



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 04:33 PM UTC

PDB ID : 7UIF / pdb_00007uif
EMDB ID : EMD-26544
Title : Mediator-PIC Early (Core B)
Authors : Gorbea Colon, J.J.; Chen, S.-F.; Tsai, K.L.; Murakami, K.
Deposited on : 2022-03-29
Resolution : 4.60 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:

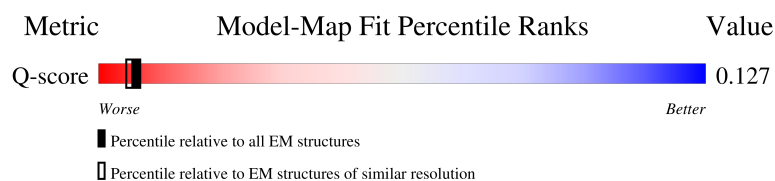
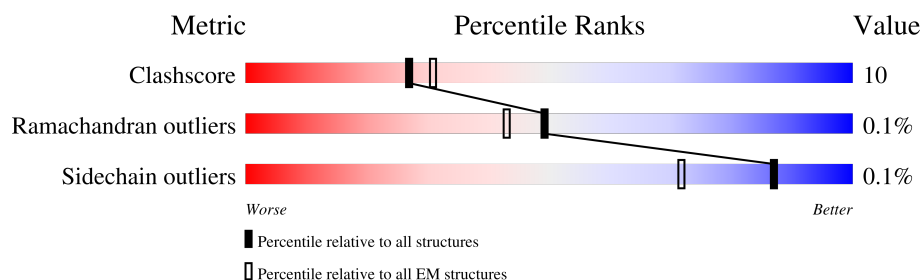
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.60 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	-
Q-score	-	25397	2407 (4.10 - 5.10)

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	A	1733	
1	z	1733	
2	B	1224	
3	C	318	

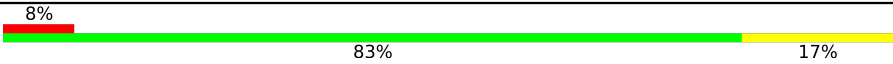
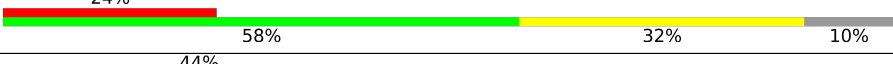
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Mol	Chain	Length	Quality of chain
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	345	
14	P	735	
15	Q	400	
16	S	309	
17	a	566	
18	d	284	
19	f	295	
20	g	222	
21	h	223	
22	i	149	
23	j	157	
24	k	115	
25	n	1082	
26	q	687	
27	r	307	
28	s	220	

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Mol	Chain	Length	Quality of chain
29	t	210	
30	u	140	
31	v	121	
32	w	127	

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 63137 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1453	Total	C	N	O	S	0	0
			11425	7192	1995	2176	62		
1	z	25	Total	C	N	O		0	0
			184	116	25	43			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1172	Total	C	N	O	S	0	0
			9336	5895	1637	1748	56		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	271	Total	C	N	O	S	0	0
			2133	1340	355	424	14		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	169	Total	C	N	O	S	0	0
			1353	838	237	275	3		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1760	1116	310	322	12		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	86	Total	C	N	O	S	0	0
			697	445	118	131	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	141	Total	C	N	O	S	0	0
			1126	706	189	226	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			943	580	171	181	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	70	Total	C	N	O	S	0	0
			578	366	102	104	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	116	Total	C	N	O	S	0	0
			929	596	158	173	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	43	Total	C	N	O	S	0	0
			344	211	69	60	4		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	35	Total	C	N	O	S	0	0
			263	169	41	49	4		

- Molecule 14 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	103	Total	C	N	O	S	0	0
			861	554	142	162	3		

- Molecule 15 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	125	Total	C	N	O	S	0	0
			1033	644	189	195	5		

- Molecule 16 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	181	Total	C	N	O	S	0	0
			1436	893	256	279	8		

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	365	Total	C	N	O	S	0	0
			3008	1932	478	588	10		

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	d	171	Total	C	N	O	S	0	0
			1388	875	233	276	4		

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	f	169	Total	C	N	O	S	0	0
			1407	905	234	262	6		

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	g	169	Total	C	N	O	S	0	0
			1409	903	238	263	5		

- Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	h	136	Total	C	N	O	S	0	0
			1126	709	199	215	3		

- Molecule 22 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	i	83	Total	C	N	O	S	0	0
			709	444	130	134	1		

- Molecule 23 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	j	146	Total	C	N	O	S	0	0
			1173	725	206	239	3		

- Molecule 24 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	k	108	Total	C	N	O	S	0	0
			876	546	149	177	4		

- Molecule 25 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	n	625	Total	C	N	O	S	0	0
			5139	3318	884	913	24		

- Molecule 26 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	q	515	Total	C	N	O	S	0	0
			4182	2674	707	788	13		

- Molecule 27 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	r	253	Total	C	N	O	S	0	0
			1995	1271	331	383	10		

- Molecule 28 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	s	81	Total	C	N	O	S	0	0
			657	415	109	132	1		

- Molecule 29 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	t	210	Total	C	N	O	S	0	0
			1609	1016	270	317	6		

- Molecule 30 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	u	122	Total	C	N	O	S	0	0
			978	611	163	199	5		

- Molecule 31 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	v	109	Total	C	N	O	S	0	0
			869	540	143	180	6		

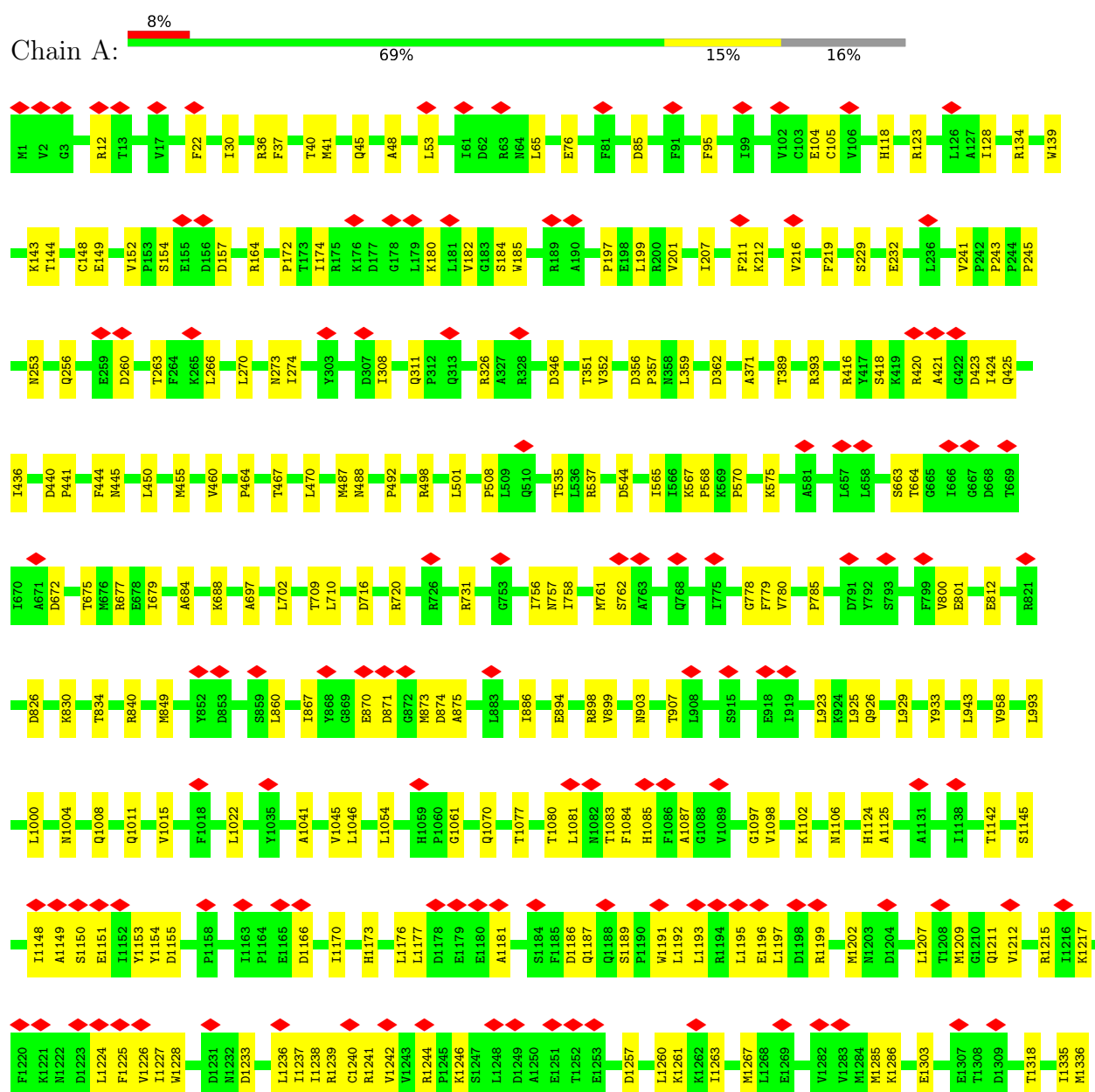
- Molecule 32 is a protein called Mediator of RNA polymerase II transcription subunit 31.

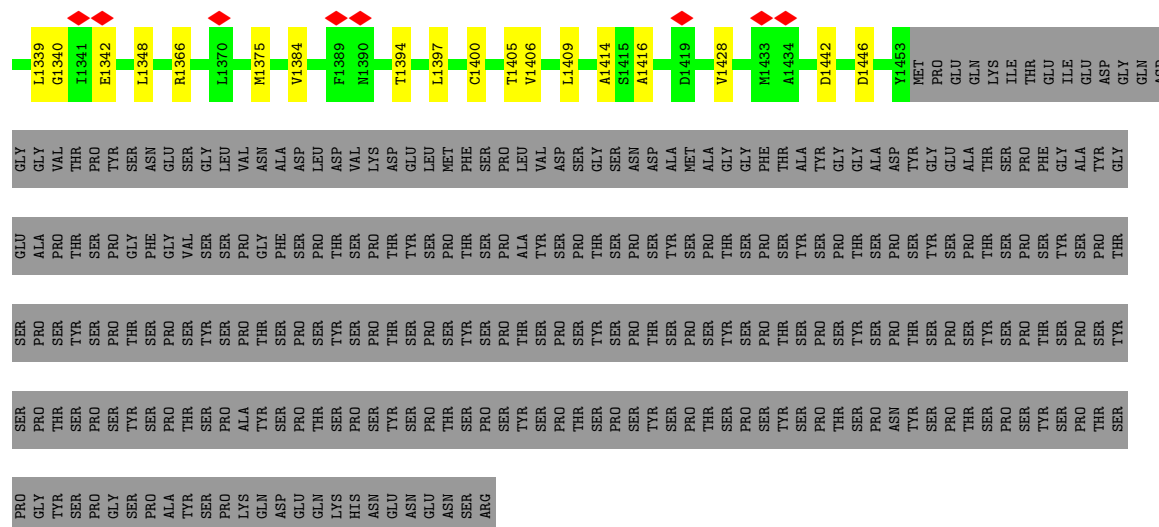
Mol	Chain	Residues	Atoms					AltConf	Trace
32	w	103	Total	C	N	O	S	0	0
			871	575	135	155	6		

3 Residue-property plots

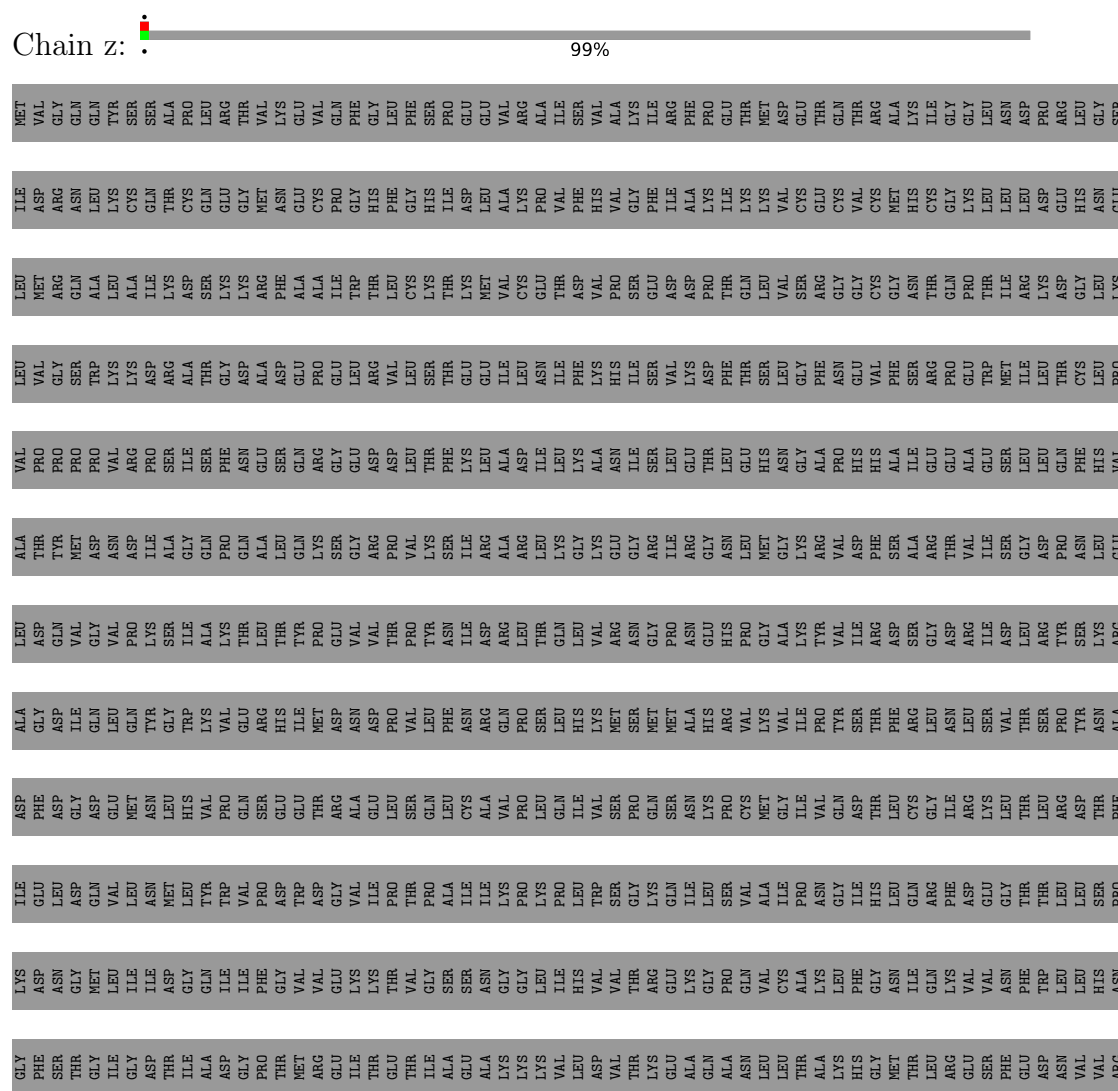
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

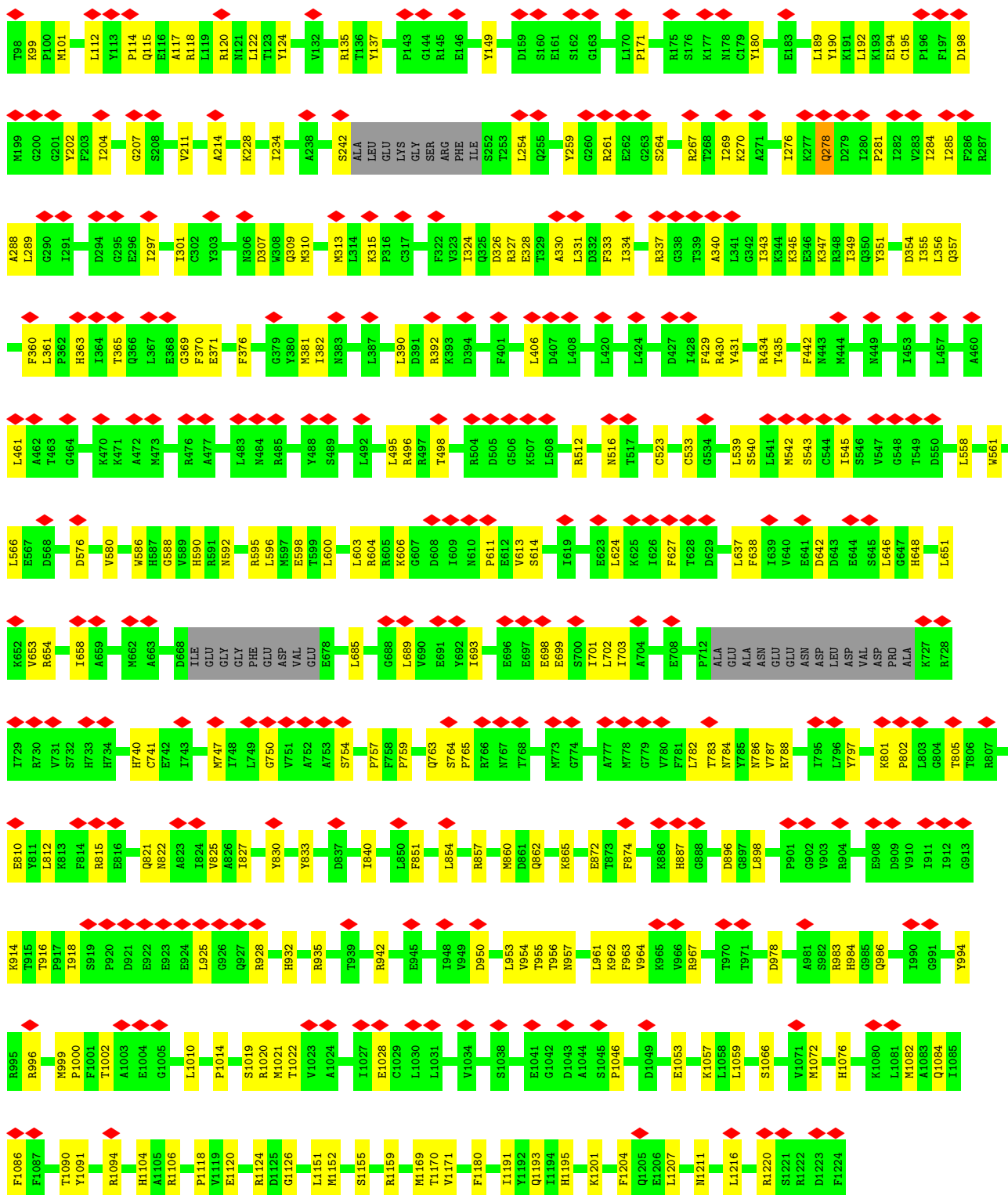
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1





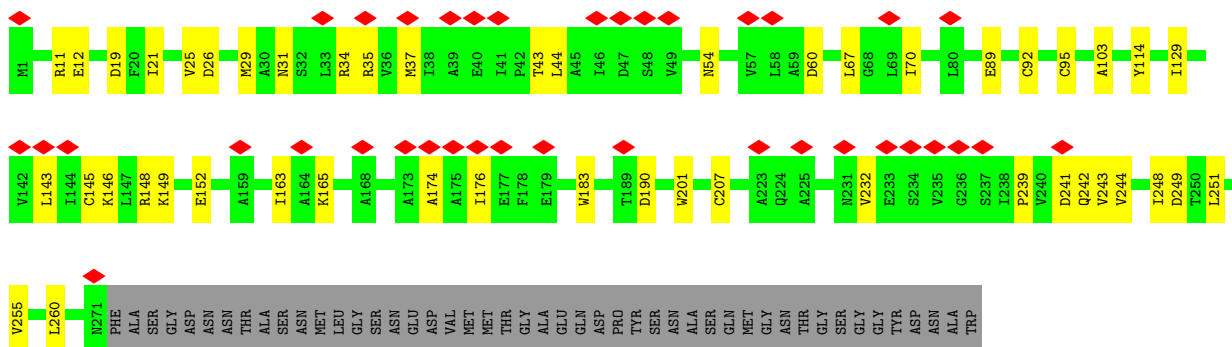
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



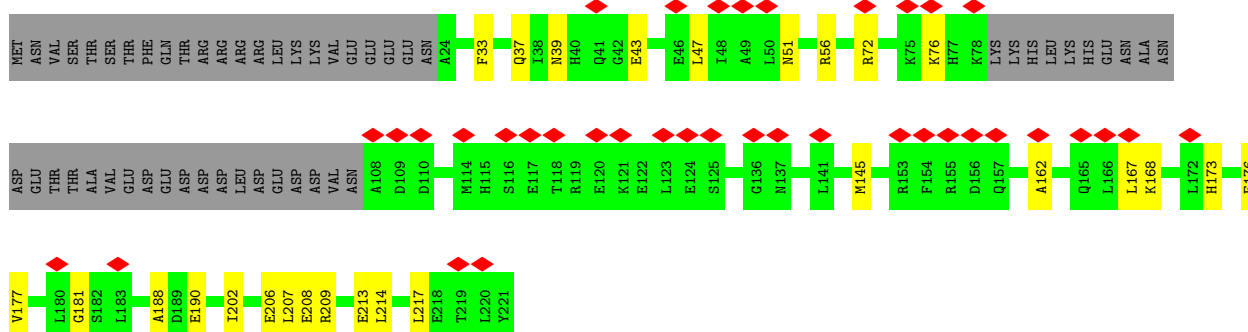


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

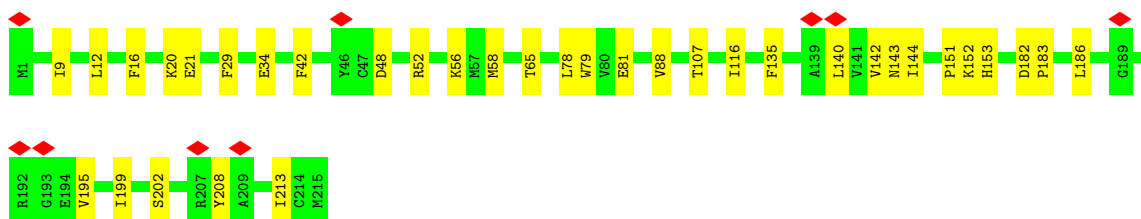
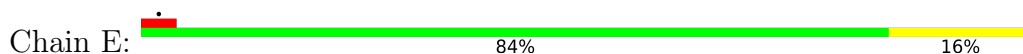




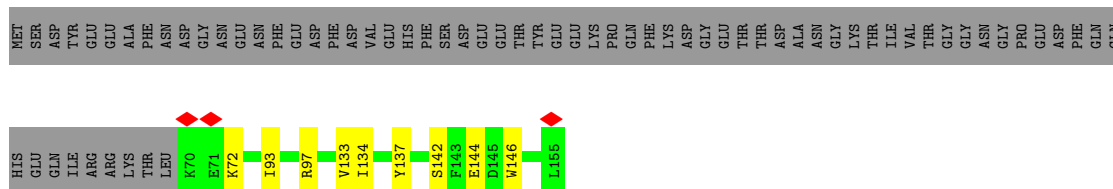
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



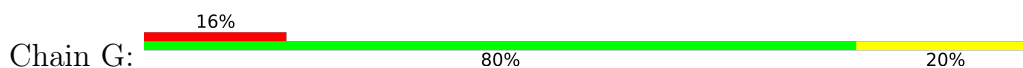
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

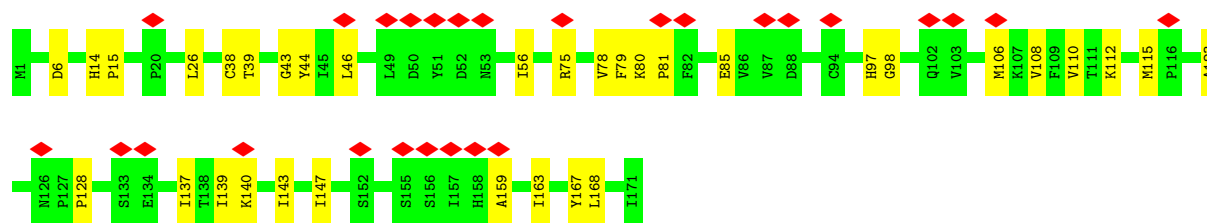


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

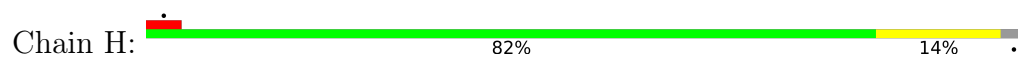


• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

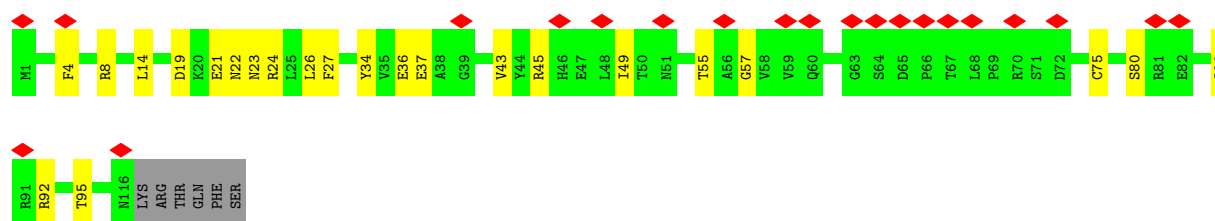
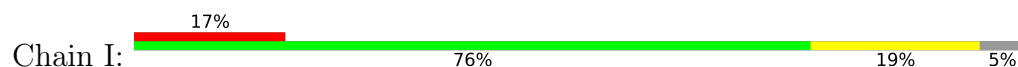




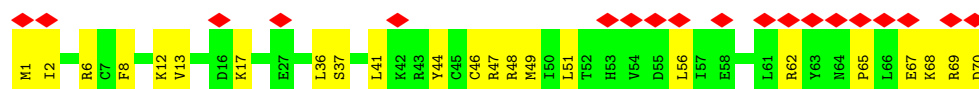
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



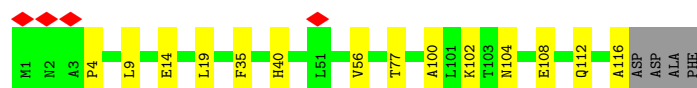
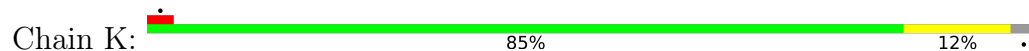
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



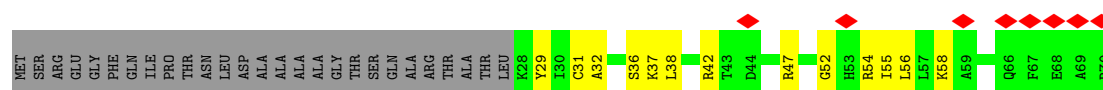
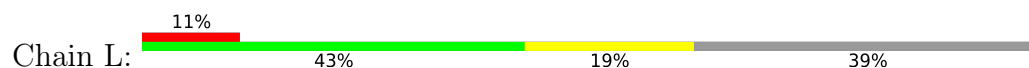
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

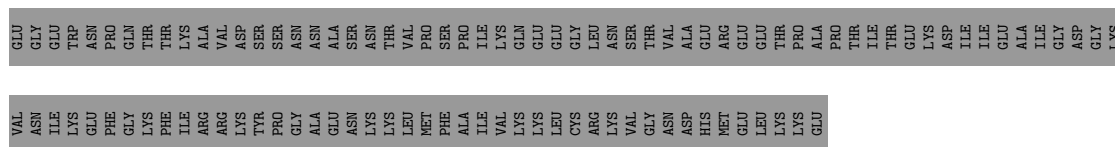


- Molecule 13: Transcription initiation factor IIB

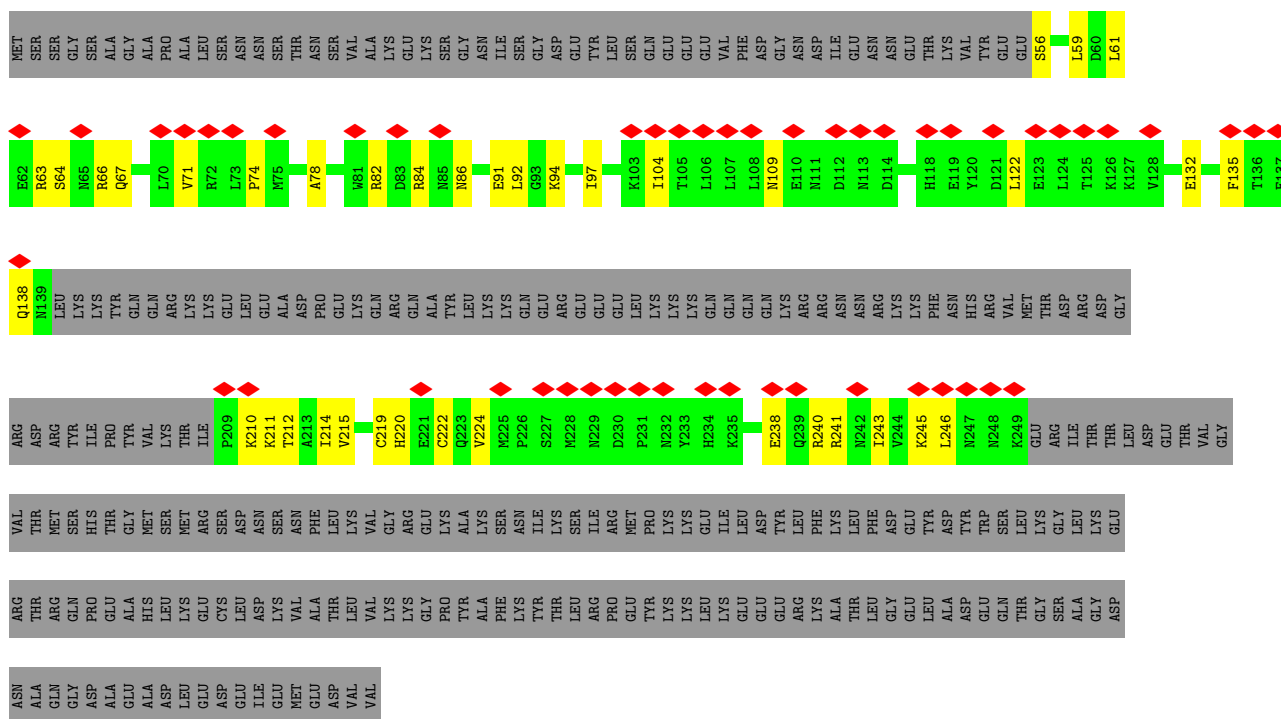
[illegible]

Chain P: 10% 86%

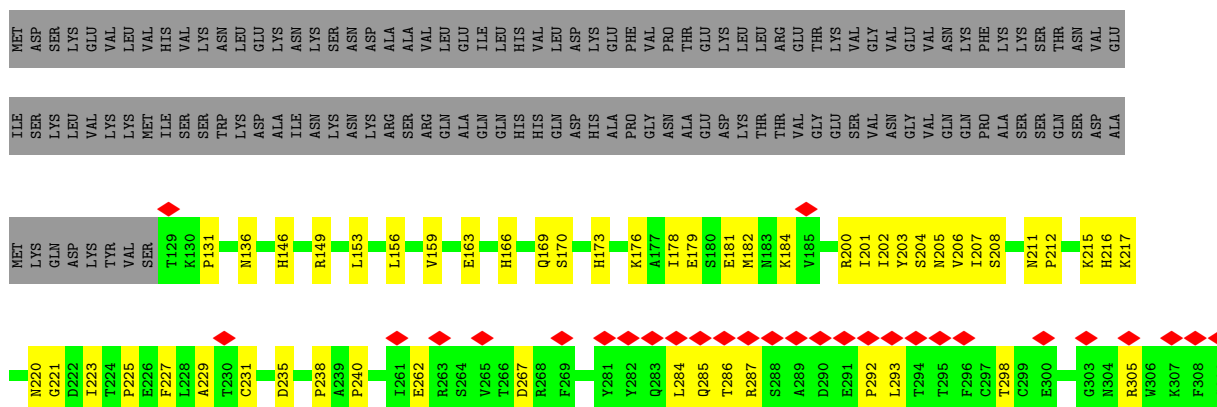
PRO	VAL	GLN	V392	GLY	LEU	VAL	ASP	THR	LYS	LYS	LYS
VAL	ALA	ALA	Y393	ASN	ALA	ASP	THR	THR	ASP	THR	LYS
LYS	PRO	MET	K394	LEU	ASN	ASP	ARG	ARG	ASP	THR	LYS
GLU	GLU	ASP	F395	ARG	GLY	VAL	THR	LEU	GLU	ASN	ASN
ASN	ASN	ASP	T396	LYS	PRO	LYS	LYS	PHE	ALA	PRO	PRO
GLU	GLU	ASP	A397	THR	LEU	ASP	LEU	ALA	ALA	GLY	GLY
SER	GLN	ASP	R398	ARG	VAL	VAL	VAL	ASN	GLY	GLY	GLY
ASP	ASP	ASP	H399	GLN	THR	THR	THR	THR	ALA	GLY	GLY
THR	GLU	ASP	LYS	LEU	LYS	LYS	LYS	THR	ALA	GLY	GLY
LEU	LEU	ASN	TYR	VAL	GLU	GLY	GLY	ALA	GLY	GLY	GLY
SER	PHE	SER	ALA	LEU	ASP	VAL	VAL	ALA	GLY	GLY	GLY
LYS	GLY	GLU	THR	LEU	ASP	ASP	ASP	ILE	LEU	LEU	GLY
SER	GLU	VAL	THR	ASP	ALA	GLY	GLY	GLN	LEU	LEU	GLY
LYS	GLU	LEU	THR	ASN	PRO	PRO	PRO	ARG	ALA	ALA	GLY
ARG	LYS	LEU	ILE	ALA	ALA	ILE	ILE	ILE	ALA	ILE	THR
SER	ASP	TYR	ASP	LYS	GLU	PRO	THR	GLN	PRO	GLN	ASN
PRO	GLU	ASP	ALA	LYS	ASP	ASP	ASP	LYS	VAL	GLY	ALA
LYS	ASP	GLU	ALA	LYS	LEU	LEU	LEU	PHE	ALA	ILE	SER
GLN	GLY	GLU	LYS	PHE	THR	THR	THR	GLY	GLY	ARG	ALA
GLN	ARG	ALA	MET	E346	VAL	VAL	SER	TYR	GLY	ALA	LYS
LYS	ILE	ASP	ASP	F347	MET	MET	LYS	LYS	ARG	ALA	LYS
LYS	LYS	ASP	LYS	Y348	VAL	VAL	LYS	LYS	SER	ASP	ASP
ALA	LYS	GLU	LYS	F349	GLU	GLU	SER	LYS	VAL	ASP	ASP
THR	ALA	LEU	ALA	GLY	ALA	TYR	ALA	ALA	PRO	VAL	THR
ASN	LEU	ALA	G350	GLU	PRO	ASP	ALA	ALA	GLY	VAL	ALA
ALA	GLN	PRO	V351	GLY	GLY	GLY	PRO	GLN	VAL	VAL	LYS
LYS	LYS	ILE	VAL	PRO	LYS	THR	THR	GLY	LYS	VAL	PHE
VAL	THR	ILE	K352	ASP	GLU	THR	THR	ARG	ASP	ASP	LEU
HIS	GLU	ASP	E353	ARG	VAL	VAL	VAL	SER	GLY	GLY	LEU
LYS	LEU	GLY	D354	TRP	ALA	THR	THR	THR	ASP	GLY	LEU
GLU	ALA	ASN	F355	LEU	ASN	ASN	ALA	PRO	ASP	ASP	ARG
PRO	ALA	GLU	MET	MET	GLU	VAL	VAL	ASN	P95	ASP	MET
THR	LEU	GLN	LYS	HIS	GLU	PRO	GLU	GLY	E100	GLY	GLY
LEU	TYR	GLU	LEU	LEU	ASN	GLU	SER	SER	K108	GLY	ASN
ARG	SER	ASN	G361	ASP	PHE	THR	ASN	GLY	K118	LYS	ASN
VAL	SER	LYS	V362	GLU	GLU	GLY	GLY	MET	K120	THR	SER
LYS	ASP	GLU	ASN	ILE	GLU	GLY	LEU	LYS	K124	VAL	GLY
ILE	ASN	GLU	G363	GLY	GLY	THR	ASN	LYS	K125	ASN	PRO
LYS	GLU	GLN	S364	THR	THR	MET	ASN	GLY	K126	ASN	GLY
ASN	ILE	ARG	Y365	THR	THR	ASP	GLY	THR	K127	THR	ASN
CYS	ASN	ILE	E366	THR	ASP	PRO	THR	VAL	K128	LYS	ASN
VAL	PRO	LYS	A367	THR	PRO	THR	THR	VAL	P129	ASP	SER
ILE	TYR	LYS	G368	ARG	LEU	SER	LEU	SER	V130	GLY	ARG
ILE	LEU	GLU	C368	THR	ALA	ALA	ALA	LEU	T131	GLY	GLY
LEU	SER	MET	H369	TYR	ASP	ASP	ALA	ASN	D132	GLN	SER
LYS	GLU	LEU	S370	ASP	VAL	VAL	ASN	ASN	F133	THR	LEU
GLY	SER	GLN	D371	THR	ALA	ALA	GLY	THR	H134	PRO	LYS
ASP	ASP	ALA	S372	ARG	PRO	PRO	LEU	VAL	R141	THR	LYS
LYS	ILE	ASN	Y373	ARG	GLY	GLY	GLY	LYS	K142	THR	LYS
GLU	GLU	ALA	V374	LYS	GLY	ASN					



- Molecule 15: Transcription initiation factor IIF subunit beta

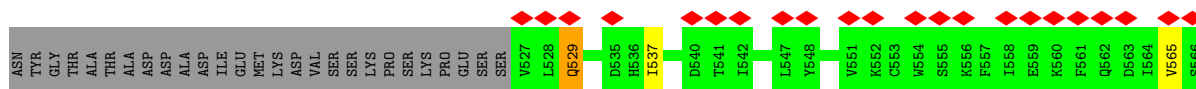


- Molecule 16: Transcription elongation factor S-II

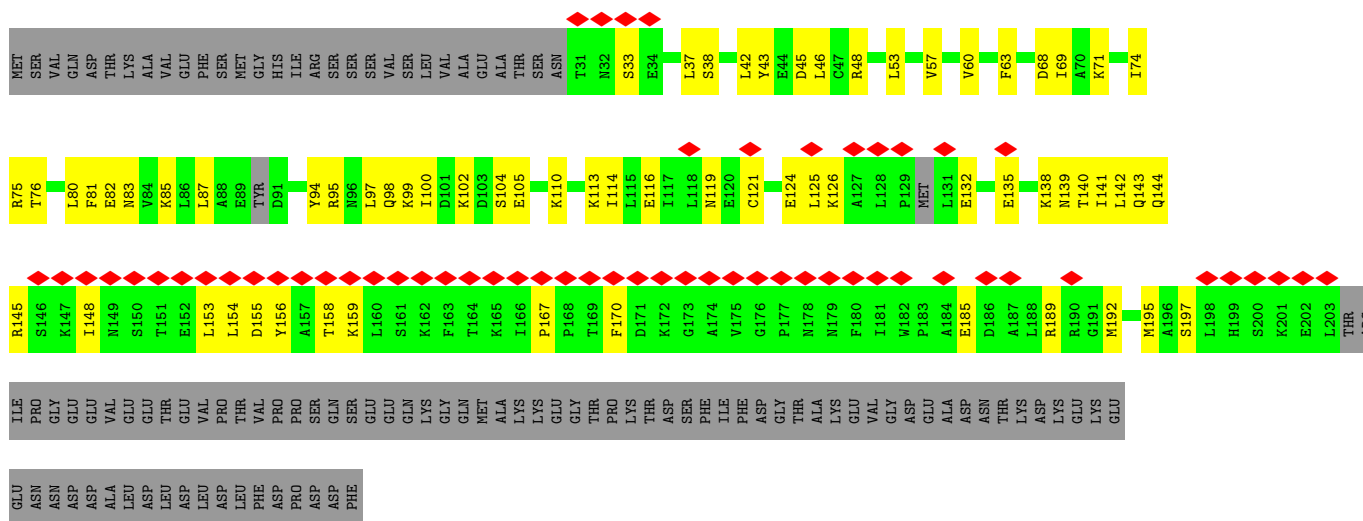


- Molecule 17: Mediator of RNA polymerase II transcription subunit 1

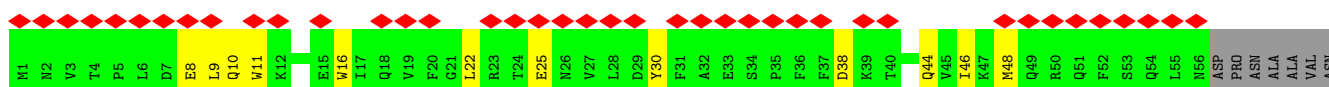


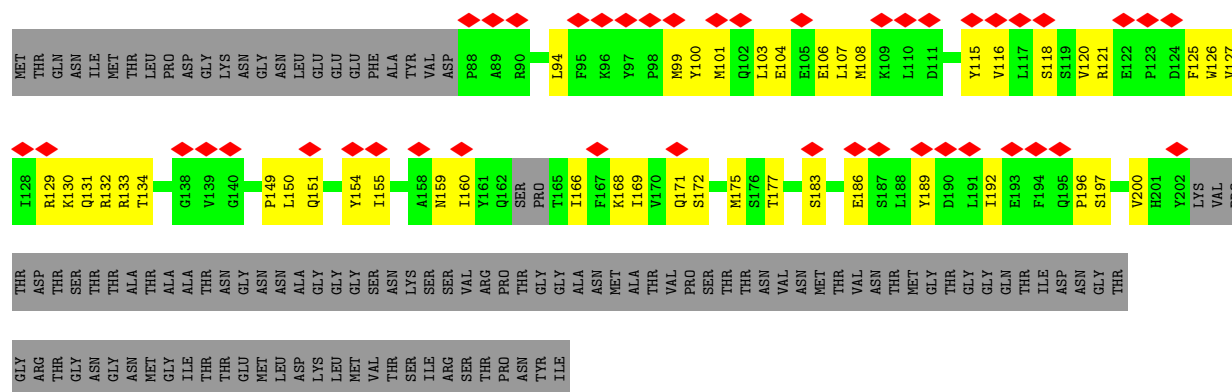


Chain d:

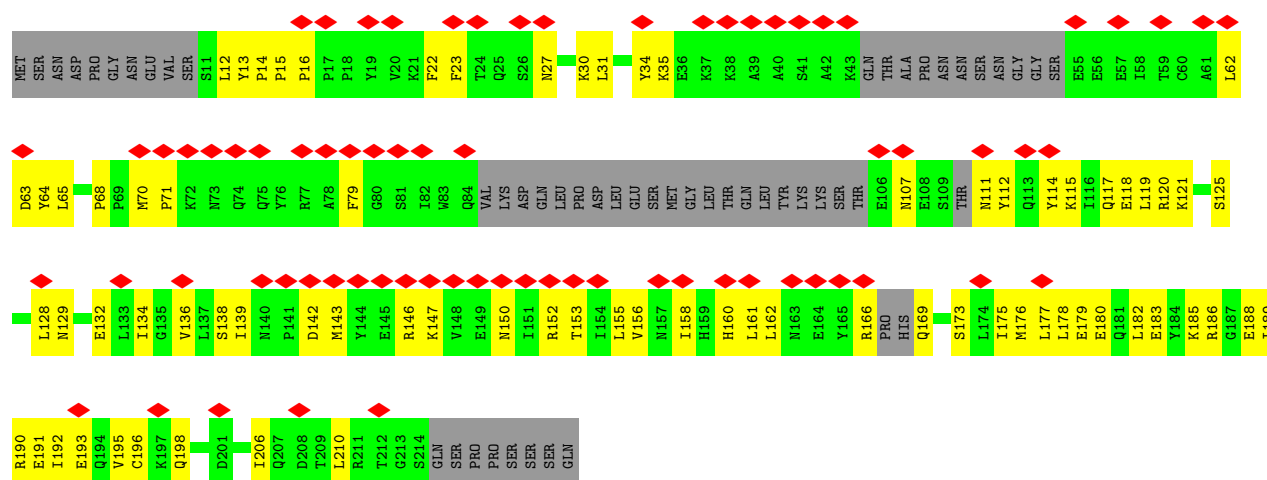


Chain f:

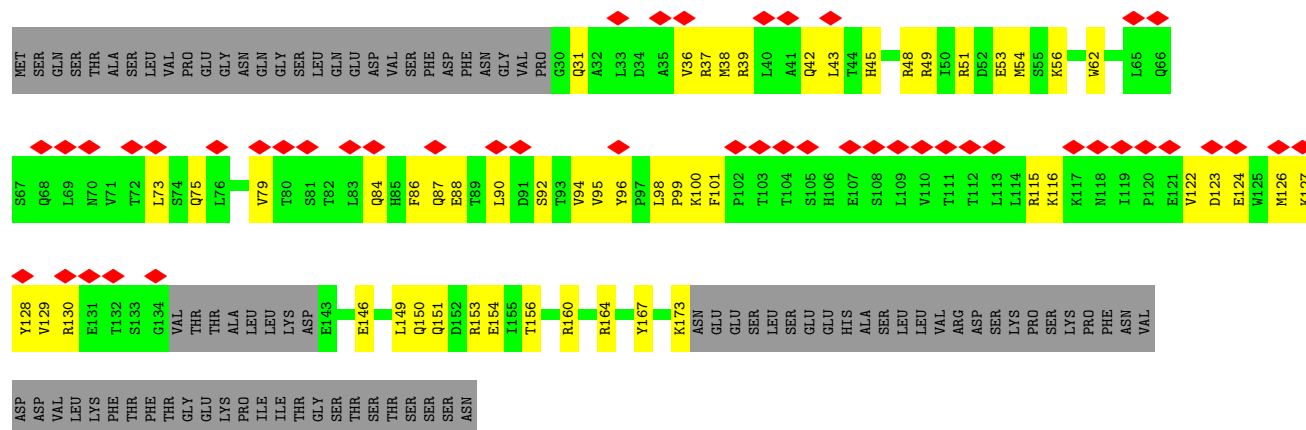




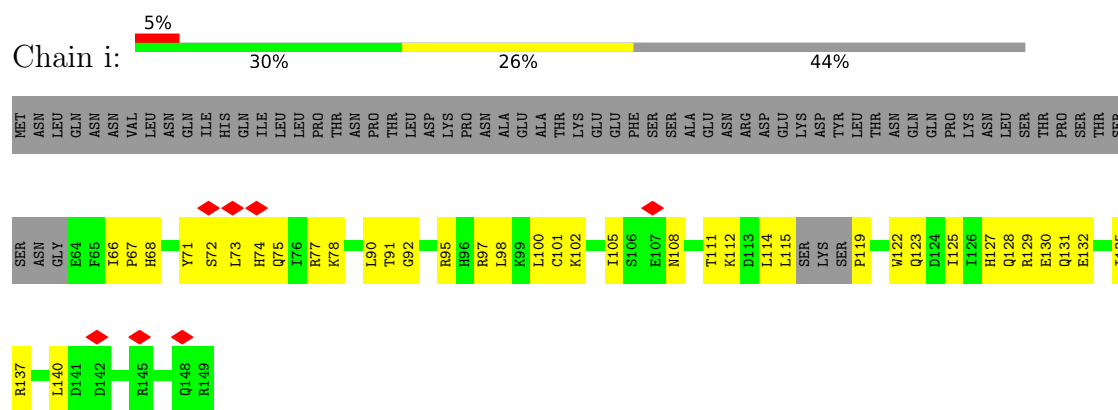
• Molecule 20: Mediator of RNA polymerase II transcription subunit 7



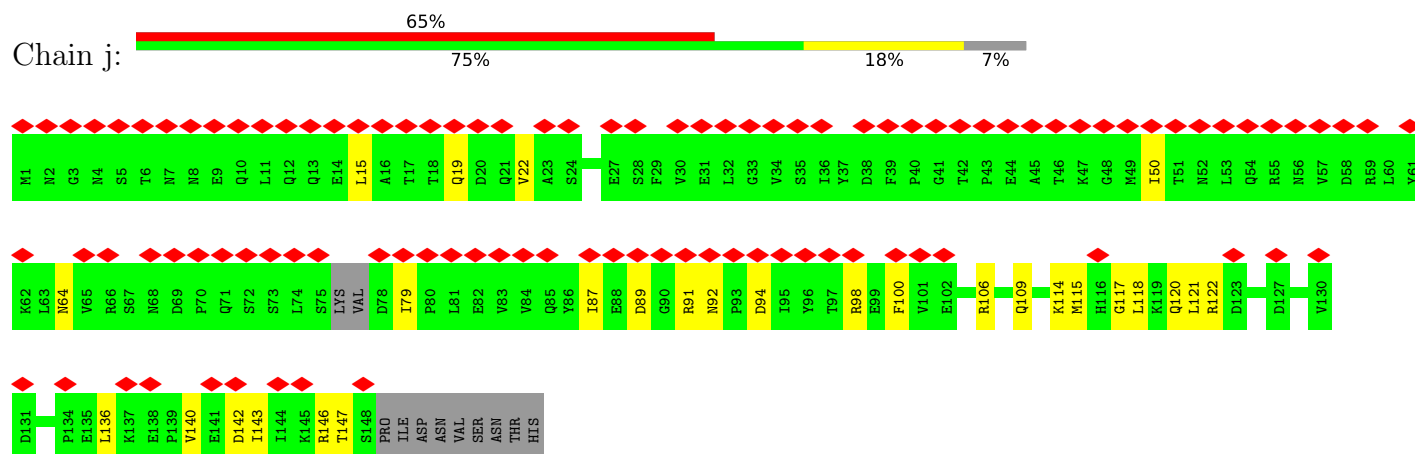
• Molecule 21: Mediator of RNA polymerase II transcription subunit 8



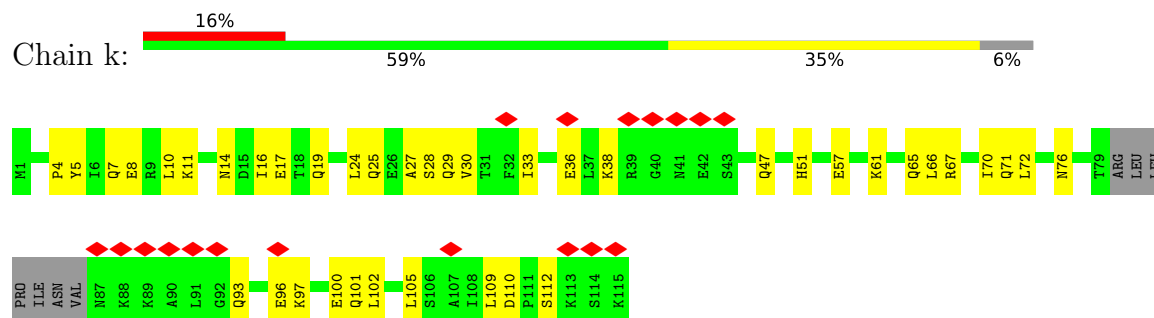
• Molecule 22: Mediator of RNA polymerase II transcription subunit 9



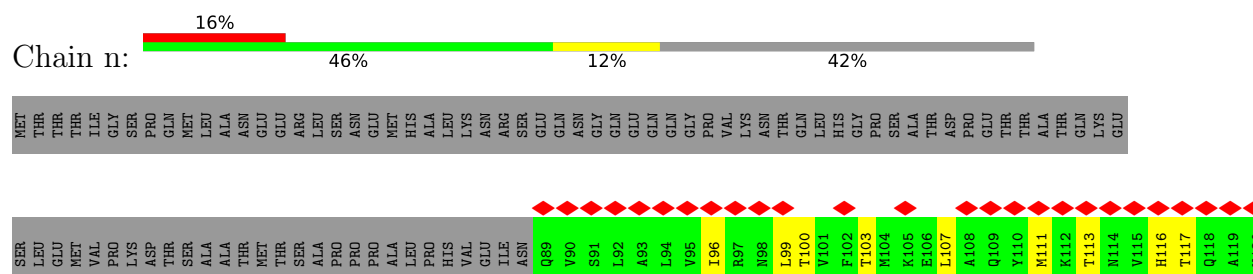
- Molecule 23: Mediator of RNA polymerase II transcription subunit 10

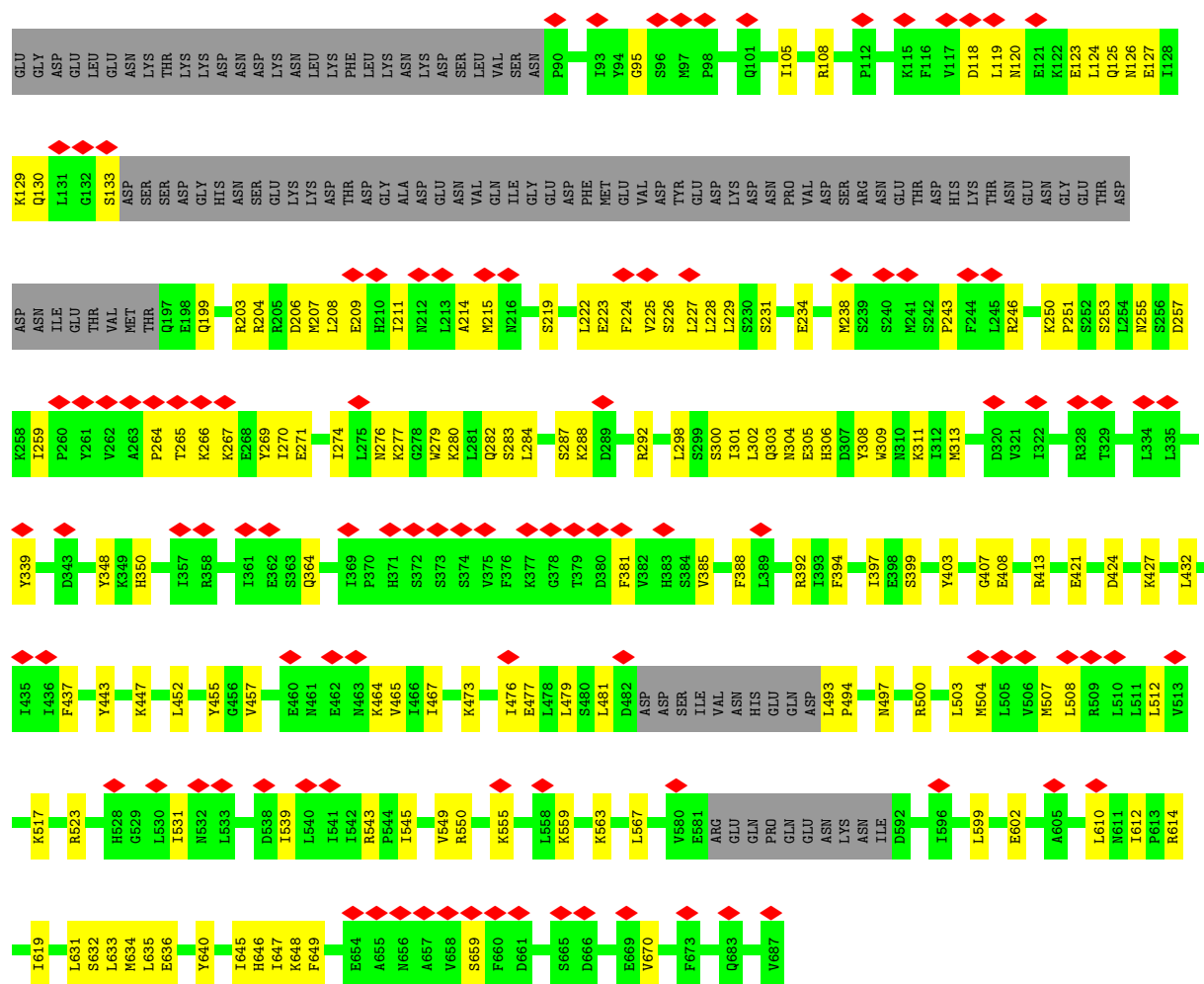


- Molecule 24: Mediator of RNA polymerase II transcription subunit 11

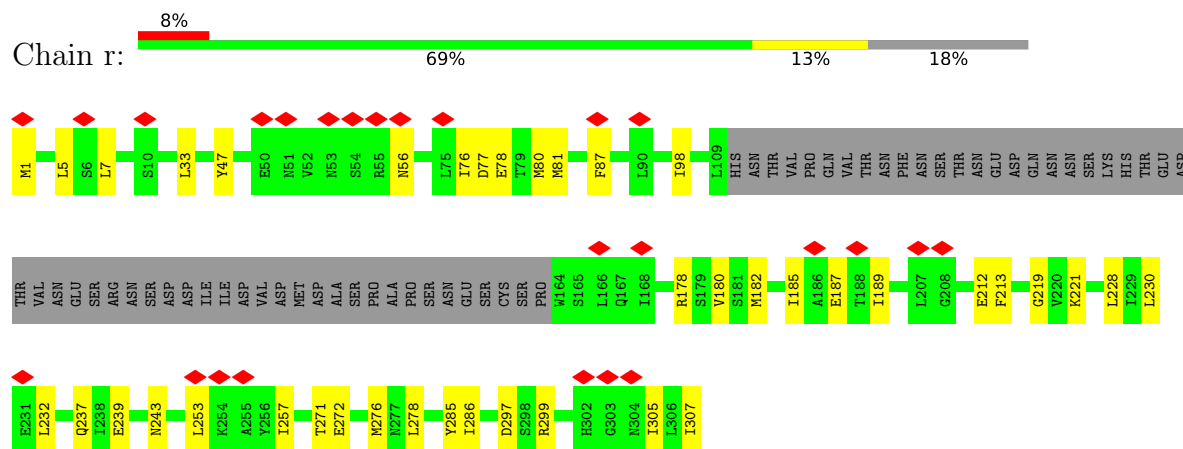


- Molecule 25: Mediator of RNA polymerase II transcription subunit 14

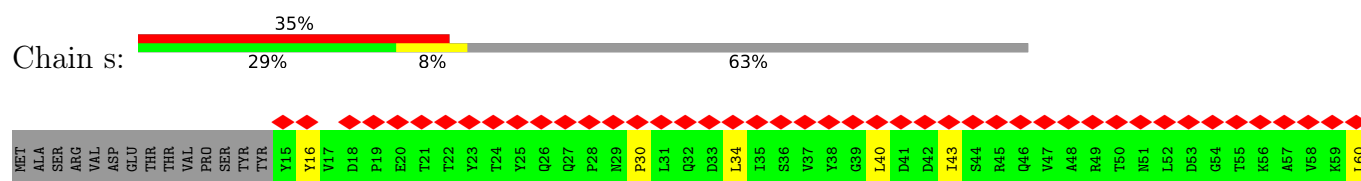


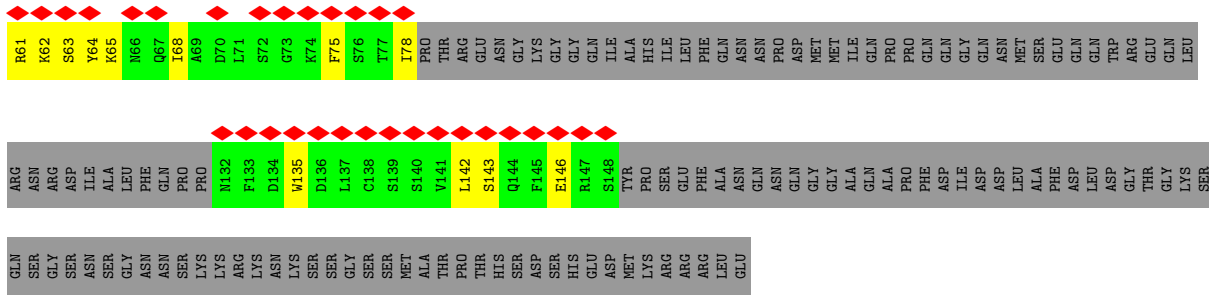


• Molecule 27: Mediator of RNA polymerase II transcription subunit 18

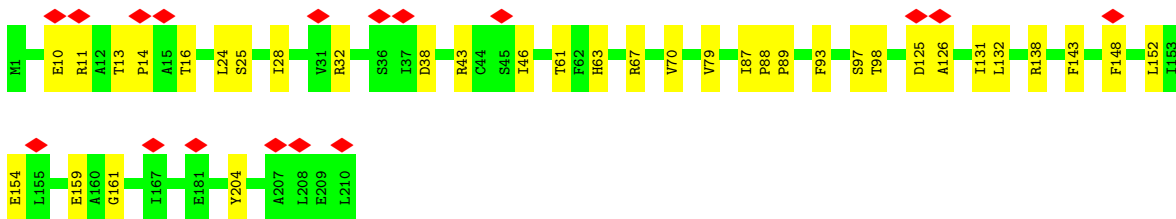
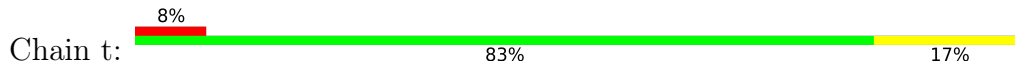


• Molecule 28: Mediator of RNA polymerase II transcription subunit 19





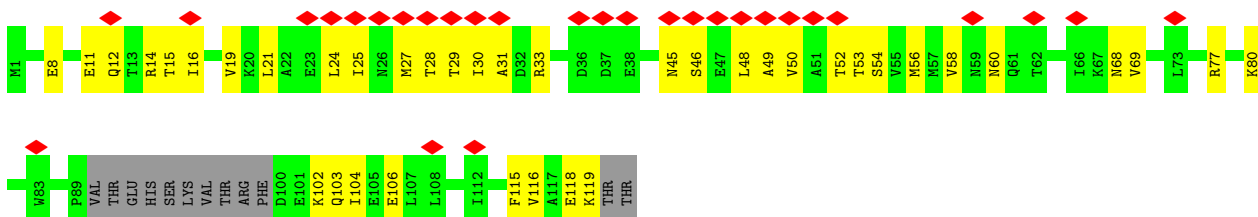
- Molecule 29: Mediator of RNA polymerase II transcription subunit 20



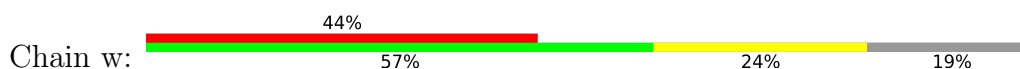
- Molecule 30: Mediator of RNA polymerase II transcription subunit 21

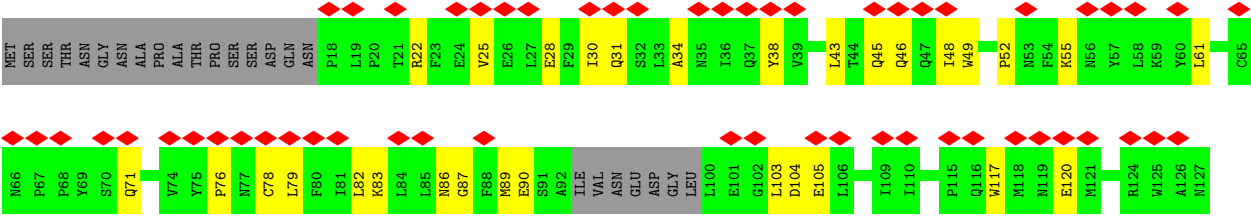


- Molecule 31: Mediator of RNA polymerase II transcription subunit 22



- Molecule 32: Mediator of RNA polymerase II transcription subunit 31





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91293	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size ($\text{\AA}$)	496.8, 496.8, 496.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.38, 1.38, 1.38	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	A	0.18	0/11632	0.35	0/15735
1	z	0.15	0/194	0.36	0/270
2	B	0.17	0/9520	0.35	2/12839 (0.0%)
3	C	0.17	0/2171	0.35	0/2941
4	D	0.10	0/1365	0.21	0/1831
5	E	0.13	0/1796	0.28	0/2416
6	F	0.16	0/709	0.31	0/956
7	G	0.13	0/1368	0.30	0/1844
8	H	0.15	0/1144	0.32	0/1548
9	I	0.13	0/961	0.35	0/1294
10	J	0.19	0/587	0.45	0/786
11	K	0.18	0/947	0.35	0/1279
12	L	0.12	0/346	0.27	0/457
13	M	0.14	0/267	0.27	0/362
14	P	0.11	0/886	0.24	0/1198
15	Q	0.11	0/1049	0.28	0/1413
16	S	0.13	0/1462	0.31	0/1973
17	a	0.67	0/3067	1.13	7/4148 (0.2%)
18	d	0.18	0/1405	0.51	0/1889
19	f	0.15	0/1440	0.35	0/1946
20	g	0.17	0/1434	0.41	1/1930 (0.1%)
21	h	0.16	0/1147	0.44	0/1552
22	i	0.21	0/720	0.54	0/965
23	j	0.13	0/1188	0.25	0/1604
24	k	0.17	0/885	0.44	0/1183
25	n	0.11	0/5226	0.28	0/7051
26	q	0.13	0/4245	0.33	0/5702
27	r	0.16	0/2030	0.33	0/2747
28	s	0.11	0/669	0.22	0/906
29	t	0.15	0/1635	0.32	0/2215
30	u	0.19	0/984	0.54	0/1317
31	v	0.18	0/873	0.46	0/1177
32	w	0.13	0/897	0.32	0/1219
All	All	0.21	0/64249	0.42	10/86693 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	278	GLN	CA-C-N	5.83	132.68	121.54
2	B	278	GLN	C-N-CA	5.83	132.68	121.54
20	g	16	PRO	CA-N-CD	-5.60	104.16	112.00
17	a	298	PRO	CA-C-N	5.45	127.43	120.56
17	a	298	PRO	C-N-CA	5.45	127.43	120.56
17	a	529	GLN	OE1-CD-NE2	-5.43	117.17	122.60
17	a	22	LYS	CA-C-N	5.12	124.79	119.56
17	a	22	LYS	C-N-CA	5.12	124.79	119.56
17	a	324	ASN	OD1-CG-ND2	-5.07	117.53	122.60
17	a	225	GLN	OE1-CD-NE2	-5.01	117.59	122.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11425	0	11482	211	0
1	z	184	0	163	6	0
2	B	9336	0	9341	213	0
3	C	2133	0	2096	37	0
4	D	1353	0	1352	21	0
5	E	1760	0	1788	23	0
6	F	697	0	720	7	0
7	G	1340	0	1357	23	0
8	H	1126	0	1094	13	0
9	I	943	0	906	17	0
10	J	578	0	593	31	0
11	K	929	0	939	12	0
12	L	344	0	367	11	0
13	M	263	0	273	3	0
14	P	861	0	819	22	0
15	Q	1033	0	1036	28	0
16	S	1436	0	1428	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	a	3008	0	2953	35	0
18	d	1388	0	1400	71	0
19	f	1407	0	1385	48	0
20	g	1409	0	1434	68	0
21	h	1126	0	1125	54	0
22	i	709	0	712	51	0
23	j	1173	0	1156	36	0
24	k	876	0	885	29	0
25	n	5139	0	5375	94	0
26	q	4182	0	4324	109	0
27	r	1995	0	2018	29	0
28	s	657	0	636	24	0
29	t	1609	0	1626	23	0
30	u	978	0	1005	52	0
31	v	869	0	881	43	0
32	w	871	0	857	20	0
All	All	63137	0	63526	1250	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 10.

All (1250) 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)
17:a:21:TYR:CE1	18:d:74:ILE:HG21	1.49	1.44
17:a:21:TYR:HE1	18:d:74:ILE:CG2	1.46	1.26
17:a:22:LYS:NZ	22:i:73:LEU:HD22	1.56	1.19
17:a:22:LYS:NZ	22:i:73:LEU:CD2	2.11	1.13
17:a:22:LYS:HD2	18:d:74:ILE:HD12	1.35	1.09
17:a:22:LYS:HZ3	22:i:73:LEU:CD2	1.69	1.00
17:a:22:LYS:HZ3	22:i:73:LEU:HD22	0.86	1.00
2:B:115:GLN:HB3	10:J:69:ARG:HG2	1.42	0.99
17:a:22:LYS:HD2	18:d:74:ILE:CD1	1.94	0.97
26:q:302:LEU:HG	26:q:306:HIS:HE1	1.29	0.94
17:a:21:TYR:CE1	18:d:74:ILE:CG2	2.31	0.92
17:a:22:LYS:HZ2	22:i:73:LEU:HD21	1.35	0.89
17:a:22:LYS:HZ2	22:i:73:LEU:CD2	1.85	0.87
1:A:185:TRP:O	1:A:197:PRO:HA	1.77	0.84
30:u:5:LEU:HG	30:u:9:GLN:HE22	1.41	0.82
2:B:435:THR:HG21	2:B:442:PHE:HB3	1.61	0.81
4:D:162:ALA:HB2	21:h:42:GLN:HE21	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	1.64	0.80
15:Q:122:LEU:HD12	15:Q:222:CYS:HB3	1.63	0.79
1:A:1217:LYS:HD2	1:A:1224:LEU:HD23	1.64	0.79
7:G:46:LEU:HD11	7:G:79:PHE:HB2	1.63	0.78
26:q:280:LYS:HB3	31:v:30:ILE:HG13	1.65	0.78
20:g:138:SER:HA	23:j:118:LEU:HD13	1.64	0.78
26:q:302:LEU:HG	26:q:306:HIS:CE1	2.17	0.78
1:A:800:VAL:HG22	1:A:812:GLU:HB2	1.66	0.77
26:q:302:LEU:O	26:q:306:HIS:ND1	2.15	0.77
1:A:346:ASP:OD1	2:B:1106:ARG:NH1	2.18	0.77
1:A:445:ASN:HD22	1:A:455:MET:HE2	1.50	0.77
23:j:91:ARG:HB3	28:s:61:ARG:HB3	1.68	0.75
2:B:118:ARG:NH1	2:B:207:GLY:O	2.20	0.75
1:A:849:MET:HE3	1:A:1061:GLY:HA2	1.68	0.75
15:Q:238:GLU:HA	15:Q:241:ARG:HD2	1.69	0.74
22:i:73:LEU:HD23	22:i:77:ARG:HE	1.52	0.74
18:d:97:LEU:HD13	18:d:100:ILE:HD11	1.70	0.74
22:i:105:ILE:HD12	22:i:115:LEU:HD11	1.69	0.73
18:d:53:LEU:HD22	22:i:98:LEU:HD12	1.69	0.73
15:Q:63:ARG:NH1	15:Q:214:ILE:O	2.20	0.73
22:i:123:GLN:O	22:i:127:HIS:ND1	2.22	0.73
2:B:788:ARG:NH1	10:J:70:ASP:OD1	2.21	0.73
24:k:19:GLN:HE22	24:k:61:LYS:HG3	1.53	0.72
17:a:22:LYS:NZ	22:i:73:LEU:HD21	1.93	0.72
2:B:496:ARG:NH2	2:B:540:SER:O	2.23	0.72
7:G:112:LYS:HA	7:G:115:MET:HE3	1.70	0.72
22:i:105:ILE:O	22:i:112:LYS:NZ	2.22	0.72
30:u:117:LYS:O	30:u:121:HIS:ND1	2.23	0.72
2:B:114:PRO:HG2	10:J:69:ARG:HD3	1.71	0.72
14:P:377:SER:OG	14:P:385:THR:OG1	2.08	0.71
27:r:1:MET:HA	27:r:185:ILE:O	1.89	0.71
19:f:25:GLU:HA	19:f:99:MET:HE1	1.70	0.71
2:B:276:ILE:HG12	2:B:334:ILE:HD12	1.70	0.71
21:h:146:GLU:HG3	21:h:150:GLN:HE22	1.55	0.71
7:G:81:PRO:HD3	7:G:106:MET:HE1	1.72	0.71
3:C:145:CYS:SG	3:C:146:LYS:N	2.64	0.71
27:r:228:LEU:HD21	27:r:278:LEU:HD22	1.73	0.71
30:u:94:ILE:O	30:u:98:GLN:NE2	2.23	0.71
22:i:92:GLY:HA2	22:i:95:ARG:HE	1.55	0.70
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.72	0.70
18:d:45:ASP:OD2	18:d:83:ASN:ND2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:q:119:LEU:HD21	26:q:124:LEU:HD13	1.73	0.70
2:B:288:ALA:HA	2:B:327:ARG:HG3	1.73	0.70
2:B:189:LEU:HB3	2:B:194:GLU:HB2	1.74	0.70
2:B:651:LEU:O	2:B:654:ARG:NH2	2.24	0.70
2:B:703:ILE:HG22	2:B:740:HIS:HB2	1.74	0.70
16:S:298:THR:HG23	16:S:305:ARG:HG2	1.73	0.70
10:J:37:SER:OG	10:J:47:ARG:NH2	2.24	0.70
3:C:54:ASN:ND2	3:C:60:ASP:OD1	2.23	0.70
17:a:21:TYR:HE1	18:d:74:ILE:HG21	0.60	0.70
1:A:41:MET:HA	1:A:48:ALA:HA	1.74	0.69
1:A:1084:PHE:O	1:A:1087:ALA:HB3	1.92	0.69
19:f:46:ILE:HD13	19:f:106:GLU:HG3	1.74	0.69
2:B:118:ARG:NE	10:J:70:ASP:OD2	2.23	0.69
2:B:261:ARG:O	2:B:267:ARG:NH2	2.25	0.69
26:q:421:GLU:HG2	26:q:427:LYS:HD3	1.74	0.69
25:n:484:LEU:HD22	25:n:491:GLU:HG2	1.74	0.69
20:g:111:ASN:OD1	20:g:115:LYS:NZ	2.25	0.69
1:A:1081:LEU:HD13	16:S:287:ARG:HA	1.73	0.68
31:v:12:GLN:HE22	31:v:16:ILE:HD11	1.58	0.68
2:B:810:GLU:OE1	2:B:815:ARG:NH1	2.26	0.68
1:A:535:THR:O	1:A:575:LYS:NZ	2.24	0.68
9:I:92:ARG:HB3	9:I:95:THR:HG23	1.75	0.68
20:g:23:PHE:HA	20:g:27:ASN:HD22	1.58	0.68
23:j:91:ARG:N	28:s:63:SER:OG	2.24	0.68
31:v:11:GLU:HA	31:v:14:ARG:HG2	1.75	0.68
4:D:168:LYS:HD2	1:z:1:PRO:H3	1.59	0.67
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.24	0.67
3:C:92:CYS:HB2	3:C:95:CYS:H	1.57	0.67
20:g:143:MET:HE2	20:g:146:ARG:HD2	1.77	0.67
29:t:32:ARG:HD2	29:t:131:ILE:HD11	1.74	0.67
1:A:40:THR:HG22	1:A:53:LEU:HB2	1.75	0.67
2:B:34:ILE:HG21	2:B:747:MET:HE3	1.76	0.67
30:u:90:GLN:HA	30:u:93:LYS:HG2	1.76	0.67
21:h:146:GLU:O	21:h:150:GLN:NE2	2.28	0.67
2:B:604:ARG:NH1	2:B:613:VAL:O	2.28	0.67
16:S:166:HIS:HE1	16:S:170:SER:HB3	1.60	0.67
1:A:393:ARG:NH1	1:A:421:ALA:O	2.27	0.66
1:A:440:ASP:OD1	1:A:498:ARG:NH1	2.27	0.66
2:B:278:GLN:OE1	2:B:337:ARG:NH1	2.27	0.66
17:a:312:ILE:HD11	17:a:565:VAL:HG22	1.76	0.66
14:P:132:ASP:O	14:P:359:ASN:ND2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:g:166:ARG:O	20:g:169:GLN:N	2.28	0.66
1:A:758:ILE:O	1:A:762:SER:OG	2.11	0.66
27:r:285:TYR:HB3	27:r:286:ILE:HD12	1.77	0.66
1:A:1260:LEU:HA	1:A:1263:ILE:HG12	1.77	0.66
2:B:786:ASN:O	2:B:967:ARG:NH1	2.23	0.66
4:D:39:ASN:HB2	7:G:75:ARG:HH22	1.60	0.66
21:h:39:ARG:HH11	21:h:79:VAL:HG22	1.60	0.66
30:u:68:LEU:O	30:u:71:ARG:HG3	1.96	0.65
1:A:779:PHE:HE2	1:A:785:PRO:HG3	1.62	0.65
2:B:264:SER:O	2:B:267:ARG:NH1	2.27	0.65
2:B:822:ASN:O	10:J:48:ARG:NH1	2.29	0.65
1:A:229:SER:OG	1:A:1414:ALA:O	2.14	0.65
18:d:167:PRO:HG2	18:d:170:PHE:HB2	1.78	0.65
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.78	0.65
29:t:13:THR:HG1	29:t:16:THR:HG1	1.40	0.65
2:B:264:SER:OG	2:B:267:ARG:NH2	2.27	0.65
14:P:375:LEU:HB2	14:P:387:ILE:HB	1.78	0.65
17:a:103:ILE:HD11	17:a:191:ASN:HB3	1.79	0.65
2:B:994:TYR:HB2	2:B:999:MET:HE3	1.78	0.65
21:h:51:ARG:HG3	26:q:215:MET:HE1	1.79	0.65
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.30	0.65
5:E:78:LEU:HD13	5:E:107:THR:HG23	1.78	0.65
14:P:129:PRO:HG2	15:Q:61:LEU:HD21	1.79	0.65
14:P:130:VAL:HG23	14:P:131:THR:HG23	1.77	0.65
15:Q:67:GLN:HB3	15:Q:219:CYS:HB3	1.79	0.65
18:d:33:SER:O	18:d:37:LEU:HG	1.97	0.64
2:B:276:ILE:HG23	2:B:337:ARG:HE	1.62	0.64
10:J:13:VAL:O	10:J:17:LYS:NZ	2.28	0.64
14:P:108:LYS:HD3	15:Q:84:ARG:HB3	1.79	0.64
19:f:100:TYR:HA	19:f:103:LEU:HD12	1.78	0.64
32:w:34:ALA:HB2	32:w:78:CYS:HB3	1.78	0.64
23:j:118:LEU:HD23	23:j:121:LEU:HD12	1.80	0.64
25:n:386:PHE:HE1	25:n:464:ILE:HG12	1.62	0.64
2:B:887:HIS:NE2	13:M:36:GLU:O	2.31	0.64
1:A:830:LYS:HD3	1:A:1080:THR:HB	1.79	0.64
2:B:91:SER:HB3	2:B:135:ARG:HH22	1.63	0.64
7:G:108:VAL:HG22	7:G:159:ALA:HB3	1.79	0.64
18:d:114:ILE:HG23	20:g:206:ILE:HD13	1.79	0.64
16:S:163:GLU:O	16:S:215:LYS:NZ	2.30	0.64
2:B:354:ASP:OD1	2:B:357:GLN:NE2	2.30	0.64
25:n:290:THR:HB	25:n:297:LEU:HD23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:LYS:HB2	9:I:4:PHE:HZ	1.63	0.63
2:B:872:GLU:HG3	2:B:916:THR:HG22	1.79	0.63
25:n:113:THR:O	25:n:117:THR:OG1	2.13	0.63
2:B:955:THR:HG22	12:L:55:ILE:HA	1.81	0.63
26:q:397:ILE:HG22	26:q:399:SER:H	1.64	0.63
1:A:184:SER:HB2	1:A:197:PRO:HB2	1.79	0.63
2:B:986:GLN:OE1	2:B:1020:ARG:NH1	2.31	0.63
21:h:39:ARG:HD2	21:h:79:VAL:HA	1.79	0.63
24:k:25:GLN:O	24:k:28:SER:OG	2.12	0.63
24:k:67:ARG:NH1	24:k:71:GLN:OE1	2.32	0.63
2:B:1152:MET:HE1	2:B:1195:HIS:HB3	1.80	0.63
20:g:189:ILE:HG12	30:u:108:LYS:HE3	1.80	0.63
21:h:37:ARG:HG2	26:q:225:VAL:HG13	1.80	0.63
22:i:137:ARG:HH21	22:i:140:LEU:HD12	1.64	0.63
2:B:69:LEU:HD21	2:B:429:PHE:HB2	1.79	0.62
20:g:112:TYR:HA	20:g:115:LYS:HE2	1.81	0.62
18:d:189:ARG:NH1	20:g:12:LEU:O	2.33	0.62
26:q:455:TYR:HB3	26:q:550:ARG:HH12	1.62	0.62
1:A:830:LYS:HB3	1:A:1080:THR:HG21	1.81	0.62
1:A:716:ASP:OD2	1:A:720:ARG:NH2	2.32	0.62
1:A:757:ASN:HD22	2:B:1021:MET:HE2	1.64	0.62
1:A:1154:TYR:HB2	9:I:43:VAL:HG22	1.80	0.62
16:S:169:GLN:O	16:S:173:HIS:ND1	2.29	0.62
19:f:177:THR:HG23	26:q:214:ALA:HB1	1.82	0.62
25:n:414:ARG:NH1	25:n:415:TYR:O	2.32	0.62
23:j:15:LEU:HD13	25:n:152:ARG:HA	1.80	0.62
32:w:43:LEU:HD23	32:w:103:LEU:HB2	1.82	0.62
19:f:189:TYR:HA	19:f:192:ILE:HD12	1.82	0.62
17:a:22:LYS:HB3	22:i:77:ARG:HD3	1.81	0.62
20:g:177:LEU:HA	20:g:180:GLU:HG2	1.82	0.62
32:w:43:LEU:HB3	32:w:103:LEU:HD13	1.81	0.62
24:k:24:LEU:HD11	31:v:69:VAL:HG11	1.81	0.61
30:u:72:GLN:HG3	30:u:75:LYS:HE3	1.82	0.61
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.81	0.61
1:A:757:ASN:O	1:A:761:MET:HG3	1.99	0.61
1:A:840:ARG:NH1	1:A:1384:VAL:O	2.30	0.61
1:A:1339:LEU:HD23	5:E:144:ILE:HG23	1.81	0.61
2:B:289:LEU:HD22	2:B:371:GLU:OE2	2.00	0.61
19:f:44:GLN:HG3	19:f:48:MET:HE1	1.81	0.61
21:h:73:LEU:HG	31:v:56:MET:SD	2.39	0.61
26:q:539:ILE:O	26:q:543:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1083:THR:HG23	1:A:1097:GLY:HA3	1.82	0.61
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.81	0.61
8:H:8:ASP:OD1	8:H:9:ILE:N	2.33	0.61
1:A:352:VAL:HG23	1:A:467:THR:HG22	1.82	0.61
2:B:1082:MET:HE2	3:C:190:ASP:HB2	1.82	0.61
3:C:35:ARG:NH1	11:K:40:HIS:HB2	2.16	0.61
23:j:91:ARG:HB3	28:s:62:LYS:H	1.66	0.61
32:w:86:ASN:O	32:w:89:MET:HG3	2.00	0.61
20:g:128:LEU:HD13	23:j:136:LEU:HD12	1.83	0.61
1:A:1173:HIS:HA	1:A:1176:LEU:HB2	1.83	0.60
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.83	0.60
18:d:185:GLU:OE2	18:d:189:ARG:NH1	2.33	0.60
25:n:498:VAL:HG22	25:n:516:LYS:HG2	1.83	0.60
1:A:1348:LEU:HD21	1:A:1375:MET:HE3	1.83	0.60
16:S:153:LEU:HD21	16:S:179:GLU:HB3	1.82	0.60
17:a:177:GLN:HE22	17:a:235:GLN:CG	2.14	0.60
2:B:586:TRP:NE1	2:B:588:GLY:O	2.34	0.60
19:f:129:ARG:HH12	19:f:149:PRO:HA	1.66	0.60
26:q:549:VAL:HG22	31:v:119:LYS:HD2	1.83	0.60
1:A:1207:LEU:HD11	1:A:1212:VAL:HG11	1.82	0.60
2:B:898:LEU:O	12:L:58:LYS:NZ	2.34	0.60
24:k:96:GLU:OE2	24:k:97:LYS:NZ	2.26	0.60
1:A:182:VAL:HG22	1:A:201:VAL:HG12	1.84	0.60
9:I:19:ASP:O	9:I:23:ASN:N	2.35	0.60
21:h:98:LEU:HB2	21:h:101:PHE:HB2	1.82	0.60
1:A:441:PRO:HG2	1:A:498:ARG:HG2	1.84	0.60
2:B:63:ILE:HD13	2:B:95:ILE:HD11	1.82	0.60
15:Q:104:ILE:HB	15:Q:122:LEU:HB2	1.84	0.60
1:A:416:ARG:NH2	27:r:56:ASN:OD1	2.35	0.60
14:P:141:ARG:NH1	14:P:345:GLU:O	2.35	0.60
31:v:25:ILE:O	31:v:29:THR:HG22	2.01	0.60
7:G:163:ILE:HG22	7:G:168:LEU:HD22	1.84	0.59
1:A:1125:ALA:HB1	1:A:1303:GLU:HG3	1.84	0.59
26:q:612:ILE:O	26:q:614:ARG:NH1	2.34	0.59
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.84	0.59
19:f:10:GLN:NE2	1:z:20:THR:OG1	2.35	0.59
5:E:20:LYS:HE3	5:E:34:GLU:HG2	1.84	0.59
18:d:95:ARG:HB3	18:d:99:LYS:NZ	2.16	0.59
22:i:101:CYS:O	22:i:105:ILE:HG12	2.02	0.59
24:k:93:GLN:O	24:k:96:GLU:HG3	2.03	0.59
2:B:862:GLN:OE1	2:B:957:ASN:ND2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:TYR:HB3	2:B:149:TYR:HB3	1.85	0.59
2:B:787:VAL:HG11	10:J:68:LYS:H	1.67	0.59
3:C:12:GLU:HB2	3:C:19:ASP:HB3	1.85	0.59
12:L:31:CYS:HB3	12:L:36:SER:H	1.67	0.59
2:B:1090:THR:HG22	2:B:1091:TYR:H	1.68	0.59
7:G:137:ILE:HG21	7:G:143:ILE:HD12	1.85	0.59
25:n:508:VAL:HG12	25:n:681:GLU:HB3	1.85	0.59
16:S:131:PRO:O	16:S:136:ASN:ND2	2.35	0.59
20:g:155:LEU:HD23	20:g:158:ILE:HD12	1.84	0.59
26:q:464:LYS:NZ	26:q:477:GLU:OE2	2.35	0.59
1:A:1195:LEU:HB3	1:A:1197:LEU:HD21	1.84	0.59
10:J:41:LEU:HD22	10:J:46:CYS:HB3	1.85	0.59
32:w:76:PRO:O	32:w:79:LEU:HB2	2.02	0.59
30:u:101:LEU:HA	30:u:104:VAL:HG12	1.85	0.58
2:B:874:PHE:HD2	2:B:962:LYS:HD2	1.67	0.58
2:B:254:LEU:HD22	2:B:361:LEU:HD11	1.84	0.58
1:A:241:VAL:HG22	1:A:266:LEU:HD21	1.86	0.58
30:u:110:GLU:HA	30:u:113:LYS:HG2	1.85	0.58
31:v:24:LEU:HD23	31:v:27:MET:HE2	1.86	0.58
2:B:431:TYR:HA	2:B:434:ARG:HD2	1.85	0.58
2:B:1120:GLU:O	2:B:1124:ARG:NH2	2.36	0.58
3:C:163:ILE:HG13	3:C:165:LYS:H	1.68	0.58
18:d:139:ASN:O	18:d:142:LEU:HG	2.04	0.58
19:f:108:MET:SD	19:f:133:ARG:NH1	2.77	0.58
2:B:950:ASP:OD2	2:B:967:ARG:NH2	2.33	0.58
26:q:634:MET:SD	26:q:646:HIS:HB3	2.44	0.58
1:A:423:ASP:O	1:A:425:GLN:NE2	2.36	0.58
25:n:502:GLN:HB3	25:n:510:MET:HE3	1.86	0.58
24:k:24:LEU:HD21	31:v:69:VAL:HG21	1.86	0.58
2:B:194:GLU:OE1	10:J:69:ARG:HB2	2.04	0.57
2:B:956:THR:OG1	12:L:54:ARG:NH2	2.36	0.57
26:q:392:ARG:HG2	26:q:408:GLU:HG3	1.85	0.57
18:d:97:LEU:HD12	22:i:125:ILE:HG22	1.85	0.57
26:q:500:ARG:HD2	31:v:118:GLU:HG3	1.86	0.57
29:t:28:ILE:HA	29:t:132:LEU:HD23	1.86	0.57
1:A:1191:TRP:CD1	1:A:1260:LEU:HD21	2.39	0.57
1:A:1211:GLN:HE22	1:A:1215:ARG:HH21	1.50	0.57
11:K:100:ALA:O	11:K:104:ASN:ND2	2.27	0.57
18:d:98:GLN:HB3	18:d:102:LYS:NZ	2.19	0.57
25:n:734:GLN:NE2	25:n:805:GLU:OE2	2.35	0.57
4:D:213:GLU:HB3	21:h:38:MET:HE3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:g:188:GLU:O	20:g:191:GLU:HG3	2.04	0.57
30:u:5:LEU:O	30:u:9:GLN:NE2	2.37	0.57
1:A:1153:TYR:OH	9:I:45:ARG:NH1	2.37	0.57
25:n:661:GLN:OE1	25:n:666:ASN:ND2	2.35	0.57
2:B:797:TYR:HE1	2:B:854:LEU:HG	1.69	0.57
25:n:171:THR:HA	25:n:174:MET:SD	2.45	0.57
1:A:118:HIS:O	1:A:123:ARG:NH2	2.38	0.57
2:B:34:ILE:HG12	2:B:542:MET:HE1	1.86	0.57
3:C:249:ASP:OD1	11:K:102:LYS:NZ	2.32	0.57
23:j:117:GLY:O	23:j:121:LEU:HG	2.04	0.57
25:n:772:ASP:O	25:n:776:SER:N	2.37	0.57
27:r:257:ILE:HD12	27:r:271:THR:HG23	1.86	0.57
2:B:333:PHE:HB3	2:B:337:ARG:HH22	1.68	0.57
25:n:652:GLU:OE1	25:n:654:ARG:NH2	2.38	0.56
1:A:779:PHE:HB3	2:B:699:GLU:OE2	2.05	0.56
1:A:1226:VAL:HG12	1:A:1228:TRP:HD1	1.70	0.56
2:B:603:LEU:HA	2:B:606:LYS:HG2	1.85	0.56
2:B:827:ILE:HG22	2:B:1014:PRO:HG3	1.88	0.56
2:B:896:ASP:OD2	12:L:29:TYR:OH	2.22	0.56
4:D:206:GLU:OE1	4:D:209:ARG:NH2	2.33	0.56
23:j:106:ARG:NH2	23:j:109:GLN:OE1	2.37	0.56
1:A:149:GLU:O	1:A:164:ARG:NE	2.36	0.56
19:f:197:SER:HA	31:v:77:ARG:HH22	1.70	0.56
22:i:68:HIS:HB3	22:i:97:ARG:HH11	1.70	0.56
2:B:1019:SER:HB3	16:S:292:PRO:HD3	1.88	0.56
32:w:46:GLN:OE1	32:w:49:TRP:NE1	2.38	0.56
1:A:993:LEU:HD22	1:A:1022:LEU:HD11	1.87	0.56
2:B:1002:THR:HG22	2:B:1072:MET:HG2	1.88	0.56
5:E:21:GLU:OE1	5:E:143:ASN:ND2	2.39	0.56
27:r:221:LYS:NZ	29:t:93:PHE:O	2.31	0.56
30:u:137:LYS:HD2	30:u:138:LYS:HE3	1.88	0.56
12:L:47:ARG:NH2	12:L:52:GLY:O	2.39	0.56
2:B:558:LEU:HD21	2:B:580:VAL:HG11	1.87	0.56
19:f:196:PRO:O	31:v:77:ARG:NH2	2.39	0.56
1:A:149:GLU:H	1:A:164:ARG:HH21	1.54	0.56
2:B:351:TYR:O	2:B:355:ILE:HG12	2.06	0.56
2:B:918:ILE:HD11	2:B:935:ARG:HB2	1.87	0.56
3:C:25:VAL:HG12	3:C:26:ASP:O	2.06	0.56
14:P:354:ASP:OD1	14:P:355:PHE:N	2.39	0.56
2:B:862:GLN:HB3	2:B:963:PHE:HD1	1.71	0.55
19:f:166:ILE:HG12	26:q:224:PHE:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ILE:O	1:A:134:ARG:NH2	2.38	0.55
3:C:92:CYS:HB2	3:C:95:CYS:N	2.21	0.55
1:A:172:PRO:HG3	1:A:185:TRP:NE1	2.21	0.55
27:r:187:GLU:OE1	29:t:98:THR:OG1	2.22	0.55
18:d:104:SER:OG	22:i:136:LYS:NZ	2.38	0.55
26:q:222:LEU:HA	26:q:225:VAL:HG12	1.89	0.55
30:u:135:ASN:O	30:u:139:SER:OG	2.19	0.55
1:A:1239:ARG:HD3	1:A:1241:ARG:HH21	1.71	0.55
7:G:163:ILE:HA	7:G:168:LEU:HD13	1.88	0.55
22:i:75:GLN:HG2	22:i:90:LEU:HD11	1.87	0.55
1:A:1148:ILE:HG13	9:I:49:ILE:HD11	1.88	0.55
4:D:167:LEU:HD21	4:D:214:LEU:HD11	1.87	0.55
6:F:144:GLU:HG2	6:F:146:TRP:HE1	1.71	0.55
14:P:100:GLU:HG3	15:Q:94:LYS:HD2	1.89	0.55
2:B:324:ILE:HG22	2:B:326:ASP:H	1.72	0.55
20:g:119:LEU:HD13	20:g:161:LEU:HD23	1.89	0.55
25:n:263:PRO:HD2	25:n:266:LEU:HD12	1.88	0.55
5:E:48:ASP:OD1	5:E:52:ARG:N	2.40	0.55
1:A:76:GLU:OE2	2:B:1159:ARG:NH2	2.28	0.55
3:C:165:LYS:HE2	11:K:9:LEU:HB3	1.89	0.55
19:f:200:VAL:HB	21:h:62:TRP:CE3	2.41	0.55
32:w:83:LYS:O	32:w:86:ASN:HB2	2.07	0.55
2:B:376:PHE:HD2	2:B:566:LEU:HG	1.72	0.55
7:G:85:GLU:O	7:G:147:ILE:N	2.36	0.55
21:h:156:THR:HG23	31:v:28:THR:HB	1.88	0.55
1:A:899:VAL:HG13	1:A:929:LEU:HD13	1.88	0.54
31:v:54:SER:O	31:v:58:VAL:HG23	2.06	0.54
32:w:30:ILE:HD11	32:w:61:LEU:HD22	1.89	0.54
2:B:978:ASP:OD2	2:B:1094:ARG:NH2	2.33	0.54
6:F:72:LYS:HB3	6:F:142:SER:HA	1.89	0.54
2:B:46:GLN:HG2	2:B:47:GLN:N	2.21	0.54
22:i:74:HIS:HA	22:i:77:ARG:HG2	1.90	0.54
25:n:530:THR:HG23	25:n:533:LEU:HD12	1.89	0.54
1:A:1209:MET:HE1	1:A:1236:LEU:HB3	1.87	0.54
4:D:162:ALA:HB2	21:h:42:GLN:NE2	2.20	0.54
1:A:1189:SER:HA	1:A:1244:ARG:HH22	1.72	0.54
1:A:1217:LYS:HZ3	1:A:1226:VAL:HG23	1.72	0.54
2:B:750:GLY:O	2:B:754:SER:OG	2.25	0.54
32:w:104:ASP:OD1	32:w:105:GLU:N	2.40	0.54
2:B:954:VAL:HG12	2:B:964:VAL:HG12	1.89	0.54
2:B:1204:PHE:HE2	2:B:1216:LEU:HD21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:h:42:GLN:HG3	21:h:75:GLN:NE2	2.23	0.54
25:n:275:ARG:NH2	26:q:118:ASP:OD1	2.40	0.54
30:u:72:GLN:HA	30:u:75:LYS:HG2	1.90	0.54
2:B:611:PRO:HG3	2:B:685:LEU:HD21	1.89	0.54
3:C:89:GLU:HB2	29:t:43:ARG:HH22	1.71	0.54
5:E:195:VAL:HG22	5:E:213:ILE:HG22	1.88	0.54
18:d:48:ARG:NH1	18:d:76:THR:HB	2.22	0.54
20:g:150:ASN:O	20:g:153:THR:OG1	2.15	0.54
1:A:1342:GLU:OE2	5:E:153:HIS:NE2	2.40	0.54
7:G:123:ALA:HA	7:G:128:PRO:HB3	1.89	0.54
16:S:149:ARG:NH2	16:S:179:GLU:OE1	2.41	0.54
18:d:45:ASP:HB3	18:d:80:LEU:HD23	1.89	0.54
19:f:169:ILE:HG12	21:h:116:LYS:HB3	1.90	0.54
25:n:161:VAL:HB	28:s:43:ILE:HD12	1.90	0.54
26:q:633:LEU:HD22	26:q:647:ILE:HG12	1.89	0.54
31:v:56:MET:HE3	31:v:60:ASN:HD21	1.73	0.54
1:A:675:THR:O	1:A:679:ILE:HG12	2.07	0.54
10:J:12:LYS:HG2	10:J:13:VAL:H	1.71	0.54
19:f:121:ARG:HH21	21:h:99:PRO:HA	1.72	0.54
24:k:100:GLU:OE2	24:k:101:GLN:NE2	2.41	0.54
26:q:465:VAL:HG12	26:q:476:ILE:HB	1.90	0.54
31:v:12:GLN:NE2	31:v:68:ASN:HB3	2.23	0.54
30:u:111:ALA:HA	30:u:114:LYS:NZ	2.24	0.53
1:A:1080:THR:HG22	1:A:1098:VAL:HG21	1.90	0.53
2:B:214:ALA:HB3	2:B:498:THR:HG22	1.90	0.53
4:D:168:LYS:HG3	4:D:177:VAL:HG11	1.91	0.53
2:B:1151:LEU:O	2:B:1155:SER:OG	2.26	0.53
9:I:55:THR:HG22	9:I:57:GLY:H	1.73	0.53
21:h:98:LEU:HD13	21:h:100:LYS:HE3	1.89	0.53
18:d:189:ARG:HH22	20:g:14:PRO:HD3	1.73	0.53
20:g:178:LEU:O	20:g:182:LEU:HD23	2.09	0.53
26:q:123:GLU:HA	26:q:126:ASN:HD22	1.73	0.53
26:q:211:ILE:HG13	26:q:215:MET:HE2	1.91	0.53
26:q:500:ARG:HE	31:v:115:PHE:HE1	1.56	0.53
2:B:328:GLU:N	2:B:328:GLU:OE1	2.42	0.53
15:Q:245:LYS:HG3	15:Q:246:LEU:HD12	1.91	0.53
25:n:515:LEU:HD11	25:n:524:PHE:HB3	1.89	0.53
25:n:586:ILE:O	25:n:622:GLN:NE2	2.42	0.53
30:u:110:GLU:HG3	30:u:113:LYS:NZ	2.24	0.53
3:C:244:VAL:O	3:C:248:ILE:HG13	2.08	0.53
8:H:36:CYS:HA	8:H:126:GLU:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:g:14:PRO:HD2	32:w:38:TYR:HE1	1.73	0.53
20:g:185:LYS:HE3	30:u:105:GLU:OE2	2.09	0.53
21:h:43:LEU:HD22	21:h:79:VAL:HG21	1.90	0.53
21:h:151:GLN:O	21:h:154:GLU:HG3	2.09	0.53
24:k:97:LYS:O	24:k:100:GLU:HG3	2.09	0.53
26:q:507:MET:HG3	26:q:545:ILE:HD11	1.90	0.53
1:A:1149:ALA:HB1	1:A:1151:GLU:CD	2.34	0.53
17:a:22:LYS:HD2	18:d:74:ILE:HD11	1.85	0.53
1:A:1242:VAL:O	1:A:1244:ARG:NH1	2.42	0.53
2:B:646:LEU:HB3	2:B:648:HIS:CE1	2.44	0.53
3:C:251:LEU:O	3:C:255:VAL:HG23	2.09	0.53
9:I:14:LEU:HB3	9:I:27:PHE:HB3	1.91	0.53
20:g:162:LEU:HD22	20:g:166:ARG:HH22	1.74	0.53
26:q:392:ARG:NH1	26:q:477:GLU:OE1	2.41	0.53
26:q:394:PHE:HB3	26:q:403:TYR:HB3	1.91	0.53
7:G:97:HIS:O	7:G:112:LYS:N	2.38	0.53
30:u:94:ILE:HG22	30:u:98:GLN:HE22	1.73	0.53
2:B:865:LYS:HB2	2:B:961:LEU:HD21	1.91	0.52
2:B:996:ARG:NH2	3:C:174:ALA:O	2.42	0.52
2:B:1053:GLU:O	2:B:1057:LYS:HG2	2.08	0.52
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.44	0.52
10:J:36:LEU:HD11	10:J:51:LEU:HD13	1.91	0.52
16:S:181:GLU:HA	16:S:184:LYS:HG2	1.90	0.52
25:n:489:PHE:HD2	25:n:499:LEU:HD13	1.74	0.52
1:A:860:LEU:HD21	1:A:1394:THR:HA	1.91	0.52
1:A:1193:LEU:HD22	1:A:1267:MET:HE1	1.90	0.52
26:q:455:TYR:O	26:q:550:ARG:NH2	2.33	0.52
15:Q:74:PRO:HD3	15:Q:224:VAL:HB	1.92	0.52
2:B:642:ASP:OD1	2:B:642:ASP:N	2.43	0.52
12:L:31:CYS:SG	12:L:32:ALA:N	2.82	0.52
26:q:199:GLN:HB2	26:q:203:ARG:HH21	1.74	0.52
18:d:57:VAL:HA	18:d:60:VAL:HG22	1.91	0.52
2:B:228:LYS:HE3	2:B:234:ILE:HG21	1.90	0.52
2:B:330:ALA:O	2:B:334:ILE:HG12	2.10	0.52
18:d:45:ASP:O	18:d:48:ARG:NH1	2.42	0.52
18:d:82:GLU:HA	18:d:85:LYS:HZ1	1.75	0.52
18:d:110:LYS:HA	18:d:113:LYS:NZ	2.24	0.52
18:d:132:GLU:O	18:d:135:GLU:HG3	2.09	0.52
22:i:72:SER:HB3	22:i:90:LEU:HD21	1.91	0.52
30:u:112:ILE:HA	30:u:115:LYS:HE2	1.91	0.52
1:A:1011:GLN:O	1:A:1015:VAL:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:34:TYR:HE1	9:I:36:GLU:HB2	1.75	0.52
2:B:198:ASP:OD2	2:B:202:TYR:OH	2.27	0.52
2:B:523:CYS:SG	2:B:750:GLY:N	2.75	0.52
15:Q:78:ALA:O	15:Q:82:ARG:HG2	2.09	0.52
26:q:305:GLU:HA	26:q:308:TYR:CD1	2.44	0.52
1:A:544:ASP:N	1:A:544:ASP:OD1	2.41	0.52
23:j:114:LYS:HZ1	25:n:176:VAL:HG11	1.74	0.51
2:B:124:TYR:HB2	2:B:204:ILE:HB	1.93	0.51
26:q:207:MET:SD	26:q:208:LEU:HD12	2.50	0.51
27:r:178:ARG:HD2	27:r:182:MET:HE3	1.91	0.51
2:B:784:ASN:O	10:J:68:LYS:HD2	2.10	0.51
17:a:312:ILE:HD11	17:a:565:VAL:CG2	2.40	0.51
18:d:94:TYR:HB2	22:i:122:TRP:HE1	1.75	0.51
18:d:138:LYS:HE2	18:d:141:ILE:HD12	1.93	0.51
20:g:107:ASN:HB2	30:u:91:LEU:HB3	1.91	0.51
20:g:125:SER:O	20:g:129:ASN:ND2	2.43	0.51
25:n:107:LEU:HD13	28:s:135:TRP:HH2	1.75	0.51
27:r:232:LEU:HG	27:r:253:LEU:HD12	1.93	0.51
29:t:70:VAL:HG22	29:t:79:VAL:HG22	1.91	0.51
2:B:115:GLN:OE1	10:J:67:GLU:HB3	2.10	0.51
2:B:787:VAL:HG21	10:J:68:LYS:H	1.74	0.51
2:B:788:ARG:HG3	10:J:68:LYS:HD3	1.92	0.51
26:q:457:VAL:HG13	26:q:467:ILE:HG13	1.93	0.51
1:A:41:MET:HE2	1:A:45:GLN:HA	1.93	0.51
2:B:297:ILE:O	2:B:301:ILE:HG12	2.11	0.51
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.92	0.51
2:B:345:LYS:O	2:B:349:ILE:HG12	2.10	0.51
26:q:243:PRO:HA	26:q:246:ARG:HD2	1.92	0.51
30:u:82:GLY:HA2	30:u:85:VAL:HB	1.93	0.51
3:C:260:LEU:HD12	29:t:14:PRO:HB3	1.92	0.51
30:u:88:GLU:HA	30:u:91:LEU:HD12	1.92	0.51
2:B:614:SER:OG	2:B:627:PHE:HB2	2.10	0.51
20:g:186:ARG:NH1	30:u:104:VAL:HG11	2.26	0.51
25:n:741:ASN:HD22	25:n:774:SER:HG	1.55	0.51
29:t:38:ASP:HB2	29:t:61:THR:HB	1.92	0.51
1:z:21:SER:H	1:z:22:PRO:CD	2.24	0.51
2:B:34:ILE:HG23	2:B:542:MET:HE3	1.93	0.51
2:B:192:LEU:HD22	10:J:69:ARG:NH2	2.25	0.51
17:a:22:LYS:HB3	22:i:77:ARG:CD	2.41	0.51
19:f:38:ASP:OD1	19:f:38:ASP:N	2.44	0.51
23:j:19:GLN:HG3	25:n:145:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:q:645:ILE:HD12	26:q:670:VAL:HG21	1.92	0.51
30:u:97:LEU:HG	30:u:100:LYS:HE3	1.93	0.51
1:A:216:VAL:HA	1:A:219:PHE:HD2	1.76	0.50
27:r:219:GLY:HA3	27:r:232:LEU:O	2.11	0.50
1:A:356:ASP:HB3	1:A:359:LEU:HD12	1.92	0.50
1:A:697:ALA:HB2	1:A:702:LEU:HD13	1.91	0.50
1:A:1197:LEU:HD11	1:A:1238:ILE:HD12	1.93	0.50
8:H:74:SER:HA	8:H:77:ARG:HB2	1.93	0.50
9:I:19:ASP:O	9:I:23:ASN:HA	2.11	0.50
17:a:21:TYR:CZ	18:d:74:ILE:CG2	2.93	0.50
18:d:95:ARG:HB3	18:d:99:LYS:HZ1	1.76	0.50
25:n:705:ILE:HA	25:n:715:ASN:HD21	1.76	0.50
1:A:270:LEU:O	1:A:274:ILE:HG23	2.12	0.50
1:A:663:SER:OG	1:A:664:THR:N	2.42	0.50
7:G:6:ASP:OD1	7:G:75:ARG:NH1	2.43	0.50
16:S:212:PRO:O	16:S:215:LYS:HG3	2.12	0.50
18:d:110:LYS:HA	18:d:113:LYS:HZ3	1.77	0.50
1:A:85:ASP:O	1:A:273:ASN:ND2	2.42	0.50
1:A:1226:VAL:HG13	1:A:1238:ILE:HG23	1.91	0.50
9:I:19:ASP:O	9:I:23:ASN:CA	2.60	0.50
17:a:177:GLN:HE22	17:a:235:GLN:HG2	1.77	0.50
19:f:183:SER:O	19:f:186:GLU:HG3	2.11	0.50
20:g:193:GLU:HA	20:g:196:CYS:SG	2.51	0.50
30:u:59:ILE:HD13	30:u:62:LEU:HD12	1.93	0.50
1:A:1285:MET:HE3	1:A:1286:LYS:H	1.76	0.50
20:g:31:LEU:HD22	20:g:65:LEU:HD13	1.94	0.50
27:r:230:LEU:HD21	27:r:253:LEU:HD11	1.92	0.50
29:t:138:ARG:HB2	29:t:154:GLU:HG3	1.93	0.50
1:A:780:VAL:HG12	2:B:699:GLU:OE2	2.12	0.50
1:A:1176:LEU:HD13	16:S:200:ARG:HG3	1.94	0.50
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.92	0.50
14:P:108:LYS:NZ	15:Q:84:ARG:O	2.43	0.50
15:Q:63:ARG:HB2	15:Q:66:ARG:HH22	1.77	0.50
17:a:274:PRO:HD3	17:a:344:TRP:CZ2	2.47	0.50
20:g:139:ILE:HD12	23:j:147:THR:HB	1.92	0.50
22:i:72:SER:OG	22:i:97:ARG:NH1	2.36	0.50
23:j:140:VAL:O	23:j:143:ILE:HB	2.11	0.50
30:u:22:THR:HG23	30:u:62:LEU:HD13	1.93	0.50
30:u:101:LEU:O	30:u:104:VAL:HG12	2.12	0.50
18:d:114:ILE:HG21	20:g:206:ILE:HG21	1.93	0.50
19:f:121:ARG:NH2	21:h:98:LEU:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1149:ALA:HB3	1:A:1196:GLU:HB3	1.93	0.50
18:d:43:TYR:O	18:d:46:LEU:HG	2.12	0.50
1:A:720:ARG:NH1	16:S:262:GLU:O	2.44	0.50
1:A:1342:GLU:CD	5:E:153:HIS:HE2	2.19	0.50
3:C:35:ARG:HH12	11:K:40:HIS:HB2	1.75	0.50
15:Q:135:PHE:HA	15:Q:214:ILE:HA	1.94	0.49
16:S:217:LYS:O	16:S:221:GLY:N	2.45	0.49
26:q:635:LEU:HD13	26:q:645:ILE:HG12	1.92	0.49
2:B:638:PHE:HE1	2:B:653:VAL:HG11	1.77	0.49
7:G:137:ILE:HD13	7:G:143:ILE:HD12	1.94	0.49
16:S:178:ILE:HG22	16:S:225:PRO:HB3	1.93	0.49
16:S:217:LYS:HB3	16:S:223:ILE:HG12	1.93	0.49
18:d:68:ASP:OD1	18:d:69:ILE:N	2.45	0.49
18:d:155:ASP:OD2	32:w:71:GLN:NE2	2.45	0.49
25:n:111:MET:HE1	28:s:142:LEU:HD11	1.93	0.49
25:n:812:LEU:HD22	25:n:832:LYS:HD3	1.94	0.49
1:A:420:ARG:HB3	1:A:424:ILE:HG13	1.93	0.49
19:f:154:TYR:OH	21:h:95:VAL:O	2.29	0.49
21:h:48:ARG:HD3	21:h:51:ARG:HH21	1.77	0.49
26:q:271:GLU:HA	26:q:274:ILE:HG22	1.93	0.49
30:u:25:TYR:O	30:u:29:ASN:HB2	2.12	0.49
30:u:117:LYS:O	30:u:120:ARG:HD3	2.12	0.49
18:d:126:LYS:HZ2	25:n:244:GLN:HG3	1.76	0.49
24:k:25:GLN:HG3	24:k:29:GLN:HE22	1.77	0.49
24:k:102:LEU:HD23	31:v:104:ILE:HD12	1.94	0.49
2:B:356:LEU:O	2:B:360:PHE:HB3	2.12	0.49
8:H:99:GLY:HA3	8:H:118:PHE:HD1	1.78	0.49
20:g:34:TYR:OH	20:g:63:ASP:OD1	2.30	0.49
22:i:73:LEU:CD2	22:i:77:ARG:HE	2.22	0.49
32:w:22:ARG:HA	32:w:25:VAL:HG22	1.93	0.49
2:B:192:LEU:HB3	10:J:69:ARG:CZ	2.42	0.49
2:B:787:VAL:HG11	10:J:68:LYS:N	2.28	0.49
7:G:39:THR:O	7:G:43:GLY:N	2.44	0.49
15:Q:240:ARG:HA	15:Q:243:ILE:HD12	1.94	0.49
22:i:111:THR:O	22:i:115:LEU:N	2.38	0.49
31:v:21:LEU:HA	31:v:24:LEU:HD12	1.94	0.49
1:A:1193:LEU:HD21	1:A:1195:LEU:HD21	1.94	0.49
18:d:145:ARG:HH22	18:d:153:LEU:HD22	1.78	0.49
20:g:210:LEU:HD13	22:i:140:LEU:HD22	1.94	0.49
26:q:266:LYS:O	26:q:270:ILE:HG12	2.12	0.49
1:A:420:ARG:HB3	1:A:423:ASP:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1191:TRP:HB2	1:A:1260:LEU:HD22	1.94	0.49
2:B:576:ASP:OD1	2:B:576:ASP:N	2.46	0.49
2:B:603:LEU:HD23	2:B:606:LYS:HD3	1.95	0.49
9:I:90:GLN:HE22	9:I:92:ARG:HB2	1.77	0.49
21:h:56:LYS:O	26:q:204:ARG:NH2	2.46	0.49
1:A:1199:ARG:NH2	1:A:1233:ASP:O	2.46	0.49
11:K:56:VAL:HG22	11:K:77:THR:HG22	1.94	0.49
20:g:134:ILE:HB	23:j:122:ARG:NH2	2.28	0.49
2:B:327:ARG:O	2:B:331:LEU:HG	2.12	0.49
2:B:825:VAL:HG22	2:B:1010:LEU:HD21	1.94	0.49
4:D:202:ILE:HD13	4:D:207:LEU:HD13	1.95	0.49
11:K:112:GLN:O	11:K:116:ALA:N	2.46	0.49
21:h:123:ASP:HA	21:h:126:MET:SD	2.53	0.49
1:A:450:LEU:O	1:A:1070:GLN:HG2	2.13	0.48
2:B:1171:VAL:HG21	2:B:1191:ILE:HG12	1.94	0.48
5:E:152:LYS:HG3	5:E:199:ILE:HB	1.95	0.48
19:f:11:TRP:CE3	1:z:22:PRO:HB2	2.48	0.48
20:g:190:ARG:HA	20:g:193:GLU:CD	2.37	0.48
23:j:98:ARG:HD3	28:s:60:LEU:HD12	1.95	0.48
24:k:30:VAL:HA	24:k:33:ILE:HG22	1.95	0.48
25:n:486:ARG:HH21	25:n:549:LEU:HD22	1.78	0.48
26:q:309:TRP:CH2	31:v:77:ARG:HG3	2.48	0.48
2:B:561:TRP:HE1	2:B:595:ARG:HH22	1.60	0.48
19:f:94:LEU:O	19:f:101:MET:HE3	2.12	0.48
23:j:114:LYS:HG3	23:j:115:MET:HE2	1.94	0.48
24:k:7:GLN:O	24:k:10:LEU:HG	2.13	0.48
1:A:785:PRO:HB2	2:B:703:ILE:HD11	1.95	0.48
4:D:37:GLN:HE21	4:D:47:LEU:HD13	1.78	0.48
18:d:192:MET:HE1	20:g:79:PHE:H	1.78	0.48
21:h:92:SER:HA	26:q:259:ILE:HG22	1.94	0.48
21:h:160:ARG:O	21:h:164:ARG:HG2	2.13	0.48
26:q:493:LEU:HD12	26:q:494:PRO:HD2	1.94	0.48
1:A:229:SER:HB2	1:A:1416:ALA:HB2	1.95	0.48
20:g:153:THR:OG1	28:s:16:TYR:OH	2.30	0.48
25:n:113:THR:HA	25:n:116:HIS:NE2	2.28	0.48
25:n:241:LEU:HD11	26:q:95:GLY:HA2	1.95	0.48
25:n:741:ASN:ND2	25:n:774:SER:OG	2.31	0.48
31:v:115:PHE:HA	31:v:118:GLU:HG2	1.95	0.48
2:B:269:ILE:HD13	2:B:382:ILE:HD11	1.95	0.48
4:D:51:ASN:HD22	4:D:181:GLY:HA3	1.79	0.48
20:g:176:MET:HA	20:g:179:GLU:CD	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:q:277:LYS:HE2	31:v:31:ALA:HB1	1.95	0.48
2:B:242:SER:HB3	2:B:363:HIS:HB3	1.94	0.48
2:B:365:THR:HG21	2:B:370:PHE:HB2	1.95	0.48
3:C:103:ALA:O	3:C:152:GLU:HG3	2.13	0.48
18:d:102:LYS:HA	18:d:105:GLU:CD	2.38	0.48
25:n:275:ARG:HE	25:n:300:VAL:HG11	1.78	0.48
1:A:870:GLU:OE1	5:E:202:SER:OG	2.26	0.48
1:A:894:GLU:OE1	1:A:933:TYR:OH	2.23	0.48
2:B:118:ARG:HH11	2:B:118:ARG:HA	1.79	0.48
21:h:153:ARG:HG2	31:v:33:ARG:NH1	2.29	0.48
31:v:46:SER:OG	31:v:49:ALA:HB3	2.14	0.48
1:A:1150:SER:HA	1:A:1195:LEU:HD23	1.95	0.48
1:A:1187:GLN:O	1:A:1244:ARG:NH1	2.46	0.48
2:B:101:MET:HA	2:B:112:LEU:H	1.77	0.48
2:B:171:PRO:HG2	2:B:461:LEU:HD12	1.95	0.48
18:d:38:SER:HA	18:d:43:TYR:CD2	2.49	0.48
22:i:66:ILE:HB	22:i:67:PRO:HD3	1.95	0.48
22:i:71:TYR:O	22:i:75:GLN:OE1	2.32	0.48
26:q:339:TYR:CE2	26:q:432:LEU:HB3	2.49	0.48
27:r:237:GLN:NE2	27:r:239:GLU:OE2	2.44	0.48
30:u:88:GLU:HB2	30:u:92:ARG:HH12	1.78	0.48
1:A:867:ILE:HD11	1:A:1000:LEU:HD11	1.96	0.48
2:B:334:ILE:HD13	2:B:337:ARG:HH21	1.78	0.48
4:D:39:ASN:ND2	4:D:43:GLU:OE2	2.47	0.48
21:h:37:ARG:HH22	26:q:229:LEU:HD22	1.78	0.48
1:A:362:ASP:HB3	1:A:508:PRO:HD3	1.95	0.48
13:M:23:THR:HG22	13:M:32:PRO:HG3	1.95	0.48
17:a:22:LYS:CD	18:d:74:ILE:CD1	2.80	0.48
18:d:45:ASP:HA	18:d:48:ARG:NE	2.28	0.48
18:d:82:GLU:HA	18:d:85:LYS:HE2	1.96	0.48
20:g:175:ILE:HG12	30:u:94:ILE:HD11	1.95	0.48
21:h:54:MET:SD	26:q:211:ILE:HG21	2.54	0.48
23:j:117:GLY:O	23:j:120:GLN:HG2	2.14	0.48
26:q:265:THR:HG23	26:q:267:LYS:H	1.79	0.48
2:B:190:TYR:CE2	10:J:62:ARG:HD2	2.48	0.47
2:B:539:LEU:HB3	2:B:543:SER:OG	2.14	0.47
23:j:91:ARG:HG2	28:s:61:ARG:HD3	1.95	0.47
23:j:94:ASP:HB3	28:s:60:LEU:HD22	1.95	0.47
2:B:289:LEU:HD22	2:B:371:GLU:CD	2.39	0.47
17:a:22:LYS:HD3	22:i:77:ARG:NE	2.29	0.47
18:d:42:LEU:HD12	18:d:45:ASP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:d:156:TYR:HA	18:d:159:LYS:HG2	1.96	0.47
31:v:8:GLU:HA	31:v:11:GLU:CD	2.40	0.47
31:v:15:THR:O	31:v:19:VAL:HG22	2.14	0.47
2:B:195:CYS:SG	2:B:782:LEU:HD22	2.54	0.47
25:n:253:VAL:HG11	25:n:276:ILE:HB	1.97	0.47
1:A:1155:ASP:HB2	1:A:1192:LEU:HB2	1.95	0.47
2:B:340:ALA:HB3	2:B:343:ILE:HD11	1.95	0.47
15:Q:56:SER:HA	15:Q:211:LYS:HB2	1.95	0.47
19:f:100:TYR:O	19:f:103:LEU:HB2	2.14	0.47
19:f:166:ILE:HD12	19:f:169:ILE:HD12	1.96	0.47
22:i:97:ARG:O	22:i:100:LEU:HG	2.14	0.47
25:n:415:TYR:OH	25:n:442:TRP:NE1	2.47	0.47
1:A:1193:LEU:HD23	1:A:1240:CYS:SG	2.55	0.47
1:A:1446:ASP:HB2	6:F:133:VAL:HG23	1.95	0.47
25:n:103:THR:HG23	25:n:137:LEU:HD22	1.95	0.47
26:q:219:SER:O	26:q:223:GLU:HG3	2.13	0.47
30:u:101:LEU:O	30:u:105:GLU:OE1	2.33	0.47
2:B:195:CYS:SG	2:B:783:THR:HG22	2.55	0.47
7:G:14:HIS:CG	7:G:15:PRO:HD2	2.50	0.47
19:f:16:TRP:CH2	19:f:30:TYR:HB2	2.49	0.47
20:g:155:LEU:HA	20:g:158:ILE:HD12	1.95	0.47
21:h:94:VAL:H	26:q:257:ASP:HB3	1.78	0.47
26:q:288:LYS:HD2	26:q:292:ARG:HH12	1.79	0.47
27:r:98:ILE:HG22	27:r:243:ASN:HD22	1.80	0.47
1:A:1193:LEU:HD22	1:A:1267:MET:CE	2.45	0.47
7:G:139:ILE:HG22	7:G:140:LYS:HG3	1.97	0.47
17:a:299:ILE:HG12	17:a:356:PHE:CE2	2.49	0.47
17:a:351:VAL:HG12	17:a:537:ILE:HD12	1.95	0.47
19:f:9:LEU:HD11	1:z:22:PRO:HG3	1.96	0.47
25:n:654:ARG:HD2	25:n:670:LEU:HD11	1.95	0.47
27:r:5:LEU:HD23	27:r:180:VAL:HG21	1.96	0.47
1:A:95:PHE:CE1	1:A:1414:ALA:HB2	2.50	0.47
1:A:199:LEU:HD23	1:A:199:LEU:H	1.80	0.47
2:B:333:PHE:HD1	2:B:337:ARG:HH12	1.63	0.47
18:d:125:LEU:HD22	30:u:119:LEU:HD13	1.97	0.47
20:g:142:ASP:OD1	20:g:142:ASP:N	2.48	0.47
25:n:187:LEU:HG	30:u:23:LEU:HD11	1.97	0.47
1:A:420:ARG:CB	1:A:424:ILE:HG13	2.44	0.47
2:B:561:TRP:NE1	2:B:595:ARG:HH12	2.13	0.47
18:d:45:ASP:O	18:d:48:ARG:HD3	2.15	0.47
21:h:156:THR:OG1	31:v:28:THR:O	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:j:87:ILE:C	28:s:63:SER:HB2	2.40	0.47
25:n:517:ILE:HG12	25:n:524:PHE:CE1	2.50	0.47
25:n:803:VAL:HG12	25:n:806:GLU:H	1.80	0.47
26:q:503:LEU:O	26:q:507:MET:HG2	2.15	0.47
1:A:1442:ASP:OD2	6:F:137:TYR:OH	2.24	0.47
26:q:206:ASP:O	26:q:209:GLU:HG3	2.15	0.47
27:r:47:TYR:HB3	29:t:46:ILE:HG21	1.97	0.47
1:A:826:ASP:OD1	1:A:830:LYS:HD2	2.15	0.46
1:A:903:ASN:O	1:A:907:THR:HG23	2.14	0.46
1:A:923:LEU:O	1:A:926:GLN:HG3	2.15	0.46
2:B:369:GLY:HA3	14:P:367:ALA:HB3	1.97	0.46
3:C:37:MET:HE1	3:C:232:VAL:HG21	1.98	0.46
16:S:201:ILE:O	16:S:205:ASN:ND2	2.48	0.46
25:n:250:ASN:ND2	25:n:274:GLY:H	2.13	0.46
25:n:304:LEU:HD11	25:n:343:LEU:HD11	1.97	0.46
30:u:105:GLU:O	30:u:109:ILE:HG13	2.15	0.46
14:P:119:LEU:HB3	14:P:395:PHE:CE2	2.49	0.46
20:g:70:MET:SD	20:g:71:PRO:HD2	2.55	0.46
20:g:132:GLU:O	20:g:136:VAL:HG23	2.14	0.46
25:n:151:THR:HA	25:n:154:ILE:HB	1.97	0.46
2:B:99:LYS:HD3	2:B:180:TYR:CE1	2.51	0.46
2:B:190:TYR:CD2	10:J:62:ARG:HD2	2.51	0.46
8:H:12:VAL:HG12	8:H:28:ALA:HB2	1.97	0.46
8:H:133:ASN:HD21	18:d:63:PHE:HZ	1.61	0.46
19:f:155:ILE:HG13	19:f:160:ILE:HD13	1.96	0.46
23:j:22:VAL:HG11	25:n:145:TYR:HB2	1.96	0.46
25:n:371:HIS:NE2	25:n:436:GLU:O	2.38	0.46
20:g:152:ARG:HD2	25:n:190:MET:HE3	1.98	0.46
20:g:188:GLU:O	20:g:192:ILE:HG13	2.15	0.46
26:q:105:ILE:O	26:q:108:ARG:HG3	2.15	0.46
26:q:413:ARG:HH12	26:q:481:LEU:HD21	1.79	0.46
31:v:53:THR:O	31:v:56:MET:HB3	2.16	0.46
1:A:834:THR:HG21	1:A:1077:THR:HA	1.98	0.46
4:D:209:ARG:HG3	21:h:31:GLN:HG3	1.97	0.46
17:a:22:LYS:CD	18:d:74:ILE:HD11	2.45	0.46
21:h:96:TYR:HE1	26:q:255:ASN:HB3	1.80	0.46
26:q:523:ARG:HE	26:q:531:ILE:HD13	1.81	0.46
30:u:85:VAL:HG13	30:u:89:GLU:OE2	2.15	0.46
2:B:71:LEU:HD23	2:B:88:TYR:HD2	1.81	0.46
32:w:52:PRO:HA	32:w:55:LYS:HE3	1.97	0.46
1:A:30:ILE:HD12	2:B:1170:THR:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:d:195:MET:SD	18:d:195:MET:N	2.89	0.46
25:n:660:SER:HB2	25:n:665:TRP:CZ3	2.51	0.46
25:n:800:ILE:HG12	25:n:812:LEU:HD21	1.96	0.46
27:r:77:ASP:OD1	27:r:77:ASP:N	2.46	0.46
2:B:309:GLN:O	2:B:313:MET:HG3	2.15	0.46
2:B:1076:HIS:O	3:C:31:ASN:ND2	2.47	0.46
5:E:29:PHE:HB2	5:E:65:THR:HG22	1.97	0.46
11:K:108:GLU:O	11:K:112:GLN:HG2	2.15	0.46
20:g:173:SER:HA	20:g:176:MET:HE3	1.98	0.46
23:j:100:PHE:HE2	25:n:166:LEU:HG	1.80	0.46
27:r:272:GLU:O	27:r:276:MET:HG2	2.16	0.46
32:w:82:LEU:O	32:w:86:ASN:N	2.46	0.46
1:A:148:CYS:SG	1:A:164:ARG:NH2	2.88	0.46
1:A:1428:VAL:HG13	2:B:1151:LEU:HD11	1.97	0.46
16:S:203:TYR:CE1	16:S:207:ILE:HD11	2.51	0.46
20:g:22:PHE:O	20:g:27:ASN:ND2	2.49	0.46
20:g:23:PHE:CE1	20:g:65:LEU:HG	2.50	0.46
21:h:130:ARG:HG2	21:h:130:ARG:HH11	1.81	0.46
26:q:123:GLU:O	26:q:126:ASN:HB2	2.15	0.46
1:A:1192:LEU:HD21	1:A:1239:ARG:HG2	1.98	0.45
2:B:592:ASN:OD1	2:B:595:ARG:HG2	2.17	0.45
8:H:83:GLN:OE1	8:H:83:GLN:HA	2.17	0.45
10:J:8:PHE:CD2	10:J:49:MET:HE1	2.51	0.45
15:Q:211:LYS:NZ	15:Q:212:THR:O	2.43	0.45
25:n:772:ASP:OD2	25:n:775:ASN:ND2	2.49	0.45
1:A:420:ARG:CB	1:A:423:ASP:HB2	2.46	0.45
1:A:1225:PHE:CG	1:A:1226:VAL:N	2.84	0.45
2:B:87:LYS:HB2	2:B:137:TYR:HB2	1.97	0.45
9:I:21:GLU:HG2	9:I:22:ASN:OD1	2.16	0.45
16:S:231:CYS:SG	16:S:235:ASP:HB3	2.56	0.45
20:g:27:ASN:HA	20:g:30:LYS:HG2	1.97	0.45
21:h:167:TYR:OH	21:h:173:LYS:NZ	2.50	0.45
23:j:87:ILE:HA	28:s:63:SER:HA	1.98	0.45
24:k:38:LYS:HG2	26:q:284:LEU:HD23	1.98	0.45
31:v:116:VAL:HG22	31:v:119:LYS:HZ3	1.80	0.45
1:A:371:ALA:HA	1:A:436:ILE:HD11	1.98	0.45
3:C:239:PRO:O	3:C:243:VAL:HG23	2.17	0.45
4:D:33:PHE:CE1	7:G:80:LYS:HD3	2.51	0.45
15:Q:97:ILE:HG12	15:Q:104:ILE:HD12	1.97	0.45
25:n:161:VAL:HG13	28:s:40:LEU:HB3	1.98	0.45
26:q:234:GLU:O	26:q:238:MET:HG2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.99	0.45
1:A:440:ASP:H	1:A:460:VAL:HG22	1.80	0.45
2:B:430:ARG:HE	2:B:434:ARG:NH2	2.15	0.45
7:G:38:CYS:HA	7:G:44:TYR:HA	1.99	0.45
20:g:23:PHE:CZ	20:g:64:TYR:HB2	2.51	0.45
20:g:147:LYS:O	20:g:150:ASN:HB2	2.15	0.45
1:A:308:ILE:HG23	1:A:311:GLN:HB2	1.98	0.45
1:A:567:LYS:NZ	8:H:90:ALA:O	2.43	0.45
2:B:874:PHE:O	12:L:42:ARG:NH2	2.47	0.45
4:D:173:HIS:HB3	4:D:176:GLU:HG3	1.99	0.45
14:P:120:LYS:HZ1	15:Q:132:GLU:HA	1.81	0.45
16:S:153:LEU:HD23	16:S:156:LEU:HD21	1.97	0.45
16:S:176:LYS:O	16:S:179:GLU:HG3	2.16	0.45
27:r:297:ASP:OD1	27:r:299:ARG:HG3	2.17	0.45
1:A:216:VAL:O	1:A:219:PHE:HB2	2.16	0.45
1:A:253:ASN:H	1:A:256:GLN:HB2	1.81	0.45
1:A:664:THR:HB	2:B:1014:PRO:HB3	1.99	0.45
1:A:1081:LEU:O	16:S:286:THR:HB	2.16	0.45
1:A:1342:GLU:HG3	5:E:151:PRO:HD2	1.99	0.45
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.97	0.45
3:C:148:ARG:HG2	3:C:149:LYS:H	1.80	0.45
4:D:188:ALA:HB2	4:D:208:GLU:HG3	1.98	0.45
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.98	0.45
20:g:118:GLU:O	20:g:121:LYS:HG3	2.17	0.45
21:h:37:ARG:HG3	26:q:226:SER:HA	1.99	0.45
23:j:142:ASP:O	23:j:146:ARG:N	2.48	0.45
1:A:993:LEU:HD13	1:A:1046:LEU:HD22	1.98	0.45
16:S:204:SER:O	16:S:208:SER:OG	2.32	0.45
20:g:195:VAL:O	20:g:198:GLN:HG3	2.17	0.45
24:k:66:LEU:O	24:k:70:ILE:HG13	2.17	0.45
25:n:146:VAL:HG21	28:s:64:TYR:CD2	2.51	0.45
25:n:146:VAL:HG21	28:s:64:TYR:HD2	1.81	0.45
25:n:251:LEU:HD11	30:u:130:VAL:HG21	1.98	0.45
1:A:1267:MET:HE2	1:A:1267:MET:HB3	1.55	0.45
2:B:561:TRP:CD1	2:B:595:ARG:HH12	2.33	0.45
8:H:103:LYS:HB3	8:H:115:TYR:CD1	2.52	0.45
18:d:53:LEU:CD2	22:i:98:LEU:HD12	2.42	0.45
19:f:132:ARG:NH1	19:f:134:THR:HG23	2.32	0.45
24:k:110:ASP:OD2	24:k:112:SER:OG	2.31	0.45
25:n:395:PHE:HA	25:n:399:ASN:HD22	1.82	0.45
30:u:80:LEU:HB2	30:u:83:VAL:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HG2	1:A:568:PRO:HA	1.99	0.45
1:A:801:GLU:OE1	1:A:801:GLU:N	2.40	0.45
1:A:1150:SER:HB2	1:A:1193:LEU:HD11	1.99	0.45
1:A:1166:ASP:O	1:A:1170:ILE:HG13	2.17	0.45
2:B:1090:THR:HG22	2:B:1091:TYR:N	2.32	0.45
3:C:176:ILE:HG22	3:C:232:VAL:HA	1.99	0.45
18:d:43:TYR:N	22:i:115:LEU:O	2.50	0.45
18:d:121:CYS:O	18:d:124:GLU:HG3	2.17	0.45
20:g:173:SER:HA	20:g:176:MET:HG2	1.97	0.45
30:u:8:LEU:HD23	30:u:12:LEU:HD23	1.99	0.45
2:B:118:ARG:HG3	10:J:70:ASP:HB2	1.98	0.45
2:B:234:ILE:HG23	2:B:259:TYR:HE1	1.82	0.45
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.52	0.45
5:E:135:PHE:HB3	5:E:140:LEU:HD21	1.99	0.45
18:d:148:ILE:HD12	18:d:153:LEU:HD11	1.97	0.45
25:n:764:GLU:HA	25:n:785:LYS:HE3	1.98	0.45
26:q:123:GLU:O	26:q:127:GLU:OE1	2.35	0.45
1:A:677:ARG:HA	1:A:677:ARG:NE	2.33	0.44
1:A:886:ILE:HG12	1:A:943:LEU:HB3	1.99	0.44
1:A:1195:LEU:HB2	1:A:1238:ILE:HB	1.98	0.44
2:B:1204:PHE:CE2	2:B:1216:LEU:HD21	2.52	0.44
20:g:210:LEU:HB2	22:i:140:LEU:HD13	1.99	0.44
24:k:27:ALA:HA	24:k:30:VAL:HG12	1.98	0.44
26:q:228:LEU:O	26:q:231:SER:OG	2.33	0.44
1:A:389:THR:O	1:A:393:ARG:HG2	2.17	0.44
1:A:444:PHE:HE2	1:A:470:LEU:HD11	1.82	0.44
1:A:1177:LEU:HD11	1:A:1227:ILE:HD11	1.97	0.44
1:A:1226:VAL:CG1	1:A:1238:ILE:HG23	2.48	0.44
3:C:143:LEU:HG	10:J:2:ILE:HD11	1.98	0.44
21:h:124:GLU:HB2	21:h:128:TYR:CZ	2.52	0.44
22:i:119:PRO:HA	22:i:122:TRP:HZ3	1.80	0.44
3:C:11:ARG:NH2	3:C:21:ILE:HD11	2.33	0.44
3:C:260:LEU:HD22	29:t:143:PHE:HZ	1.82	0.44
14:P:119:LEU:HB3	14:P:395:PHE:HE2	1.81	0.44
18:d:81:PHE:CD2	18:d:85:LYS:NZ	2.86	0.44
26:q:407:GLY:HA3	26:q:497:ASN:HB2	1.98	0.44
1:A:873:MET:HB2	1:A:1366:ARG:HH21	1.82	0.44
1:A:1224:LEU:HA	1:A:1242:VAL:HA	1.99	0.44
7:G:26:LEU:HD13	7:G:56:ILE:HD11	2.00	0.44
10:J:68:LYS:HG2	10:J:69:ARG:N	2.32	0.44
16:S:166:HIS:CE1	16:S:170:SER:HB3	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:g:120:ARG:CZ	30:u:77:ILE:HG21	2.48	0.44
24:k:14:ASN:HA	24:k:17:GLU:CD	2.42	0.44
25:n:539:LYS:O	25:n:542:ARG:NH1	2.51	0.44
26:q:264:PRO:HB3	26:q:269:TYR:OH	2.17	0.44
30:u:129:PHE:CZ	30:u:133:ILE:HD11	2.52	0.44
1:A:1209:MET:SD	1:A:1238:ILE:HD11	2.58	0.44
1:A:1257:ASP:HA	1:A:1260:LEU:HG	2.00	0.44
1:A:1340:GLY:HA2	5:E:182:ASP:OD1	2.18	0.44
2:B:122:LEU:O	2:B:207:GLY:N	2.51	0.44
11:K:14:GLU:OE1	11:K:14:GLU:HA	2.18	0.44
21:h:87:GLN:HG3	21:h:88:GLU:N	2.33	0.44
14:P:118:LEU:HB2	14:P:392:VAL:HA	1.99	0.44
17:a:278:ILE:HD11	17:a:341:ILE:HG12	1.98	0.44
25:n:526:PHE:HB2	25:n:529:PRO:HB3	1.98	0.44
26:q:277:LYS:CE	31:v:31:ALA:HB1	2.47	0.44
26:q:394:PHE:HB2	26:q:473:LYS:HB3	1.99	0.44
27:r:76:ILE:HG23	27:r:80:MET:HB2	1.99	0.44
2:B:63:ILE:HG13	2:B:64:CYS:N	2.32	0.44
2:B:953:LEU:HD11	12:L:55:ILE:HG23	1.98	0.44
3:C:67:LEU:HD23	3:C:70:ILE:HD12	1.99	0.44
18:d:87:LEU:HD11	22:i:114:LEU:HB3	2.00	0.44
19:f:116:VAL:HG13	19:f:129:ARG:HB3	2.00	0.44
21:h:123:ASP:O	21:h:127:LYS:HG2	2.17	0.44
25:n:99:LEU:HD23	25:n:144:LEU:HD22	1.99	0.44
25:n:257:ILE:HG21	25:n:276:ILE:HD13	2.00	0.44
26:q:300:SER:O	26:q:303:GLN:HG3	2.17	0.44
27:r:81:MET:SD	27:r:81:MET:N	2.91	0.44
1:A:894:GLU:O	1:A:898:ARG:HB3	2.18	0.44
1:A:1318:THR:HG22	5:E:142:VAL:HG23	2.00	0.44
6:F:144:GLU:HG2	6:F:146:TRP:NE1	2.33	0.44
23:j:121:LEU:HD21	30:u:59:ILE:HG13	2.00	0.44
24:k:16:ILE:HD11	24:k:65:GLN:HB3	1.99	0.44
26:q:280:LYS:HD3	31:v:30:ILE:O	2.17	0.44
27:r:212:GLU:HG2	27:r:213:PHE:HD2	1.82	0.44
30:u:94:ILE:CG2	30:u:98:GLN:HE22	2.30	0.44
30:u:117:LYS:C	30:u:121:HIS:HD1	2.20	0.44
1:A:65:LEU:HG	2:B:925:LEU:HD23	1.99	0.44
1:A:830:LYS:CD	1:A:1080:THR:HB	2.48	0.44
1:A:840:ARG:HG2	1:A:1384:VAL:HG12	1.99	0.44
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.18	0.44
1:A:1428:VAL:HG13	2:B:1151:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:8:ARG:HH21	14:P:124:LYS:HD2	1.83	0.44
14:P:120:LYS:NZ	15:Q:132:GLU:HA	2.33	0.44
20:g:68:PRO:HD3	32:w:22:ARG:HH22	1.82	0.44
21:h:48:ARG:NH2	26:q:215:MET:HB3	2.33	0.44
26:q:270:ILE:HG13	26:q:271:GLU:N	2.33	0.44
29:t:24:LEU:O	29:t:28:ILE:HG13	2.17	0.44
29:t:63:HIS:CE1	29:t:67:ARG:HH12	2.36	0.44
31:v:48:LEU:O	31:v:52:THR:HG23	2.18	0.44
1:A:216:VAL:HA	1:A:219:PHE:CD2	2.52	0.43
1:A:492:PRO:HG3	1:A:501:LEU:HD12	2.00	0.43
1:A:684:ALA:O	1:A:688:LYS:HG2	2.17	0.43
15:Q:86:ASN:HB3	15:Q:92:LEU:HD11	1.99	0.43
17:a:22:LYS:CD	22:i:73:LEU:HD21	2.47	0.43
20:g:31:LEU:HG	20:g:35:LYS:NZ	2.33	0.43
23:j:64:ASN:HB2	25:n:100:THR:HG21	2.00	0.43
26:q:614:ARG:HG3	26:q:636:GLU:HG3	1.99	0.43
1:A:104:GLU:HG2	1:A:174:ILE:HD12	1.99	0.43
1:A:1202:MET:HE2	1:A:1202:MET:HB2	1.82	0.43
3:C:43:THR:HG22	3:C:44:LEU:H	1.83	0.43
5:E:16:PHE:CE2	5:E:20:LYS:HE2	2.53	0.43
17:a:177:GLN:HE22	17:a:235:GLN:CB	2.31	0.43
19:f:120:VAL:HG22	19:f:126:TRP:HD1	1.83	0.43
25:n:127:LYS:HE2	28:s:146:GLU:HG2	2.00	0.43
26:q:500:ARG:O	26:q:504:MET:HG2	2.18	0.43
1:A:1342:GLU:CD	1:A:1342:GLU:H	2.24	0.43
5:E:56:LYS:HD3	5:E:56:LYS:HA	1.67	0.43
7:G:98:GLY:HA3	7:G:110:VAL:O	2.18	0.43
15:Q:138:GLN:N	15:Q:138:GLN:OE1	2.51	0.43
21:h:49:ARG:HG3	21:h:53:GLU:OE2	2.18	0.43
25:n:629:LEU:HB2	25:n:632:TRP:CD1	2.53	0.43
26:q:313:MET:HE1	31:v:80:LYS:HZ3	1.83	0.43
26:q:348:TYR:CZ	26:q:350:HIS:HB2	2.53	0.43
1:A:731:ARG:HA	1:A:731:ARG:HD3	1.83	0.43
3:C:114:TYR:HA	3:C:143:LEU:HA	1.99	0.43
22:i:125:ILE:O	22:i:128:GLN:HG2	2.16	0.43
25:n:718:CYS:HB3	25:n:728:LEU:HD11	1.99	0.43
26:q:649:PHE:O	26:q:659:SER:OG	2.28	0.43
28:s:65:LYS:O	28:s:68:ILE:HG12	2.18	0.43
29:t:10:GLU:HG3	29:t:11:ARG:HG2	2.01	0.43
2:B:313:MET:SD	2:B:390:LEU:HD21	2.59	0.43
2:B:390:LEU:HD12	2:B:392:ARG:HH12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:168:LYS:HG2	4:D:177:VAL:HG21	2.00	0.43
4:D:190:GLU:HA	7:G:167:TYR:CD2	2.54	0.43
17:a:30:ASN:O	22:i:78:LYS:NZ	2.51	0.43
19:f:8:GLU:HB3	21:h:115:ARG:HH22	1.84	0.43
20:g:186:ARG:HH12	30:u:104:VAL:HG11	1.83	0.43
23:j:114:LYS:HB2	30:u:30:HIS:HB2	2.01	0.43
23:j:118:LEU:HA	23:j:121:LEU:HD12	1.99	0.43
27:r:80:MET:HE3	27:r:80:MET:HA	1.99	0.43
27:r:305:ILE:HG22	27:r:307:ILE:HG13	1.99	0.43
2:B:523:CYS:HG	2:B:750:GLY:H	1.63	0.43
2:B:595:ARG:O	2:B:598:GLU:HG2	2.18	0.43
2:B:872:GLU:HG2	2:B:914:LYS:HE2	2.01	0.43
3:C:44:LEU:HD22	3:C:129:ILE:HG12	2.01	0.43
8:H:37:LYS:HG3	8:H:126:GLU:HB3	2.00	0.43
18:d:116:GLU:OE1	25:n:293:ARG:HD3	2.19	0.43
19:f:121:ARG:CG	19:f:125:PHE:HB3	2.49	0.43
19:f:192:ILE:HG23	19:f:200:VAL:HG13	2.01	0.43
20:g:143:MET:O	20:g:146:ARG:HB2	2.19	0.43
21:h:37:ARG:HH12	26:q:229:LEU:HB3	1.83	0.43
21:h:42:GLN:OE1	21:h:45:HIS:ND1	2.38	0.43
25:n:162:LEU:O	25:n:166:LEU:HB2	2.19	0.43
26:q:555:LYS:HE2	26:q:559:LYS:HE3	2.00	0.43
29:t:88:PRO:HA	29:t:89:PRO:HD3	1.93	0.43
32:w:87:GLY:HA2	32:w:90:GLU:OE2	2.18	0.43
1:A:537:ARG:HH21	8:H:122:LEU:HD12	1.84	0.43
1:A:1142:THR:O	1:A:1145:SER:OG	2.34	0.43
1:A:1226:VAL:HG22	1:A:1240:CYS:HA	2.00	0.43
2:B:698:GLU:HA	2:B:701:ILE:HG12	2.00	0.43
23:j:89:ASP:HB3	23:j:91:ARG:HH21	1.82	0.43
25:n:173:ASN:HD22	25:n:173:ASN:C	2.27	0.43
25:n:266:LEU:HB3	25:n:278:PHE:CE2	2.54	0.43
26:q:619:ILE:HD12	26:q:631:LEU:HD23	2.00	0.43
27:r:7:LEU:HD23	27:r:7:LEU:HA	1.90	0.43
27:r:187:GLU:OE2	29:t:97:SER:OG	2.32	0.43
27:r:189:ILE:HD12	29:t:87:ILE:HG12	2.01	0.43
30:u:68:LEU:O	30:u:72:GLN:OE1	2.36	0.43
1:A:143:LYS:HG3	1:A:144:THR:HG23	1.99	0.43
1:A:149:GLU:N	1:A:164:ARG:HH21	2.16	0.43
1:A:212:LYS:HG3	1:A:232:GLU:OE1	2.19	0.43
13:M:37:ARG:HA	13:M:37:ARG:HD2	1.86	0.43
15:Q:219:CYS:SG	15:Q:220:HIS:N	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:n:480:ARG:NH1	25:n:484:LEU:HD11	2.34	0.43
1:A:1195:LEU:HB3	1:A:1197:LEU:CD2	2.49	0.43
2:B:365:THR:HG21	2:B:370:PHE:CB	2.49	0.43
2:B:512:ARG:NH1	2:B:533:CYS:O	2.51	0.43
2:B:1104:HIS:NE2	2:B:1126:GLY:O	2.46	0.43
9:I:19:ASP:OD2	9:I:24:ARG:NH1	2.51	0.43
16:S:216:HIS:O	16:S:220:ASN:N	2.45	0.43
18:d:139:ASN:O	18:d:143:GLN:OE1	2.37	0.43
19:f:11:TRP:H	19:f:160:ILE:HG22	1.84	0.43
19:f:115:TYR:CE1	19:f:130:LYS:HD3	2.54	0.43
20:g:30:LYS:HD2	20:g:62:LEU:HD11	2.01	0.43
20:g:128:LEU:HG	23:j:143:ILE:HD11	2.00	0.43
20:g:169:GLN:HE21	30:u:5:LEU:HD22	1.84	0.43
22:i:98:LEU:O	22:i:102:LYS:HG2	2.19	0.43
25:n:822:ILE:HA	25:n:825:TYR:HD2	1.83	0.43
26:q:119:LEU:HD12	26:q:120:ASN:N	2.34	0.43
3:C:29:MET:HE3	3:C:29:MET:HB2	1.96	0.43
21:h:129:VAL:HG11	26:q:282:GLN:CD	2.44	0.43
25:n:486:ARG:NH2	25:n:549:LEU:HD22	2.34	0.43
26:q:443:TYR:O	26:q:447:LYS:HG2	2.18	0.43
28:s:30:PRO:HA	28:s:34:LEU:HD11	2.00	0.43
1:A:871:ASP:OD1	1:A:871:ASP:N	2.52	0.42
2:B:787:VAL:HG22	10:J:65:PRO:C	2.44	0.42
19:f:130:LYS:HB3	19:f:151:GLN:O	2.19	0.42
23:j:92:ASN:H	28:s:61:ARG:CB	2.32	0.42
25:n:714:ARG:H	25:n:751:SER:HB2	1.84	0.42
26:q:504:MET:O	26:q:508:LEU:HG	2.19	0.42
26:q:599:LEU:HD23	26:q:599:LEU:HA	1.89	0.42
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.18	0.42
1:A:672:ASP:N	1:A:672:ASP:OD1	2.52	0.42
2:B:580:VAL:HG22	2:B:624:LEU:HD12	2.01	0.42
2:B:759:PRO:HD2	2:B:1046:PRO:HB3	2.02	0.42
4:D:72:ARG:HH11	4:D:76:LYS:HD2	1.83	0.42
14:P:119:LEU:HD22	14:P:395:PHE:HZ	1.84	0.42
18:d:71:LYS:HA	18:d:74:ILE:HG22	2.00	0.42
24:k:105:LEU:O	24:k:109:LEU:N	2.50	0.42
25:n:718:CYS:SG	25:n:746:THR:HG23	2.59	0.42
26:q:301:ILE:O	26:q:304:ASN:HB2	2.19	0.42
31:v:103:GLN:HA	31:v:106:GLU:CD	2.43	0.42
31:v:103:GLN:HA	31:v:106:GLU:OE2	2.19	0.42
1:A:444:PHE:CE2	1:A:487:MET:HE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1004:ASN:O	1:A:1008:GLN:HG2	2.20	0.42
1:A:1177:LEU:HD13	1:A:1181:ALA:HB1	2.01	0.42
2:B:381:MET:HE3	2:B:381:MET:HB2	1.87	0.42
2:B:757:PRO:HG3	2:B:983:ARG:NH2	2.34	0.42
2:B:1020:ARG:HB3	2:B:1022:THR:HG23	2.01	0.42
6:F:93:ILE:HD11	6:F:134:ILE:HD11	2.01	0.42
14:P:376:LEU:HD11	15:Q:71:VAL:HG12	2.00	0.42
16:S:285:GLN:HB2	16:S:293:LEU:HD22	2.01	0.42
19:f:22:LEU:HB3	19:f:126:TRP:CH2	2.54	0.42
19:f:172:SER:O	19:f:175:MET:HG3	2.20	0.42
22:i:91:THR:O	22:i:95:ARG:HG3	2.19	0.42
24:k:57:GLU:O	24:k:61:LYS:HG2	2.19	0.42
25:n:575:SER:OG	25:n:628:ARG:O	2.34	0.42
32:w:45:GLN:HB2	32:w:48:ILE:HD12	2.00	0.42
3:C:43:THR:HG22	3:C:44:LEU:N	2.34	0.42
23:j:121:LEU:HD22	30:u:59:ILE:HG21	2.00	0.42
24:k:7:GLN:O	24:k:11:LYS:HG2	2.19	0.42
25:n:564:VAL:O	25:n:568:MET:HG2	2.19	0.42
26:q:301:ILE:O	26:q:305:GLU:OE1	2.36	0.42
32:w:28:GLU:O	32:w:31:GLN:HG3	2.20	0.42
1:A:445:ASN:OD1	1:A:488:ASN:HB2	2.19	0.42
1:A:1054:LEU:HD23	1:A:1054:LEU:HA	1.85	0.42
2:B:234:ILE:HG12	2:B:259:TYR:CZ	2.54	0.42
2:B:590:HIS:CE1	2:B:596:LEU:HD13	2.54	0.42
19:f:129:ARG:NH1	19:f:131:GLN:HB3	2.34	0.42
22:i:132:GLU:HA	22:i:135:ILE:HG22	2.01	0.42
23:j:50:ILE:HD11	28:s:143:SER:HB3	2.00	0.42
24:k:47:GLN:O	24:k:51:HIS:ND1	2.33	0.42
25:n:255:ILE:O	25:n:259:LEU:HG	2.20	0.42
26:q:279:TRP:O	26:q:282:GLN:HB3	2.19	0.42
26:q:311:LYS:NZ	26:q:364:GLN:HG2	2.34	0.42
26:q:452:LEU:HD21	26:q:543:ARG:HE	1.84	0.42
26:q:610:LEU:O	26:q:640:TYR:OH	2.36	0.42
1:A:1233:ASP:OD1	1:A:1233:ASP:N	2.53	0.42
2:B:118:ARG:HA	2:B:118:ARG:HD2	1.72	0.42
2:B:821:GLN:HB2	2:B:851:PHE:CE1	2.55	0.42
2:B:928:ARG:NE	2:B:932:HIS:O	2.50	0.42
17:a:189:ARG:HH21	17:a:209:GLU:CD	2.28	0.42
20:g:189:ILE:O	20:g:193:GLU:OE1	2.37	0.42
26:q:348:TYR:CE2	26:q:350:HIS:HB2	2.54	0.42
26:q:563:LYS:HA	26:q:567:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:801:LYS:HE2	2:B:815:ARG:HB3	2.01	0.42
2:B:860:MET:HE2	2:B:963:PHE:CE1	2.54	0.42
2:B:1106:ARG:NH1	2:B:1118:PRO:HB3	2.34	0.42
3:C:34:ARG:HB2	3:C:176:ILE:CD1	2.49	0.42
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.90	0.42
8:H:113:ALA:HA	8:H:125:LEU:O	2.20	0.42
9:I:75:CYS:HB3	9:I:80:SER:H	1.85	0.42
11:K:19:LEU:HD22	11:K:35:PHE:CD1	2.55	0.42
19:f:103:LEU:O	19:f:107:LEU:HB2	2.19	0.42
22:i:108:ASN:HB3	22:i:111:THR:HG22	2.00	0.42
25:n:286:ILE:HD13	25:n:302:LEU:HD12	2.01	0.42
26:q:227:LEU:HB3	26:q:253:SER:HB2	2.01	0.42
26:q:283:SER:O	26:q:287:SER:OG	2.33	0.42
1:A:565:ILE:O	1:A:570:PRO:HA	2.20	0.42
1:A:1148:ILE:HG22	1:A:1196:GLU:O	2.20	0.42
1:A:1186:ASP:HB2	1:A:1246:LYS:HE2	2.02	0.42
2:B:918:ILE:HB	2:B:928:ARG:NH2	2.35	0.42
10:J:1:MET:H3	10:J:56:LEU:HB2	1.85	0.42
15:Q:91:GLU:HG2	15:Q:109:ASN:HD21	1.85	0.42
25:n:821:ILE:O	25:n:821:ILE:HG22	2.20	0.42
29:t:25:SER:HA	29:t:28:ILE:HD12	2.02	0.42
1:A:1192:LEU:HD11	1:A:1239:ARG:HA	2.02	0.42
2:B:860:MET:HE2	2:B:963:PHE:HE1	1.85	0.42
10:J:44:TYR:HA	10:J:47:ARG:HD2	2.02	0.42
15:Q:210:LYS:HA	15:Q:210:LYS:HD3	1.80	0.42
18:d:37:LEU:HD13	22:i:112:LYS:HD2	2.01	0.42
19:f:100:TYR:O	19:f:104:GLU:OE1	2.38	0.42
20:g:136:VAL:HG21	20:g:147:LYS:HD2	2.02	0.42
22:i:119:PRO:HA	22:i:122:TRP:CZ3	2.55	0.42
22:i:129:ARG:O	22:i:132:GLU:HG2	2.20	0.42
24:k:33:ILE:HG13	24:k:36:GLU:OE2	2.19	0.42
1:A:12:ARG:NH2	2:B:1220:ARG:HB2	2.34	0.42
1:A:418:SER:C	1:A:420:ARG:H	2.28	0.42
1:A:756:ILE:HG21	16:S:293:LEU:HD12	2.01	0.42
1:A:1085:HIS:NE2	16:S:286:THR:HG21	2.34	0.42
2:B:653:VAL:HG12	2:B:689:LEU:HD23	2.01	0.42
2:B:754:SER:HB2	2:B:812:LEU:HD11	2.02	0.42
3:C:239:PRO:HB2	3:C:242:GLN:HG2	2.01	0.42
25:n:96:ILE:HG12	25:n:144:LEU:HD21	2.01	0.42
26:q:130:GLN:O	26:q:133:SER:OG	2.38	0.42
29:t:125:ASP:OD1	29:t:126:ALA:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:LEU:O	1:A:929:LEU:HG	2.20	0.41
1:A:1015:VAL:HG22	1:A:1015:VAL:O	2.20	0.41
1:A:1226:VAL:HG12	1:A:1228:TRP:CD1	2.51	0.41
2:B:211:VAL:HG21	2:B:495:LEU:HD23	2.02	0.41
2:B:637:LEU:HD12	2:B:693:ILE:HG13	2.03	0.41
5:E:79:TRP:HE1	5:E:81:GLU:HB2	1.84	0.41
19:f:196:PRO:CD	26:q:305:GLU:HG2	2.50	0.41
25:n:795:ILE:HG22	25:n:795:ILE:O	2.20	0.41
27:r:33:LEU:HD13	27:r:87:PHE:HA	2.02	0.41
7:G:46:LEU:HG	7:G:78:VAL:HA	2.02	0.41
18:d:119:ASN:OD1	25:n:293:ARG:NH2	2.53	0.41
18:d:192:MET:HA	18:d:195:MET:HE2	2.01	0.41
21:h:86:PHE:O	21:h:90:LEU:HG	2.20	0.41
24:k:72:LEU:O	24:k:76:ASN:ND2	2.36	0.41
26:q:381:PHE:CZ	26:q:385:VAL:HG21	2.56	0.41
26:q:437:PHE:CE1	26:q:512:LEU:HD23	2.55	0.41
31:v:45:ASN:C	31:v:45:ASN:HD22	2.28	0.41
1:A:351:THR:HG22	1:A:352:VAL:N	2.34	0.41
1:A:1405:THR:OG1	1:A:1406:VAL:N	2.53	0.41
2:B:354:ASP:HA	2:B:357:GLN:NE2	2.34	0.41
2:B:954:VAL:HG23	12:L:56:LEU:HB2	2.02	0.41
2:B:1059:LEU:HD22	2:B:1066:SER:HA	2.02	0.41
17:a:299:ILE:HG23	17:a:356:PHE:CZ	2.56	0.41
19:f:118:SER:HB3	19:f:127:VAL:HG23	2.02	0.41
23:j:19:GLN:OE1	25:n:152:ARG:NH1	2.51	0.41
24:k:4:PRO:O	24:k:7:GLN:HB2	2.21	0.41
25:n:716:LYS:HB3	25:n:746:THR:OG1	2.20	0.41
26:q:309:TRP:HH2	31:v:77:ARG:HG3	1.84	0.41
28:s:75:PHE:HB3	28:s:78:ILE:HD11	2.02	0.41
30:u:51:PRO:HA	30:u:52:PRO:HD3	1.99	0.41
1:A:180:LYS:HA	1:A:180:LYS:HD2	1.73	0.41
1:A:709:THR:HG22	1:A:710:LEU:N	2.36	0.41
2:B:29:ASP:HB3	2:B:658:ILE:HG13	2.01	0.41
2:B:702:LEU:HD12	2:B:702:LEU:HA	1.90	0.41
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.56	0.41
10:J:6:ARG:HG2	10:J:13:VAL:HG22	2.02	0.41
15:Q:59:LEU:HD23	15:Q:61:LEU:HD11	2.03	0.41
16:S:227:PHE:O	16:S:231:CYS:HB2	2.20	0.41
19:f:121:ARG:HG3	19:f:125:PHE:HB3	2.02	0.41
1:A:393:ARG:HD3	1:A:421:ALA:O	2.21	0.41
2:B:802:PRO:HG2	2:B:805:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.84	0.41
5:E:12:LEU:HD21	5:E:58:MET:HE1	2.03	0.41
5:E:88:VAL:HB	5:E:116:ILE:HG12	2.02	0.41
17:a:315:MET:SD	17:a:529:GLN:NE2	2.93	0.41
18:d:197:SER:HB2	20:g:15:PRO:HG2	2.02	0.41
20:g:156:VAL:HG12	20:g:160:HIS:CE1	2.55	0.41
25:n:287:GLN:O	25:n:300:VAL:HB	2.20	0.41
25:n:503:LEU:HD11	25:n:557:LYS:HA	2.02	0.41
27:r:78:GLU:O	27:r:81:MET:HE1	2.20	0.41
31:v:12:GLN:HE21	31:v:68:ASN:HB3	1.83	0.41
31:v:46:SER:O	31:v:50:VAL:HG23	2.20	0.41
1:A:778:GLY:HA3	2:B:516:ASN:HB2	2.03	0.41
2:B:833:TYR:HB2	2:B:840:ILE:HD11	2.01	0.41
18:d:71:LYS:O	18:d:75:ARG:HG2	2.20	0.41
20:g:107:ASN:HB3	30:u:95:ASP:HB2	2.03	0.41
22:i:72:SER:HA	22:i:75:GLN:CD	2.46	0.41
24:k:5:TYR:HA	24:k:8:GLU:OE2	2.21	0.41
24:k:102:LEU:CD2	31:v:104:ILE:HD12	2.50	0.41
25:n:479:ILE:O	25:n:483:LEU:HG	2.20	0.41
26:q:125:GLN:OE1	26:q:129:LYS:NZ	2.50	0.41
26:q:250:LYS:H	26:q:250:LYS:HG3	1.62	0.41
26:q:298:LEU:O	26:q:302:LEU:HB2	2.20	0.41
1:A:118:HIS:CG	1:A:152:VAL:HG11	2.56	0.41
2:B:120:ARG:NH2	2:B:956:THR:O	2.52	0.41
2:B:234:ILE:HG12	2:B:259:TYR:CE1	2.56	0.41
2:B:328:GLU:HG3	2:B:349:ILE:HD12	2.01	0.41
2:B:857:ARG:HD3	2:B:942:ARG:NH1	2.36	0.41
3:C:241:ASP:N	3:C:241:ASP:OD1	2.51	0.41
5:E:183:PRO:HA	5:E:186:LEU:HD12	2.03	0.41
12:L:37:LYS:O	12:L:38:LEU:HD23	2.20	0.41
14:P:134:HIS:HB2	14:P:354:ASP:OD1	2.21	0.41
16:S:202:ILE:O	16:S:206:VAL:HG23	2.20	0.41
16:S:267:ASP:OD1	16:S:267:ASP:N	2.52	0.41
18:d:140:THR:HA	18:d:143:GLN:NE2	2.36	0.41
21:h:36:VAL:HA	21:h:39:ARG:NH2	2.36	0.41
22:i:128:GLN:O	22:i:131:GLN:HG3	2.21	0.41
29:t:152:LEU:HD21	29:t:204:TYR:CE2	2.56	0.41
1:z:1:PRO:HB2	1:z:2:SER:H	1.63	0.41
16:S:182:MET:HE1	16:S:229:ALA:HA	2.03	0.41
21:h:84:GLN:HG2	31:v:45:ASN:HB3	2.02	0.41
21:h:122:VAL:HG12	21:h:126:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:h:153:ARG:HG2	31:v:33:ARG:CZ	2.51	0.41
25:n:705:ILE:HG12	25:n:715:ASN:ND2	2.36	0.41
26:q:632:SER:OG	26:q:648:LYS:HB3	2.21	0.41
31:v:102:LYS:HA	31:v:102:LYS:HD2	1.97	0.41
1:A:207:ILE:HG22	1:A:211:PHE:CE1	2.56	0.41
1:A:326:ARG:HG3	1:A:1406:VAL:HG11	2.03	0.41
1:A:357:PRO:HD2	2:B:833:TYR:CE1	2.56	0.41
1:A:1336:MET:HA	1:A:1340:GLY:O	2.21	0.41
2:B:259:TYR:HB2	2:B:270:LYS:HZ1	1.85	0.41
2:B:288:ALA:HA	2:B:327:ARG:CG	2.48	0.41
2:B:600:LEU:HD23	2:B:600:LEU:HA	1.91	0.41
2:B:651:LEU:HD21	2:B:741:CYS:SG	2.61	0.41
5:E:9:ILE:HG23	5:E:42:PHE:HE2	1.85	0.41
18:d:144:GLN:O	18:d:148:ILE:HG12	2.20	0.41
19:f:159:ASN:OD1	19:f:160:ILE:N	2.53	0.41
20:g:114:TYR:O	20:g:117:GLN:HG3	2.21	0.41
20:g:180:GLU:O	20:g:183:GLU:HG3	2.21	0.41
22:i:98:LEU:HD23	22:i:98:LEU:HA	1.83	0.41
25:n:161:VAL:HG13	28:s:40:LEU:HD22	2.03	0.41
25:n:241:LEU:HA	25:n:244:GLN:NE2	2.35	0.41
25:n:782:ALA:HB3	25:n:810:PHE:CZ	2.56	0.41
26:q:388:PHE:CZ	26:q:479:LEU:HB2	2.56	0.41
26:q:424:ASP:HB3	26:q:427:LYS:HD2	2.03	0.41
1:A:36:ARG:HB3	1:A:37:PHE:HD1	1.86	0.41
2:B:561:TRP:HE1	2:B:595:ARG:HH12	1.67	0.41
4:D:217:LEU:HD11	21:h:38:MET:HE1	2.03	0.41
10:J:68:LYS:NZ	10:J:69:ARG:O	2.39	0.41
18:d:98:GLN:HB3	18:d:102:LYS:HZ1	1.84	0.41
29:t:159:GLU:CD	29:t:161:GLY:H	2.28	0.41
30:u:111:ALA:HA	30:u:114:LYS:HZ2	1.85	0.41
1:A:154:SER:OG	1:A:157:ASP:O	2.32	0.40
1:A:260:ASP:O	1:A:263:THR:HG22	2.21	0.40
1:A:464:PRO:HB3	11:K:4:PRO:HD3	2.02	0.40
2:B:370:PHE:CZ	14:P:368:GLY:HA3	2.56	0.40
2:B:406:LEU:HD12	2:B:545:ILE:HD11	2.02	0.40
7:G:14:HIS:CD2	7:G:15:PRO:HD2	2.56	0.40
16:S:159:VAL:HG11	16:S:203:TYR:HE1	1.85	0.40
16:S:211:ASN:OD1	16:S:211:ASN:N	2.54	0.40
21:h:149:LEU:O	21:h:153:ARG:HG3	2.21	0.40
24:k:4:PRO:O	24:k:7:GLN:N	2.54	0.40
25:n:753:LEU:HB3	25:n:756:SER:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:q:238:MET:HE1	26:q:251:PRO:HG2	2.02	0.40
26:q:276:ASN:HA	26:q:279:TRP:HE3	1.86	0.40
32:w:117:TRP:O	32:w:120:GLU:HG2	2.21	0.40
1:A:873:MET:HB2	1:A:1366:ARG:NH2	2.36	0.40
1:A:874:ASP:OD1	1:A:875:ALA:N	2.54	0.40
2:B:347:LYS:HA	2:B:347:LYS:HD3	1.60	0.40
9:I:26:LEU:HD23	9:I:37:GLU:HA	2.03	0.40
11:K:19:LEU:HD22	11:K:35:PHE:CE1	2.56	0.40
16:S:238:PRO:HB2	16:S:240:PRO:HD2	2.03	0.40
20:g:13:TYR:HD2	32:w:38:TYR:CD1	2.40	0.40
23:j:79:ILE:HD13	25:n:147:LEU:HD13	2.03	0.40
1:A:1166:ASP:OD1	1:A:1237:ILE:HG21	2.21	0.40
1:A:1192:LEU:HD12	1:A:1240:CYS:O	2.22	0.40
1:A:1397:LEU:HA	1:A:1400:CYS:SG	2.62	0.40
2:B:307:ASP:OD2	2:B:310:MET:HB2	2.21	0.40
2:B:461:LEU:HD23	2:B:461:LEU:HA	1.89	0.40
2:B:764:SER:OG	2:B:765:PRO:HD3	2.21	0.40
4:D:56:ARG:HG3	4:D:145:MET:HE1	2.03	0.40
19:f:169:ILE:HG12	21:h:116:LYS:CB	2.51	0.40
20:g:150:ASN:O	28:s:16:TYR:OH	2.38	0.40
25:n:689:MET:O	25:n:693:ARG:HG3	2.21	0.40
27:r:98:ILE:HG22	27:r:243:ASN:ND2	2.35	0.40
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.57	0.40
1:A:1187:GLN:NE2	1:A:1244:ARG:O	2.43	0.40
2:B:1169:MET:HE1	2:B:1201:LYS:HG2	2.04	0.40
16:S:146:HIS:ND1	16:S:149:ARG:HG3	2.36	0.40
19:f:8:GLU:HB3	21:h:115:ARG:HH12	1.86	0.40
19:f:132:ARG:HB2	19:f:150:LEU:HD11	2.04	0.40
22:i:127:HIS:O	22:i:130:GLU:HG3	2.21	0.40
29:t:143:PHE:HD1	29:t:148:PHE:HA	1.86	0.40
1:A:105:CYS:SG	1:A:139:TRP:HA	2.61	0.40
1:A:1257:ASP:OD1	1:A:1261:LYS:HG3	2.22	0.40
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	2.04	0.40
2:B:29:ASP:O	2:B:33:VAL:HG23	2.22	0.40
2:B:281:PRO:O	2:B:285:ILE:HG12	2.21	0.40
10:J:1:MET:N	10:J:56:LEU:HB2	2.37	0.40
14:P:141:ARG:NH1	14:P:348:TYR:O	2.55	0.40
15:Q:64:SER:HA	15:Q:215:VAL:O	2.22	0.40
16:S:284:LEU:HB3	16:S:286:THR:HG23	2.03	0.40
18:d:138:LYS:HD2	30:u:105:GLU:HG2	2.04	0.40
18:d:154:LEU:O	18:d:158:THR:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:f:168:LYS:O	19:f:171:GLN:HG3	2.21	0.40
23:j:87:ILE:O	28:s:63:SER:HB2	2.22	0.40
26:q:517:LYS:NZ	26:q:602:GLU:OE1	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1451/1733 (84%)	1407 (97%)	43 (3%)	1 (0%)	48	83
1	z	23/1733 (1%)	21 (91%)	1 (4%)	1 (4%)	2	17
2	B	1164/1224 (95%)	1132 (97%)	32 (3%)	0	100	100
3	C	269/318 (85%)	261 (97%)	8 (3%)	0	100	100
4	D	165/221 (75%)	163 (99%)	2 (1%)	0	100	100
5	E	213/215 (99%)	210 (99%)	3 (1%)	0	100	100
6	F	84/155 (54%)	83 (99%)	1 (1%)	0	100	100
7	G	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
8	H	137/146 (94%)	134 (98%)	3 (2%)	0	100	100
9	I	114/122 (93%)	113 (99%)	1 (1%)	0	100	100
10	J	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
11	K	114/120 (95%)	112 (98%)	2 (2%)	0	100	100
12	L	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
13	M	33/345 (10%)	33 (100%)	0	0	100	100
14	P	99/735 (14%)	98 (99%)	1 (1%)	0	100	100
15	Q	121/400 (30%)	121 (100%)	0	0	100	100
16	S	179/309 (58%)	177 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	a	357/566 (63%)	343 (96%)	11 (3%)	3 (1%)	16	53
18	d	165/284 (58%)	164 (99%)	1 (1%)	0	100	100
19	f	163/295 (55%)	161 (99%)	2 (1%)	0	100	100
20	g	159/222 (72%)	158 (99%)	1 (1%)	0	100	100
21	h	132/223 (59%)	129 (98%)	3 (2%)	0	100	100
22	i	79/149 (53%)	79 (100%)	0	0	100	100
23	j	142/157 (90%)	137 (96%)	5 (4%)	0	100	100
24	k	104/115 (90%)	104 (100%)	0	0	100	100
25	n	611/1082 (56%)	607 (99%)	4 (1%)	0	100	100
26	q	505/687 (74%)	500 (99%)	5 (1%)	0	100	100
27	r	249/307 (81%)	244 (98%)	5 (2%)	0	100	100
28	s	77/220 (35%)	76 (99%)	1 (1%)	0	100	100
29	t	208/210 (99%)	206 (99%)	2 (1%)	0	100	100
30	u	116/140 (83%)	115 (99%)	1 (1%)	0	100	100
31	v	105/121 (87%)	105 (100%)	0	0	100	100
32	w	99/127 (78%)	97 (98%)	2 (2%)	0	100	100
All	All	7715/12992 (59%)	7560 (98%)	150 (2%)	5 (0%)	49	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	z	21	SER
17	a	291	SER
17	a	306	ASN
17	a	289	CYS
1	A	958	VAL

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	A	1268/1520 (83%)	1267 (100%)	1 (0%)	88	88
1	z	25/1520 (2%)	25 (100%)	0	100	100
2	B	1018/1061 (96%)	1018 (100%)	0	100	100
3	C	239/274 (87%)	239 (100%)	0	100	100
4	D	150/200 (75%)	150 (100%)	0	100	100
5	E	197/197 (100%)	197 (100%)	0	100	100
6	F	76/137 (56%)	76 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	124/128 (97%)	124 (100%)	0	100	100
9	I	110/116 (95%)	110 (100%)	0	100	100
10	J	65/65 (100%)	65 (100%)	0	100	100
11	K	99/102 (97%)	99 (100%)	0	100	100
12	L	38/57 (67%)	38 (100%)	0	100	100
13	M	32/299 (11%)	32 (100%)	0	100	100
14	P	95/641 (15%)	95 (100%)	0	100	100
15	Q	119/363 (33%)	119 (100%)	0	100	100
16	S	158/274 (58%)	158 (100%)	0	100	100
17	a	350/528 (66%)	347 (99%)	3 (1%)	70	76
18	d	158/258 (61%)	158 (100%)	0	100	100
19	f	158/259 (61%)	158 (100%)	0	100	100
20	g	160/208 (77%)	160 (100%)	0	100	100
21	h	128/207 (62%)	128 (100%)	0	100	100
22	i	82/144 (57%)	82 (100%)	0	100	100
23	j	134/145 (92%)	134 (100%)	0	100	100
24	k	101/108 (94%)	101 (100%)	0	100	100
25	n	591/1001 (59%)	591 (100%)	0	100	100
26	q	482/642 (75%)	482 (100%)	0	100	100
27	r	228/280 (81%)	228 (100%)	0	100	100
28	s	75/195 (38%)	75 (100%)	0	100	100
29	t	178/178 (100%)	178 (100%)	0	100	100
30	u	115/132 (87%)	115 (100%)	0	100	100
31	v	101/113 (89%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	w	97/117 (83%)	97 (100%)	0	100	100
All	All	7103/11621 (61%)	7099 (100%)	4 (0%)	87	88

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

Mol	Chain	Res	Type
1	A	1124	HIS
17	a	288	THR
17	a	290	SER
17	a	296	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	ASN
1	A	471	ASN
1	A	490	HIS
1	A	510	GLN
1	A	589	GLN
1	A	742	ASN
1	A	760	GLN
1	A	1211	GLN
1	A	1232	ASN
1	A	1427	ASN
2	B	60	GLN
2	B	516	ASN
2	B	821	GLN
3	C	242	GLN
4	D	138	ASN
4	D	179	GLN
6	F	100	GLN
7	G	122	ASN
7	G	131	GLN
8	H	133	ASN
8	H	137	GLN
9	I	89	GLN
10	J	23	ASN
11	K	89	ASN
14	P	359	ASN
15	Q	242	ASN
16	S	166	HIS

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Mol	Chain	Res	Type
16	S	169	GLN
16	S	304	ASN
17	a	30	ASN
17	a	106	ASN
17	a	177	GLN
17	a	235	GLN
17	a	250	ASN
17	a	292	ASN
18	d	144	GLN
19	f	10	GLN
19	f	180	HIS
20	g	129	ASN
20	g	169	GLN
20	g	194	GLN
21	h	150	GLN
24	k	14	ASN
24	k	19	GLN
25	n	173	ASN
25	n	250	ASN
25	n	502	GLN
25	n	541	ASN
25	n	622	GLN
25	n	715	ASN
26	q	360	ASN
26	q	365	ASN
27	r	226	HIS
27	r	243	ASN
30	u	9	GLN
30	u	98	GLN
31	v	4	GLN
31	v	43	GLN
31	v	68	ASN
31	v	86	ASN
32	w	119	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
26	q	1
30	u	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	q	318:ASN	C	319:LYS	N	5.82
1	u	80:LEU	C	81:PRO	N	3.17

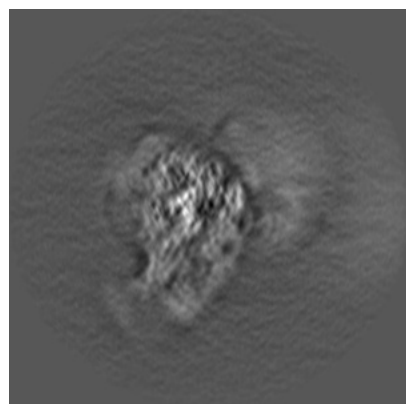
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26544. These allow visual inspection of the internal detail of the map and identification of artifacts.

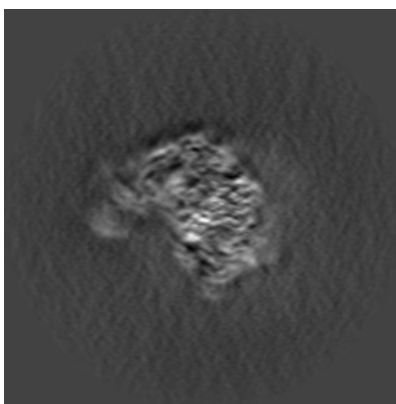
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

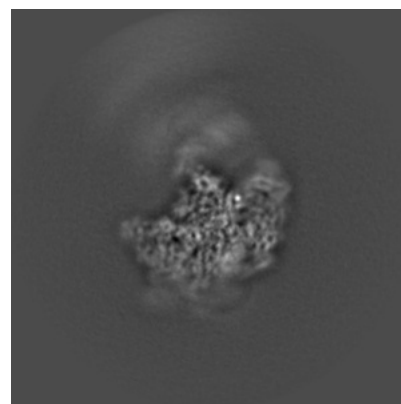
6.1.1 Primary map



X

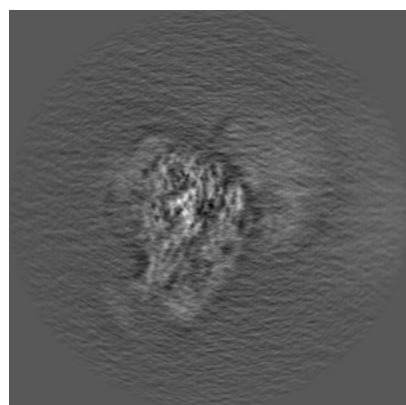


Y

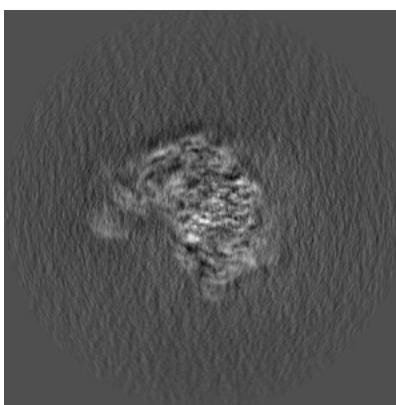


Z

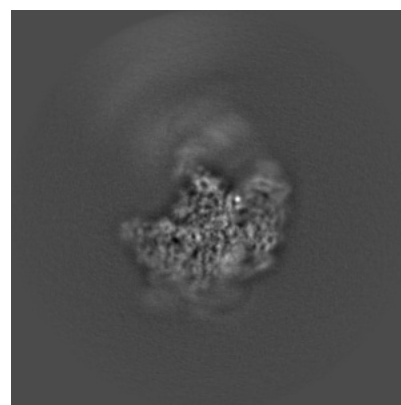
6.1.2 Raw map



X



Y

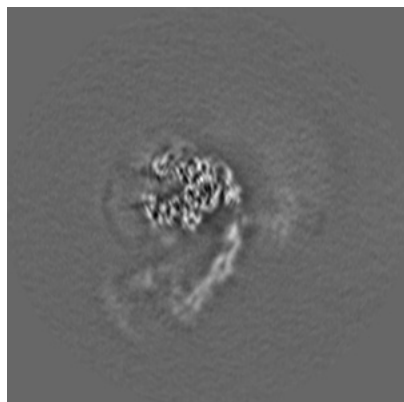


Z

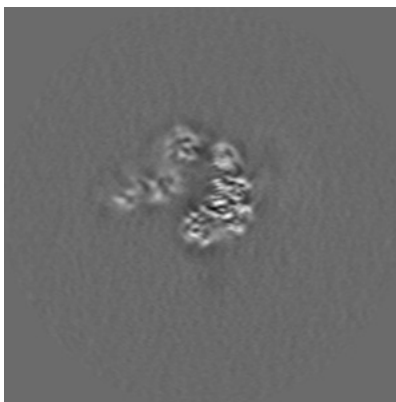
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

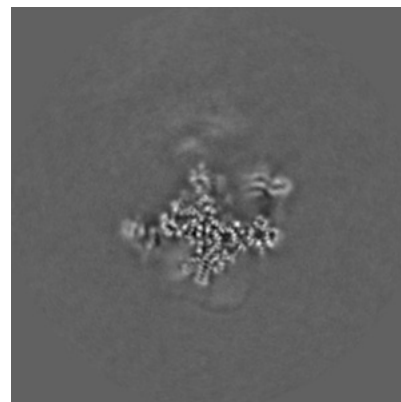
6.2.1 Primary map



X Index: 180

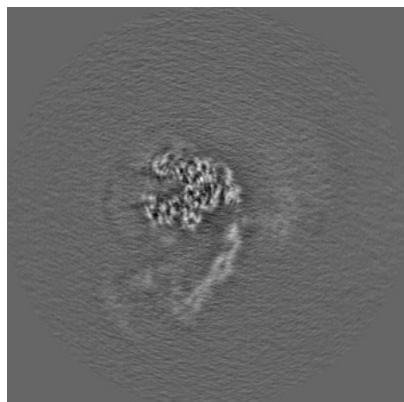


Y Index: 180

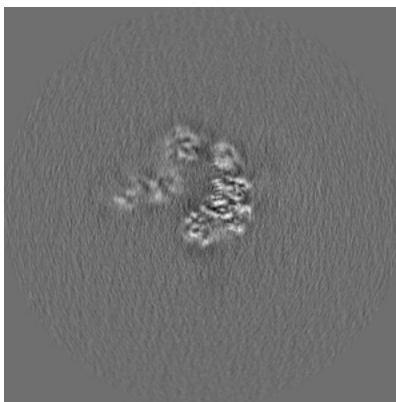


Z Index: 180

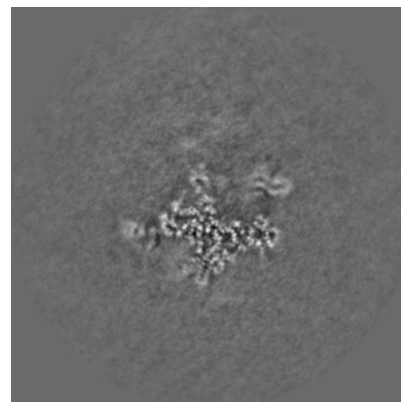
6.2.2 Raw map



X Index: 180



Y Index: 180

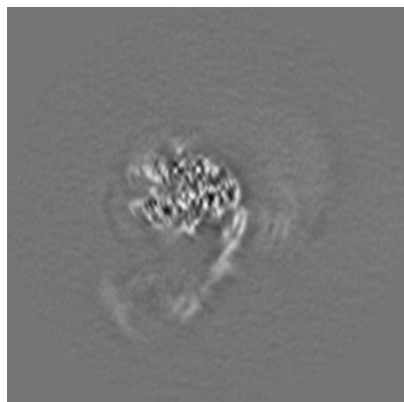


Z Index: 180

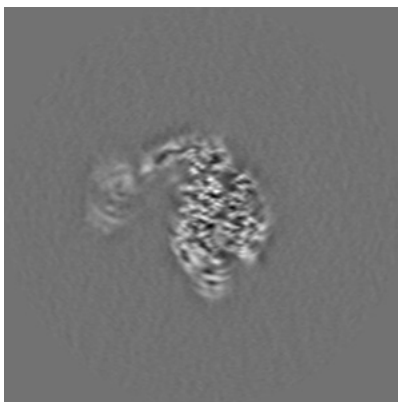
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

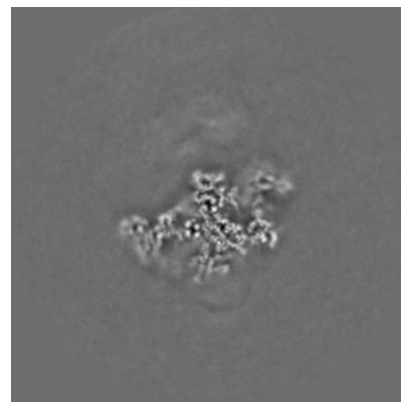
6.3.1 Primary map



X Index: 176

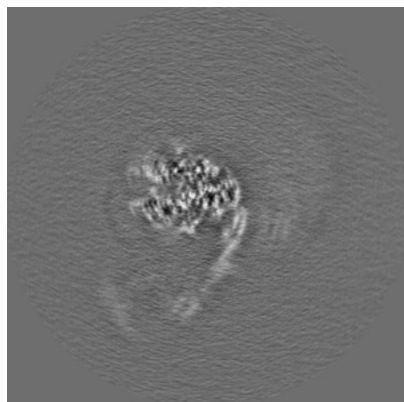


Y Index: 160

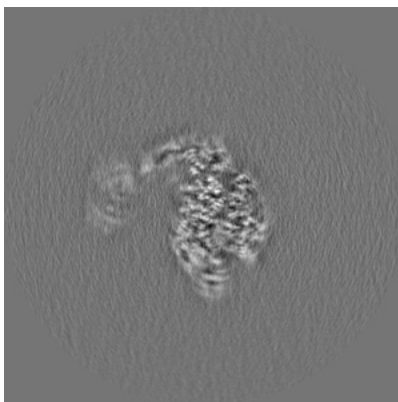


Z Index: 187

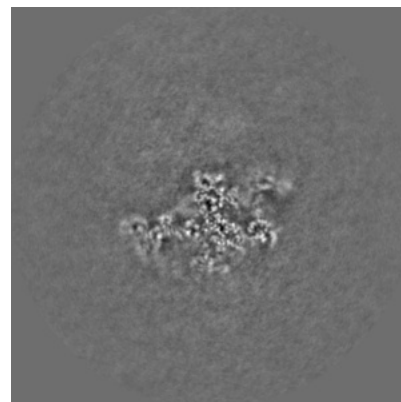
6.3.2 Raw map



X Index: 176



Y Index: 160

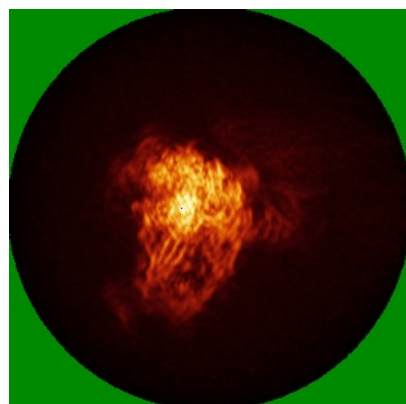


Z Index: 188

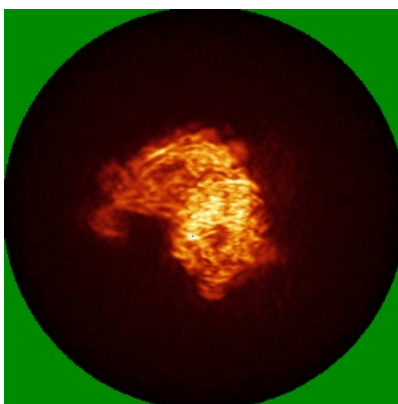
The images above show the largest variance slices of the map in three orthogonal directions.

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

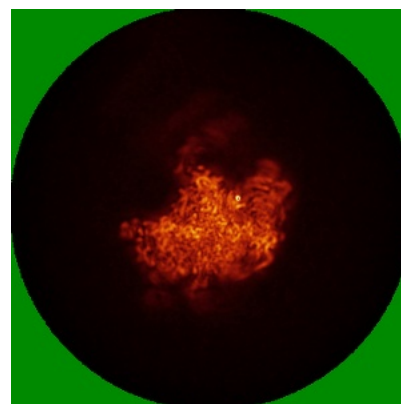
6.4.1 Primary map



X

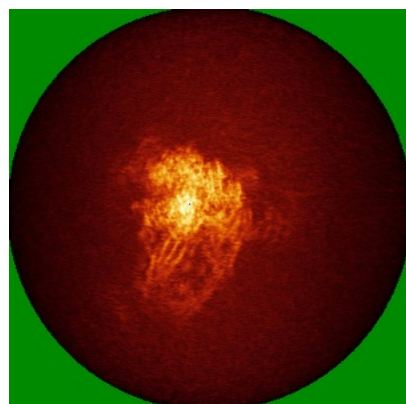


Y

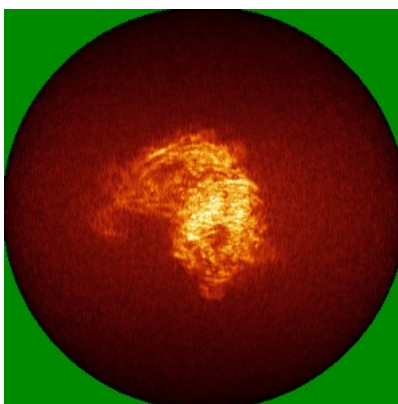


Z

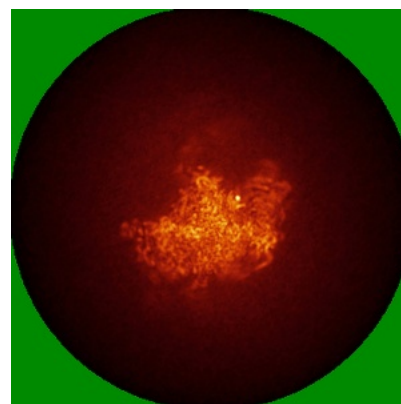
6.4.2 Raw map



X



Y



Z

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

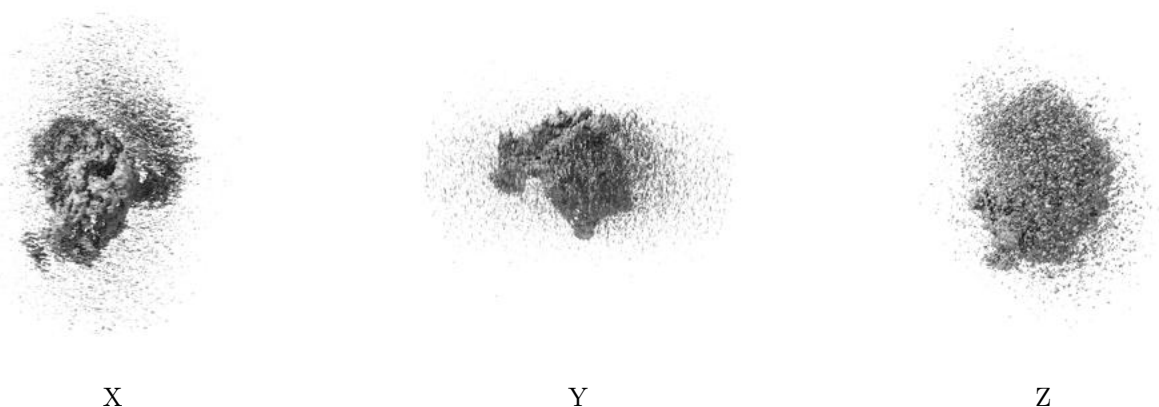
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

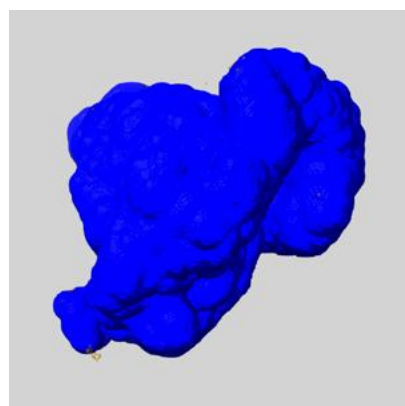
6.6 Mask visualisation [i](#)

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

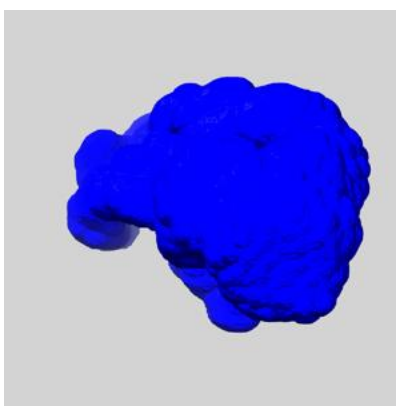
A mask typically either:

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

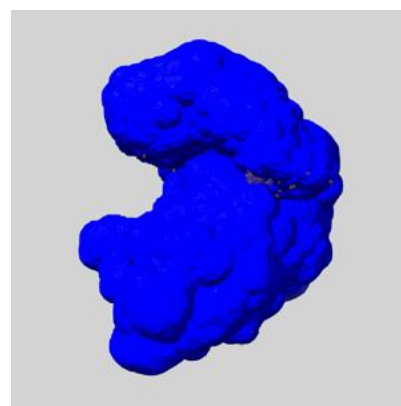
6.6.1 emd_26544_msk_1.map [i](#)



X



Y

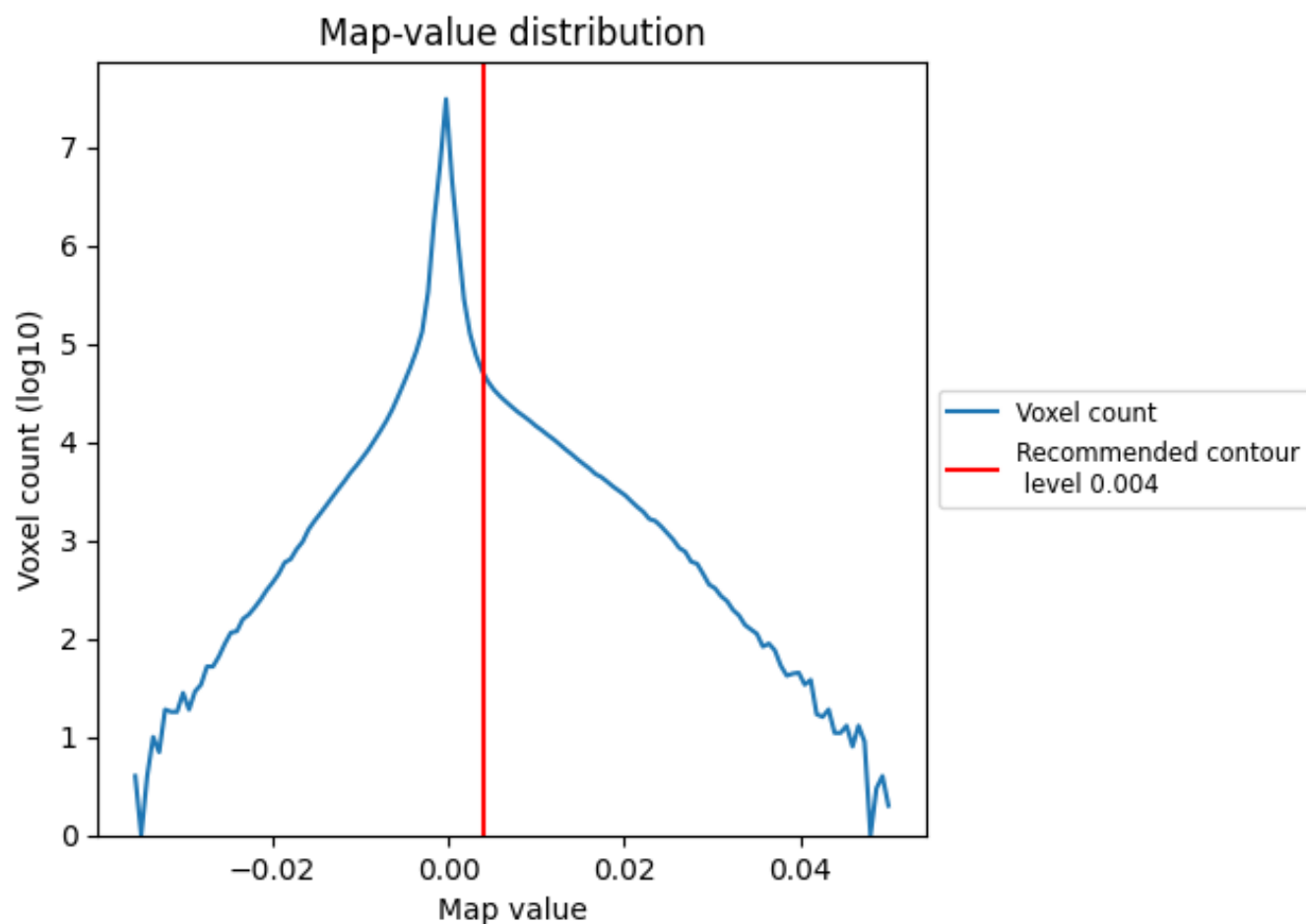


Z

7 Map analysis [i](#)

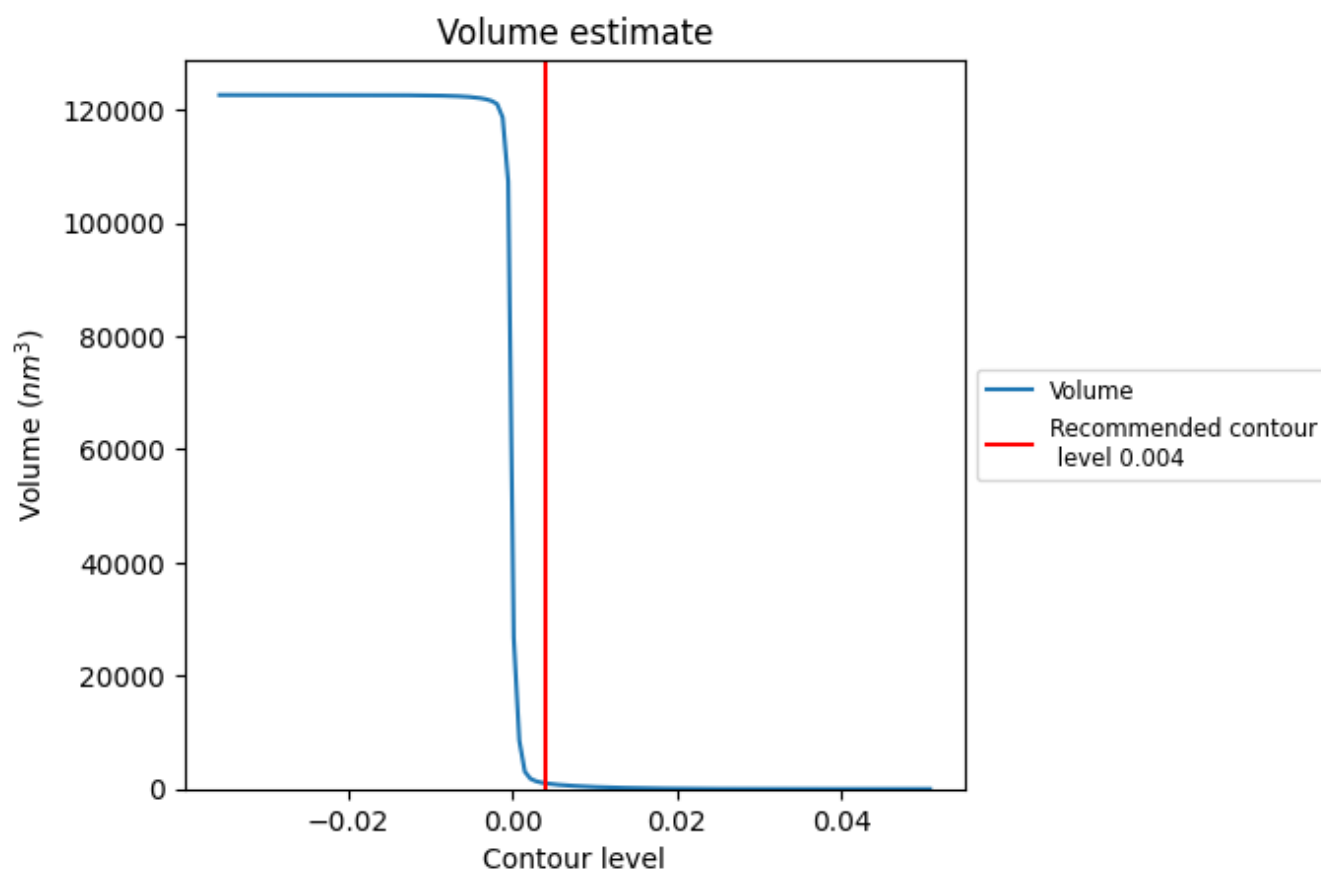
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

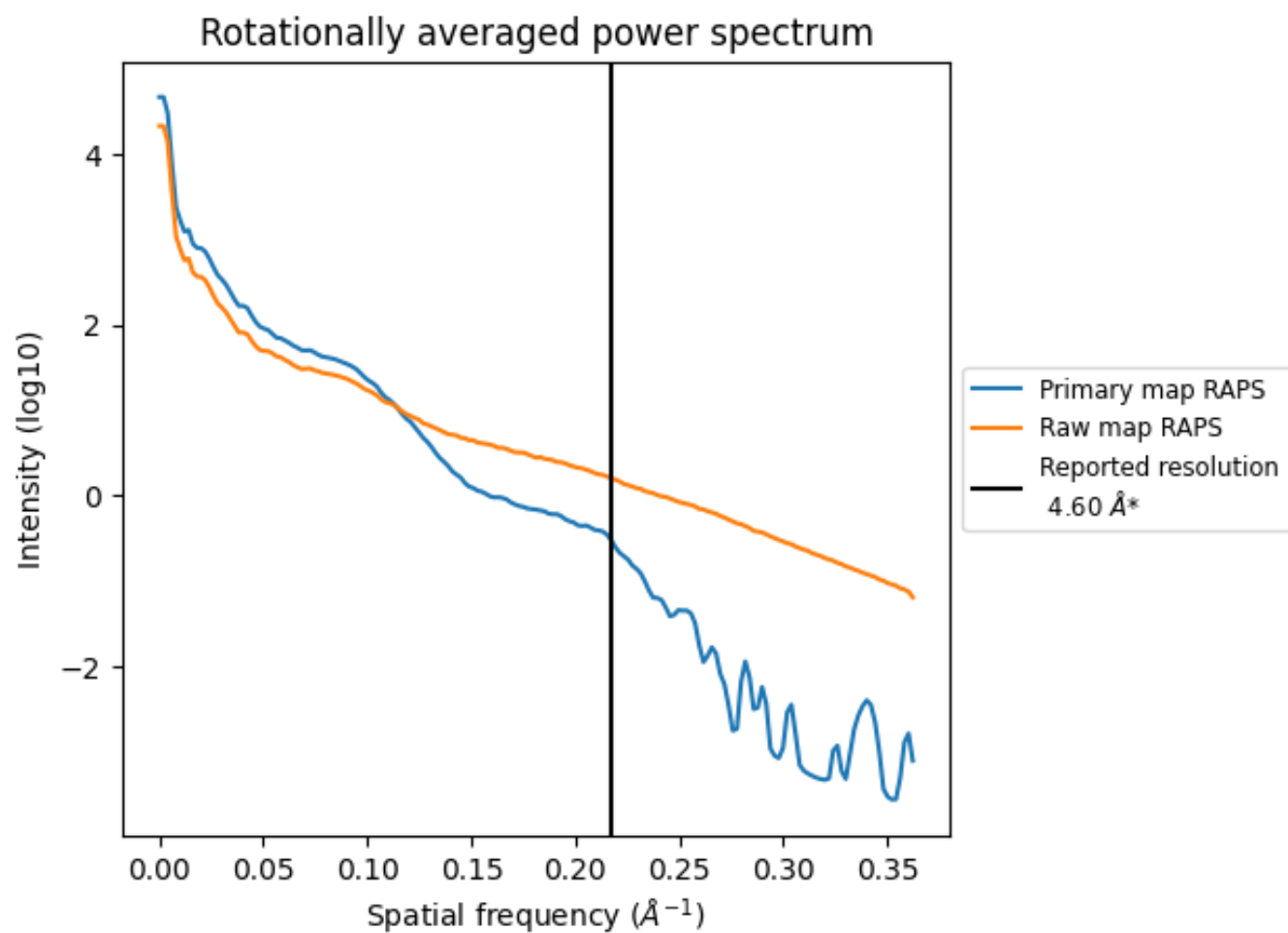
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1005 nm³; this corresponds to an approximate mass of 908 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 ⓘ

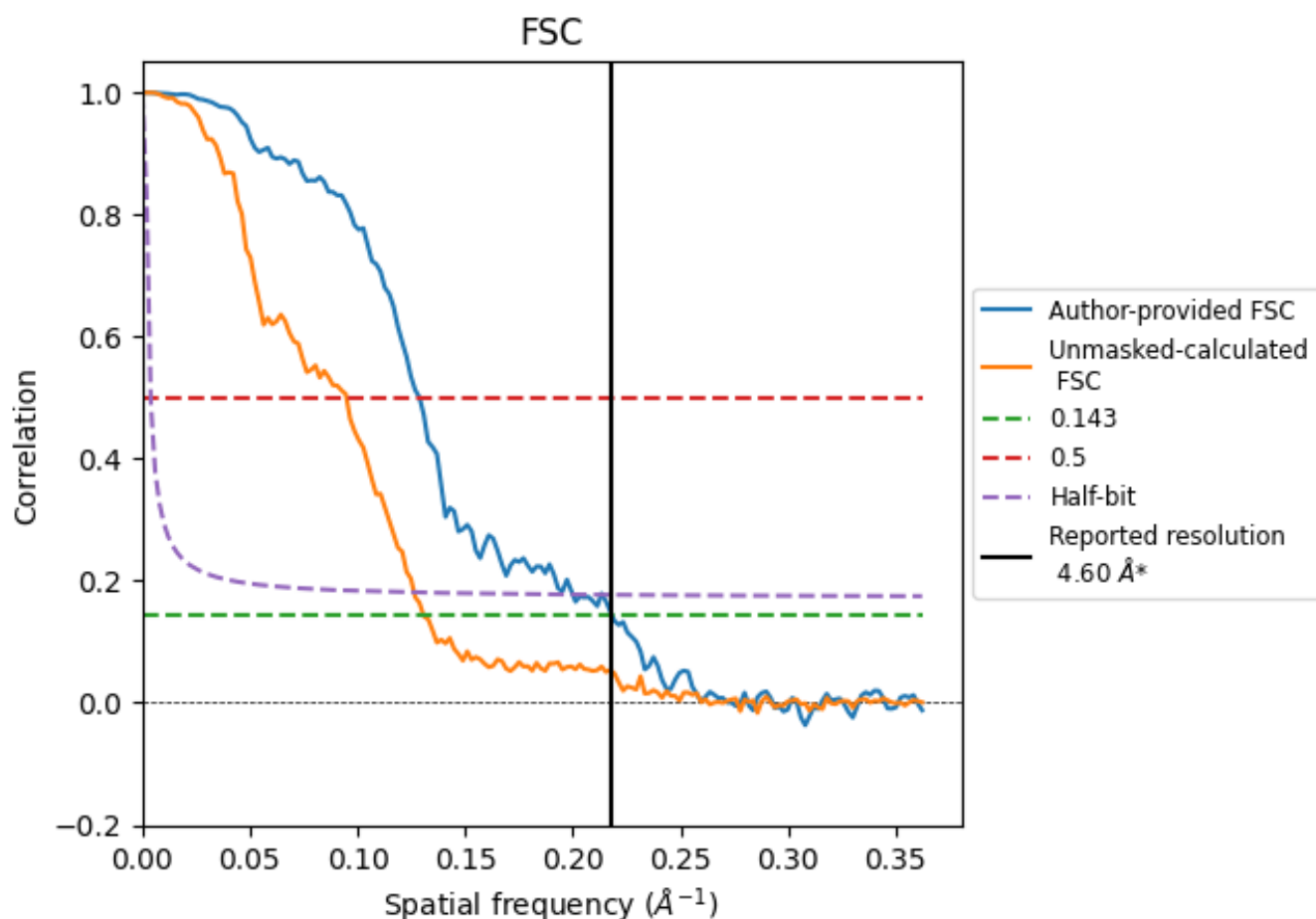


*Reported resolution corresponds to spatial frequency of 0.217 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.217 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

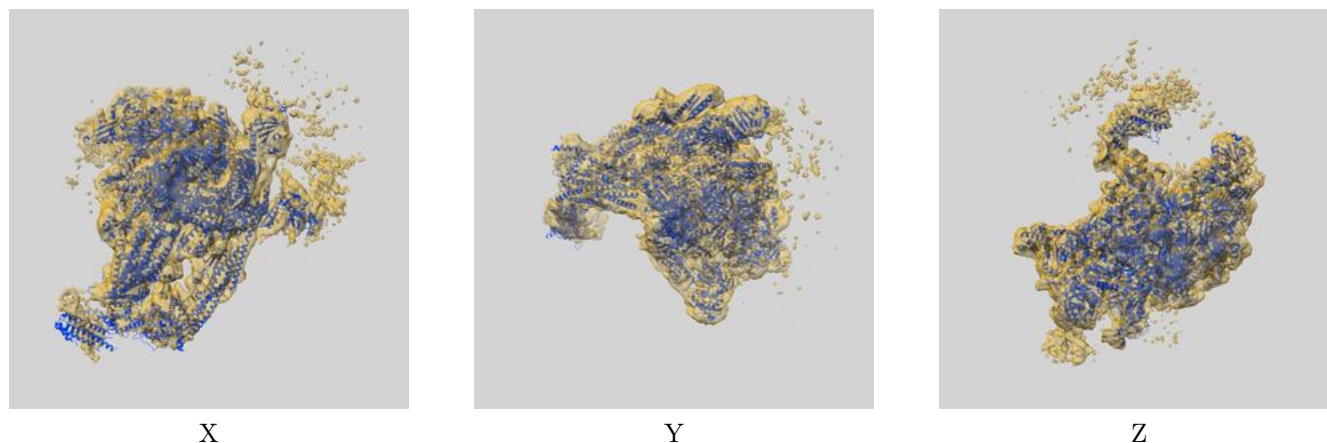
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.58	7.76	5.00
Unmasked-calculated*	7.65	10.54	7.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.65 differs from the reported value 4.6 by more than 10 %

9 Map-model fit [i](#)

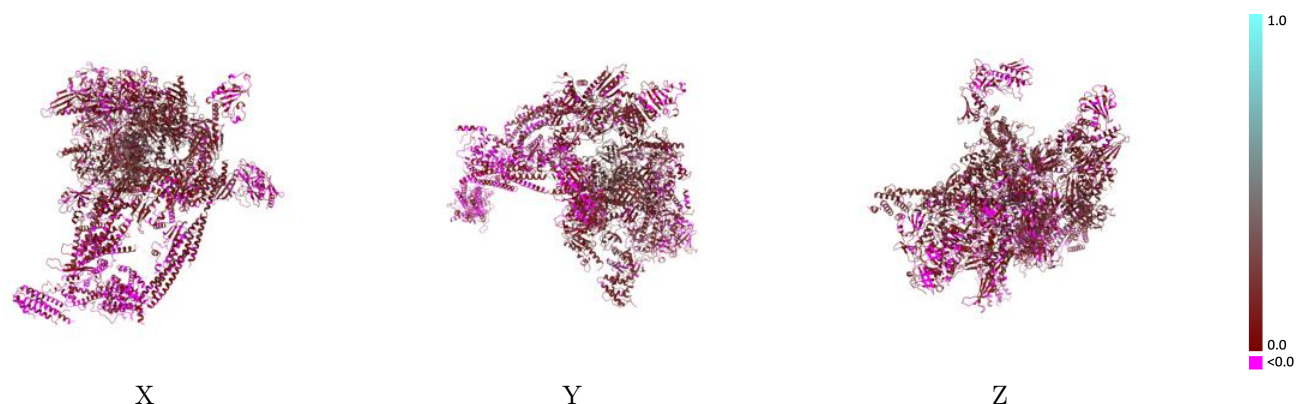
This section contains information regarding the fit between EMDB map EMD-26544 and PDB model 7UIF. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



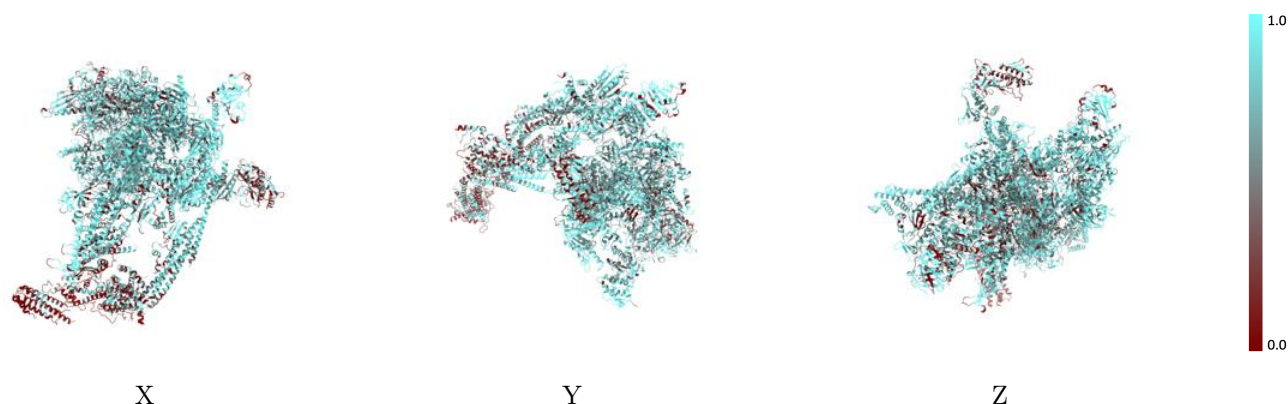
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



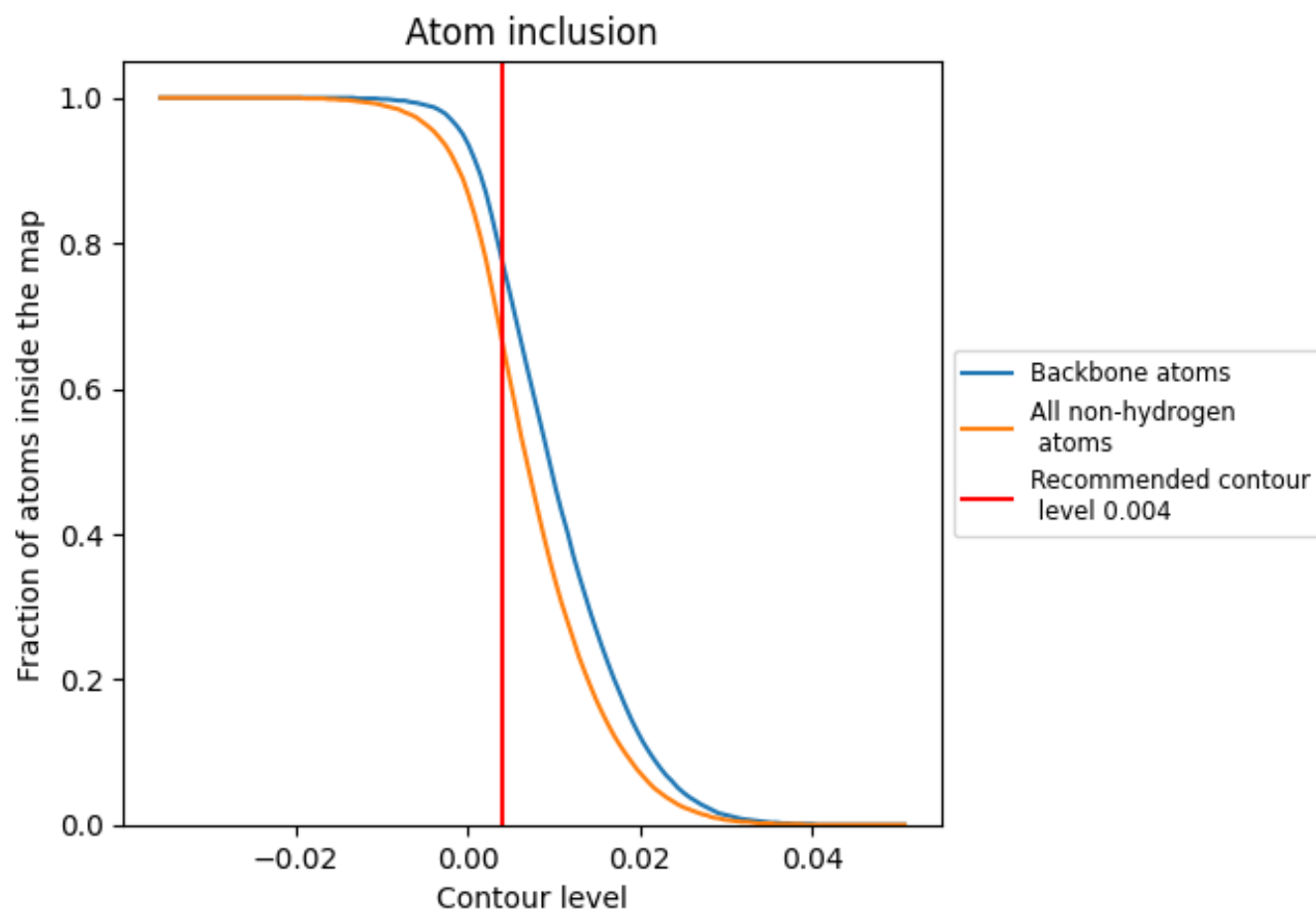
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 67% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6660	 0.1270
A	 0.7460	 0.2120
B	 0.6400	 0.1190
C	 0.7500	 0.1590
D	 0.6820	 0.0850
E	 0.8280	 0.1850
F	 0.7780	 0.2120
G	 0.7350	 0.1250
H	 0.8210	 0.2300
I	 0.7460	 0.1490
J	 0.5930	 0.0660
K	 0.7780	 0.2310
L	 0.6830	 0.0900
M	 0.7960	 0.2840
P	 0.6520	 0.0890
Q	 0.5050	 0.0270
S	 0.7260	 0.1410
a	 0.5300	 0.0480
d	 0.5980	 0.0650
f	 0.4640	 0.0360
g	 0.5340	 0.0110
h	 0.5950	 0.0450
i	 0.7770	 0.1330
j	 0.2830	 0.0210
k	 0.7530	 0.1220
n	 0.6590	 0.0750
q	 0.6910	 0.1120
r	 0.7730	 0.2220
s	 0.0890	 0.0160
t	 0.7820	 0.2000
u	 0.6690	 0.0670
v	 0.6410	 0.0800
w	 0.4040	 -0.0340
z	 0.3330	 0.0140

