SER:H	6:B:214:GLU:HG2	1.76	0.50
11:L:39:HIS:NE2	11:L:154:GLU:OE2	2.43	0.50
3:6:20:A:O2'	14:Q:120:ARG:NH1	2.44	0.50
5:A:898:PHE:HD2	5:A:905:LEU:HB3	1.76	0.50
17:T:463:ILE:HD11	17:T:493:ILE:HG22	1.93	0.50
20:p:281:GLY:O	20:p:309:ARG:NH1	2.45	0.50
6:B:564:THR:HG21	6:B:576:ILE:HA	1.93	0.50
5:A:162:LYS:NZ	5:A:1690:ASP:OD2	2.43	0.50
5:A:405:LEU:O	6:B:413:ARG:NH2	2.45	0.50
8:D:314:ILE:HD12	8:D:324:HIS:HB2	1.92	0.50
20:p:180:HIS:HB2	20:p:207:LYS:HG3	1.92	0.50
13:P:182:ARG:HG2	13:P:184:GLU:HG3	1.94	0.50
10:F:231:MET:HE2	10:F:272:ARG:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:338:GLU:OE1	6:B:342:ARG:NH1	2.45	0.50
14:Q:105:CYS:HB3	14:Q:117:CYS:HB2	1.94	0.50
8:D:497:GLU:OE1	8:D:497:GLU:N	2.44	0.50
5:A:318:TYR:O	6:B:645:ARG:NH1	2.44	0.49
12:O:409:GLU:O	12:O:416:TYR:OH	2.27	0.49
5:A:511:LYS:HB2	5:A:513:LEU:HD23	1.94	0.49
5:A:956:CYS:HB3	5:A:1216:LEU:HD13	1.94	0.49
6:B:200:PHE:HB3	6:B:202:ILE:HG13	1.93	0.49
7:C:177:ILE:HD12	7:C:199:MET:HE3	1.93	0.49
24:u:58:ALA:HB2	24:u:78:ILE:HG22	1.94	0.49
5:A:1257:THR:HA	5:A:1260:VAL:HG12	1.94	0.49
15:R:213:ASP:OD1	15:R:214:THR:N	2.45	0.49
5:A:657:ALA:O	5:A:661:GLU:HB2	2.12	0.49
6:B:389:ASP:OD1	6:B:389:ASP:N	2.41	0.49
6:B:664:GLU:HG2	6:B:779:LEU:HB2	1.94	0.49
10:F:187:ILE:HG22	10:F:188:GLN:HG2	1.94	0.49
5:A:758:ARG:HD3	5:A:779:LEU:HD11	1.94	0.49
6:B:664:GLU:HB3	6:B:779:LEU:HD12	1.95	0.49
6:B:932:GLU:OE1	6:B:936:LYS:HD2	2.12	0.49
8:D:291:VAL:HA	8:D:307:SER:HA	1.93	0.49
10:F:75:HIS:CE1	10:F:77:ASN:HB2	2.48	0.49
5:A:681:PHE:HE2	5:A:746:LYS:HG3	1.78	0.49
17:T:603:LEU:HD12	17:T:612:PHE:HE2	1.77	0.49
5:A:65:HIS:HD2	14:Q:46:LEU:HD22	1.77	0.49
5:A:623:LYS:NZ	5:A:623:LYS:CB	2.73	0.49
6:B:277:LYS:NZ	6:B:864:PRO:O	2.42	0.49
10:F:105:LEU:HB3	10:F:136:TRP:CZ3	2.48	0.49
20:p:446:ARG:HH12	20:p:472:ALA:HB2	1.77	0.49
6:B:828:MET:HB3	6:B:906:ILE:HD13	1.95	0.48
11:L:215:PRO:O	12:O:267:ARG:NH2	2.46	0.48
12:O:227:LYS:HD2	12:O:251:TRP:CE2	2.47	0.48
5:A:680:HIS:NE2	5:A:684:GLU:OE2	2.45	0.48
5:A:717:TRP:CD2	5:A:746:LYS:HD3	2.48	0.48
9:E:90:ALA:O	18:V:72:ARG:NH1	2.46	0.48
10:F:71:CYS:HB2	10:F:84:ALA:HB3	1.95	0.48
10:F:114:GLU:OE2	10:F:116:HIS:NE2	2.46	0.48
7:C:173:PRO:HG2	7:C:201:GLU:HG3	1.95	0.48
24:u:48:GLU:OE2	24:u:80:CYS:SG	2.72	0.48
5:A:1289:VAL:HG13	5:A:1357:MET:HG3	1.94	0.48
5:A:1667:ARG:NH2	5:A:1673:SER:O	2.40	0.48
3:6:17:C:H2'	3:6:18:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:797:ALA:O	6:B:803:ARG:NH2	2.47	0.48
20:p:188:LEU:HD23	20:p:197:LEU:HD21	1.96	0.48
3:6:78:A:H4'	12:O:237:LYS:HE2	1.95	0.48
5:A:1254:THR:HG21	5:A:1258:LYS:HE2	1.95	0.48
13:P:207:ASP:OD1	13:P:209:VAL:N	2.47	0.48
17:T:596:LEU:O	17:T:600:ASN:HB2	2.12	0.48
5:A:979:SER:OG	5:A:980:ARG:N	2.46	0.48
5:A:1237:MET:HE3	5:A:1284:LEU:HB2	1.96	0.48
10:F:113:MET:HE3	10:F:129:THR:HG21	1.96	0.48
11:L:231:ASN:HD22	12:O:258:ILE:HB	1.79	0.48
20:p:288:THR:HG21	20:p:337:THR:HG23	1.96	0.48
3:6:29:A:N6	19:Y:73:U:O3'	2.47	0.47
5:A:946:GLU:HB2	5:A:950:LEU:HD22	1.96	0.47
5:A:1553:VAL:HG21	24:u:7:LEU:HD13	1.95	0.47
6:B:674:CYS:HG	6:B:818:SER:HG	1.59	0.47
10:F:68:GLU:HB2	10:F:347:SER:HA	1.96	0.47
5:A:1048:MET:HA	5:A:1048:MET:HE2	1.96	0.47
5:A:1488:THR:OG1	5:A:1537:TRP:O	2.26	0.47
20:p:292:HIS:CE1	20:p:295:ILE:HD12	2.47	0.47
5:A:90:GLY:HA3	7:C:209:PRO:HD3	1.95	0.47
5:A:138:PRO:HG2	5:A:235:MET:HE1	1.95	0.47
6:B:365:SER:OG	6:B:366:GLN:N	2.42	0.47
9:E:128:GLN:HE22	9:E:139:LEU:HD23	1.79	0.47
10:F:210:SER:O	10:F:218:LYS:N	2.44	0.47
3:6:52:U:OP1	24:u:55:LYS:NZ	2.43	0.47
6:B:271:PRO:HB2	6:B:370:VAL:HG13	1.97	0.47
12:O:262:ARG:NH2	12:O:286:GLU:OE1	2.47	0.47
20:p:183:LYS:HB2	20:p:203:ASP:HB3	1.96	0.47
2:5:36:C:O2	16:S:11:ARG:NH1	2.43	0.47
5:A:1260:VAL:HG11	5:A:1325:LEU:HB3	1.96	0.47
11:L:49:ARG:HG3	11:L:54:LEU:HD13	1.97	0.47
5:A:86:ARG:NH2	7:C:211:ARG:HA	2.29	0.47
5:A:231:THR:OG1	6:B:389:ASP:OD2	2.31	0.47
5:A:377:GLU:HA	5:A:381:PRO:HD3	1.97	0.47
5:A:1204:TYR:CE2	5:A:1206:GLU:HB3	2.49	0.47
6:B:220:ARG:HH11	6:B:452:THR:HG22	1.79	0.47
6:B:235:VAL:HG21	6:B:284:GLU:HG2	1.97	0.47
8:D:351:ASP:HB3	8:D:353:THR:HG22	1.96	0.47
8:D:427:LEU:HB3	8:D:439:TRP:HB2	1.96	0.47
12:O:373:HIS:HB2	12:O:378:ASN:HD21	1.78	0.47
5:A:167:PRO:HA	5:A:168:PRO:HD3	1.81	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1405:LEU:HD11	5:A:1412:TRP:HD1	1.80	0.47
10:F:343:ILE:HG22	10:F:353:MET:HA	1.97	0.47
24:u:43:CYS:SG	24:u:83:CYS:SG	3.13	0.47
6:B:142:LYS:NZ	6:B:205:THR:O	2.43	0.47
5:A:758:ARG:HD2	5:A:758:ARG:HA	1.76	0.47
5:A:1581:LEU:HD22	5:A:1746:ARG:HH11	1.80	0.47
6:B:174:GLU:HG2	6:B:181:ILE:HD12	1.97	0.47
12:O:242:ILE:HD11	12:O:278:LEU:HD22	1.97	0.47
2:5:66:A:H2'	2:5:67:A:H8	1.80	0.46
5:A:962:LEU:HB2	5:A:965:VAL:HB	1.97	0.46
5:A:1350:ILE:HD11	17:T:470:GLU:HB2	1.96	0.46
6:B:302:PRO:HB2	6:B:320:LEU:HD11	1.97	0.46
5:A:710:LEU:HA	5:A:710:LEU:HD23	1.63	0.46
5:A:776:LEU:HD11	5:A:900:ASP:HB2	1.97	0.46
5:A:1701:VAL:HA	5:A:1716:GLY:HA3	1.98	0.46
6:B:696:LEU:O	6:B:700:ILE:HD12	2.14	0.46
10:F:221:ASP:OD2	10:F:228:THR:OG1	2.33	0.46
24:u:100:MET:HE3	24:u:101:GLU:N	2.30	0.46
5:A:395:THR:OG1	5:A:396:ASP:N	2.39	0.46
9:E:128:GLN:HE22	9:E:139:LEU:CD2	2.28	0.46
21:r:382:MET:HE3	21:r:388:VAL:HG21	1.96	0.46
5:A:1381:ASP:OD2	5:A:1414:ARG:NH1	2.42	0.46
5:A:1545:ALA:O	25:x:255:ARG:HD2	2.15	0.46
17:T:588:GLN:O	17:T:592:GLU:HG2	2.15	0.46
5:A:516:LEU:HG	5:A:524:LEU:HD11	1.98	0.46
5:A:532:THR:HG21	19:Y:60:U:H3'	1.97	0.46
5:A:863:GLU:HB2	5:A:913:PRO:HB3	1.97	0.46
6:B:166:CYS:HB3	6:B:169:ASP:HB2	1.97	0.46
8:D:246:ILE:HB	8:D:267:ASP:OD2	2.15	0.46
10:F:243:LEU:HD12	10:F:247:GLY:HA2	1.98	0.46
23:t:39:GLU:OE2	23:t:40:LEU:HD23	2.15	0.46
8:D:213:GLU:HA	8:D:254:VAL:HG11	1.98	0.46
8:D:473:SER:OG	8:D:475:SER:OG	2.26	0.46
5:A:570:ASP:HB3	5:A:573:GLN:HG3	1.98	0.46
12:O:299:TRP:O	12:O:302:ALA:N	2.48	0.46
20:p:337:THR:HG21	20:p:383:CYS:HA	1.97	0.46
4:9:112:MET:SD	4:9:112:MET:N	2.88	0.46
5:A:950:LEU:HD23	5:A:954:LYS:HG3	1.98	0.46
8:D:257:ARG:HH21	8:D:301:ASP:CG	2.24	0.46
8:D:455:GLN:OE1	8:D:485:THR:OG1	2.34	0.46
6:B:137:HIS:HB3	6:B:140:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:52:GLU:HA	15:R:55:ARG:NH1	2.31	0.46
18:V:28:TYR:OH	18:V:131:ARG:NE	2.33	0.46
5:A:731:LEU:HB3	7:C:248:PRO:HD2	1.97	0.45
6:B:841:ASP:OD1	6:B:842:CYS:N	2.49	0.45
8:D:436:MET:HE1	8:D:479:THR:HG21	1.98	0.45
9:E:145:ASN:OD1	9:E:146:HIS:N	2.46	0.45
10:F:113:MET:HE3	10:F:129:THR:CG2	2.47	0.45
13:P:191:ASP:OD1	13:P:191:ASP:N	2.46	0.45
17:T:538:ARG:HH21	17:T:538:ARG:HD2	1.28	0.45
20:p:333:VAL:HG11	20:p:353:ASN:HB2	1.98	0.45
5:A:224:THR:HG23	5:A:226:GLN:HG2	1.98	0.45
5:A:946:GLU:HB2	5:A:950:LEU:HB3	1.98	0.45
5:A:1351:THR:HG23	5:A:1352:HIS:ND1	2.31	0.45
6:B:301:SER:HB3	6:B:304:LEU:HD13	1.98	0.45
7:C:142:GLU:HB3	7:C:146:LYS:NZ	2.31	0.45
8:D:309:ASP:OD1	8:D:309:ASP:N	2.48	0.45
24:u:97:ASP:OD1	24:u:98:TYR:N	2.44	0.45
6:B:259:LYS:HB3	6:B:262:ARG:HB2	1.98	0.45
6:B:833:PHE:HB2	6:B:902:HIS:CD2	2.51	0.45
24:u:92:ASP:HB2	24:u:99:THR:HG23	1.97	0.45
9:E:120:ILE:HD13	10:F:284:PHE:HZ	1.81	0.45
18:V:56:ILE:HG23	18:V:62:ILE:HG22	1.98	0.45
6:B:605:ASP:OD1	6:B:608:ARG:NH1	2.50	0.45
17:T:493:ILE:HD11	17:T:525:PHE:HZ	1.82	0.45
17:T:515:CYS:SG	17:T:516:MET:N	2.89	0.45
5:A:1370:ARG:NH1	17:T:467:LEU:O	2.50	0.45
6:B:157:ILE:O	6:B:158:ARG:HD2	2.15	0.45
6:B:436:GLN:HG3	6:B:437:HIS:ND1	2.31	0.45
10:F:264:VAL:CA	10:F:272:ARG:HH22	2.23	0.45
10:F:304:SER:H	10:F:330:ILE:HB	1.82	0.45
20:p:306:ALA:HA	20:p:334:ILE:HA	1.97	0.45
20:p:358:ILE:HB	20:p:368:LYS:HB2	1.97	0.45
23:t:31:GLU:HA	23:t:34:ARG:HG2	1.99	0.45
6:B:733:TRP:CZ3	6:B:763:LYS:HA	2.52	0.45
17:T:476:LEU:HD23	17:T:476:LEU:HA	1.84	0.45
5:A:1533:ARG:NH1	5:A:1752:GLN:OE1	2.44	0.45
8:D:481:GLU:OE1	8:D:487:LYS:NZ	2.33	0.45
10:F:243:LEU:HA	10:F:250:LEU:HA	1.99	0.45
11:L:82:TRP:CZ3	11:L:85:ILE:HD11	2.52	0.45
5:A:701:ILE:O	7:C:242:GLN:NE2	2.50	0.45
5:A:812:THR:HG23	5:A:1055:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:474:LEU:HB3	6:B:567:GLU:HG2	1.98	0.45
7:C:189:ASN:HD21	7:C:195:ARG:HG3	1.82	0.45
8:D:354:ILE:HG13	8:D:375:VAL:HG11	1.98	0.45
5:A:29:LYS:O	5:A:33:LYS:HG3	2.17	0.45
6:B:705:VAL:HG22	6:B:717:PHE:HE2	1.81	0.45
8:D:287:HIS:CD2	8:D:313:ARG:HD2	2.52	0.45
8:D:462:GLU:OE2	8:D:462:GLU:N	2.47	0.45
10:F:111:ALA:N	10:F:129:THR:OG1	2.50	0.45
10:F:210:SER:N	10:F:218:LYS:O	2.48	0.45
13:P:16:GLU:H	13:P:41:TYR:HE1	1.64	0.45
1:2:38:A:H4'	22:s:10:THR:HG22	1.98	0.44
3:6:19:C:O2'	14:Q:95:GLN:O	2.30	0.44
5:A:61:MET:HE1	14:Q:104:ARG:HB3	1.98	0.44
5:A:444:ARG:NH1	19:Z:49:C:OP1	2.51	0.44
5:A:1274:PHE:HB3	5:A:1277:ALA:HB3	2.00	0.44
5:A:1644:LEU:HG	5:A:1715:TYR:HD1	1.82	0.44
5:A:799:PRO:HB2	5:A:801:ILE:HG22	1.98	0.44
5:A:1653:ASP:OD1	5:A:1653:ASP:N	2.50	0.44
6:B:600:LEU:HD11	6:B:627:HIS:HE2	1.82	0.44
8:D:399:LYS:HG2	8:D:400:PHE:H	1.82	0.44
9:E:98:PRO:HG2	18:V:121:TRP:HE1	1.83	0.44
6:B:186:VAL:HG12	6:B:535:ALA:HB2	1.98	0.44
6:B:239:THR:O	6:B:243:ILE:HG12	2.17	0.44
8:D:200:ILE:HG13	8:D:486:ILE:HB	2.00	0.44
10:F:171:SER:OG	10:F:172:ASP:N	2.51	0.44
10:F:244:SER:N	10:F:249:TYR:O	2.50	0.44
18:V:147:THR:HA	18:V:153:PRO:HA	1.99	0.44
5:A:1457:HIS:HB3	5:A:1460:HIS:HB2	1.99	0.44
5:A:1718:TRP:HZ3	5:A:1726:ILE:HD12	1.83	0.44
6:B:193:THR:HB	6:B:325:LYS:HD2	1.99	0.44
24:u:39:PHE:CE2	24:u:100:MET:HG2	2.52	0.44
6:B:109:LEU:HD23	6:B:537:TYR:CD1	2.52	0.44
17:T:535:THR:OG1	17:T:538:ARG:NH2	2.51	0.44
5:A:732:PRO:HB3	7:C:244:GLU:OE2	2.18	0.44
6:B:829:GLU:OE2	6:B:854:ARG:NH2	2.44	0.44
7:C:119:LEU:HD12	7:C:230:MET:CG	2.47	0.44
8:D:496:THR:HG22	8:D:499:THR:HG22	1.99	0.44
20:p:414:LEU:HG	20:p:415:PHE:H	1.83	0.44
3:6:58:G:O6	3:6:76:A:N6	2.51	0.44
11:L:14:THR:HG21	11:L:152:LEU:HD21	1.98	0.44
20:p:317:LYS:HA	20:p:317:LYS:HD3	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:29:LYS:O	5:A:32:GLU:HG3	2.18	0.44
5:A:450:LEU:HD23	5:A:450:LEU:HA	1.75	0.44
5:A:625:PRO:HB3	25:x:258:LYS:HD2	1.98	0.44
5:A:854:SER:OG	5:A:855:ARG:N	2.49	0.44
5:A:1133:CYS:SG	5:A:1231:ARG:NE	2.91	0.44
6:B:189:VAL:HG12	6:B:199:LEU:HA	2.00	0.44
20:p:282:HIS:CE1	20:p:309:ARG:HD3	2.53	0.44
5:A:531:THR:O	5:A:535:ARG:N	2.51	0.44
5:A:609:LYS:NZ	27:A:3001:IHP:O44	2.50	0.44
5:A:998:ARG:HE	5:A:1003:HIS:HB2	1.82	0.44
5:A:1589:ILE:HD13	5:A:1705:ILE:HD13	2.00	0.44
18:V:28:TYR:HH	18:V:131:ARG:HE	1.60	0.44
3:6:29:A:H62	19:Y:73:U:H1'	1.82	0.43
5:A:66:VAL:HA	5:A:69:ILE:HG22	1.99	0.43
6:B:561:LYS:NZ	6:B:614:TYR:O	2.51	0.43
9:E:104:MET:HE1	13:P:132:ARG:HG3	2.00	0.43
21:r:380:ASN:C	21:r:380:ASN:HD22	2.26	0.43
24:u:101:GLU:HG3	24:u:102:HIS:ND1	2.33	0.43
5:A:231:THR:HG22	5:A:234:MET:HE2	2.00	0.43
5:A:490:VAL:HG21	5:A:565:ARG:HG3	2.00	0.43
5:A:609:LYS:CE	27:A:3001:IHP:O44	2.66	0.43
5:A:975:VAL:HG22	5:A:1177:VAL:HG22	2.00	0.43
5:A:1215:ASN:O	5:A:1224:ARG:NE	2.45	0.43
5:A:1604:LEU:HD23	5:A:1719:PHE:HE2	1.83	0.43
5:A:1647:ASP:OD1	5:A:1647:ASP:N	2.52	0.43
6:B:903:HIS:HE1	6:B:905:GLN:HG3	1.83	0.43
8:D:290:ALA:O	8:D:308:ARG:N	2.48	0.43
8:D:424:ASP:OD1	8:D:425:GLY:N	2.50	0.43
24:u:16:ASP:HB3	24:u:19:LYS:HD3	2.00	0.43
5:A:1142:LEU:O	5:A:1143:MET:HE2	2.18	0.43
24:u:101:GLU:HG3	24:u:102:HIS:CG	2.53	0.43
6:B:745:LEU:HD23	6:B:789:PHE:HB2	2.00	0.43
12:O:291:GLN:OE1	12:O:291:GLN:N	2.51	0.43
20:p:446:ARG:HH22	20:p:472:ALA:HB2	1.84	0.43
24:u:90:LYS:HB2	24:u:90:LYS:HE3	1.66	0.43
5:A:768:ASP:N	5:A:768:ASP:OD1	2.50	0.43
6:B:530:LEU:HG	6:B:552:ILE:HG22	2.00	0.43
9:E:124:MET:HB2	9:E:124:MET:HE2	1.69	0.43
20:p:438:ILE:O	20:p:456:PHE:N	2.46	0.43
5:A:1057:ARG:HD2	5:A:1057:ARG:HA	1.73	0.43
5:A:1729:ALA:O	5:A:1733:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V:12:PRO:HG2	18:V:165:SER:HB3	2.01	0.43
18:V:18:THR:N	18:V:21:GLY:O	2.51	0.43
24:u:38:PRO:HA	24:u:52:LYS:HG3	1.99	0.43
5:A:1106:ALA:O	5:A:1110:ILE:HD12	2.18	0.43
5:A:1528:GLN:HG2	5:A:1533:ARG:HH22	1.84	0.43
6:B:193:THR:OG1	6:B:432:ASP:OD2	2.26	0.43
6:B:833:PHE:HZ	6:B:872:LYS:HD3	1.83	0.43
8:D:214:PRO:HG2	8:D:256:THR:HA	2.01	0.43
8:D:218:TRP:HZ3	8:D:220:VAL:HB	1.83	0.43
13:P:80:VAL:HG21	13:P:94:ILE:HD11	2.01	0.43
3:6:2:U:O2	14:Q:95:GLN:NE2	2.33	0.43
5:A:422:LEU:HD12	5:A:422:LEU:H	1.82	0.43
5:A:1430:LEU:HD11	5:A:1459:ARG:HB3	2.01	0.43
6:B:237:LEU:HD21	6:B:900:VAL:HG21	2.00	0.43
6:B:705:VAL:HG22	6:B:717:PHE:CE2	2.54	0.43
20:p:264:MET:HG2	20:p:313:VAL:HG13	2.01	0.43
3:6:69:A:OP1	5:A:671:THR:OG1	2.37	0.43
5:A:684:GLU:OE1	8:D:308:ARG:NE	2.52	0.43
5:A:689:VAL:HG11	5:A:710:LEU:HD21	2.00	0.43
5:A:842:ALA:HB2	5:A:924:GLN:HG3	2.01	0.43
5:A:1072:LEU:HD22	5:A:1087:LEU:HD22	2.01	0.43
6:B:598:SER:OG	6:B:599:GLU:OE1	2.37	0.43
6:B:737:PRO:HD2	6:B:741:GLY:HA3	2.00	0.43
14:Q:9:LYS:NZ	14:Q:10:ALA:O	2.40	0.43
5:A:163:ARG:HE	5:A:163:ARG:HB3	1.65	0.43
6:B:80:ILE:HB	8:D:200:ILE:HG22	2.01	0.43
6:B:366:GLN:O	6:B:368:SER:N	2.51	0.43
6:B:473:PRO:O	6:B:498:SER:OG	2.31	0.43
8:D:383:ARG:HG3	8:D:383:ARG:HH11	1.83	0.43
13:P:92:LEU:HD22	13:P:213:LEU:HD21	2.01	0.43
23:t:20:VAL:HA	23:t:23:VAL:HG12	2.01	0.43
5:A:850:TYR:CE2	5:A:864:LEU:HD21	2.52	0.42
5:A:1410:ASP:OD1	5:A:1410:ASP:N	2.50	0.42
6:B:168:THR:HG21	6:B:204:ASP:OD1	2.19	0.42
17:T:616:LEU:HA	17:T:618:ARG:HG3	2.00	0.42
6:B:637:LEU:HA	6:B:640:VAL:HG22	2.01	0.42
10:F:217:ILE:HD11	10:F:234:HIS:HD2	1.84	0.42
5:A:912:GLU:CD	5:A:913:PRO:HD2	2.45	0.42
5:A:1749:LYS:HE2	5:A:1749:LYS:HB2	1.86	0.42
6:B:130:ARG:NH2	6:B:435:VAL:O	2.52	0.42
6:B:448:LYS:HA	6:B:448:LYS:HD3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:261:LEU:HD23	8:D:275:LEU:HD11	2.00	0.42
10:F:71:CYS:SG	10:F:114:GLU:HA	2.59	0.42
5:A:159:ARG:HD2	5:A:159:ARG:HA	1.86	0.42
5:A:173:GLU:HB3	20:p:273:ILE:HB	2.01	0.42
5:A:820:ARG:NH1	5:A:1063:GLY:O	2.52	0.42
6:B:192:ASP:OD1	6:B:192:ASP:N	2.51	0.42
7:C:232:SER:HB2	8:D:372:LYS:NZ	2.35	0.42
13:P:30:GLU:OE2	13:P:30:GLU:N	2.53	0.42
13:P:93:PRO:HD3	19:Y:78:A:N6	2.34	0.42
13:P:150:LEU:HD21	13:P:213:LEU:HG	2.02	0.42
16:S:24:SER:O	17:T:513:ARG:NH1	2.52	0.42
20:p:480:HIS:CD2	20:p:483:LEU:H	2.37	0.42
5:A:68:LYS:NZ	14:Q:45:SER:O	2.48	0.42
5:A:1021:ASP:OD1	5:A:1021:ASP:N	2.53	0.42
10:F:224:GLN:HE21	10:F:228:THR:HG21	1.84	0.42
11:L:165:LYS:HD3	11:L:165:LYS:HA	1.85	0.42
13:P:45:CYS:HB2	13:P:71:CYS:HB3	2.02	0.42
20:p:224:LEU:H	20:p:224:LEU:HD23	1.84	0.42
1:2:30:A:H1'	5:A:861:ARG:NH2	2.35	0.42
6:B:93:ILE:HB	8:D:275:LEU:HB3	2.01	0.42
6:B:938:ARG:HG3	6:B:943:LEU:HB2	2.00	0.42
10:F:209:ILE:HG22	10:F:219:VAL:HG22	2.01	0.42
20:p:187:ALA:HA	20:p:476:ARG:HG2	2.01	0.42
21:r:387:VAL:HG13	21:r:388:VAL:HG23	2.01	0.42
5:A:187:PRO:HB2	5:A:564:TYR:CZ	2.54	0.42
5:A:240:ARG:HB3	5:A:240:ARG:HH21	1.85	0.42
5:A:1237:MET:HE1	5:A:1283:GLU:HB2	2.01	0.42
5:A:1310:ARG:NH2	5:A:1563:HIS:O	2.46	0.42
5:A:1545:ALA:N	5:A:1670:ASP:OD2	2.53	0.42
8:D:419:LEU:HD22	8:D:427:LEU:HD21	2.02	0.42
17:T:611:PHE:CE2	17:T:612:PHE:HE1	2.38	0.42
20:p:237:TYR:CZ	20:p:244:ILE:HD11	2.55	0.42
12:O:232:GLU:HA	12:O:235:ILE:HG12	2.02	0.42
20:p:185:VAL:HG23	20:p:493:GLY:HA2	2.02	0.42
20:p:282:HIS:NE2	20:p:301:THR:OG1	2.47	0.42
5:A:590:GLY:HA2	5:A:592:TYR:CE2	2.55	0.42
7:C:119:LEU:HD12	7:C:230:MET:HG3	2.02	0.42
8:D:354:ILE:HD11	8:D:375:VAL:HG21	2.01	0.42
5:A:1673:SER:O	5:A:1673:SER:OG	2.37	0.42
6:B:672:LEU:HB2	6:B:822:MET:HE2	2.02	0.42
7:C:229:VAL:O	8:D:369:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:125:PHE:HE2	10:F:159:PRO:HB3	1.84	0.42
11:L:74:LEU:HD23	11:L:77:LEU:HD23	2.02	0.42
5:A:567:GLY:HA3	20:p:331:LYS:HE3	2.02	0.41
5:A:727:LYS:HD2	5:A:727:LYS:HA	1.94	0.41
5:A:830:LEU:HD11	24:u:151:LEU:HG	2.02	0.41
5:A:1026:ASN:HD22	5:A:1031:ILE:HG23	1.85	0.41
6:B:451:HIS:O	6:B:578:ARG:NH2	2.53	0.41
10:F:88:ARG:HG2	10:F:110:GLY:C	2.45	0.41
10:F:200:THR:HB	10:F:209:ILE:HD11	2.02	0.41
10:F:249:TYR:CE1	10:F:263:ASP:HB3	2.55	0.41
12:O:363:ARG:HB2	12:O:363:ARG:HH11	1.85	0.41
13:P:193:LEU:O	19:Y:77:G:N2	2.53	0.41
18:V:13:ASN:HA	18:V:26:GLU:HA	2.01	0.41
18:V:54:HIS:NE2	18:V:63:GLN:OE1	2.53	0.41
20:p:432:SER:OG	20:p:433:PRO:HD3	2.19	0.41
7:C:198:ARG:HE	7:C:198:ARG:HB2	1.70	0.41
10:F:150:HIS:CE1	10:F:177:LYS:HG3	2.56	0.41
14:Q:42:LYS:HE3	14:Q:42:LYS:HB2	1.89	0.41
20:p:403:LYS:HE2	20:p:405:TRP:CZ2	2.55	0.41
27:A:3001:IHP:P6	27:A:3001:IHP:O45	2.79	0.41
8:D:260:TYR:OH	15:R:41:ILE:HG23	2.20	0.41
10:F:112:VAL:HG12	10:F:128:SER:OG	2.20	0.41
5:A:543:ALA:HB2	5:A:651:TRP:HB3	2.03	0.41
5:A:1322:LEU:HD11	5:A:1481:VAL:HG13	2.02	0.41
6:B:516:LEU:HD13	6:B:575:GLN:HB3	2.01	0.41
6:B:678:THR:O	6:B:680:ASN:N	2.52	0.41
6:B:680:ASN:ND2	6:B:802:HIS:O	2.54	0.41
8:D:334:ALA:HB2	8:D:350:HIS:CE1	2.55	0.41
9:E:98:PRO:HG2	18:V:121:TRP:NE1	2.36	0.41
20:p:432:SER:HB2	20:p:479:TRP:CD2	2.56	0.41
24:u:39:PHE:CE1	24:u:98:TYR:HB2	2.55	0.41
5:A:341:LYS:HE3	5:A:341:LYS:HB3	1.90	0.41
5:A:1624:SER:O	5:A:1624:SER:OG	2.35	0.41
24:u:46:CYS:SG	24:u:48:GLU:HG3	2.61	0.41
3:6:24:A:N3	3:6:26:U:O2'	2.52	0.41
5:A:946:GLU:CB	5:A:950:LEU:HD22	2.50	0.41
6:B:93:ILE:HD11	8:D:240:LEU:CD2	2.50	0.41
15:R:222:LYS:HE3	15:R:222:LYS:HB2	1.86	0.41
3:6:19:C:O2	14:Q:95:GLN:NE2	2.42	0.41
5:A:689:VAL:CG1	5:A:710:LEU:HD21	2.51	0.41
8:D:458:SER:HB2	8:D:462:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:293:ASN:HA	12:O:296:ARG:HD2	2.03	0.41
20:p:300:MET:HE2	20:p:338:CYS:SG	2.61	0.41
3:6:14:C:H2'	3:6:15:A:C8	2.56	0.41
5:A:76:MET:HE1	5:A:84:ASP:HB2	2.03	0.41
5:A:93:LYS:O	5:A:649:GLU:HG2	2.20	0.41
5:A:231:THR:HG23	5:A:233:PRO:HD2	2.03	0.41
5:A:246:LEU:HD23	5:A:246:LEU:HA	1.90	0.41
5:A:936:PHE:HB3	5:A:940:ILE:HD11	2.03	0.41
5:A:1556:ASP:OD1	5:A:1556:ASP:N	2.53	0.41
5:A:1650:ASP:OD2	5:A:1723:LYS:NZ	2.37	0.41
6:B:92:PRO:HB3	8:D:276:GLU:HA	2.03	0.41
6:B:359:LYS:HE3	6:B:359:LYS:HB3	1.95	0.41
6:B:679:PRO:HD3	6:B:811:THR:HG21	2.02	0.41
8:D:263:SER:HB3	8:D:273:TRP:HE1	1.85	0.41
8:D:492:ASP:OD1	8:D:492:ASP:N	2.49	0.41
10:F:88:ARG:HB3	10:F:88:ARG:HH11	1.85	0.41
10:F:299:LYS:HE3	10:F:299:LYS:HB3	1.82	0.41
14:Q:120:ARG:HH21	14:Q:142:CYS:HB3	1.86	0.41
18:V:14:VAL:N	18:V:25:LEU:O	2.40	0.41
20:p:196:ARG:HH11	20:p:258:ARG:HH21	1.67	0.41
5:A:888:GLN:O	5:A:889:ARG:NH1	2.49	0.41
5:A:936:PHE:HA	5:A:937:PRO:HD3	1.86	0.41
5:A:1683:LYS:HD3	5:A:1683:LYS:HA	1.93	0.41
6:B:341:LYS:HB3	6:B:341:LYS:HE2	1.77	0.41
6:B:369:PHE:O	6:B:373:ILE:HB	2.21	0.41
6:B:662:PHE:HB3	6:B:827:LEU:HD22	2.03	0.41
12:O:403:VAL:HG13	12:O:416:TYR:HE1	1.86	0.41
20:p:175:GLU:HA	20:p:498:TYR:HD1	1.86	0.41
20:p:282:HIS:HA	20:p:309:ARG:HH12	1.86	0.41
5:A:1106:ALA:O	5:A:1109:LEU:N	2.54	0.40
6:B:366:GLN:HA	6:B:370:VAL:HB	2.02	0.40
8:D:409:LEU:HD22	8:D:444:GLY:HA2	2.03	0.40
15:R:23:LEU:HD23	15:R:26:LEU:HD21	2.03	0.40
20:p:300:MET:HB2	20:p:300:MET:HE3	1.86	0.40
24:u:136:VAL:HG12	24:u:140:ARG:NH2	2.36	0.40
5:A:638:LEU:HA	5:A:638:LEU:HD23	1.89	0.40
5:A:862:GLU:O	5:A:866:LEU:HD23	2.21	0.40
5:A:1419:ILE:HD13	5:A:1419:ILE:HG21	1.88	0.40
5:A:1604:LEU:HD23	5:A:1719:PHE:CE2	2.56	0.40
6:B:688:ILE:HG22	6:B:790:LYS:HB2	2.03	0.40
7:C:132:LEU:HD23	7:C:132:LEU:HA	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:92:LEU:HG	10:F:103:ALA:HB3	2.03	0.40
11:L:222:LEU:HD13	11:L:222:LEU:HA	1.95	0.40
12:O:317:THR:O	12:O:321:GLU:HG2	2.22	0.40
17:T:465:SER:OG	17:T:466:SER:N	2.54	0.40
20:p:322:VAL:O	20:p:364:THR:OG1	2.34	0.40
5:A:606:LYS:HD2	5:A:1548:TYR:CZ	2.57	0.40
5:A:886:LEU:HD12	24:u:151:LEU:HD12	2.03	0.40
6:B:124:ASP:HA	6:B:545:PRO:HG2	2.02	0.40
6:B:465:MET:HE1	6:B:475:MET:CG	2.44	0.40
12:O:282:TYR:O	12:O:285:MET:HG3	2.22	0.40
17:T:563:SER:HA	17:T:611:PHE:CE2	2.56	0.40
20:p:190:LEU:HD23	20:p:190:LEU:HA	1.92	0.40
5:A:1202:THR:OG1	5:A:1204:TYR:O	2.31	0.40
6:B:719:GLN:HA	6:B:724:TRP:H	1.87	0.40
17:T:574:THR:HG23	17:T:575:THR:H	1.85	0.40
1:2:23:A:H4'	5:A:777:GLY:HA3	2.04	0.40
5:A:95:MET:HE2	5:A:551:LEU:HD21	2.03	0.40
5:A:451:LEU:O	5:A:455:VAL:HG12	2.22	0.40
5:A:641:MET:HE2	5:A:641:MET:HB3	1.73	0.40
6:B:679:PRO:HD2	6:B:807:GLN:HB3	2.03	0.40
7:C:195:ARG:HG2	13:P:32:PRO:HA	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	
4	9	12/450 (3%)	10 (83%)	2 (17%)	0	100	100
5	A	1718/1755 (98%)	1567 (91%)	150 (9%)	1 (0%)	48	78
6	B	893/952 (94%)	809 (91%)	84 (9%)	0	100	100
7	C	220/536 (41%)	187 (85%)	33 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	D	313/514 (61%)	277 (88%)	36 (12%)	0	100	100
9	E	76/579 (13%)	66 (87%)	10 (13%)	0	100	100
10	F	297/357 (83%)	262 (88%)	35 (12%)	0	100	100
11	L	198/802 (25%)	176 (89%)	22 (11%)	0	100	100
12	O	248/848 (29%)	229 (92%)	19 (8%)	0	100	100
13	P	191/218 (88%)	175 (92%)	16 (8%)	0	100	100
14	Q	140/144 (97%)	126 (90%)	14 (10%)	0	100	100
15	R	83/229 (36%)	77 (93%)	6 (7%)	0	100	100
16	S	28/2752 (1%)	23 (82%)	5 (18%)	0	100	100
17	T	201/908 (22%)	184 (92%)	17 (8%)	0	100	100
18	V	161/166 (97%)	149 (92%)	12 (8%)	0	100	100
20	p	321/654 (49%)	273 (85%)	48 (15%)	0	100	100
21	r	33/1227 (3%)	30 (91%)	3 (9%)	0	100	100
22	s	18/285 (6%)	16 (89%)	2 (11%)	0	100	100
23	t	54/425 (13%)	54 (100%)	0	0	100	100
24	u	153/178 (86%)	131 (86%)	22 (14%)	0	100	100
25	x	28/258 (11%)	26 (93%)	2 (7%)	0	100	100
All	All	5386/14237 (38%)	4847 (90%)	538 (10%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	803	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	9	11/411 (3%)	11 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	A	1528/1584 (96%)	1526 (100%)	2 (0%)	88	89
6	B	756/847 (89%)	756 (100%)	0	100	100
7	C	173/459 (38%)	173 (100%)	0	100	100
8	D	271/441 (62%)	271 (100%)	0	100	100
9	E	65/502 (13%)	65 (100%)	0	100	100
10	F	231/300 (77%)	231 (100%)	0	100	100
11	L	158/709 (22%)	158 (100%)	0	100	100
12	O	201/751 (27%)	201 (100%)	0	100	100
13	P	175/197 (89%)	175 (100%)	0	100	100
14	Q	125/130 (96%)	125 (100%)	0	100	100
15	R	64/203 (32%)	64 (100%)	0	100	100
16	S	24/2432 (1%)	24 (100%)	0	100	100
17	T	186/838 (22%)	186 (100%)	0	100	100
18	V	87/134 (65%)	87 (100%)	0	100	100
20	p	234/572 (41%)	234 (100%)	0	100	100
21	r	23/1074 (2%)	23 (100%)	0	100	100
22	s	14/240 (6%)	13 (93%)	1 (7%)	13	39
23	t	36/381 (9%)	36 (100%)	0	100	100
24	u	139/167 (83%)	138 (99%)	1 (1%)	76	78
25	x	23/223 (10%)	23 (100%)	0	100	100
All	All	4524/12595 (36%)	4520 (100%)	4 (0%)	87	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	617	ASN
5	A	623	LYS
22	s	4	ASN
24	u	136	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	83	HIS

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Mol	Chain	Res	Type
5	A	97	HIS
5	A	105	ASN
5	A	160	HIS
5	A	210	HIS
5	A	357	ASN
5	A	461	HIS
5	A	483	GLN
5	A	514	ASN
5	A	587	GLN
5	A	664	HIS
5	A	675	GLN
5	A	757	ASN
5	A	775	ASN
5	A	1026	ASN
5	A	1069	ASN
5	A	1083	HIS
5	A	1124	ASN
5	A	1217	GLN
5	A	1623	ASN
5	A	1665	GLN
6	B	175	GLN
6	B	366	GLN
6	B	451	HIS
6	B	548	ASN
6	B	557	GLN
6	B	807	GLN
6	B	903	HIS
6	B	905	GLN
7	C	189	ASN
7	C	256	ASN
8	D	278	ASN
8	D	287	HIS
8	D	344	GLN
8	D	384	HIS
8	D	394	ASN
8	D	407	GLN
9	E	121	ASN
10	F	188	GLN
10	F	207	GLN
10	F	215	ASN
10	F	225	ASN
11	L	13	ASN

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Mol	Chain	Res	Type
11	L	45	GLN
11	L	231	ASN
12	O	250	GLN
12	O	325	ASN
13	P	163	HIS
13	P	206	ASN
14	Q	54	HIS
17	T	532	GLN
17	T	542	ASN
20	p	252	GLN
20	p	287	HIS
20	p	411	ASN
23	t	30	HIS
24	u	95	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	26/188 (13%)	13 (50%)	2 (7%)
19	Y	39/324 (12%)	23 (58%)	0
19	Z	12/324 (3%)	1 (8%)	0
2	5	73/116 (62%)	11 (15%)	1 (1%)
3	6	78/79 (98%)	22 (28%)	0
All	All	228/1031 (22%)	70 (30%)	3 (1%)

All (70) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	19	G
1	2	22	U
1	2	24	A
1	2	25	G
1	2	29	A
1	2	30	A
1	2	31	G
1	2	33	G
1	2	39	U
1	2	40	C
1	2	42	G
1	2	43	U
1	2	44	U

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Mol	Chain	Res	Type
2	5	8	G
2	5	10	U
2	5	22	U
2	5	23	C
2	5	24	G
2	5	25	C
2	5	28	A
2	5	35	U
2	5	53	U
2	5	68	C
2	5	76	A
3	6	3	G
3	6	6	C
3	6	7	G
3	6	9	U
3	6	13	G
3	6	26	U
3	6	28	A
3	6	29	A
3	6	37	C
3	6	40	U
3	6	41	A
3	6	43	A
3	6	46	G
3	6	47	A
3	6	49	G
3	6	54	G
3	6	62	C
3	6	68	C
3	6	69	A
3	6	71	G
3	6	74	U
3	6	79	C
19	Y	61	A
19	Y	63	G
19	Y	65	G
19	Y	66	C
19	Y	68	U
19	Y	69	A
19	Y	70	G
19	Y	71	C
19	Y	72	A

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Mol	Chain	Res	Type
19	Y	74	G
19	Y	75	U
19	Y	78	A
19	Y	79	A
19	Y	142	U
19	Y	144	A
19	Y	145	U
19	Y	146	G
19	Y	147	U
19	Y	148	C
19	Y	149	A
19	Y	152	C
19	Y	159	U
19	Y	160	G
19	Z	58	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	28	C
1	2	39	U
2	5	23	C

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 14 ligands modelled in this entry, 12 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	$\# Z > 2$
27	IHP	A	3001	-	36,36,36	0.86	0	60,60,60	1.45	8 (13%)
28	GTP	B	1001	-	33,34,34	1.04	1 (3%)	50,54,54	1.91	9 (18%)

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
27	IHP	A	3001	-	-	7/30/54/54	0/1/1/1
28	GTP	B	1001	-	-	7/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	1001	GTP	C5-N7	-2.88	1.33	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	1001	GTP	C5-C4-N3	-6.04	118.78	128.39
28	B	1001	GTP	C2-N3-C4	5.61	121.96	112.30
28	B	1001	GTP	N9-C4-N3	3.82	133.59	125.95
27	A	3001	IHP	C6-C1-C2	3.78	118.72	110.43
28	B	1001	GTP	C2-N1-C6	-3.51	118.75	125.11
28	B	1001	GTP	C3'-C2'-C1'	3.46	108.00	101.46
27	A	3001	IHP	C5-C6-C1	3.19	117.42	110.43
28	B	1001	GTP	N2-C2-N1	3.05	123.19	116.76
28	B	1001	GTP	O6-C6-C5	-2.76	119.24	126.53
28	B	1001	GTP	C5-C6-N1	2.73	120.20	113.25
27	A	3001	IHP	C3-C2-C1	2.52	115.97	110.43
27	A	3001	IHP	O12-C2-C1	2.43	113.92	108.76
27	A	3001	IHP	O16-C6-C1	2.37	113.80	108.76
27	A	3001	IHP	O15-C5-C6	2.20	113.45	108.76
27	A	3001	IHP	P1-O11-C1	-2.16	117.66	123.43
28	B	1001	GTP	C8-N7-C5	2.13	108.05	104.26
27	A	3001	IHP	O13-C3-C2	2.08	113.19	108.76

There are no chirality outliers.

All (14) torsion outliers are listed below:

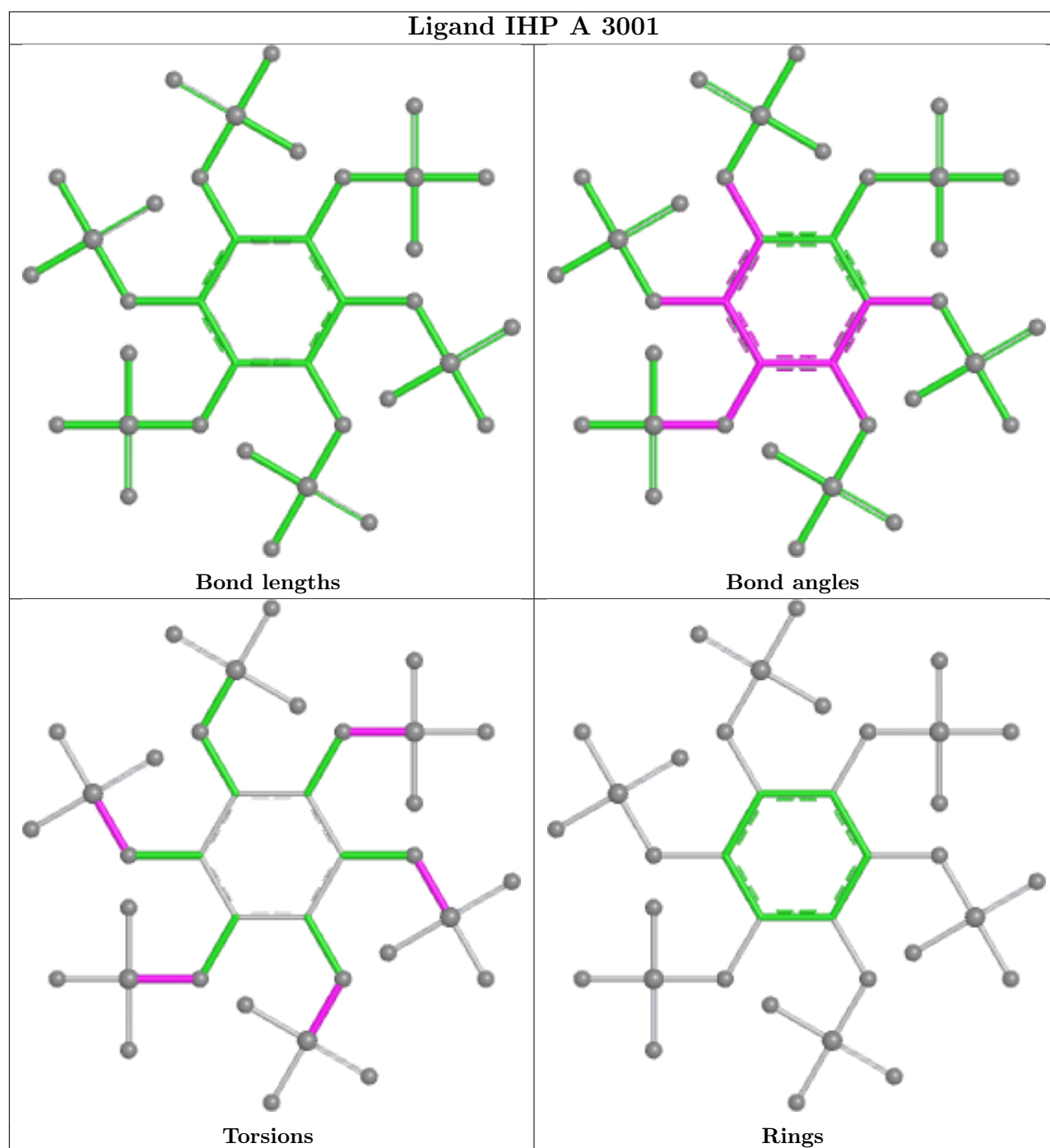
Mol	Chain	Res	Type	Atoms
28	B	1001	GTP	C5'-O5'-PA-O3A
28	B	1001	GTP	C5'-O5'-PA-O1A
28	B	1001	GTP	C5'-O5'-PA-O2A
28	B	1001	GTP	PB-O3B-PG-O1G
28	B	1001	GTP	PB-O3B-PG-O3G
27	A	3001	IHP	C1-O11-P1-O21
27	A	3001	IHP	C4-O14-P4-O24
28	B	1001	GTP	PB-O3A-PA-O2A
27	A	3001	IHP	C2-O12-P2-O42
27	A	3001	IHP	C2-O12-P2-O22
27	A	3001	IHP	C5-O15-P5-O25
27	A	3001	IHP	C5-O15-P5-O45
27	A	3001	IHP	C6-O16-P6-O46
28	B	1001	GTP	C4'-C5'-O5'-PA

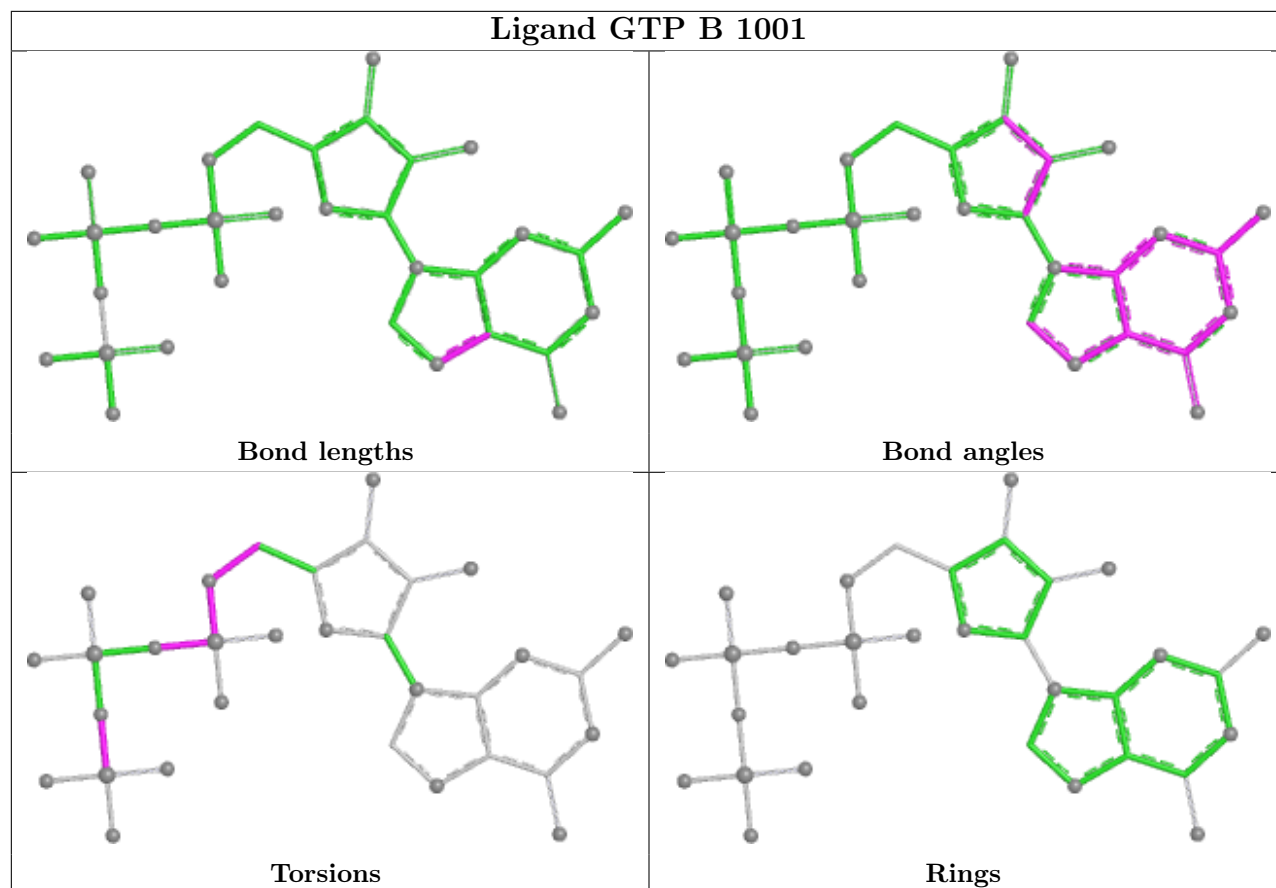
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	3001	IHP	5	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.

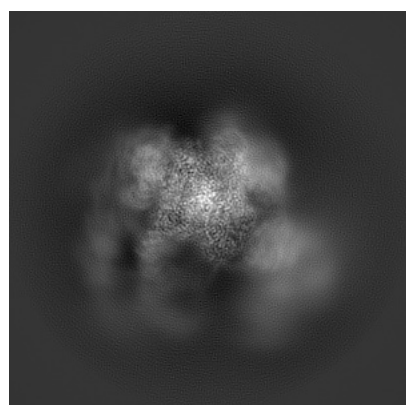
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11569. These allow visual inspection of the internal detail of the map and identification of artifacts.

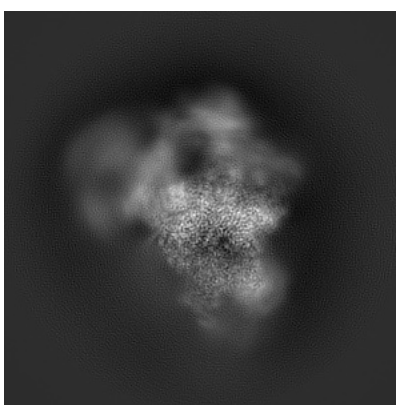
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

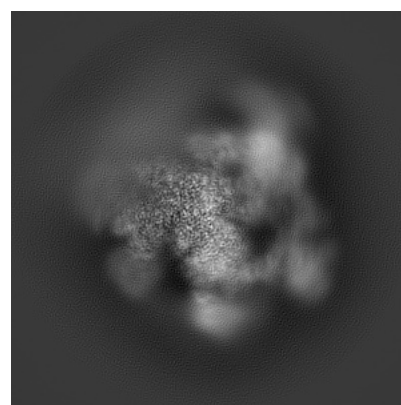
6.1.1 Primary map



X



Y

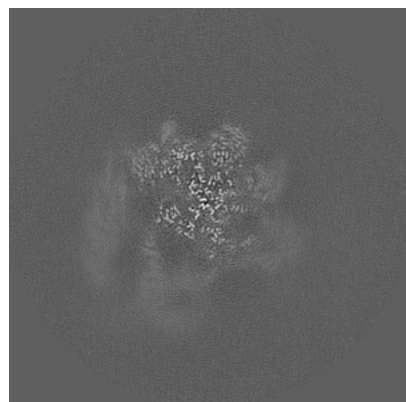


Z

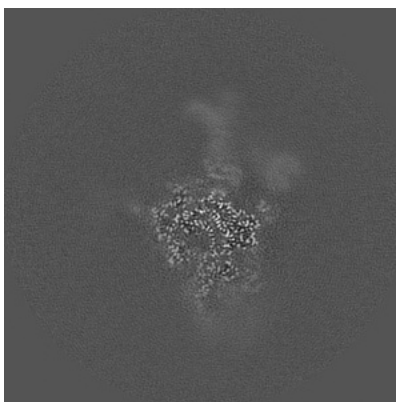
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

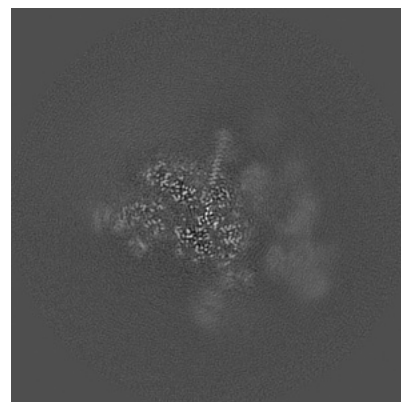
6.2.1 Primary map



X Index: 220



Y Index: 220

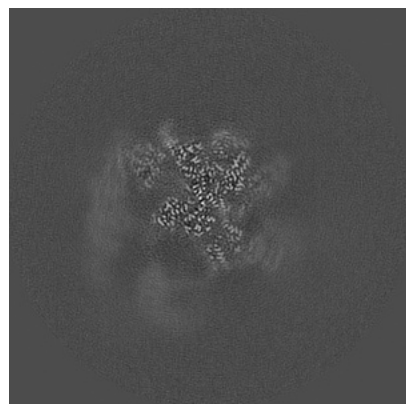


Z Index: 220

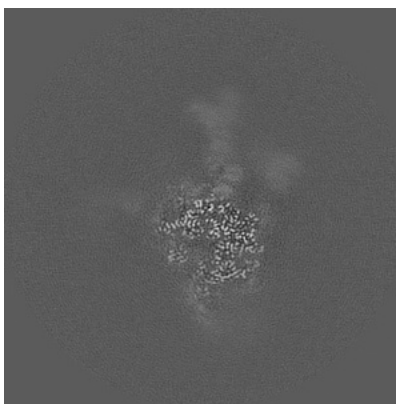
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

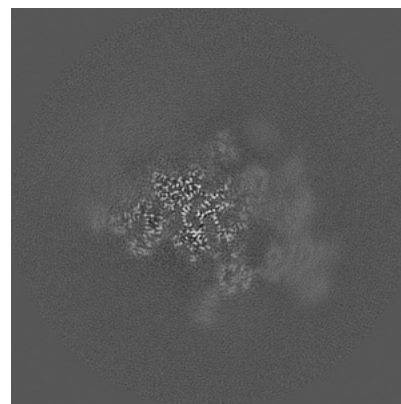
6.3.1 Primary map



X Index: 213



Y Index: 216

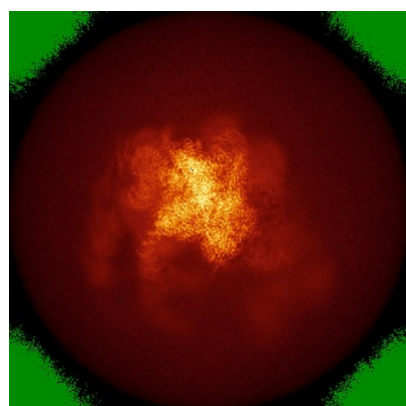


Z Index: 227

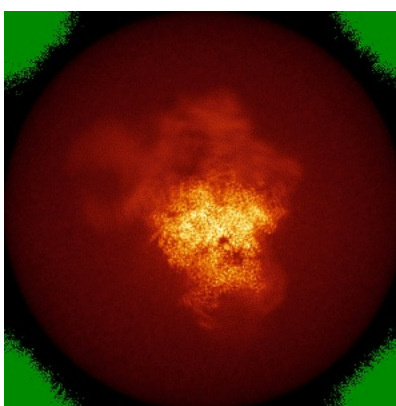
The images above show the largest variance slices of the map in three orthogonal directions.

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

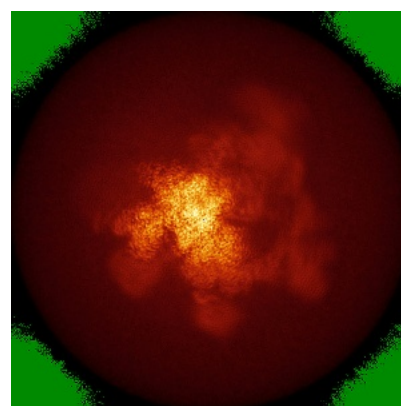
6.4.1 Primary map



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

This section was not generated.

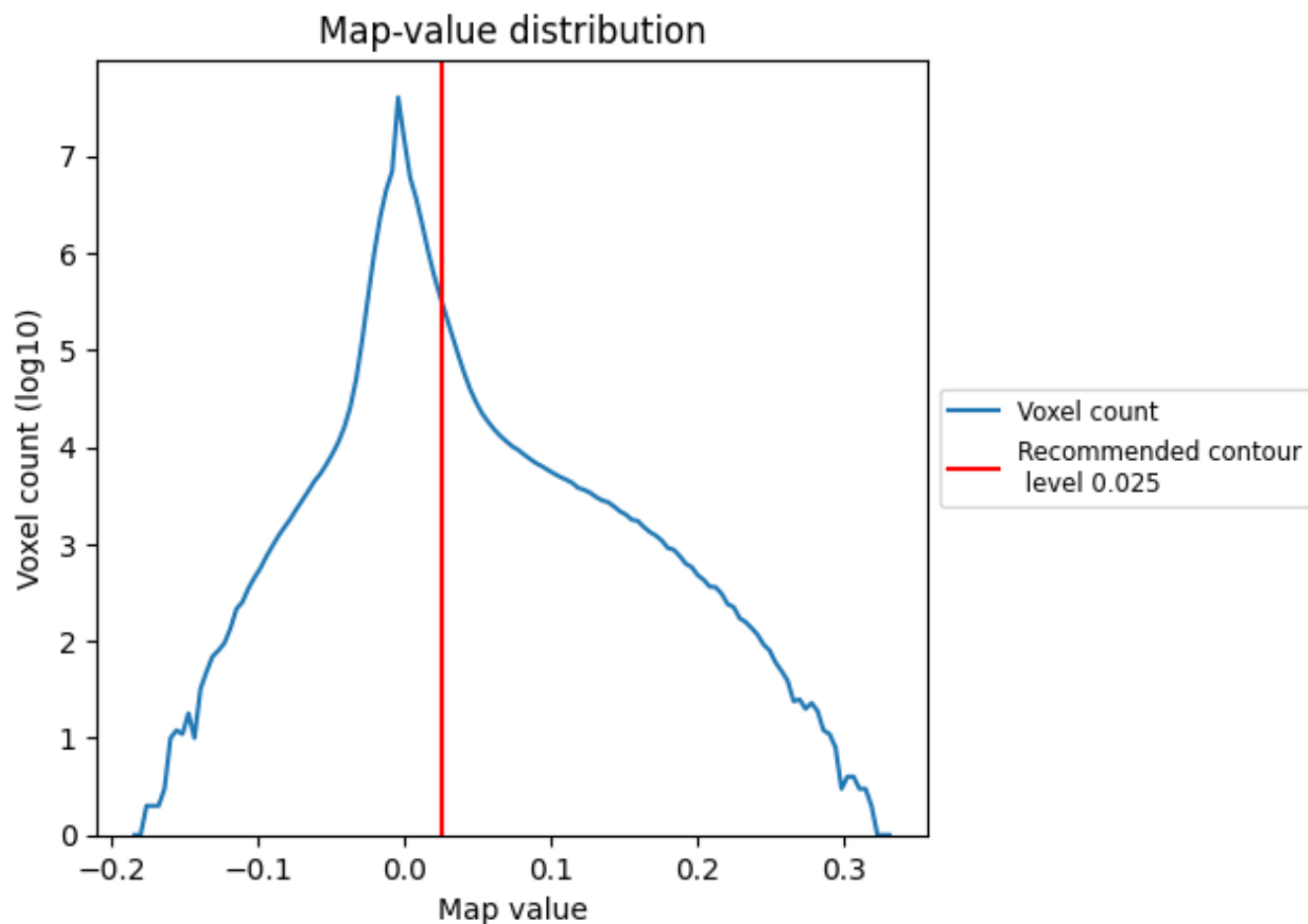
6.6 Mask visualisation

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

7 Map analysis [i](#)

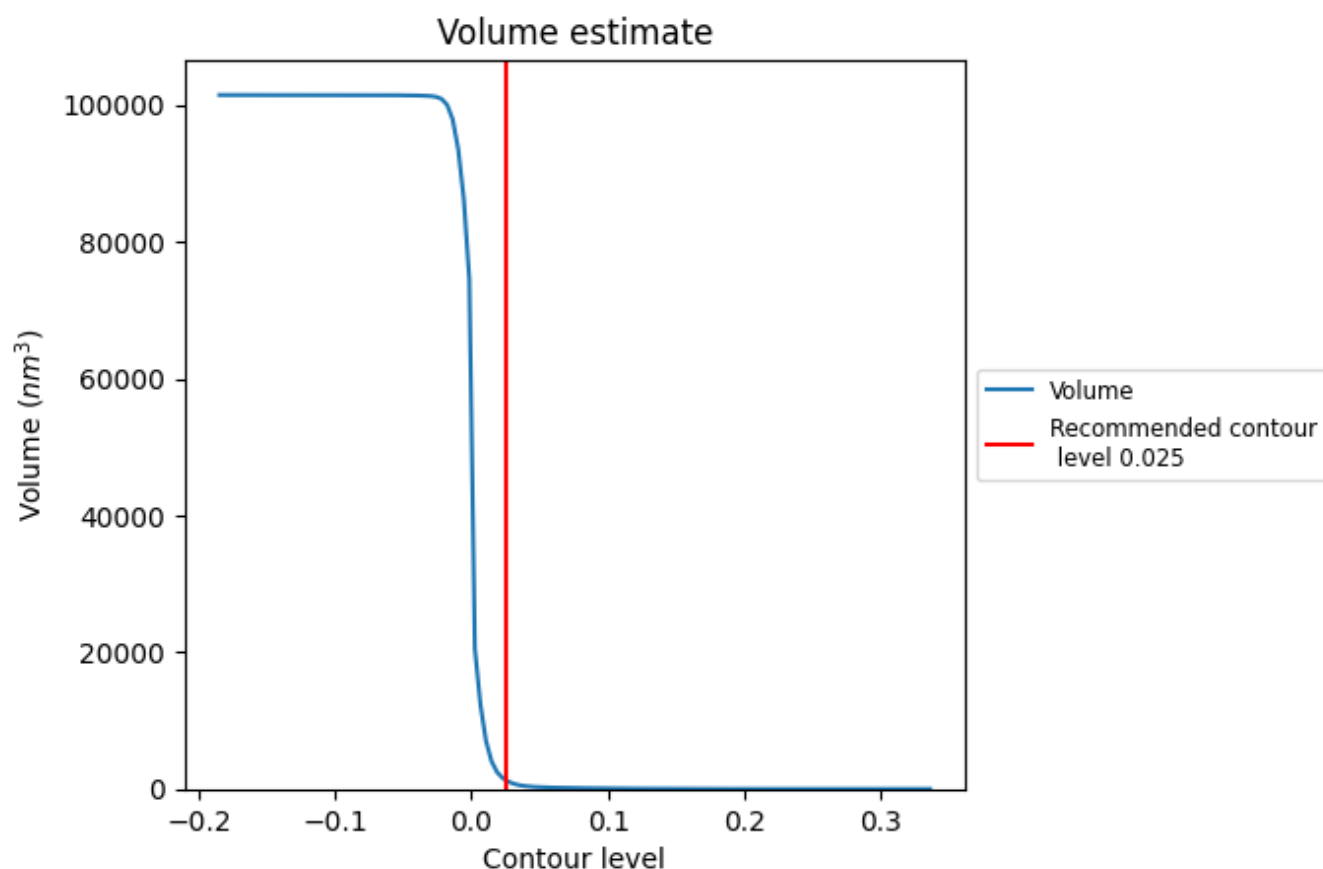
This section contains the results of statistical analysis of the map.

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.

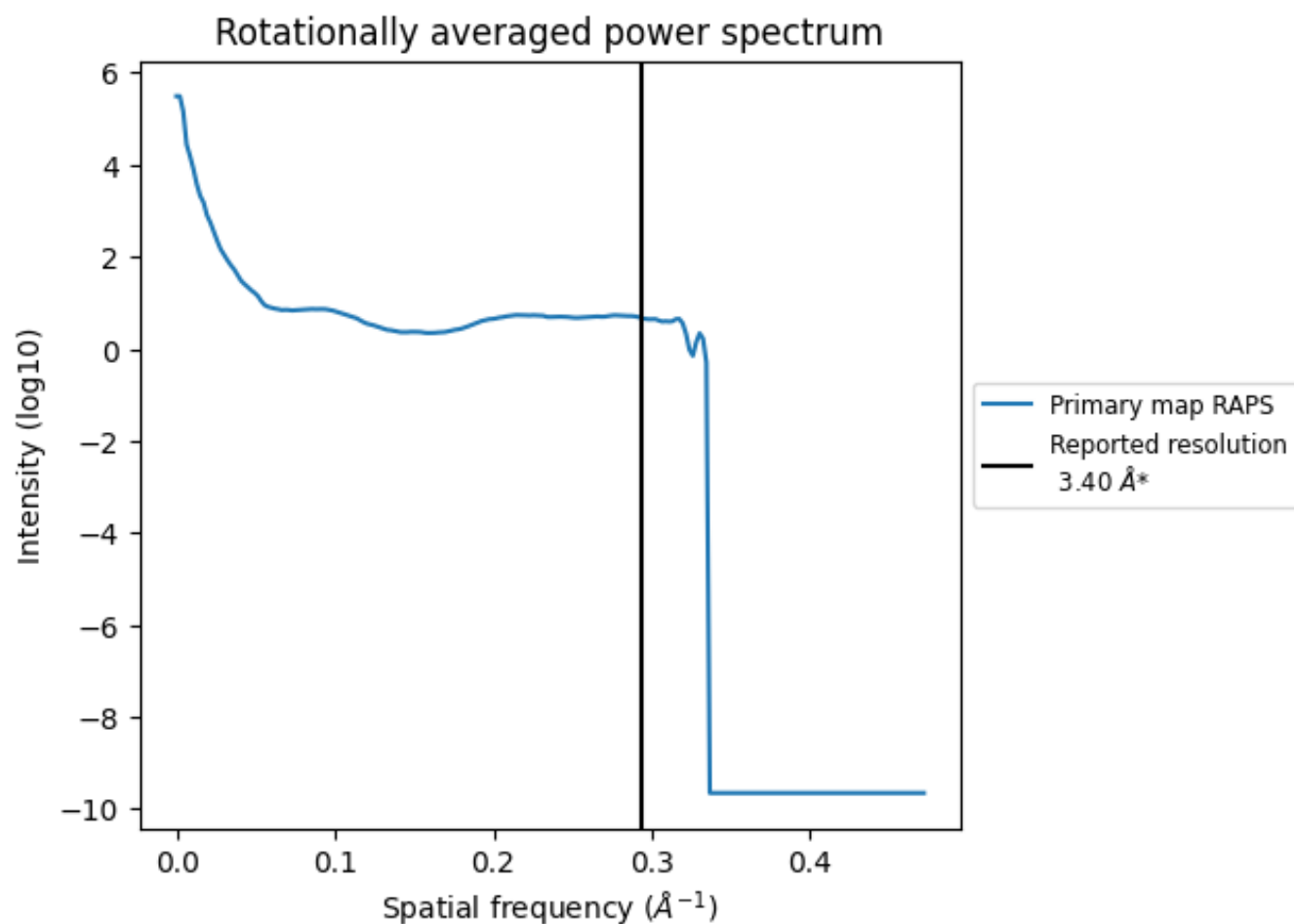
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1311 nm³; this corresponds to an approximate mass of 1184 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 0.294 $\text{\AA}^{-1}$

8 Fourier-Shell correlation

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

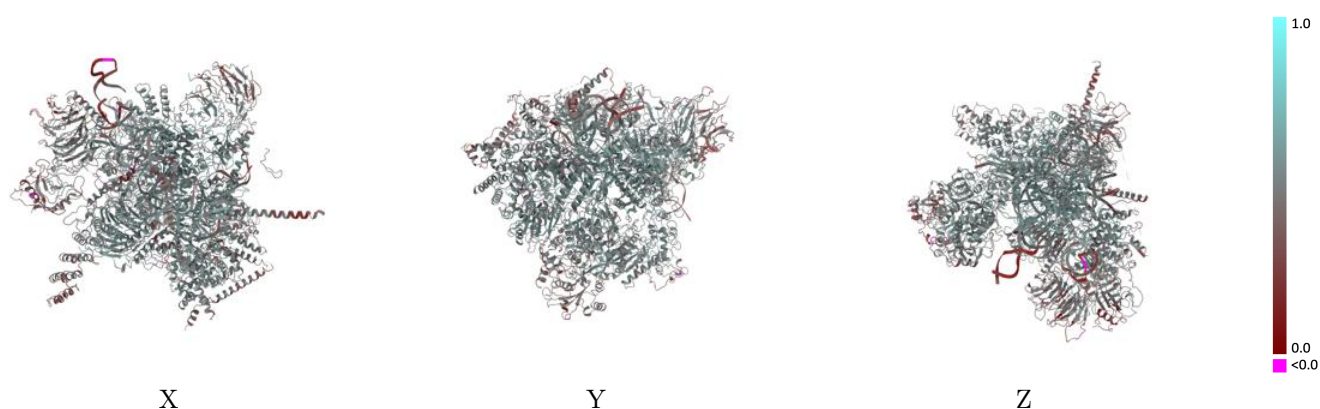
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11569 and PDB model 6ZYM. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)

This section was not generated.

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

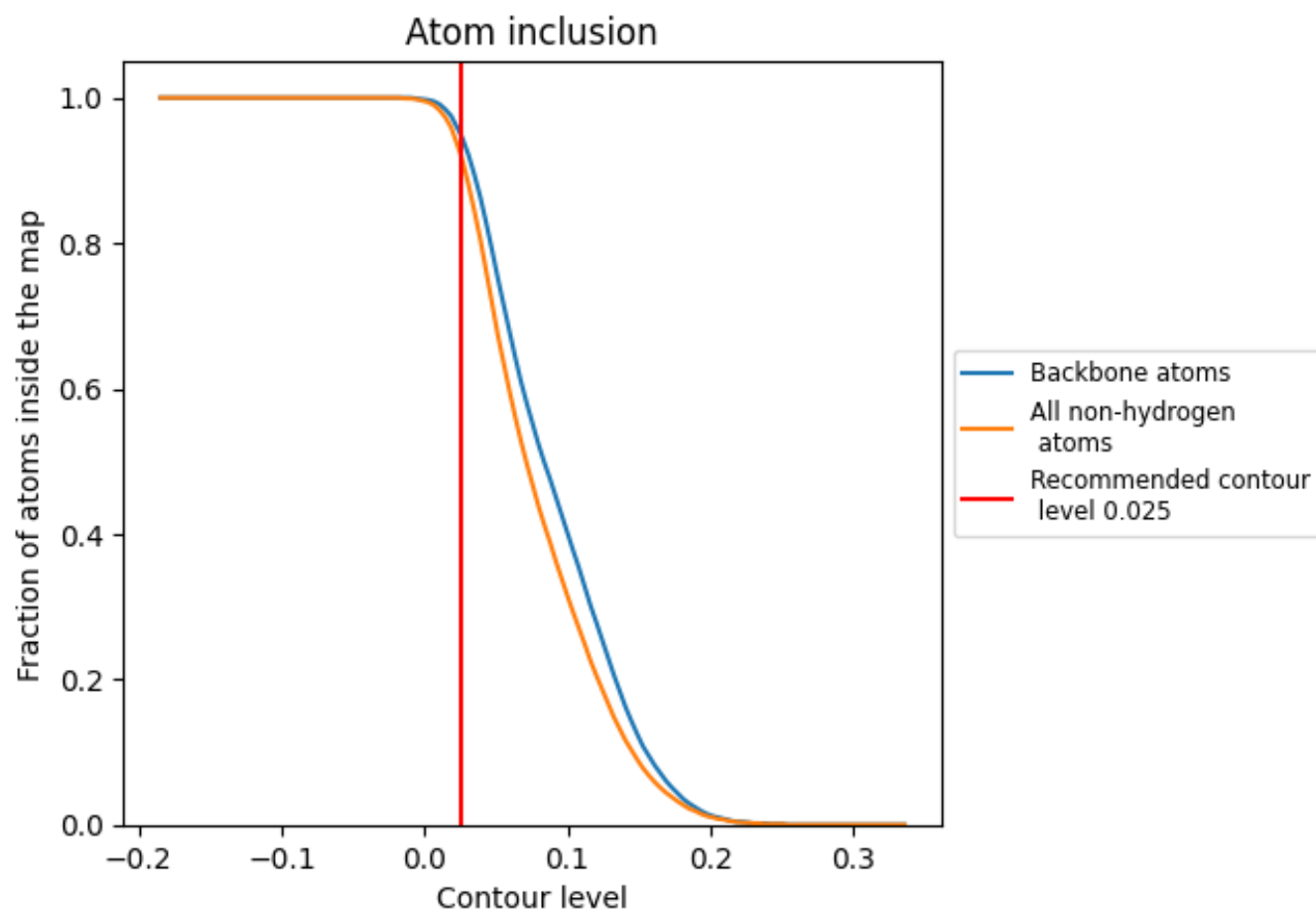


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9240	 0.4980
2	 0.9040	 0.4570
5	 0.9350	 0.4550
6	 0.9500	 0.4720
9	 0.6790	 0.4240
A	 0.9350	 0.5390
B	 0.9220	 0.4880
C	 0.8900	 0.4710
D	 0.9570	 0.5520
E	 0.9060	 0.4900
F	 0.9260	 0.4340
L	 0.8910	 0.4840
O	 0.9080	 0.4660
P	 0.9150	 0.5070
Q	 0.9490	 0.5260
R	 0.8840	 0.4980
S	 0.9080	 0.5290
T	 0.9030	 0.4820
V	 0.9290	 0.4170
Y	 0.9270	 0.4580
Z	 0.9460	 0.5490
p	 0.9350	 0.4540
r	 0.8330	 0.4610
s	 0.9340	 0.5570
t	 0.8910	 0.4500
u	 0.8930	 0.4830
x	 0.8960	 0.5330

