



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 02:53 PM UTC

PDB ID : 6MZL / pdb_00006mzl
EMDB ID : EMD-9305
Title : Human TFIID canonical state
Authors : Patel, A.B.; Louder, R.K.; Greber, B.J.; Grunberg, S.; Luo, J.; Fang, J.; Liu, Y.; Ranish, J.; Hahn, S.; Nogales, E.
Deposited on : 2018-11-05
Resolution : 23.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

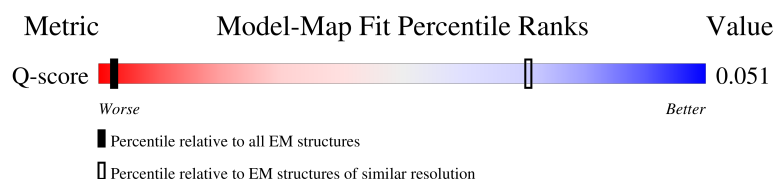
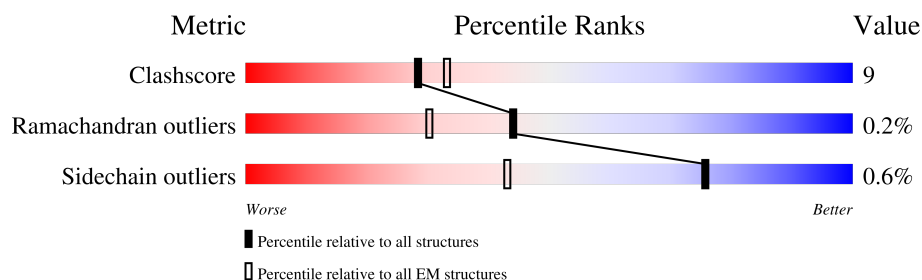
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 23.00 Å.

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



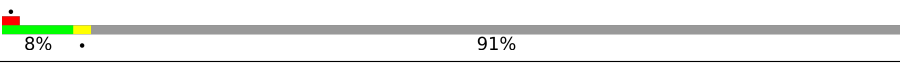
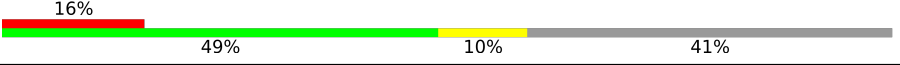
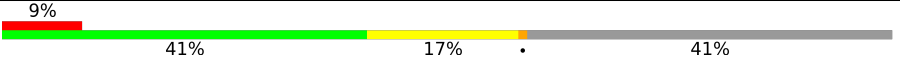
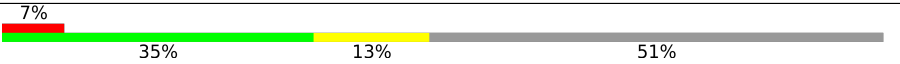
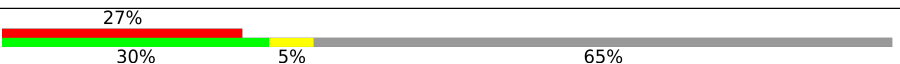
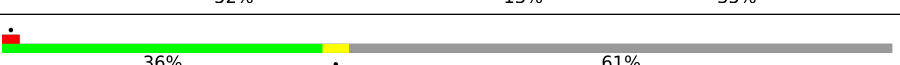
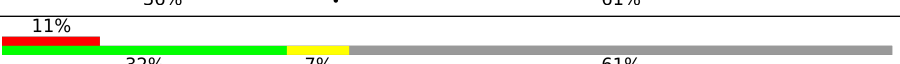
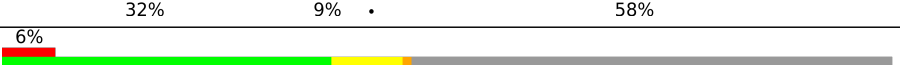
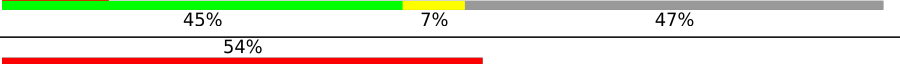
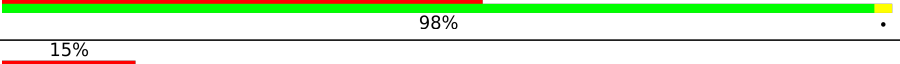
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	17 (22.90 - 23.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1872	14% 22% 75%
2	B	1199	16% 52% 28% 19%
3	C	929	9% 90%
4	D	1085	9% 91%

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Mol	Chain	Length	Quality of chain
4	E	1085	
5	F	800	
5	G	800	
6	H	677	
7	I	677	
8	J	349	
9	K	310	
10	L	264	
10	M	264	
11	N	218	
11	O	218	
12	P	211	
13	Q	161	
13	R	161	
14	S	124	
15	T	339	
16	Y	96	
17	Z	238	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 36618 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 Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	472	Total	C	N	O	S	0	0
			3772	2397	659	693	23		

- Molecule 2 is a protein called Transcription initiation factor TFIID subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	968	Total	C	N	O	S	0	0
			7832	5031	1322	1421	58		

- Molecule 3 is a protein called Transcription initiation factor TFIID subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	93	Total	C	N	O	S	0	0
			742	467	128	141	6		

- Molecule 4 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	102	Total	C	N	O	0	0
			686	423	130	133		
4	E	102	Total	C	N	O	0	0
			686	423	130	133		

- Molecule 5 is a protein called Transcription initiation factor TFIID subunit 5,TAF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	473	Total	C	N	O	S	0	0
			3646	2314	638	679	15		
5	G	473	Total	C	N	O	S	0	0
			3646	2314	638	679	15		

- Molecule 6 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	329	Total	C	N	O	S	0	0
			2494	1575	439	464	16		

- Molecule 7 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	339	Total	C	N	O	S	0	0
			2520	1585	445	474	16		

- Molecule 8 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	123	Total	C	N	O	S	0	0
			998	638	184	172	4		

- Molecule 9 is a protein called Transcription initiation factor TFIID subunit 8, TAF8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	202	Total	C	N	O	S	0	0
			1449	906	260	278	5		

- Molecule 10 is a protein called Transcription initiation factor TFIID subunit 9, TAF9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	104	Total	C	N	O	S	0	0
			732	456	129	142	5		
10	M	104	Total	C	N	O	S	0	0
			732	456	129	142	5		

- Molecule 11 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	82	Total	C	N	O	S	0	0
			645	413	102	126	4		
11	O	82	Total	C	N	O	S	0	0
			645	413	102	126	4		

- Molecule 12 is a protein called Transcription initiation factor TFIID subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	89	Total	C	N	O	S	0	0
			707	447	127	128	5		

- Molecule 13 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	74	Total	C	N	O	S	0	0
			611	381	107	120	3		
13	R	74	Total	C	N	O	S	0	0
			611	381	107	120	3		

- Molecule 14 is a protein called Transcription initiation factor TFIID subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	45	Total	C	N	O	S	0	0
			365	233	54	73	5		

- Molecule 15 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	180	Total	C	N	O	S	0	0
			1429	927	252	243	7		

- Molecule 16 is a protein called poly(UNK).

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Y	96	Total	C	N	O	0	0
			480	288	96	96		

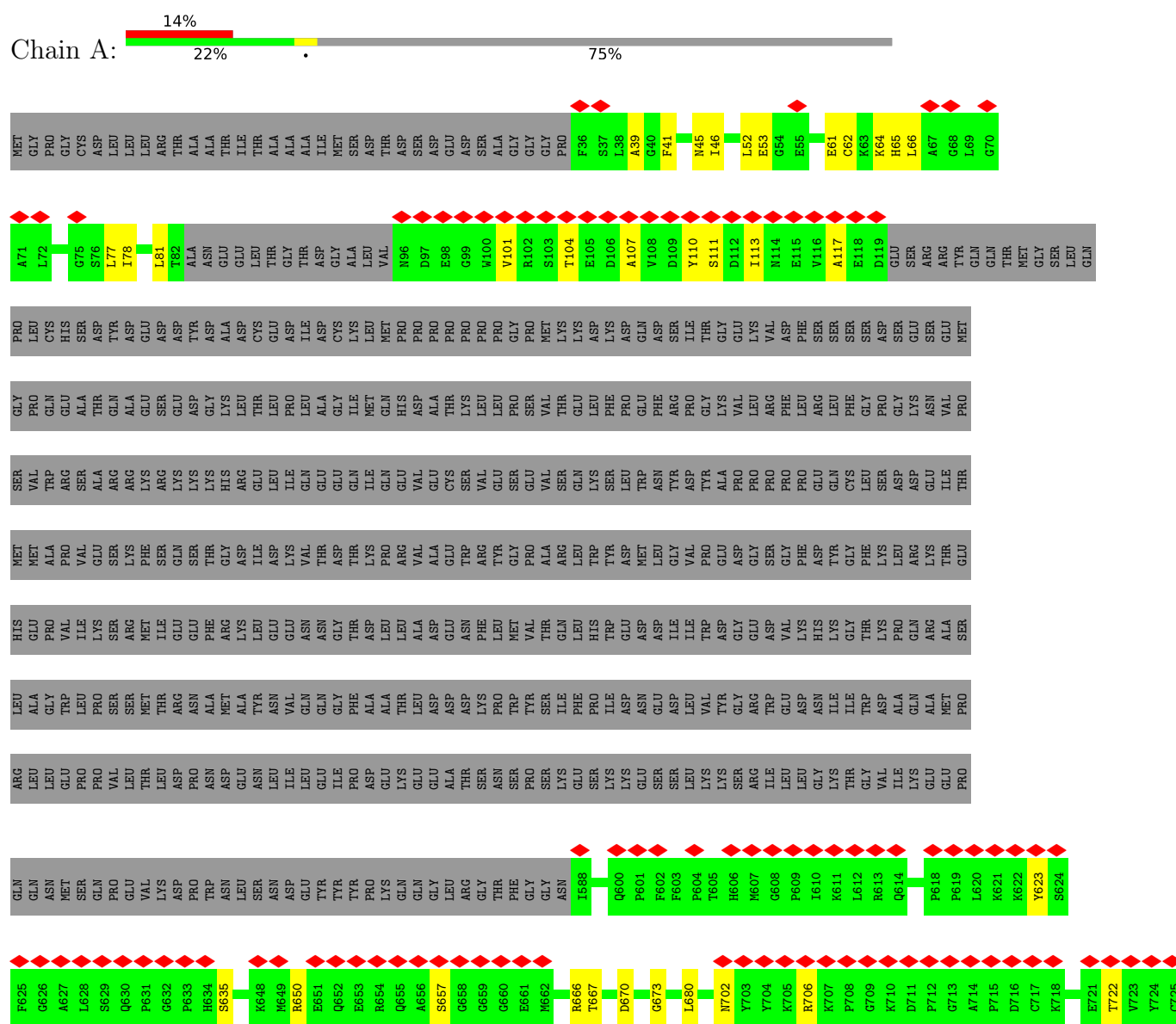
- Molecule 17 is a protein called poly(UNK).

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Z	238	Total	C	N	O	0	0
			1190	714	238	238		

3 Residue-property plots

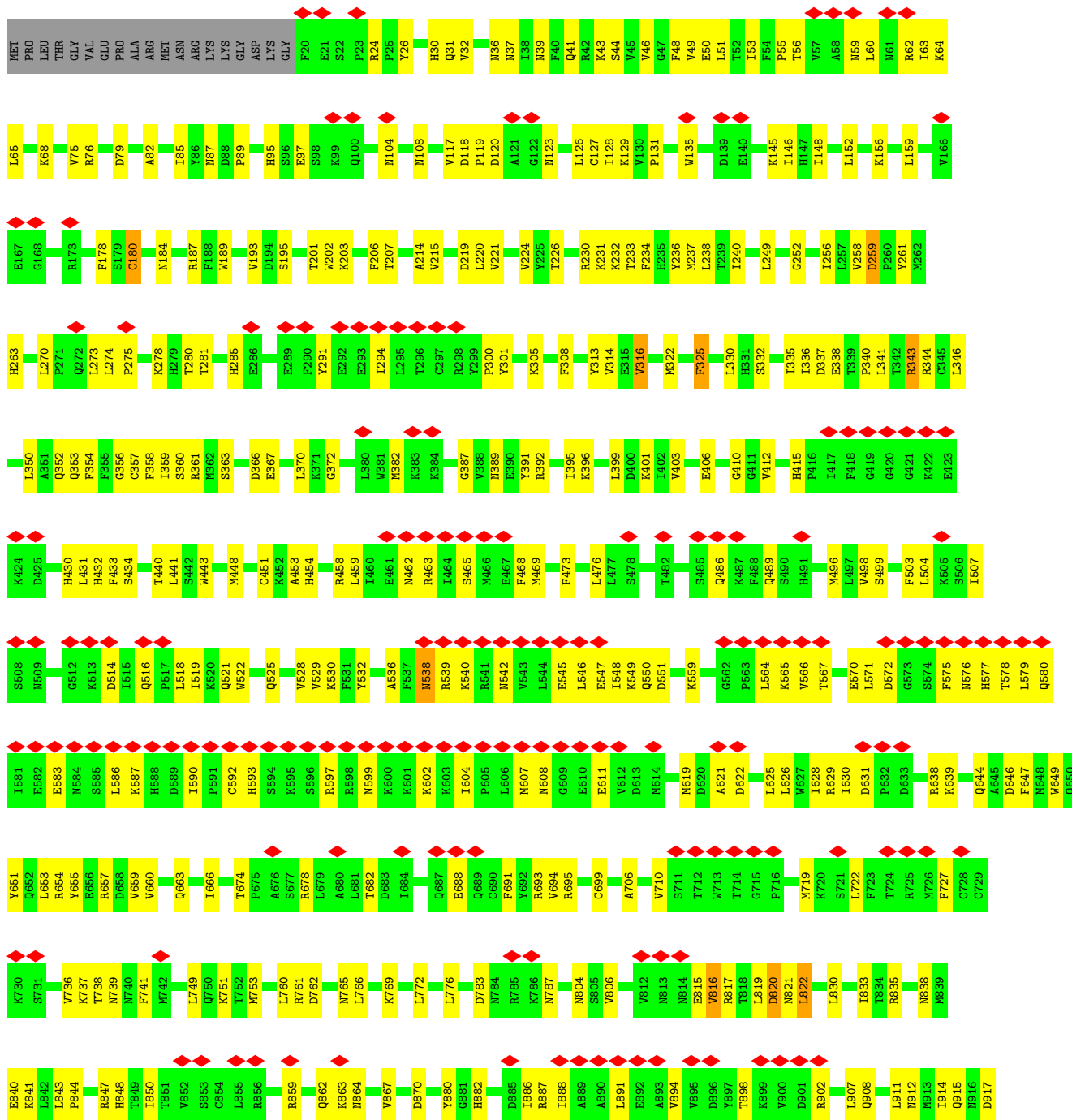
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

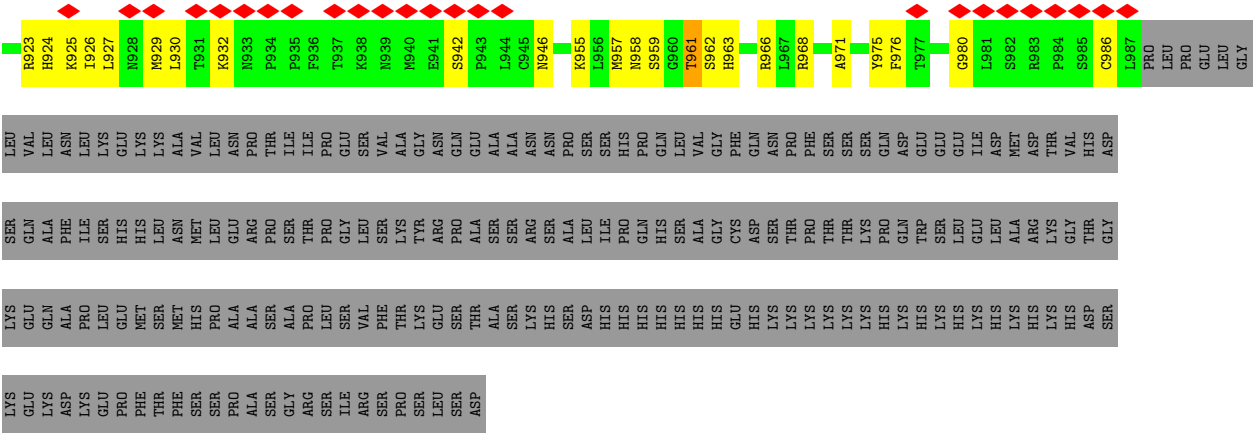
- Molecule 1: Transcription initiation factor TFIID subunit 1



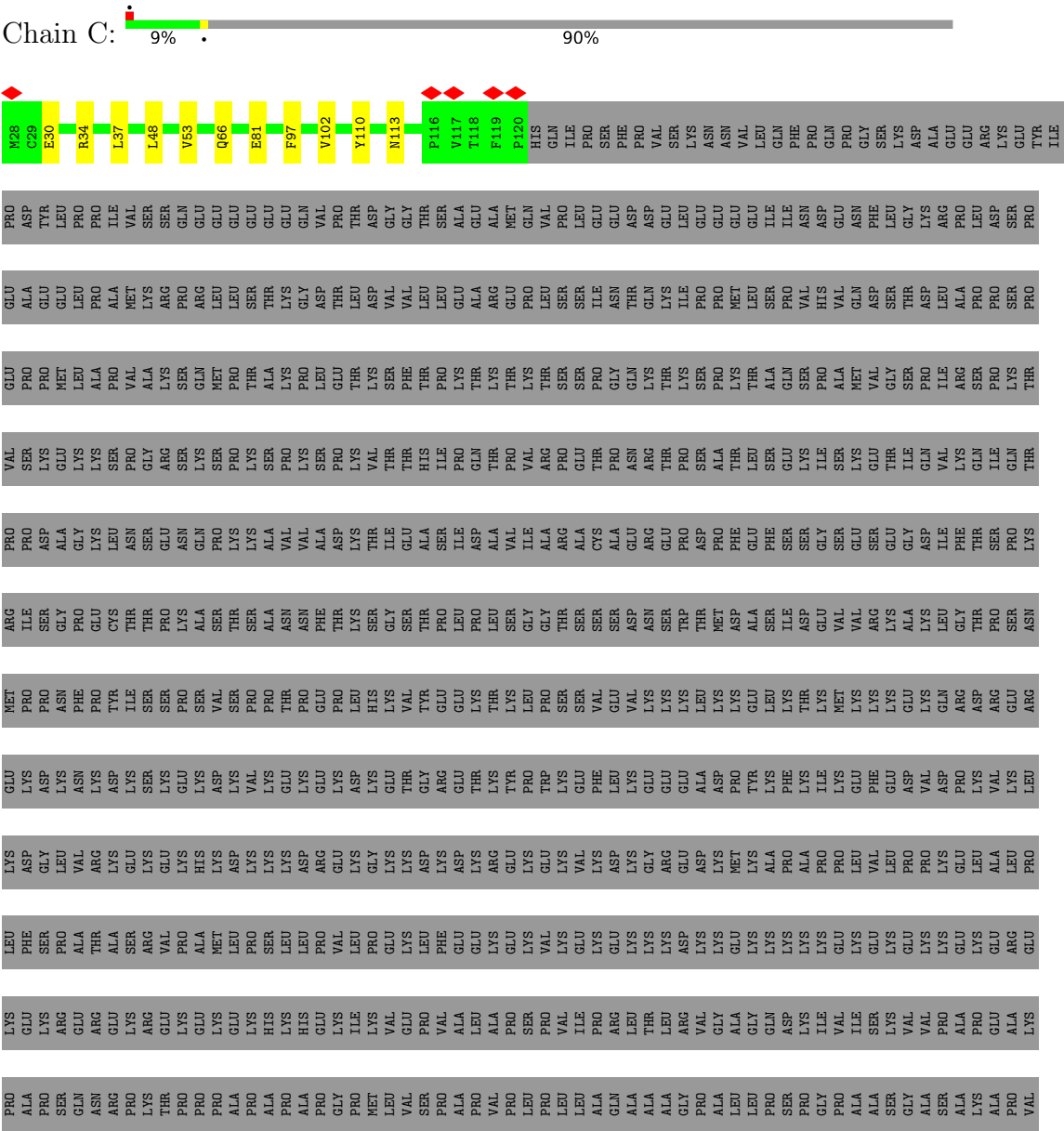


- Molecule 2: Transcription initiation factor TFIID subunit 2



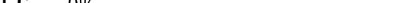


● Molecule 3: Transcription initiation factor TFIID subunit 3



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

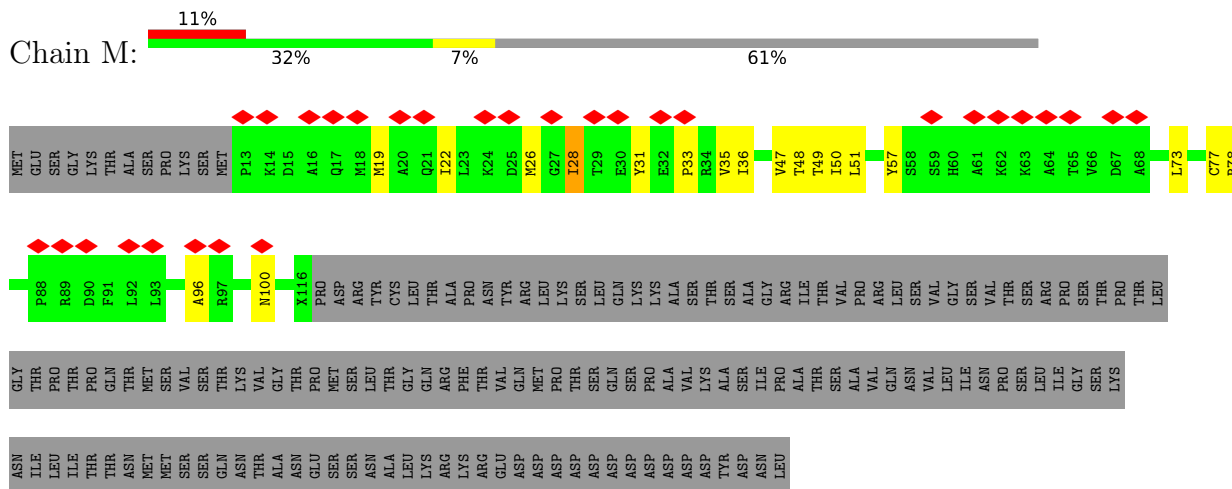
- Molecule 4: Transcription initiation factor TFIID subunit 4

Chain D:  9% 91%

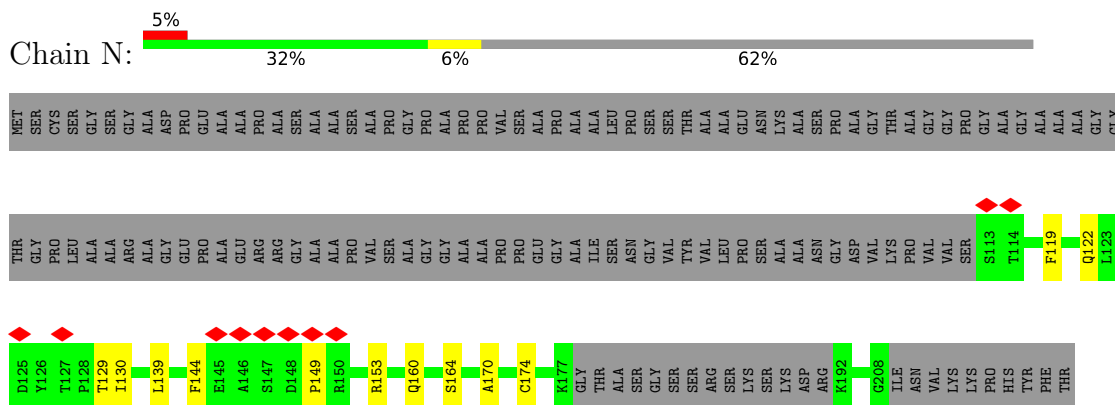
Y934	ALA	GLN	VAL	LEU	LEU	SER	GLN	HIS	SER	LEU	ALA	PRO	GLY	PRO	ALA	VAL	HIS	MET
E935	VAL	ILE	SER	LEU	ALA	THR	ARG	ALA	GLN	ILE	ALA	PRO	PHE	GLY	ALA	VAL	VAL	ALA
Q936	ASN	GLN	LEU	ARG	LEU	ILE	GLY	PRO	GLN	ARG	GLN	LEU	VAL	GLY	ALA	GLY	GLY	SER
A937	LEU	ASN	GLN	GLN	LEU	VAL	VAL	THR	GLN	ALA	PRO	PRO	ALA	PRO	LEU	SER	SER	ASP
S938	SER	PRO	PRO	GLN	LEU	ALA	GLN	THR	THR	LEU	ALA	ALA	ALA	GLY	ARG	PRO	PRO	LEU
D939	GLU	LEU	THR	THR	THR	SER	THR	MET	THR	THR	SER	THR	ALA	LYS	ALA	ALA	ALA	LEU
I953	ALA	VAL	LYS	PHE	ALA	THR	GLY	THR	THR	PRO	MET	THR	ALA	GLY	GLY	GLY	PHE	ASN
E954	ARG	VAL	VAL	SER	ALA	VAL	GLN	ARG	PRO	VAL	SER	ALA	ALA	ALA	ALA	VAL	ALA	GLU
K955	ILE	VAL	GLY	ALA	GLN	SER	GLY	PRO	ALA	LEU	ALA	ALA	PRO	PRO	GLY	GLY	ALA	PHE
Q956	LEU	VAL	GLY	ALA	GLN	SER	THR	ALA	THR	LEU	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ASN
R957	THR	VAL	GLN	ILE	GLU	THR	ALA	PRO	ARG	ILE	VAL	THR	ALA	ALA	GLY	PRO	GLY	SER
K958	ASN	PRO	GLN	THR	THR	THR	ALA	THR	SER	THR	GLY	PRO	SER	GLN	SER	ALA	ALA	GLY
D959	SER	ALA	GLN	GLN	ALA	ALA	GLN	SER	SER	PRO	THR	PRO	PRO	THR	CYS	ALA	ALA	VAL
E960	GLU	VAL	THR	SER	ALA	ASN	THR	ALA	PRO	GLN	ALA	ALA	ALA	PRO	ALA	PRO	PRO	ASP
Q961	LEU	LEU	THR	GLN	VAL	ASN	VAL	PRO	PRO	MET	GLN	ALA	ALA	ASN	ALA	GLY	GLY	GLU
E962	VAL	PRO	PRO	PRO	VAL	LYS	SER	VAL	VAL	GLN	GLY	GLY	PRO	SER	VAL	ALA	ALA	VAL
R963	THR	THR	VAL	VAL	GLU	GLU	GLY	GLN	GLN	ASN	ALA	ALA	ALA	ALA	ALA	ALA	ALA	SER
E964	LEU	LYS	ILE	ILE	PRO	LEU	THR	ILE	ILE	THR	LEU	ALA	PRO	ALA	ALA	ALA	GLY	ASP
E965	THR	ALA	GLN	GLN	VAL	VAL	GLN	SER	THR	THR	SER	SER	VAL	ALA	ALA	ALA	ALA	LEU
I966	ARG	LEU	GLN	PRO	THR	GLN	THR	THR	THR	ASN	THR	ASN	ALA	ALA	ALA	ALA	ALA	SER
S967	SER	ALA	PRO	ASN	LEU	LEU	GLN	VAL	GLN	GLN	ALA	ALA	GLY	SER	ALA	GLY	GLY	VAL
M967	CYS	VAL	VAL	SER	SER	THR	VAL	ALA	ALA	ILE	ALA	PRO	ALA	ASN	VAL	ALA	ALA	GLY
R968	LYS	VAL	VAL	LYS	GLN	ASP	THR	PRO	GLY	GLY	VAL	PRO	ALA	HIS	PRO	ALA	ALA	SER
A969	ASP	ALA	PRO	ALA	THR	THR	GLY	THR	THR	LEU	GLN	PRO	PRO	ALA	PRO	PRO	PRO	GLU
E970	E970	GLN	ALA	THR	ALA	LYS	THR	THR	THR	PRO	PRO	PRO	PRO	ALA	ALA	ALA	ALA	SER
K971	L873	GLN	ALA	ILE	ILE	GLU	GLN	PRO	PRO	PRO	GLY	GLY	PRO	PRO	PRO	GLY	GLY	GLN
S984	E984	GLN	PRO	VAL	GLU	THR	ARG	ALA	THR	VAL	THR	THR	THR	SER	ALA	ALA	ARG	SER
I885	I885	LYS	GLN	VAL	VAL	PHE	GLU	GLN	GLN	LEU	LEU	THR	THR	LEU	LEU	GLY	GLY	ALA
Q886	Q886	LYS	ASN	VAL	VAL	THR	THR	VAL	VAL	VAL	VAL	VAL	VAL	SER	GLY	GLY	GLY	ALA
R887	R887	LYS	ASN	VAL	VAL	SER	SER	THR	THR	GLY	ARG	THR	THR	THR	ALA	ALA	ALA	ALA
K888	K888	LYS	LEU	THR	ARG	LEU	THR	PRO	THR	ILE	SER	PRO	LEU	ASN	PRO	ARG	ARG	HIS
H889	H889	LYS	THR	SER	SER	THR	THR	THR	THR	THR	GLY	ALA	ALA	ALA	GLY	GLY	GLY	HIS
T892	T892	GLU	PRO	GLN	VAL	TYR	THR	THR	THR	ASN	LYS	THR	VAL	ARG	PRO	PRO	PRO	HIS
E893	E893	PRO	GLY	THR	GLN	ARG	SER	ILE	THR	ILE	GLY	GLY	PRO	ALA	ALA	GLN	GLN	LEU
L894	L894	GLY	THR	MET	THR	LEU	ALA	LYS	GLY	GLN	ALA	ALA	GLY	GLY	PRO	PRO	ARG	ALA
V899	V899	GLY	VAL	ALA	ALA	ASN	ALA	GLN	LEU	LEU	GLY	GLY	SER	HIS	LEU	LEU	GLY	ARG
H904	H904	PHE	LEU	ALA	GLY	SER	THR	VAL	THR	ILE	VAL	PRO	ALA	ALA	ALA	PRO	PRO	THR
Q907	Q907	ASP	GLN	GLN	GLU	GLN	MET	GLN	GLN	GLN	VAL	VAL	VAL	LYS	ALA	ALA	ARG	GLY
Q908	Q908	ASP	ASN	THR	THR	TYR	ASN	THR	THR	ALA	LEU	THR	THR	ALA	PRO	ARG	ARG	ASN
Q911	Q911	ILE	ARG	THR	VAL	VAL	VAL	THR	VAL	THR	SER	VAL	VAL	ALA	ALA	PRO	ALA	ALA
V914	V914	ASN	ILE	SER	ALA	PHE	THR	GLN	GLN	GLN	THR	THR	PRO	GLY	ALA	VAL	VAL	ALA
K929	K929	ALA	VAL	LEU	LEU	LYS	LEU	SER	PRO	THR	ARG	THR	THR	GLY	LEU	GLY	GLY	LEU
D930	D930	THR	THR	PRO	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	PRO	ASN



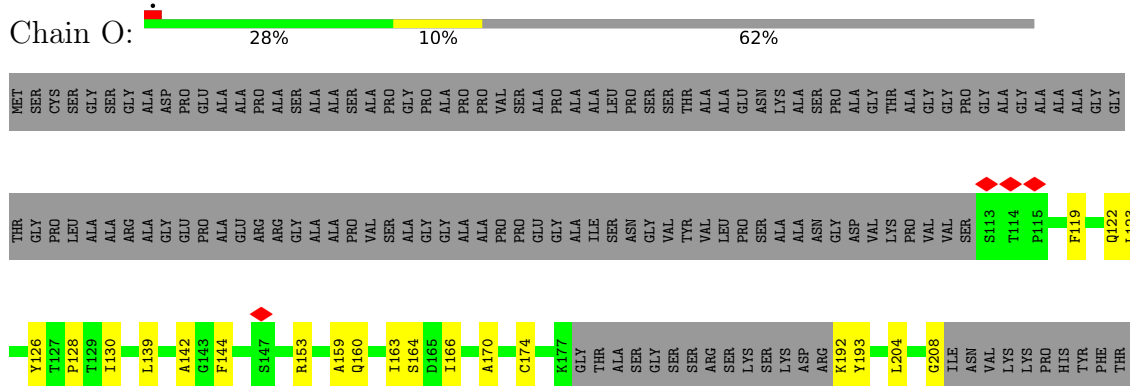
Chain M:



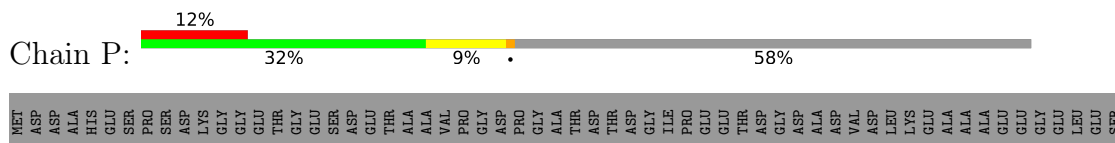
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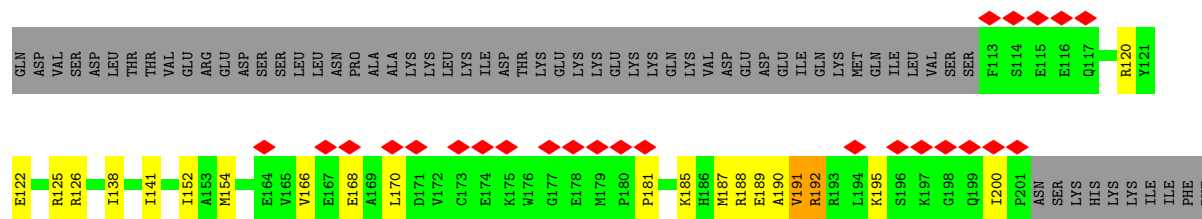


Chain 0:

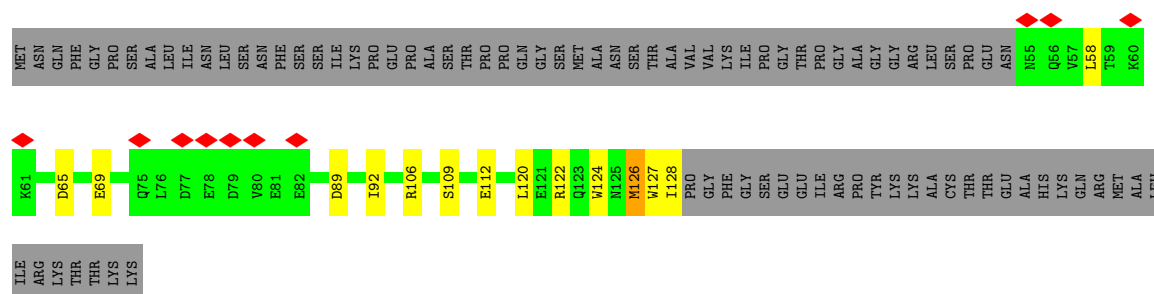
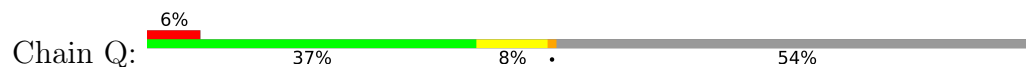


Chain P:

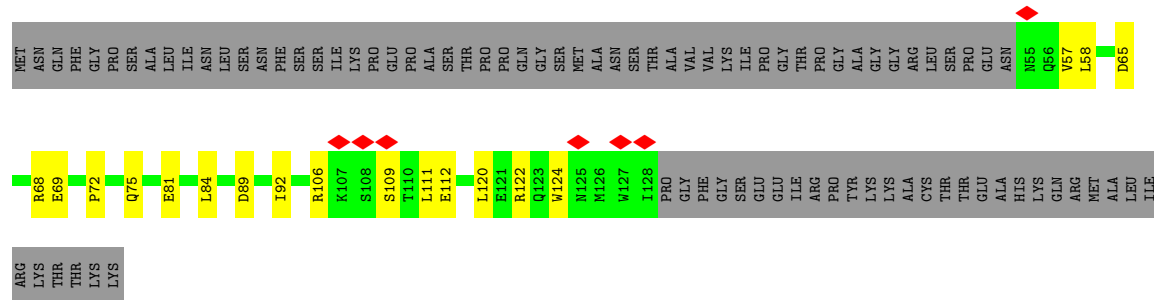
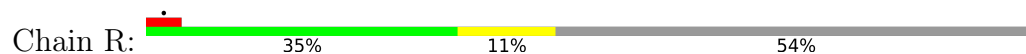




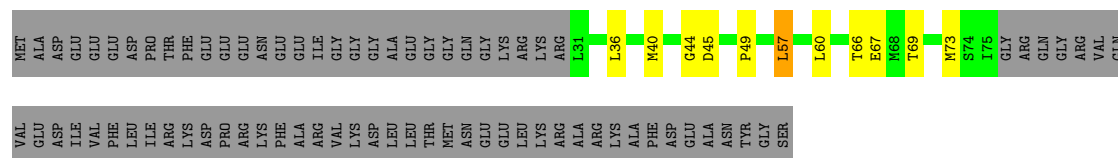
• Molecule 13: Transcription initiation factor TFIID subunit 12



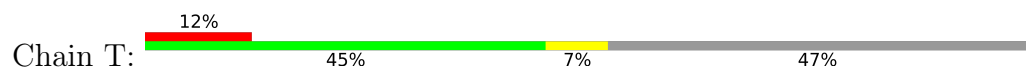
• Molecule 13: Transcription initiation factor TFIID subunit 12

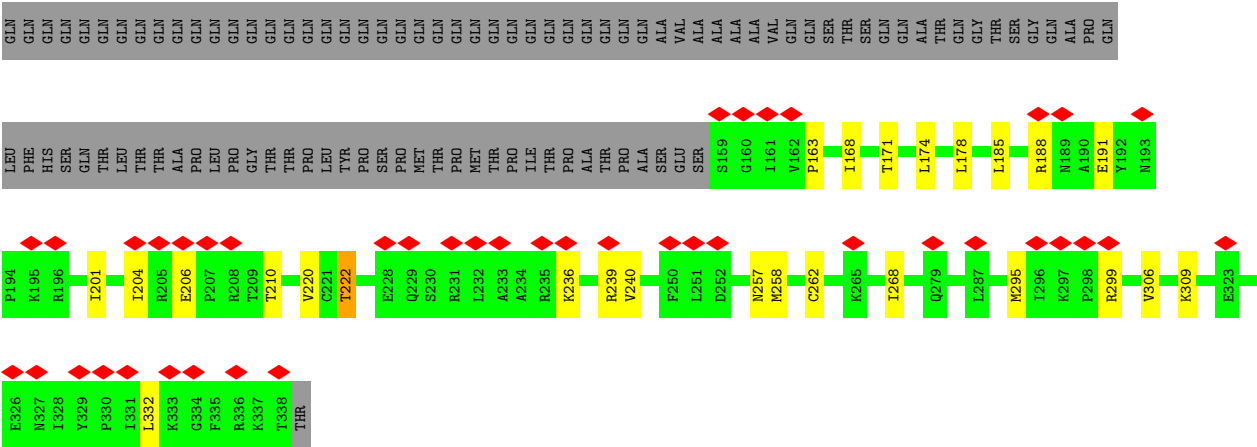


• Molecule 14: Transcription initiation factor TFIID subunit 13

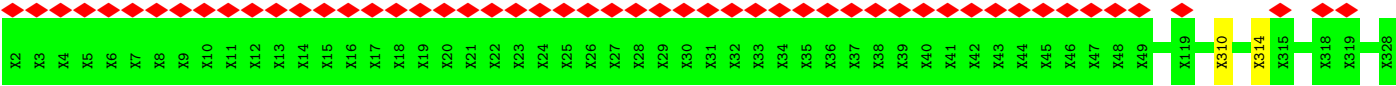


• Molecule 15: TATA-box-binding protein

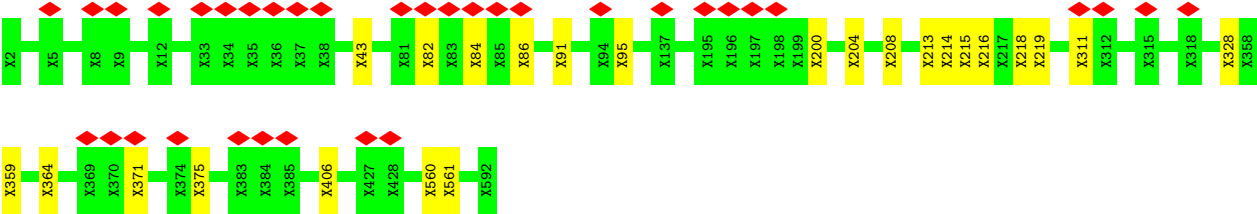
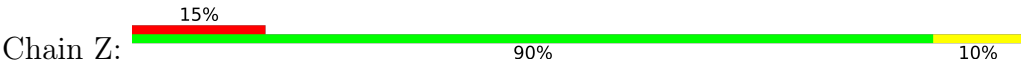




● Molecule 16: poly(UNK)



● Molecule 17: poly(UNK)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	107900	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	144, 144, 144	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.64, 2.64, 2.64	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	0.19	0/3858	0.51	3/5193 (0.1%)
2	B	0.53	0/8029	0.85	7/10882 (0.1%)
3	C	0.24	0/757	0.53	0/1027
4	D	0.31	0/692	0.70	3/945 (0.3%)
4	E	0.29	0/692	0.52	0/945
5	F	0.22	0/3537	0.59	0/4802
5	G	0.50	0/3537	0.81	4/4802 (0.1%)
6	H	0.46	0/2533	0.75	1/3439 (0.0%)
7	I	0.42	0/2506	0.77	3/3402 (0.1%)
8	J	0.23	0/1017	0.52	0/1370
9	K	0.41	0/1212	0.65	0/1640
10	L	0.18	0/705	0.50	0/955
10	M	0.32	0/705	0.69	0/955
11	N	0.21	0/657	0.48	0/891
11	O	0.32	0/657	0.55	0/891
12	P	0.34	0/719	0.89	3/965 (0.3%)
13	Q	0.26	0/618	0.65	1/835 (0.1%)
13	R	0.27	0/618	0.59	0/835
14	S	0.24	0/371	0.68	0/498
15	T	0.28	0/1455	0.59	0/1958
All	All	0.39	0/34875	0.71	25/47230 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	17
5	F	0	3
5	G	0	8
6	H	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	I	0	4
9	K	0	2
10	M	0	1
17	Z	0	1
All	All	0	43

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	908	GLN	CB-CG-CD	7.70	125.69	112.60
7	I	261	THR	CA-C-N	-7.45	109.75	122.56
7	I	261	THR	C-N-CA	-7.45	109.75	122.56
1	A	657	SER	N-CA-C	6.79	120.81	111.71
12	P	192	ARG	CB-CG-CD	-6.25	96.92	111.30
12	P	192	ARG	CG-CD-NE	6.23	125.71	112.00
7	I	392	ILE	N-CA-C	-6.18	106.41	111.91
12	P	192	ARG	CA-CB-CG	5.85	125.81	114.10
1	A	657	SER	CA-C-N	5.46	131.53	121.70
1	A	657	SER	C-N-CA	5.46	131.53	121.70
2	B	252	GLY	N-CA-C	5.37	123.28	112.34
5	G	607	ARG	CA-CB-CG	5.34	124.79	114.10
6	H	312	ILE	N-CA-CB	-5.32	106.17	112.39
2	B	741	PHE	CA-C-N	5.23	131.53	121.54
2	B	741	PHE	C-N-CA	5.23	131.53	121.54
2	B	765	ASN	CA-C-N	5.23	131.53	121.54
2	B	765	ASN	C-N-CA	5.23	131.53	121.54
5	G	589	TRP	N-CA-C	5.22	116.82	111.03
5	G	730	SER	CA-C-N	5.14	131.37	121.54
5	G	730	SER	C-N-CA	5.14	131.37	121.54
13	Q	126	MET	CB-CG-SD	5.13	128.08	112.70
4	D	907	GLN	CA-C-N	-5.12	113.10	122.38
4	D	907	GLN	C-N-CA	-5.12	113.10	122.38
2	B	226	THR	CA-C-N	5.04	131.16	121.54
2	B	226	THR	C-N-CA	5.04	131.16	121.54

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	949	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	B	193	VAL	Peptide
2	B	259	ASP	Peptide
2	B	316	VAL	Peptide
2	B	325	PHE	Peptide
2	B	340	PRO	Peptide
2	B	415	HIS	Peptide
2	B	434	SER	Peptide
2	B	538	ASN	Peptide
2	B	540	LYS	Peptide
2	B	583	GLU	Peptide
2	B	674	THR	Peptide
2	B	737	LYS	Peptide
2	B	816	VAL	Peptide
2	B	820	ASP	Peptide
2	B	821	ASN	Peptide
2	B	822	LEU	Peptide
2	B	843	LEU	Peptide
5	F	668	HIS	Peptide
5	F	721	ARG	Peptide
5	F	783	LEU	Peptide
5	G	275	TYR	Peptide
5	G	467	LEU	Peptide
5	G	479	THR	Peptide
5	G	489	PHE	Peptide
5	G	615	ASP	Peptide
5	G	668	HIS	Peptide
5	G	711	THR	Peptide
5	G	721	ARG	Peptide
6	H	313	VAL	Peptide
6	H	320	ARG	Peptide
6	H	347	THR	Peptide
6	H	348	THR	Peptide
6	H	384	GLY	Peptide
6	H	441	PRO	Peptide
7	I	216	UNK	Peptide
7	I	254	GLN	Peptide
7	I	256	LEU	Peptide
7	I	262	PHE	Peptide
9	K	144	UNK	Peptide
9	K	217	ARG	Peptide
10	M	28	ILE	Peptide
17	Z	364	UNK	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3772	0	3742	43	0
2	B	7832	0	7789	223	0
3	C	742	0	719	8	0
4	D	686	0	572	8	0
4	E	686	0	572	13	0
5	F	3646	0	3312	47	0
5	G	3646	0	3312	94	0
6	H	2494	0	2474	58	0
7	I	2520	0	2422	65	0
8	J	998	0	1055	12	0
9	K	1449	0	1281	34	0
10	L	732	0	624	6	0
10	M	732	0	624	13	0
11	N	645	0	640	7	0
11	O	645	0	640	15	0
12	P	707	0	730	26	0
13	Q	611	0	610	16	0
13	R	611	0	610	16	0
14	S	365	0	351	12	0
15	T	1429	0	1521	19	0
16	Y	480	0	112	1	0
17	Z	1190	0	280	17	0
All	All	36618	0	33992	667	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 9.

All (667) 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)
1:A:874:GLU:HG2	2:B:468:PHE:HZ	1.27	0.99
2:B:566:VAL:O	2:B:577:HIS:HA	1.64	0.97
2:B:532:TYR:O	2:B:551:ASP:HB2	1.67	0.94
2:B:50:GLU:HA	2:B:146:ILE:O	1.70	0.92
1:A:874:GLU:HG2	2:B:468:PHE:CZ	2.04	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:309:ILE:O	5:G:341:ILE:HA	1.73	0.88
2:B:567:THR:O	2:B:629:ARG:HB3	1.73	0.87
2:B:350:LEU:O	2:B:353:GLN:HB3	1.77	0.84
4:D:908:GLN:HG2	12:P:192:ARG:HD3	1.61	0.83
6:H:329:LEU:O	6:H:332:PHE:HB3	1.79	0.80
12:P:195:LYS:HE2	13:Q:127:TRP:H	1.45	0.80
7:I:350:ASN:O	7:I:354:ARG:HB2	1.82	0.79
4:D:904:HIS:HA	12:P:192:ARG:HH21	1.50	0.76
1:A:62:CYS:O	1:A:66:LEU:HB2	1.84	0.76
3:C:34:ARG:HG2	3:C:66:GLN:HE22	1.53	0.73
2:B:538:ASN:HA	2:B:542:ASN:HD22	1.51	0.73
2:B:39:ASN:HB3	2:B:44:SER:H	1.52	0.73
2:B:835:ARG:HH22	9:K:184:ARG:HE	1.36	0.73
5:G:474:THR:O	5:G:486:ALA:HB3	1.89	0.72
7:I:392:ILE:HA	7:I:395:ARG:HB2	1.71	0.71
2:B:305:LYS:O	2:B:322:MET:HA	1.91	0.70
5:G:726:LEU:HB2	5:G:738:TRP:HB2	1.73	0.70
9:K:112:LYS:HA	9:K:116:ARG:HD2	1.74	0.70
2:B:564:LEU:H	2:B:580:GLN:HB2	1.57	0.69
11:N:139:LEU:HB3	11:N:144:PHE:HB3	1.73	0.69
5:F:718:ARG:HG2	5:F:771:GLY:H	1.58	0.68
5:G:475:ALA:HA	5:G:484:LEU:O	1.93	0.68
9:K:195:ALA:HB1	9:K:212:PRO:HG2	1.76	0.68
5:F:586:TYR:HB3	5:F:605:HIS:HB3	1.75	0.68
7:I:338:ALA:HB2	7:I:382:GLU:HB3	1.76	0.67
2:B:463:ARG:NH1	2:B:514:ASP:O	2.27	0.67
11:O:130:ILE:HG13	11:O:160:GLN:HE21	1.59	0.66
2:B:64:LYS:HA	2:B:126:LEU:O	1.96	0.66
6:H:330:ARG:O	6:H:333:ALA:HB3	1.95	0.66
6:H:333:ALA:O	6:H:336:LEU:HB2	1.94	0.66
6:H:325:ASN:O	6:H:328:ALA:HB3	1.95	0.66
7:I:323:VAL:HA	7:I:326:HIS:HD2	1.60	0.66
1:A:101:VAL:HG21	15:T:191:GLU:HA	1.78	0.66
1:A:666:ARG:HG3	1:A:667:THR:HG23	1.77	0.66
2:B:62:ARG:HG2	2:B:129:LYS:HG2	1.76	0.66
2:B:815:GLU:HA	2:B:819:LEU:HD12	1.79	0.65
2:B:835:ARG:HH21	9:K:188:ARG:HD2	1.61	0.65
2:B:354:PHE:O	2:B:357:CYS:HB2	1.97	0.65
5:F:321:LEU:HD22	5:F:327:ASN:HD21	1.61	0.65
6:H:323:VAL:O	6:H:327:TRP:N	2.29	0.65
2:B:359:ILE:HG23	2:B:498:VAL:HB	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:888:ILE:HD11	2:B:925:LYS:HG3	1.79	0.64
5:G:733:ASN:HB3	5:G:761:LEU:HB2	1.80	0.64
4:E:892:THR:H	13:R:109:SER:HB2	1.63	0.64
12:P:185:LYS:O	12:P:189:GLU:HB2	1.97	0.63
5:G:586:TYR:HB3	5:G:605:HIS:HB3	1.79	0.63
10:L:77:CYS:SG	13:Q:122:ARG:NH2	2.71	0.63
2:B:396:LYS:HD2	2:B:660:VAL:HA	1.80	0.63
2:B:630:ILE:O	2:B:638:ARG:NH1	2.31	0.63
5:F:472:GLY:HA3	5:F:783:LEU:HD13	1.80	0.63
5:F:726:LEU:HB2	5:F:738:TRP:HB2	1.81	0.63
9:K:108:PRO:O	9:K:111:ALA:HB3	1.99	0.63
12:P:122:GLU:OE2	12:P:125:ARG:NH2	2.32	0.63
2:B:118:ASP:O	2:B:123:ASN:ND2	2.32	0.63
1:A:874:GLU:CG	2:B:468:PHE:HZ	2.06	0.62
2:B:32:VAL:HA	2:B:203:LYS:O	1.99	0.62
2:B:459:LEU:HD23	2:B:462:ASN:HD22	1.63	0.62
15:T:191:GLU:HB2	15:T:201:ILE:HB	1.81	0.62
2:B:63:ILE:O	2:B:127:CYS:HA	2.00	0.62
2:B:646:ASP:HA	2:B:649:TRP:HD1	1.65	0.62
5:G:229:LEU:HB2	5:G:232:HIS:HD2	1.64	0.62
5:G:684:LEU:HB2	5:G:696:TRP:HB2	1.80	0.62
2:B:338:GLU:OE2	2:B:847:ARG:NH2	2.32	0.62
2:B:651:TYR:OH	2:B:654:ARG:NH2	2.33	0.62
5:F:286:THR:HG22	5:F:287:LYS:HG3	1.82	0.61
10:M:57:TYR:OH	13:R:122:ARG:NH2	2.33	0.61
1:A:77:LEU:HD23	15:T:257:ASN:HD21	1.64	0.61
2:B:206:PHE:O	2:B:233:THR:HA	2.00	0.61
2:B:550:GLN:HB2	2:B:586:LEU:HB2	1.83	0.61
5:F:546:VAL:HA	5:F:562:SER:HA	1.83	0.61
2:B:955:LYS:O	2:B:959:SER:N	2.31	0.61
5:G:464:TYR:HE1	9:K:151:UNK:HA	1.66	0.61
13:R:65:ASP:O	13:R:69:GLU:HB2	2.01	0.61
5:G:718:ARG:HG2	5:G:771:GLY:H	1.64	0.61
6:H:427:LEU:O	6:H:431:CYS:HB3	2.01	0.61
9:K:65:LEU:HD11	11:O:159:ALA:HB1	1.83	0.60
11:N:130:ILE:HG13	11:N:160:GLN:HE21	1.65	0.60
15:T:236:LYS:HG2	15:T:239:ARG:HH12	1.66	0.60
2:B:433:PHE:HB3	2:B:440:THR:HG21	1.84	0.60
6:H:55:LEU:HD13	10:L:28:ILE:HD12	1.83	0.60
2:B:911:LEU:HA	2:B:914:ILE:HD12	1.82	0.60
5:F:229:LEU:HB2	5:F:232:HIS:HD2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:R:120:LEU:O	13:R:124:TRP:N	2.32	0.60
2:B:691:PHE:HD2	2:B:694:VAL:H	1.48	0.60
6:H:292:ASN:HD22	6:H:295:LEU:HG	1.67	0.60
2:B:41:GLN:O	2:B:43:LYS:NZ	2.35	0.60
5:F:651:VAL:HB	5:F:665:PHE:HB2	1.84	0.60
9:K:31:LEU:HD11	9:K:34:ARG:HH21	1.67	0.59
1:A:927:VAL:O	1:A:933:ASN:ND2	2.35	0.59
7:I:429:LYS:NZ	7:I:458:LEU:O	2.33	0.59
13:Q:106:ARG:HH22	13:Q:112:GLU:HB2	1.66	0.59
7:I:55:LEU:HD13	10:M:28:ILE:HD12	1.84	0.59
2:B:24:ARG:NH1	2:B:120:ASP:OD1	2.33	0.59
5:G:787:ARG:NH2	17:Z:328:UNK:O	2.35	0.59
2:B:538:ASN:HD22	2:B:547:GLU:HB2	1.68	0.59
2:B:219:ASP:O	2:B:236:TYR:HA	2.02	0.59
1:A:117:ALA:H	15:T:239:ARG:HH21	1.50	0.59
2:B:352:GLN:O	2:B:356:GLY:N	2.35	0.59
6:H:233:GLY:O	6:H:239:ARG:NH1	2.35	0.59
10:M:77:CYS:SG	13:R:122:ARG:NH2	2.76	0.59
5:F:733:ASN:HB3	5:F:761:LEU:HB2	1.84	0.58
2:B:230:ARG:HG3	2:B:231:LYS:HG3	1.84	0.58
2:B:915:GLN:O	2:B:923:ARG:NH2	2.37	0.58
5:G:287:LYS:H	5:G:290:HIS:HD2	1.49	0.58
5:G:321:LEU:HD22	5:G:327:ASN:HD21	1.69	0.58
9:K:115:GLN:HE22	11:O:126:TYR:HB3	1.67	0.58
1:A:635:SER:HB3	8:J:40:LYS:HB2	1.84	0.58
5:F:609:ALA:HB3	5:F:623:PHE:HB2	1.86	0.58
7:I:414:ASN:HA	7:I:417:ARG:HB2	1.85	0.58
2:B:401:LYS:HD3	2:B:448:MET:HE1	1.85	0.58
5:G:472:GLY:HA3	5:G:783:LEU:HD13	1.85	0.58
17:Z:82:UNK:O	17:Z:86:UNK:N	2.37	0.58
2:B:917:ASP:OD1	2:B:923:ARG:NE	2.33	0.58
12:P:126:ARG:HG3	15:T:306:VAL:HB	1.84	0.58
2:B:391:TYR:OH	2:B:458:ARG:NH1	2.33	0.58
2:B:608:ASN:O	2:B:657:ARG:NH2	2.37	0.58
2:B:341:LEU:O	2:B:344:ARG:HB3	2.04	0.57
5:G:552:SER:HB3	5:G:557:TYR:HB2	1.86	0.57
5:G:465:THR:HA	5:G:788:ARG:HG2	1.86	0.57
5:G:646:SER:OG	5:G:647:ALA:N	2.36	0.57
12:P:191:VAL:HG12	12:P:195:LYS:HE3	1.85	0.57
5:G:635:PHE:HA	5:G:642:VAL:HG12	1.85	0.57
9:K:73:GLY:HA3	11:O:142:ALA:HB1	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:550:GLN:HE22	2:B:580:GLN:HA	1.69	0.57
3:C:110:TYR:HH	11:N:164:SER:HG	1.52	0.57
2:B:929:MET:HG2	2:B:932:LYS:HD2	1.87	0.57
5:G:278:ASP:O	5:G:282:LEU:HB2	2.04	0.57
6:H:324:ASP:O	6:H:327:TRP:HB2	2.04	0.57
2:B:184:ASN:OD1	2:B:195:SER:OG	2.23	0.57
2:B:599:ASN:HA	2:B:602:LYS:HB2	1.87	0.57
5:G:562:SER:OG	5:G:563:GLU:N	2.37	0.57
2:B:367:GLU:HG3	2:B:370:LEU:HD12	1.86	0.57
5:F:277:ASP:OD1	5:F:649:ARG:NH2	2.38	0.57
2:B:337:ASP:OD2	2:B:751:LYS:NZ	2.33	0.57
2:B:917:ASP:H	2:B:923:ARG:HH21	1.53	0.57
9:K:51:GLU:OE1	11:O:192:LYS:N	2.38	0.57
2:B:783:ASP:OD2	2:B:787:ASN:ND2	2.38	0.57
5:F:240:PHE:HB3	5:F:271:GLN:HE22	1.70	0.57
2:B:51:LEU:HB2	2:B:146:ILE:HB	1.86	0.56
5:G:564:ASP:HB2	5:G:566:THR:HG22	1.86	0.56
12:P:200:ILE:HD12	13:Q:127:TRP:HD1	1.70	0.56
15:T:168:ILE:HG12	15:T:258:MET:HG2	1.87	0.56
6:H:404:ARG:NH2	6:H:452:PHE:O	2.38	0.56
2:B:530:LYS:HE2	2:B:639:LYS:HD3	1.88	0.56
5:G:332:ILE:HA	5:G:336:HIS:HD2	1.71	0.56
5:G:476:VAL:HG22	5:G:768:LEU:HD22	1.87	0.56
7:I:363:TRP:NE1	7:I:399:GLU:OE2	2.38	0.56
9:K:75:SER:O	9:K:79:TYR:HB2	2.04	0.56
5:G:235:GLU:O	5:G:238:GLN:NE2	2.38	0.56
6:H:253:TYR:O	9:K:182:GLN:NE2	2.39	0.56
2:B:678:ARG:NH1	2:B:682:THR:OG1	2.39	0.56
5:F:237:SER:HA	5:F:240:PHE:HD2	1.71	0.56
6:H:306:PRO:HB3	17:Z:406:UNK:HA	1.86	0.56
2:B:631:ASP:O	2:B:638:ARG:NH1	2.38	0.56
9:K:191:THR:O	9:K:195:ALA:HB2	2.06	0.56
2:B:344:ARG:NH1	2:B:382:MET:SD	2.79	0.55
5:G:594:SER:HB2	5:G:597:GLY:H	1.71	0.55
2:B:946:ASN:ND2	2:B:986:CYS:SG	2.76	0.55
5:F:692:ARG:NH2	5:F:706:GLU:OE1	2.39	0.55
7:I:246:ILE:O	7:I:292:ASN:ND2	2.39	0.55
4:E:894:LEU:HA	13:R:111:LEU:H	1.71	0.55
5:G:613:ALA:HB2	5:G:620:LEU:HD11	1.89	0.55
6:H:57:PHE:O	6:H:61:GLY:N	2.38	0.55
9:K:196:LYS:HE2	9:K:208:VAL:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:139:LEU:HB3	11:O:144:PHE:HB3	1.88	0.55
3:C:30:GLU:OE2	5:F:471:GLN:NE2	2.37	0.55
2:B:597:ARG:NH1	2:B:621:ALA:O	2.37	0.55
1:A:903:TYR:HE2	1:A:926:GLU:HB3	1.72	0.55
2:B:806:VAL:HG13	2:B:864:ASN:HD21	1.70	0.55
3:C:81:GLU:OE2	5:F:568:ARG:NH2	2.39	0.55
4:D:873:LEU:HD23	13:Q:58:LEU:HD13	1.88	0.55
1:A:961:GLU:OE1	8:J:147:ARG:NH1	2.40	0.55
2:B:820:ASP:HB2	2:B:822:LEU:HA	1.88	0.55
4:E:924:LYS:NZ	13:R:75:GLN:O	2.40	0.55
5:F:468:ASN:HA	5:F:786:THR:HG23	1.87	0.55
5:G:286:THR:HG22	5:G:287:LYS:HG3	1.87	0.55
7:I:337:VAL:HA	7:I:340:ILE:HD12	1.88	0.55
2:B:840:GLU:HG3	2:B:850:ILE:HB	1.87	0.55
4:E:873:LEU:HD23	13:R:58:LEU:HD13	1.87	0.55
1:A:61:GLU:O	1:A:65:HIS:HB2	2.06	0.55
7:I:233:GLY:O	7:I:239:ARG:NH1	2.37	0.55
2:B:44:SER:OG	2:B:152:LEU:O	2.23	0.54
10:L:57:TYR:OH	13:Q:122:ARG:NH2	2.33	0.54
12:P:120:ARG:NH1	14:S:45:ASP:O	2.39	0.54
17:Z:204:UNK:O	17:Z:208:UNK:N	2.40	0.54
6:H:217:SER:OG	6:H:218:VAL:N	2.41	0.54
9:K:172:TYR:OH	9:K:176:ARG:NH1	2.40	0.54
2:B:504:LEU:HA	2:B:507:ILE:HD12	1.89	0.54
2:B:536:ALA:H	2:B:548:ILE:HG12	1.72	0.54
2:B:32:VAL:HG22	2:B:203:LYS:HB3	1.87	0.54
5:G:609:ALA:HB3	5:G:623:PHE:HB2	1.88	0.54
7:I:345:SER:HB3	7:I:351:ILE:HB	1.90	0.54
5:F:684:LEU:HB2	5:F:696:TRP:HB2	1.88	0.54
7:I:208:UNK:HA	17:Z:560:UNK:HA	1.89	0.54
5:G:309:ILE:HD11	5:G:339:ILE:HG12	1.90	0.54
5:G:549:ALA:HA	5:G:559:LEU:O	2.07	0.54
15:T:163:PRO:HA	15:T:262:CYS:HB3	1.90	0.54
4:E:940:VAL:O	4:E:944:LEU:N	2.40	0.53
15:T:268:ILE:HD13	15:T:332:LEU:HD22	1.90	0.53
2:B:82:ALA:HB3	2:B:128:ILE:HD11	1.88	0.53
5:G:240:PHE:HB3	5:G:271:GLN:HE22	1.73	0.53
7:I:224:TYR:HA	7:I:227:ILE:HD12	1.91	0.53
12:P:187:MET:HE3	14:S:40:MET:HE3	1.91	0.53
2:B:902:ARG:NH2	2:B:942:SER:O	2.42	0.53
5:G:468:ASN:HA	5:G:786:THR:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:185:LYS:O	12:P:189:GLU:CB	2.57	0.53
2:B:406:GLU:OE2	2:B:412:VAL:N	2.42	0.53
2:B:663:GLN:HA	2:B:666:ILE:HB	1.91	0.53
5:F:491:ASP:HA	5:F:540:TYR:HB3	1.90	0.53
2:B:761:ARG:NH2	2:B:804:ASN:O	2.41	0.53
5:G:653:LEU:HD12	5:G:663:ARG:HB2	1.90	0.53
1:A:680:LEU:HD11	8:J:91:ILE:HD12	1.91	0.53
2:B:206:PHE:HB2	2:B:234:PHE:HB2	1.91	0.53
7:I:368:THR:OG1	7:I:373:ARG:NE	2.42	0.53
13:Q:65:ASP:O	13:Q:69:GLU:HB2	2.09	0.53
13:R:106:ARG:HH22	13:R:112:GLU:HB2	1.74	0.53
1:A:104:THR:HG23	15:T:185:LEU:HB3	1.91	0.52
2:B:392:ARG:HD3	2:B:395:ILE:HD12	1.91	0.52
2:B:486:GLN:OE1	2:B:489:GLN:NE2	2.41	0.52
5:G:692:ARG:NH2	5:G:706:GLU:OE1	2.41	0.52
11:N:170:ALA:O	11:N:174:CYS:HB2	2.10	0.52
14:S:57:LEU:HA	14:S:60:LEU:HD12	1.91	0.52
5:F:332:ILE:HA	5:F:336:HIS:HD2	1.74	0.52
13:Q:120:LEU:HD13	13:Q:126:MET:HG3	1.90	0.52
1:A:753:TYR:OH	1:A:1074:ASN:OD1	2.27	0.52
7:I:276:LEU:HA	7:I:279:LEU:HD12	1.91	0.52
5:F:671:PRO:O	5:F:689:THR:OG1	2.27	0.52
6:H:410:PRO:O	6:H:417:ARG:NH2	2.43	0.52
13:R:89:ASP:HA	13:R:92:ILE:HD12	1.91	0.52
1:A:706:ARG:CZ	2:B:263:HIS:NE2	2.72	0.52
5:F:767:GLU:O	6:H:62:LYS:NZ	2.41	0.52
5:G:300:PHE:HB3	5:G:301:ARG:HH11	1.75	0.52
2:B:224:VAL:O	2:B:232:LYS:NZ	2.43	0.52
2:B:859:ARG:HE	2:B:863:LYS:HE3	1.75	0.52
7:I:311:CYS:O	7:I:316:GLN:NE2	2.42	0.52
5:G:459:PRO:O	17:Z:359:UNK:N	2.43	0.52
7:I:22:VAL:O	7:I:25:SER:OG	2.28	0.52
2:B:270:LEU:HB2	2:B:273:LEU:HD12	1.91	0.52
5:G:608:VAL:HG12	5:G:624:ALA:HB2	1.91	0.52
7:I:23:ALA:HB1	7:I:28:ILE:HD12	1.91	0.52
2:B:525:GLN:O	2:B:559:LYS:NZ	2.34	0.51
2:B:530:LYS:HG2	2:B:639:LYS:HB3	1.93	0.51
1:A:784:GLN:H	1:A:1073:GLN:HE22	1.58	0.51
2:B:76:ARG:NH1	2:B:79:ASP:OD1	2.43	0.51
2:B:232:LYS:HE3	2:B:234:PHE:HE1	1.76	0.51
5:G:693:VAL:HB	5:G:707:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:256:LEU:HD22	6:H:295:LEU:HD22	1.92	0.51
1:A:670:ASP:O	8:J:78:LYS:NZ	2.37	0.51
17:Z:371:UNK:O	17:Z:375:UNK:N	2.44	0.51
1:A:702:ASN:HB2	1:A:722:THR:HA	1.92	0.51
2:B:353:GLN:O	2:B:357:CYS:N	2.44	0.51
4:D:894:LEU:HD22	4:D:899:VAL:HG21	1.92	0.51
6:H:328:ALA:O	6:H:331:ASP:HB2	2.10	0.51
2:B:392:ARG:HA	2:B:395:ILE:HD12	1.92	0.51
3:C:37:LEU:HD12	3:C:66:GLN:HE21	1.76	0.51
9:K:63:GLU:OE1	9:K:66:GLN:NE2	2.44	0.51
2:B:118:ASP:OD1	2:B:187:ARG:NH2	2.44	0.50
5:G:472:GLY:HA2	5:G:487:GLY:HA2	1.93	0.50
7:I:410:PRO:HG2	7:I:417:ARG:HE	1.76	0.50
12:P:170:LEU:HD11	14:S:44:GLY:HA3	1.93	0.50
1:A:111:SER:HA	15:T:204:ILE:HG22	1.93	0.50
2:B:366:ASP:HB3	2:B:499:SER:HB2	1.92	0.50
2:B:539:ARG:HG3	2:B:545:GLU:HA	1.92	0.50
2:B:565:LYS:HA	2:B:578:THR:O	2.12	0.50
9:K:66:GLN:HA	9:K:69:ILE:HD12	1.93	0.50
12:P:189:GLU:HA	12:P:192:ARG:HD2	1.94	0.50
2:B:48:PHE:HA	2:B:148:ILE:O	2.11	0.50
2:B:688:GLU:H	2:B:695:ARG:HH12	1.60	0.50
5:F:298:LEU:O	5:F:302:THR:OG1	2.25	0.50
7:I:207:UNK:O	17:Z:561:UNK:N	2.44	0.50
14:S:57:LEU:HG	14:S:60:LEU:HD12	1.92	0.50
6:H:387:VAL:O	6:H:391:LEU:HB2	2.11	0.50
6:H:457:PRO:O	6:H:461:SER:N	2.42	0.50
7:I:223:TYR:OH	7:I:249:ASP:OD2	2.28	0.50
2:B:156:LYS:O	2:B:963:HIS:ND1	2.34	0.50
2:B:360:SER:OG	2:B:496:MET:O	2.26	0.50
7:I:43:VAL:HG21	10:M:47:VAL:HG22	1.92	0.50
9:K:110:TYR:HH	11:O:164:SER:HG	1.55	0.50
1:A:46:ILE:HG22	1:A:52:LEU:HA	1.94	0.50
7:I:410:PRO:O	7:I:417:ARG:NH2	2.44	0.50
17:Z:91:UNK:O	17:Z:95:UNK:N	2.45	0.50
2:B:24:ARG:HD3	2:B:120:ASP:HA	1.93	0.50
2:B:387:GLY:O	2:B:391:TYR:N	2.38	0.50
2:B:604:ILE:HG23	2:B:607:MET:HE3	1.93	0.50
2:B:958:ASN:O	2:B:968:ARG:NH2	2.43	0.50
5:F:783:LEU:HD21	5:F:787:ARG:HG3	1.93	0.50
5:G:769:LEU:HD13	5:G:780:VAL:HG13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:369:PRO:O	6:H:372:THR:OG1	2.30	0.50
10:M:48:THR:HA	10:M:51:LEU:HD12	1.92	0.50
5:G:298:LEU:O	5:G:302:THR:OG1	2.28	0.50
7:I:217:SER:H	7:I:220:GLN:HG2	1.77	0.49
13:Q:120:LEU:O	13:Q:124:TRP:N	2.38	0.49
2:B:55:PRO:HB3	2:B:60:LEU:HD23	1.93	0.49
2:B:104:ASN:O	2:B:108:ASN:ND2	2.45	0.49
2:B:256:ILE:HD11	2:B:274:LEU:HB3	1.93	0.49
5:F:730:SER:OG	5:F:732:ASP:OD1	2.29	0.49
13:Q:128:ILE:HA	14:S:60:LEU:HD23	1.95	0.49
2:B:841:LYS:HZ3	9:K:217:ARG:H	1.60	0.49
5:G:244:PHE:HZ	5:G:264:PHE:HA	1.78	0.49
6:H:419:GLY:HA2	6:H:422:HIS:CE1	2.47	0.49
7:I:267:VAL:HG11	7:I:307:ALA:HB1	1.95	0.49
7:I:354:ARG:O	7:I:358:THR:OG1	2.29	0.49
1:A:62:CYS:O	1:A:66:LEU:CB	2.56	0.49
1:A:752:ILE:HG22	1:A:782:VAL:HG22	1.92	0.49
2:B:313:TYR:O	2:B:966:ARG:NH2	2.45	0.49
5:G:644:THR:HB	5:G:654:TRP:HE1	1.78	0.49
2:B:314:VAL:HG12	2:B:316:VAL:H	1.77	0.49
5:G:558:LEU:O	5:G:569:LEU:HA	2.13	0.49
12:P:120:ARG:HD3	14:S:44:GLY:HA2	1.95	0.49
12:P:200:ILE:HB	13:Q:127:TRP:HE1	1.77	0.49
1:A:41:PHE:HB3	1:A:81:LEU:HD23	1.95	0.49
2:B:215:VAL:HA	2:B:236:TYR:HE2	1.78	0.49
6:H:260:SER:HA	6:H:263:ILE:HD12	1.94	0.49
7:I:216:UNK:HA	7:I:220:GLN:HE21	1.78	0.49
13:R:106:ARG:NH1	13:R:112:GLU:OE1	2.41	0.49
2:B:451:CYS:HA	2:B:454:HIS:HD2	1.78	0.49
2:B:546:LEU:HB3	2:B:590:ILE:HB	1.93	0.49
2:B:727:PHE:HB3	2:B:736:VAL:HG11	1.94	0.49
5:G:601:VAL:HG11	5:G:642:VAL:HG11	1.95	0.49
1:A:110:TYR:HD1	1:A:113:ILE:HD11	1.78	0.49
2:B:220:LEU:HD23	2:B:236:TYR:HE1	1.78	0.49
2:B:570:GLU:OE1	2:B:593:HIS:ND1	2.38	0.49
2:B:291:TYR:HA	2:B:294:ILE:HD12	1.95	0.48
2:B:431:LEU:HD13	2:B:976:PHE:HB2	1.95	0.48
2:B:76:ARG:HD2	2:B:79:ASP:HA	1.95	0.48
6:H:371:THR:HG23	6:H:372:THR:HG23	1.95	0.48
7:I:270:ASN:HA	7:I:273:GLN:HB2	1.95	0.48
1:A:64:LYS:HD3	12:P:152:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:410:GLY:HA3	2:B:430:HIS:CD2	2.48	0.48
2:B:521:GLN:O	2:B:559:LYS:NZ	2.40	0.48
6:H:427:LEU:O	6:H:431:CYS:CB	2.61	0.48
10:M:96:ALA:O	10:M:100:ASN:CB	2.61	0.48
5:G:296:THR:O	5:G:300:PHE:HB3	2.13	0.48
6:H:337:VAL:HA	6:H:340:ILE:HD12	1.95	0.48
4:E:878:LEU:HD13	13:R:57:VAL:HG21	1.94	0.48
4:E:967:MET:O	4:E:971:LYS:N	2.44	0.48
7:I:374:TYR:HD1	7:I:423:VAL:HG13	1.79	0.48
1:A:45:ASN:HB3	1:A:53:GLU:HB2	1.95	0.48
2:B:26:TYR:HB2	2:B:53:ILE:HD11	1.96	0.48
6:H:336:LEU:O	6:H:340:ILE:N	2.47	0.48
10:L:49:THR:OG1	10:L:78:ARG:NH1	2.45	0.48
13:R:81:GLU:HA	13:R:84:LEU:HD12	1.95	0.48
15:T:295:MET:O	15:T:299:ARG:HA	2.13	0.48
2:B:258:VAL:HG11	2:B:281:THR:HB	1.95	0.48
2:B:259:ASP:O	2:B:261:TYR:N	2.47	0.48
2:B:655:TYR:OH	17:Z:84:UNK:O	2.28	0.48
7:I:222:LEU:HD23	7:I:225:LYS:HD2	1.95	0.48
2:B:830:LEU:HD23	2:B:833:ILE:HD11	1.95	0.48
11:O:170:ALA:O	11:O:174:CYS:N	2.47	0.48
4:E:894:LEU:HD22	4:E:899:VAL:HG21	1.95	0.48
10:M:33:PRO:HA	10:M:36:ILE:HD12	1.96	0.48
15:T:174:LEU:HD12	15:T:178:LEU:HD11	1.96	0.48
5:F:735:VAL:HG22	5:F:766:GLN:HE22	1.79	0.47
11:O:128:PRO:HG3	11:O:153:ARG:HG2	1.95	0.47
6:H:324:ASP:HA	6:H:327:TRP:HD1	1.78	0.47
2:B:275:PRO:O	2:B:278:LYS:HB2	2.13	0.47
6:H:323:VAL:HA	6:H:326:HIS:HB2	1.94	0.47
6:H:332:PHE:O	6:H:335:ARG:HB3	2.14	0.47
2:B:403:VAL:HG22	2:B:528:VAL:HG11	1.96	0.47
2:B:607:MET:HG3	2:B:611:GLU:HB2	1.97	0.47
2:B:769:LYS:HA	2:B:772:LEU:HD12	1.95	0.47
5:F:695:LEU:HB3	5:F:705:GLY:H	1.79	0.47
6:H:370:TRP:O	6:H:374:TYR:CB	2.63	0.47
12:P:166:VAL:HG22	12:P:187:MET:HE1	1.97	0.47
14:S:69:THR:HG22	14:S:73:MET:HE2	1.95	0.47
5:G:542:HIS:CD2	5:G:562:SER:HB2	2.50	0.47
6:H:455:LEU:O	6:H:459:LEU:N	2.43	0.47
10:M:28:ILE:O	10:M:31:TYR:OH	2.21	0.47
1:A:765:ILE:HB	1:A:772:TYR:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:287:LYS:H	5:G:290:HIS:CD2	2.30	0.47
2:B:346:LEU:HD23	2:B:346:LEU:HA	1.76	0.47
2:B:389:ASN:HB3	2:B:659:VAL:HG21	1.97	0.47
2:B:565:LYS:HG2	2:B:579:LEU:HA	1.96	0.47
2:B:738:THR:HG22	2:B:739:ASN:HB2	1.97	0.47
2:B:820:ASP:HB2	2:B:822:LEU:HD23	1.96	0.47
5:G:786:THR:HG22	5:G:788:ARG:HG3	1.97	0.47
10:M:49:THR:OG1	10:M:78:ARG:NH1	2.40	0.47
1:A:110:TYR:HB3	15:T:240:VAL:HG22	1.95	0.47
2:B:37:ASN:HB2	2:B:46:VAL:HG22	1.97	0.47
2:B:89:PRO:HG2	2:B:117:VAL:HG22	1.96	0.47
2:B:529:VAL:HG22	2:B:559:LYS:HB3	1.96	0.47
4:E:879:GLN:HG3	4:E:894:LEU:HD21	1.96	0.47
11:O:119:PHE:HA	11:O:122:GLN:HG2	1.97	0.47
1:A:107:ALA:O	15:T:188:ARG:NE	2.41	0.47
1:A:929:THR:HG22	1:A:954:ALA:HA	1.97	0.47
2:B:119:PRO:HA	2:B:123:ASN:HD22	1.80	0.47
2:B:459:LEU:HA	2:B:462:ASN:HD22	1.80	0.47
6:H:276:LEU:HA	6:H:279:LEU:HD12	1.97	0.47
5:F:552:SER:HB3	5:F:557:TYR:HB2	1.97	0.47
14:S:36:LEU:HD11	14:S:57:LEU:HD22	1.96	0.47
5:F:653:LEU:HD12	5:F:663:ARG:HB2	1.97	0.46
4:D:892:THR:H	13:Q:109:SER:HB2	1.80	0.46
5:G:636:HIS:HA	5:G:677:PHE:HD2	1.79	0.46
6:H:292:ASN:HB3	6:H:295:LEU:HB2	1.97	0.46
8:J:21:PRO:HB2	8:J:24:TYR:HD2	1.80	0.46
2:B:880:TYR:HD1	2:B:887:ARG:HH22	1.63	0.46
7:I:387:VAL:O	7:I:390:THR:OG1	2.28	0.46
2:B:473:PHE:HA	2:B:476:LEU:HD12	1.97	0.46
7:I:370:TRP:HA	7:I:373:ARG:HD3	1.97	0.46
1:A:1083:LEU:O	8:J:141:LYS:NZ	2.49	0.46
2:B:961:THR:HB	2:B:968:ARG:HE	1.80	0.46
5:G:590:ASP:HB3	5:G:633:THR:HG22	1.97	0.46
5:G:631:ASN:ND2	5:G:672:ILE:O	2.49	0.46
6:H:381:ALA:HA	6:H:388:ILE:HD11	1.98	0.46
6:H:414:ASN:HA	6:H:417:ARG:HB3	1.97	0.46
5:G:684:LEU:O	5:G:695:LEU:HA	2.16	0.46
2:B:59:ASN:H	2:B:135:TRP:HE1	1.64	0.46
5:F:475:ALA:HB3	5:F:781:VAL:HG11	1.98	0.46
5:G:631:ASN:H	5:G:646:SER:HA	1.81	0.46
5:G:636:HIS:HD2	5:G:638:ASN:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:904:HIS:NE2	12:P:188:ARG:HB3	2.31	0.46
5:F:779:PRO:HA	5:F:791:VAL:HA	1.98	0.46
6:H:383:LEU:HB3	6:H:387:VAL:HG21	1.98	0.46
7:I:263:ILE:HG23	7:I:282:LEU:HD22	1.97	0.46
11:O:126:TYR:O	11:O:153:ARG:NE	2.45	0.46
12:P:141:ILE:HD13	14:S:66:THR:HA	1.98	0.46
2:B:221:VAL:HG11	2:B:237:MET:HB3	1.98	0.46
5:G:636:HIS:HA	5:G:677:PHE:CD2	2.51	0.46
7:I:326:HIS:HA	7:I:329:LEU:HD12	1.98	0.46
7:I:395:ARG:O	7:I:399:GLU:HB2	2.16	0.46
9:K:222:PRO:O	9:K:225:THR:OG1	2.33	0.46
10:M:47:VAL:HA	10:M:50:ILE:HD12	1.97	0.46
11:O:123:LEU:HA	11:O:126:TYR:HD2	1.81	0.46
1:A:673:GLY:O	1:A:774:ARG:NH1	2.49	0.46
2:B:539:ARG:HH11	2:B:592:CYS:HB3	1.80	0.46
11:N:129:THR:HB	11:N:160:GLN:HE22	1.81	0.45
2:B:300:PRO:HB2	2:B:358:PHE:HE2	1.81	0.45
6:H:370:TRP:O	6:H:374:TYR:HB2	2.16	0.45
9:K:219:PHE:HE2	9:K:222:PRO:HA	1.80	0.45
2:B:64:LYS:HD3	2:B:119:PRO:HB3	1.97	0.45
5:G:467:LEU:H	5:G:495:ARG:HH12	1.65	0.45
5:G:470:TYR:CD2	5:G:471:GLN:HG3	2.52	0.45
6:H:402:ARG:O	6:H:405:SER:OG	2.28	0.45
1:A:39:ALA:HB2	1:A:78:ILE:HD11	1.99	0.45
2:B:85:ILE:HD11	2:B:129:LYS:HE3	1.97	0.45
2:B:518:LEU:HD12	2:B:522:TRP:HD1	1.82	0.45
12:P:192:ARG:HA	12:P:195:LYS:HD2	1.98	0.45
2:B:159:LEU:HD21	2:B:189:TRP:CD1	2.51	0.45
5:F:461:ILE:HG12	5:F:792:LEU:HB3	1.99	0.45
7:I:456:GLY:HA2	7:I:457:PRO:HA	1.78	0.45
2:B:908:GLN:HE21	2:B:912:ASN:HD21	1.63	0.45
5:G:783:LEU:HD21	5:G:787:ARG:HG3	1.98	0.45
2:B:26:TYR:N	2:B:56:THR:OG1	2.46	0.45
4:E:912:ASN:HB2	13:R:124:TRP:HH2	1.81	0.45
1:A:706:ARG:NH1	2:B:263:HIS:NE2	2.63	0.45
2:B:343:ARG:HA	2:B:346:LEU:HB2	1.99	0.45
2:B:880:TYR:HA	2:B:887:ARG:CZ	2.47	0.45
2:B:570:GLU:OE2	2:B:576:ASN:ND2	2.47	0.45
2:B:68:LYS:HZ3	2:B:962:SER:HB2	1.81	0.44
2:B:95:HIS:CE1	2:B:97:GLU:HB2	2.52	0.44
4:D:908:GLN:HG2	12:P:192:ARG:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:389:LYS:HG3	6:H:438:LEU:HD11	1.98	0.44
11:O:204:LEU:HB3	11:O:208:GLY:HA3	1.99	0.44
5:F:558:LEU:HB3	5:F:570:TRP:HB2	2.00	0.44
9:K:194:MET:HA	9:K:197:THR:HB	2.00	0.44
2:B:572:ASP:HA	2:B:607:MET:HA	1.99	0.44
4:E:910:LEU:HD23	4:E:913:LEU:HD12	2.00	0.44
5:G:668:HIS:HD2	5:G:688:ALA:HB3	1.81	0.44
2:B:848:HIS:CD2	2:B:886:ILE:HD11	2.53	0.44
5:G:251:LEU:HB3	5:G:260:ALA:HB2	1.98	0.44
5:G:254:ASN:HB3	5:G:256:HIS:HD2	1.82	0.44
7:I:55:LEU:HD23	7:I:55:LEU:HA	1.83	0.44
2:B:280:THR:OG1	2:B:330:LEU:O	2.30	0.44
5:F:241:TYR:HD1	5:F:271:GLN:HG3	1.83	0.44
5:F:716:SER:HB2	5:F:769:LEU:HB2	2.00	0.44
5:G:504:UNK:HA	5:G:529:UNK:HA	1.99	0.44
6:H:334:ALA:O	6:H:337:VAL:HB	2.17	0.44
7:I:369:PRO:O	7:I:372:THR:OG1	2.30	0.44
10:M:22:ILE:O	10:M:26:MET:N	2.50	0.44
2:B:65:LEU:O	2:B:126:LEU:HB2	2.17	0.44
5:G:768:LEU:HB3	5:G:769:LEU:H	1.49	0.44
2:B:26:TYR:HA	2:B:55:PRO:HA	2.00	0.44
2:B:31:GLN:HB3	2:B:202:TRP:CD1	2.52	0.44
2:B:201:THR:OG1	2:B:238:LEU:O	2.26	0.44
5:G:638:ASN:HD22	17:Z:43:UNK:HA	1.83	0.44
7:I:68:THR:HG23	10:M:35:VAL:HG22	2.00	0.44
11:N:119:PHE:HA	11:N:122:GLN:HG2	1.99	0.44
2:B:95:HIS:HE1	2:B:97:GLU:HB2	1.82	0.44
2:B:372:GLY:HA2	2:B:453:ALA:HB1	2.00	0.44
2:B:626:LEU:HD23	2:B:626:LEU:HA	1.84	0.44
5:G:236:LEU:HD22	5:G:239:LEU:HD11	2.00	0.44
5:G:542:HIS:CE1	5:G:568:ARG:HD2	2.53	0.44
7:I:457:PRO:O	7:I:461:SER:N	2.43	0.44
1:A:623:TYR:HE2	1:A:766:ARG:HE	1.66	0.43
1:A:926:GLU:OE1	8:J:149:ARG:NH1	2.39	0.43
2:B:51:LEU:O	2:B:145:LYS:HA	2.18	0.43
2:B:332:SER:H	2:B:335:ILE:HD12	1.83	0.43
2:B:597:ARG:NH2	2:B:622:ASP:OD1	2.51	0.43
5:F:636:HIS:HA	5:F:677:PHE:HD2	1.83	0.43
5:F:764:ASN:HB2	5:F:782:HIS:HB3	1.99	0.43
6:H:333:ALA:HA	6:H:336:LEU:HD12	1.98	0.43
7:I:417:ARG:O	7:I:421:ASP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:89:ASP:HA	13:Q:92:ILE:HD12	2.00	0.43
2:B:214:ALA:HB1	2:B:249:LEU:HD11	1.98	0.43
2:B:628:ILE:H	2:B:644:GLN:NE2	2.16	0.43
5:F:615:ASP:HB3	10:L:113:UNK:HA	1.99	0.43
5:G:479:THR:O	5:G:555:ARG:NH2	2.48	0.43
5:G:542:HIS:HD2	5:G:562:SER:HB2	1.83	0.43
2:B:862:GLN:NE2	2:B:870:ASP:H	2.16	0.43
2:B:891:LEU:HA	2:B:894:VAL:HG12	1.99	0.43
3:C:110:TYR:HA	3:C:113:ASN:HD22	1.82	0.43
5:F:605:HIS:ND1	5:F:629:ASP:OD1	2.51	0.43
5:G:571:SER:HB2	5:G:575:PHE:N	2.33	0.43
8:J:65:SER:HA	8:J:96:VAL:O	2.18	0.43
2:B:36:ASN:OD1	2:B:207:THR:OG1	2.36	0.43
2:B:549:LYS:HG2	2:B:587:LYS:HG2	2.01	0.43
2:B:914:ILE:HD13	2:B:927:LEU:HD21	2.00	0.43
5:G:464:TYR:OH	9:K:150:UNK:O	2.25	0.43
8:J:77:LEU:HG	8:J:87:LYS:HA	2.01	0.43
2:B:835:ARG:NH2	9:K:184:ARG:HE	2.12	0.43
5:G:590:ASP:OD2	5:G:633:THR:N	2.40	0.43
5:G:732:ASP:N	5:G:732:ASP:OD1	2.49	0.43
7:I:314:SER:OG	17:Z:200:UNK:O	2.30	0.43
4:E:892:THR:HG22	4:E:893:GLU:HG3	2.00	0.43
5:F:768:LEU:HB3	5:F:769:LEU:H	1.65	0.43
6:H:403:ILE:HG23	6:H:420:ALA:HB1	2.01	0.43
2:B:308:PHE:HA	2:B:325:PHE:O	2.18	0.43
2:B:503:PHE:CE2	2:B:507:ILE:HD11	2.54	0.43
7:I:313:VAL:HG12	7:I:314:SER:HB3	2.00	0.43
12:P:187:MET:O	12:P:191:VAL:HG23	2.19	0.43
17:Z:213:UNK:O	17:Z:216:UNK:CB	2.67	0.43
1:A:874:GLU:HA	1:A:877:ARG:HD2	2.01	0.43
2:B:567:THR:HG23	2:B:577:HIS:HE1	1.83	0.43
2:B:611:GLU:OE2	2:B:657:ARG:NE	2.51	0.43
2:B:957:MET:HG2	2:B:971:ALA:HB1	2.01	0.43
2:B:975:TYR:O	2:B:980:GLY:HA2	2.19	0.43
5:G:566:THR:HA	5:G:581:TYR:O	2.18	0.43
1:A:650:ARG:HH11	8:J:80:ILE:HD11	1.84	0.43
2:B:180:CYS:HB3	2:B:313:TYR:HB2	2.01	0.43
2:B:443:TRP:CG	2:B:924:HIS:HE1	2.37	0.43
2:B:699:CYS:SG	2:B:753:MET:HG2	2.59	0.43
15:T:262:CYS:O	15:T:309:LYS:HA	2.18	0.43
2:B:516:GLN:HA	2:B:519:ILE:HD12	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:594:SER:HB2	5:G:597:GLY:N	2.32	0.42
6:H:411:VAL:HA	6:H:417:ARG:HH21	1.84	0.42
8:J:39:LEU:HA	8:J:42:ARG:HB2	2.00	0.42
2:B:706:ALA:HB3	2:B:760:LEU:HD22	2.01	0.42
6:H:43:VAL:HG21	10:L:47:VAL:HG22	2.01	0.42
6:H:385:HIS:HE1	6:H:437:LYS:HD2	1.84	0.42
6:H:418:ILE:O	6:H:422:HIS:ND1	2.38	0.42
2:B:30:HIS:ND1	2:B:201:THR:HG23	2.35	0.42
2:B:75:VAL:HG13	2:B:148:ILE:HG12	2.00	0.42
2:B:575:PHE:HB3	2:B:577:HIS:CE1	2.55	0.42
9:K:51:GLU:O	17:Z:311:UNK:N	2.51	0.42
2:B:363:SER:H	2:B:366:ASP:HB2	1.85	0.42
5:G:605:HIS:ND1	5:G:629:ASP:OD1	2.52	0.42
15:T:171:THR:HG22	15:T:220:VAL:HG22	2.00	0.42
5:F:564:ASP:HB2	5:F:566:THR:HG22	2.01	0.42
5:G:241:TYR:HD1	5:G:271:GLN:HG3	1.83	0.42
5:G:467:LEU:O	5:G:787:ARG:NE	2.41	0.42
6:H:23:ALA:HB1	6:H:28:ILE:HD12	2.02	0.42
6:H:308:VAL:O	6:H:311:CYS:HB2	2.19	0.42
15:T:206:GLU:O	15:T:236:LYS:NZ	2.42	0.42
2:B:604:ILE:HG12	2:B:607:MET:HE3	2.01	0.42
6:H:320:ARG:O	6:H:323:VAL:HB	2.18	0.42
7:I:309:MET:HA	7:I:312:ILE:HD12	2.02	0.42
7:I:400:GLY:HA2	7:I:403:ILE:HD12	2.00	0.42
2:B:688:GLU:H	2:B:695:ARG:NH1	2.18	0.42
2:B:749:LEU:HD12	2:B:749:LEU:HA	1.87	0.42
5:G:730:SER:OG	5:G:734:THR:OG1	2.34	0.42
9:K:79:TYR:HA	9:K:82:HIS:HD2	1.85	0.42
17:Z:214:UNK:O	17:Z:218:UNK:N	2.52	0.42
2:B:87:ASN:HB3	2:B:89:PRO:HD3	2.02	0.42
2:B:261:TYR:HB2	2:B:285:HIS:CG	2.55	0.42
5:G:695:LEU:O	5:G:704:VAL:N	2.53	0.42
6:H:446:ASP:O	6:H:450:ALA:N	2.50	0.42
7:I:276:LEU:HB3	7:I:326:HIS:CE1	2.55	0.42
11:O:163:ILE:HD13	11:O:166:ILE:HD12	2.01	0.42
13:R:68:ARG:NH1	13:R:72:PRO:O	2.53	0.42
2:B:238:LEU:HD11	2:B:240:ILE:HB	2.01	0.42
2:B:571:LEU:HD23	2:B:626:LEU:HG	2.02	0.42
2:B:772:LEU:O	2:B:776:LEU:HG	2.20	0.42
4:D:911:GLN:HA	4:D:914:VAL:HB	2.01	0.42
5:F:251:LEU:HB3	5:F:260:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:783:LEU:HD23	5:F:783:LEU:HA	1.84	0.42
5:G:623:PHE:HB3	5:G:654:TRP:CE2	2.55	0.42
5:G:730:SER:OG	5:G:732:ASP:OD1	2.37	0.42
2:B:51:LEU:HD21	2:B:65:LEU:HD21	2.01	0.42
2:B:867:VAL:HA	9:K:204:PHE:HE1	1.85	0.42
4:E:922:GLN:HA	4:E:925:ASN:HD22	1.85	0.42
7:I:252:LEU:O	7:I:254:GLN:N	2.53	0.42
1:A:680:LEU:HD23	1:A:776:LEU:HD22	2.01	0.41
1:A:749:ARG:HB3	1:A:786:CYS:HB2	2.02	0.41
2:B:653:LEU:HA	2:B:653:LEU:HD23	1.83	0.41
13:R:65:ASP:O	13:R:69:GLU:CB	2.68	0.41
3:C:48:LEU:HD23	3:C:48:LEU:HA	1.94	0.41
7:I:53:ASP:HA	7:I:56:LYS:HE3	2.01	0.41
7:I:403:ILE:O	7:I:407:LEU:N	2.37	0.41
12:P:168:GLU:HB3	12:P:190:ALA:HB1	2.02	0.41
13:Q:120:LEU:HB3	13:Q:126:MET:HG2	2.02	0.41
2:B:838:ASN:HD22	9:K:191:THR:HG23	1.85	0.41
6:H:366:GLU:HG2	6:H:367:LYS:H	1.84	0.41
7:I:224:TYR:HE1	7:I:259:PHE:HD1	1.67	0.41
7:I:320:ARG:HD3	7:I:415:ILE:HD13	2.02	0.41
9:K:51:GLU:N	11:O:193:TYR:O	2.53	0.41
5:F:730:SER:OG	5:F:734:THR:OG1	2.37	0.41
5:G:584:HIS:HB3	5:G:586:TYR:HB2	2.03	0.41
8:J:17:ILE:O	8:J:94:MET:HA	2.20	0.41
12:P:181:PRO:HB3	14:S:49:PRO:HA	2.01	0.41
2:B:26:TYR:HB3	2:B:60:LEU:HD21	2.02	0.41
2:B:49:VAL:HG12	2:B:148:ILE:HB	2.01	0.41
2:B:926:ILE:O	2:B:930:LEU:HB2	2.20	0.41
5:G:286:THR:H	5:G:290:HIS:CD2	2.39	0.41
7:I:274:ASN:HD21	7:I:317:LEU:H	1.67	0.41
7:I:302:HIS:CD2	17:Z:213:UNK:HA	2.55	0.41
9:K:227:LEU:HA	9:K:227:LEU:HD12	1.84	0.41
13:Q:127:TRP:CZ3	14:S:67:GLU:HB3	2.55	0.41
2:B:178:PHE:HA	2:B:249:LEU:O	2.21	0.41
5:G:761:LEU:HD11	5:G:766:GLN:HE21	1.85	0.41
15:T:210:THR:O	15:T:222:THR:OG1	2.35	0.41
2:B:816:VAL:HB	2:B:817:ARG:HG3	2.02	0.41
2:B:882:HIS:CE1	9:K:216:ALA:HB1	2.56	0.41
6:H:286:VAL:HA	6:H:289:LEU:HD12	2.03	0.41
7:I:24:GLU:C	7:I:27:GLY:H	2.29	0.41
9:K:110:TYR:CD1	9:K:113:ARG:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:19:MET:HA	10:M:22:ILE:HD12	2.02	0.41
11:N:149:PRO:HG2	11:N:153:ARG:HH12	1.86	0.41
12:P:200:ILE:HB	13:Q:127:TRP:NE1	2.35	0.41
2:B:465:SER:O	2:B:469:MET:HG3	2.21	0.41
2:B:619:MET:HG3	2:B:647:PHE:CE2	2.56	0.41
2:B:678:ARG:O	2:B:682:THR:OG1	2.34	0.41
5:G:477:ASP:OD1	5:G:477:ASP:N	2.51	0.41
5:G:675:LEU:HG	5:G:686:THR:HG22	2.03	0.41
6:H:219:GLU:HA	6:H:222:LEU:HD12	2.03	0.41
6:H:304:LEU:O	6:H:308:VAL:N	2.41	0.41
7:I:411:VAL:O	7:I:417:ARG:NH2	2.53	0.41
12:P:138:ILE:HD11	12:P:154:MET:HG2	2.03	0.41
16:Y:310:UNK:O	16:Y:314:UNK:N	2.54	0.41
2:B:31:GLN:HE21	2:B:49:VAL:HG21	1.86	0.41
2:B:432:HIS:NE2	2:B:441:LEU:HA	2.35	0.41
2:B:691:PHE:HE2	2:B:693:ARG:HB2	1.85	0.41
5:F:479:THR:O	5:F:555:ARG:NH2	2.53	0.41
5:G:473:LEU:HD21	5:G:489:PHE:HE1	1.86	0.41
5:G:763:GLU:O	5:G:784:HIS:HB3	2.21	0.41
7:I:383:LEU:HB2	7:I:387:VAL:HG11	2.01	0.41
2:B:131:PRO:O	2:B:135:TRP:N	2.50	0.40
2:B:719:MET:HA	2:B:722:LEU:HG	2.02	0.40
7:I:218:VAL:HA	7:I:221:GLN:HG2	2.03	0.40
7:I:241:GLU:OE2	9:K:135:UNK:N	2.54	0.40
7:I:270:ASN:O	7:I:274:ASN:N	2.49	0.40
2:B:898:THR:HG21	2:B:907:LEU:HB2	2.03	0.40
3:C:97:PHE:HB3	3:C:102:VAL:HB	2.04	0.40
5:F:558:LEU:HD23	5:F:572:LEU:HD21	2.03	0.40
6:H:386:ASP:HA	6:H:389:LYS:HB3	2.02	0.40
17:Z:215:UNK:O	17:Z:219:UNK:N	2.55	0.40
1:A:851:ASP:OD1	1:A:865:LYS:NZ	2.41	0.40
2:B:546:LEU:HD22	2:B:625:LEU:HD21	2.02	0.40
2:B:710:VAL:HG22	2:B:762:ASP:HA	2.04	0.40
2:B:761:ARG:HB3	2:B:766:LEU:HB3	2.03	0.40
7:I:252:LEU:HD12	7:I:252:LEU:HA	1.90	0.40
7:I:380:LEU:HD13	7:I:391:LEU:HD13	2.02	0.40
7:I:383:LEU:HB3	7:I:387:VAL:HG21	2.02	0.40
5:G:305:PHE:HD2	5:G:337:LEU:HD23	1.85	0.40
5:G:572:LEU:HD13	5:G:575:PHE:HE1	1.87	0.40
5:G:783:LEU:HA	5:G:783:LEU:HD23	1.77	0.40
7:I:280:ILE:HB	7:I:329:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:341:LEU:HA	2:B:341:LEU:HD23	1.90	0.40
2:B:399:LEU:HD23	2:B:399:LEU:HA	1.83	0.40
5:G:248:TYR:HE2	5:G:285:LEU:HD12	1.85	0.40
5:G:474:THR:O	5:G:486:ALA:CB	2.65	0.40
6:H:309:MET:HA	6:H:312:ILE:HD12	2.04	0.40
7:I:58:MET:HE3	7:I:63:ARG:HB2	2.02	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	462/1872 (25%)	454 (98%)	7 (2%)	1 (0%)	43	78
2	B	966/1199 (81%)	781 (81%)	183 (19%)	2 (0%)	43	78
3	C	91/929 (10%)	89 (98%)	2 (2%)	0	100	100
4	D	100/1085 (9%)	93 (93%)	7 (7%)	0	100	100
4	E	100/1085 (9%)	94 (94%)	6 (6%)	0	100	100
5	F	429/800 (54%)	382 (89%)	47 (11%)	0	100	100
5	G	429/800 (54%)	352 (82%)	77 (18%)	0	100	100
6	H	325/677 (48%)	293 (90%)	31 (10%)	1 (0%)	36	72
7	I	326/677 (48%)	292 (90%)	32 (10%)	2 (1%)	21	59
8	J	119/349 (34%)	117 (98%)	2 (2%)	0	100	100
9	K	149/310 (48%)	133 (89%)	15 (10%)	1 (1%)	18	56
10	L	96/264 (36%)	93 (97%)	3 (3%)	0	100	100
10	M	96/264 (36%)	89 (93%)	7 (7%)	0	100	100
11	N	78/218 (36%)	75 (96%)	3 (4%)	0	100	100
11	O	78/218 (36%)	74 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	P	87/211 (41%)	86 (99%)	1 (1%)	0	100	100
13	Q	72/161 (45%)	71 (99%)	1 (1%)	0	100	100
13	R	72/161 (45%)	68 (94%)	4 (6%)	0	100	100
14	S	43/124 (35%)	43 (100%)	0	0	100	100
15	T	178/339 (52%)	177 (99%)	1 (1%)	0	100	100
All	All	4296/11743 (37%)	3856 (90%)	433 (10%)	7 (0%)	44	78

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	950	VAL
7	I	256	LEU
6	H	321	PRO
7	I	257	PRO
9	K	218	PRO
2	B	336	ILE
2	B	844	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	407/1665 (24%)	407 (100%)	0	100	100
2	B	879/1083 (81%)	874 (99%)	5 (1%)	78	83
3	C	83/833 (10%)	82 (99%)	1 (1%)	63	75
4	D	52/815 (6%)	51 (98%)	1 (2%)	50	67
4	E	52/815 (6%)	52 (100%)	0	100	100
5	F	367/619 (59%)	366 (100%)	1 (0%)	86	86
5	G	367/619 (59%)	360 (98%)	7 (2%)	50	67
6	H	260/574 (45%)	259 (100%)	1 (0%)	84	84
7	I	252/564 (45%)	251 (100%)	1 (0%)	84	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	J	113/322 (35%)	113 (100%)	0	100	100
9	K	132/223 (59%)	132 (100%)	0	100	100
10	L	61/229 (27%)	60 (98%)	1 (2%)	55	70
10	M	61/229 (27%)	60 (98%)	1 (2%)	55	70
11	N	71/154 (46%)	71 (100%)	0	100	100
11	O	71/154 (46%)	71 (100%)	0	100	100
12	P	78/182 (43%)	77 (99%)	1 (1%)	61	74
13	Q	70/141 (50%)	70 (100%)	0	100	100
13	R	70/141 (50%)	70 (100%)	0	100	100
14	S	42/106 (40%)	41 (98%)	1 (2%)	43	64
15	T	155/293 (53%)	154 (99%)	1 (1%)	78	83
All	All	3643/9761 (37%)	3621 (99%)	22 (1%)	76	83

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	180	CYS
2	B	301	TYR
2	B	343	ARG
2	B	361	ARG
2	B	961	THR
3	C	53	VAL
4	D	908	GLN
5	F	558	LEU
5	G	558	LEU
5	G	559	LEU
5	G	627	LEU
5	G	637	PRO
5	G	657	LEU
5	G	768	LEU
5	G	780	VAL
6	H	347	THR
7	I	347	THR
10	L	73	LEU
10	M	73	LEU
12	P	191	VAL
14	S	57	LEU
15	T	222	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	802	HIS
1	A	1073	GLN
2	B	36	ASN
2	B	61	ASN
2	B	108	ASN
2	B	123	ASN
2	B	137	HIS
2	B	160	HIS
2	B	352	GLN
2	B	430	HIS
2	B	437	HIS
2	B	454	HIS
2	B	462	ASN
2	B	486	GLN
2	B	489	GLN
2	B	538	ASN
2	B	542	ASN
2	B	550	GLN
2	B	577	HIS
2	B	792	ASN
2	B	838	ASN
2	B	864	ASN
2	B	912	ASN
2	B	915	GLN
2	B	924	HIS
3	C	66	GLN
3	C	113	ASN
4	D	879	GLN
4	D	925	ASN
4	E	912	ASN
4	E	925	ASN
5	F	223	HIS
5	F	232	HIS
5	F	246	HIS
5	F	271	GLN
5	F	290	HIS
5	F	320	HIS
5	F	331	ASN
5	F	336	HIS
5	F	585	ASN

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Mol	Chain	Res	Type
5	F	626	HIS
5	F	710	HIS
5	F	733	ASN
5	F	766	GLN
5	G	232	HIS
5	G	246	HIS
5	G	256	HIS
5	G	290	HIS
5	G	320	HIS
5	G	327	ASN
5	G	331	ASN
5	G	334	GLN
5	G	336	HIS
5	G	542	HIS
5	G	556	ASN
5	G	585	ASN
5	G	636	HIS
5	G	638	ASN
5	G	784	HIS
6	H	270	ASN
6	H	343	HIS
6	H	385	HIS
6	H	397	GLN
7	I	52	GLN
7	I	64	GLN
7	I	220	GLN
7	I	244	GLN
7	I	326	HIS
7	I	343	HIS
7	I	430	HIS
9	K	30	HIS
9	K	82	HIS
9	K	103	ASN
9	K	173	GLN
10	M	37	ASN
11	N	122	GLN
11	N	160	GLN
11	N	168	ASN
11	O	122	GLN
11	O	160	GLN
11	O	168	ASN
12	P	119	ASN

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Mol	Chain	Res	Type
13	Q	119	HIS
13	Q	125	ASN
13	R	125	ASN
14	S	48	ASN
15	T	193	ASN
15	T	327	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
17	Z	8
16	Y	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	95:UNK	C	119:UNK	N	129.81
1	Z	52:UNK	C	81:UNK	N	116.40
1	Z	143:UNK	C	195:UNK	N	95.92
1	Z	223:UNK	C	309:UNK	N	54.56
1	Y	143:UNK	C	309:UNK	N	54.12
1	Y	52:UNK	C	119:UNK	N	47.22
1	Z	386:UNK	C	401:UNK	N	34.09
1	Z	328:UNK	C	358:UNK	N	33.32
1	Z	428:UNK	C	551:UNK	N	24.82
1	Z	571:UNK	C	573:UNK	N	4.23

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9305. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 72



Y Index: 72



Z Index: 72

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: 79



Y Index: 62

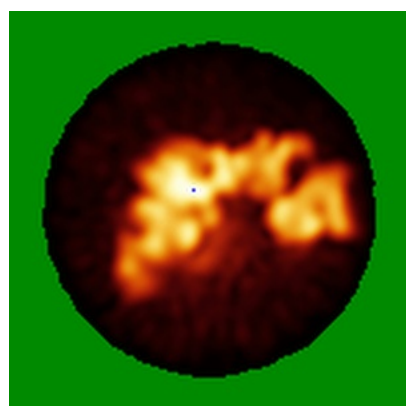


Z Index: 80

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

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

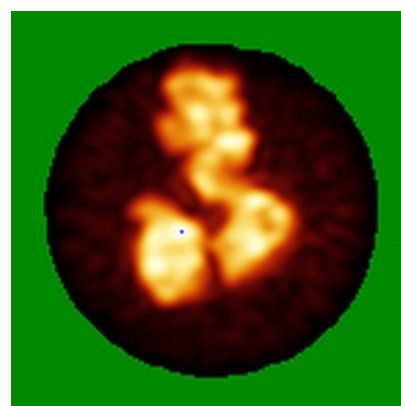
6.4.1 Primary map



X



Y

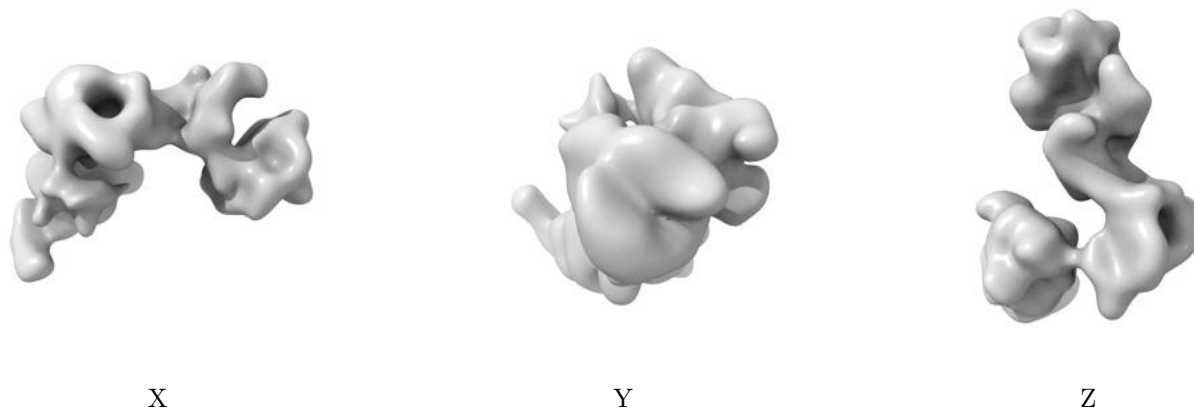


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

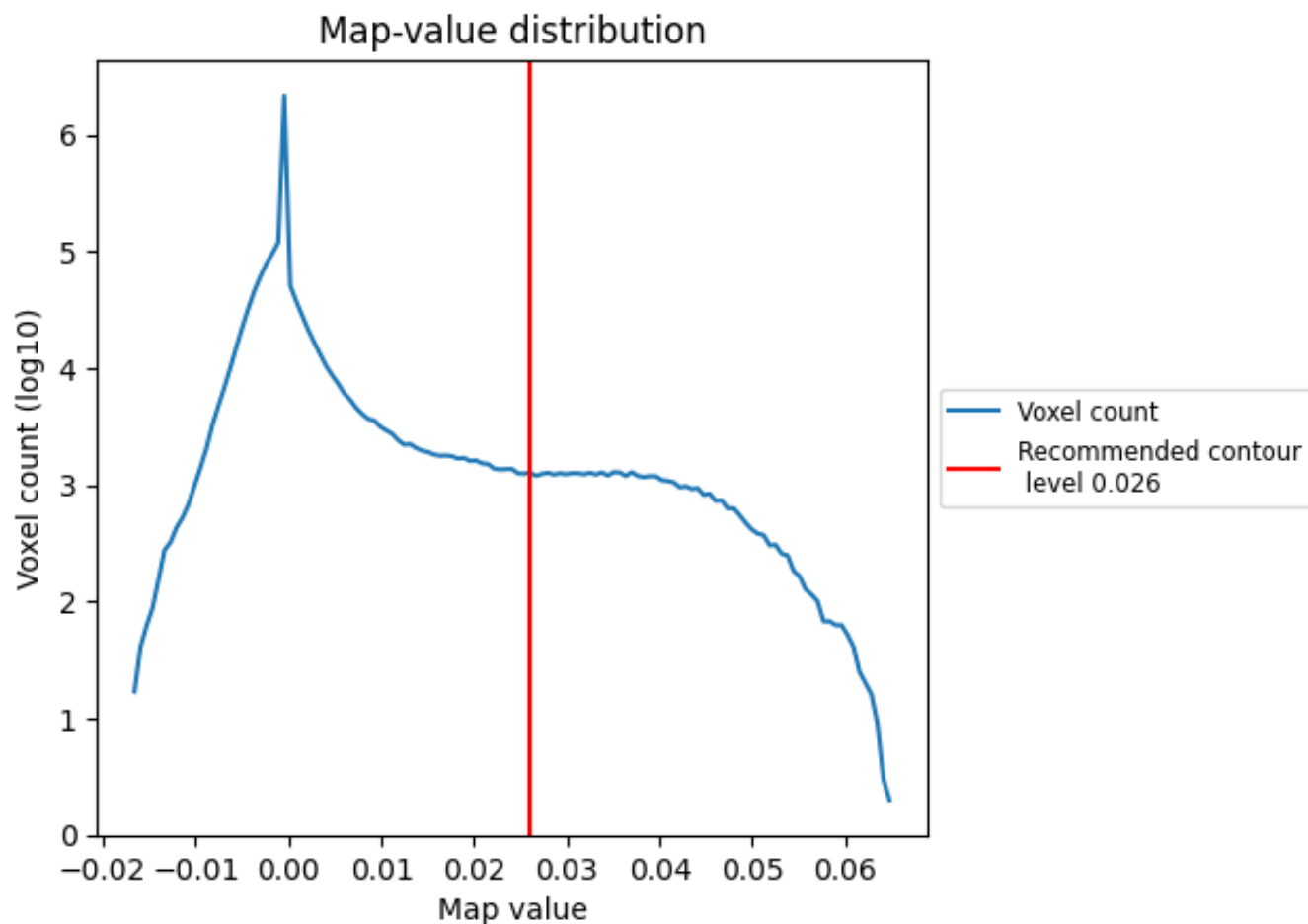
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

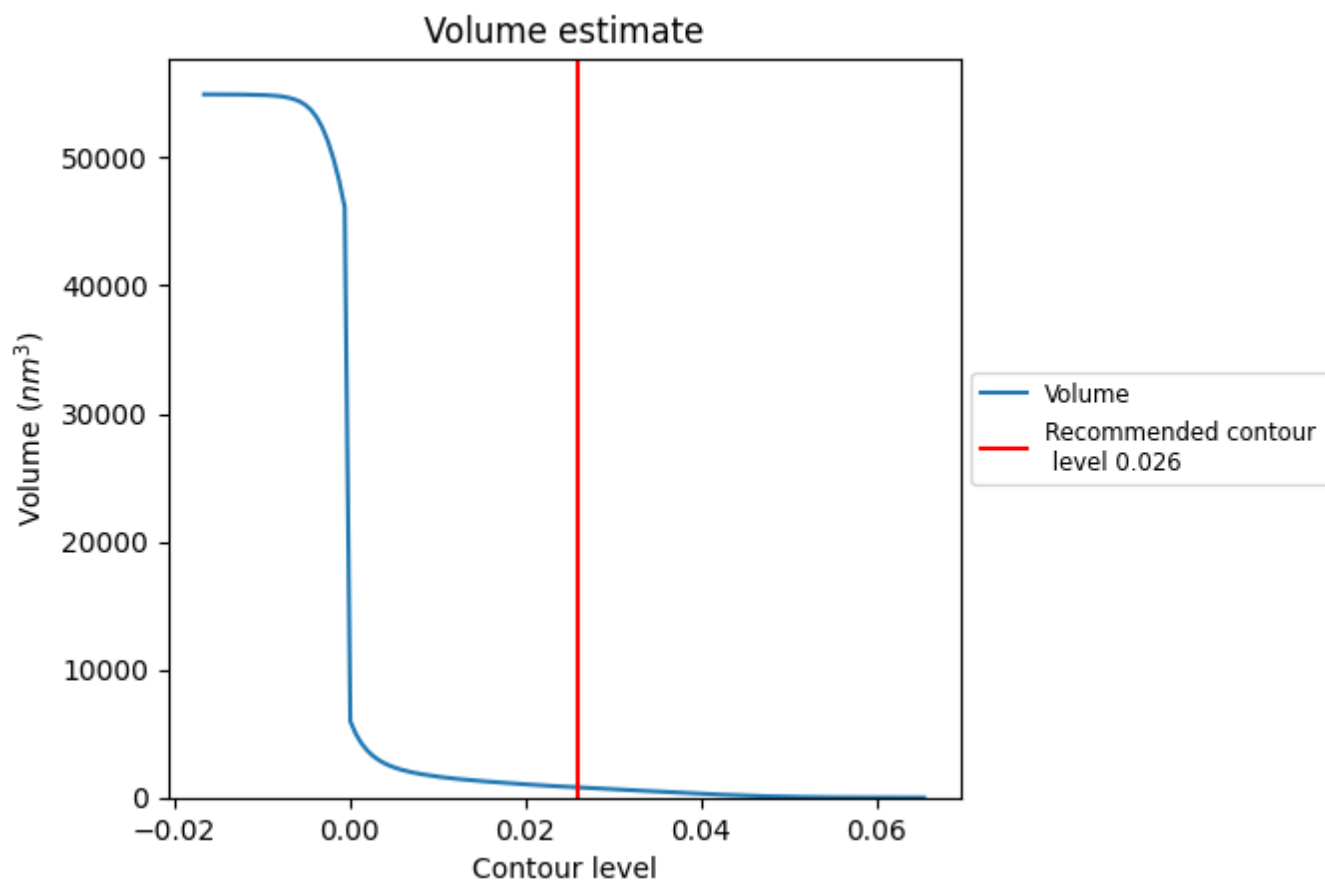
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

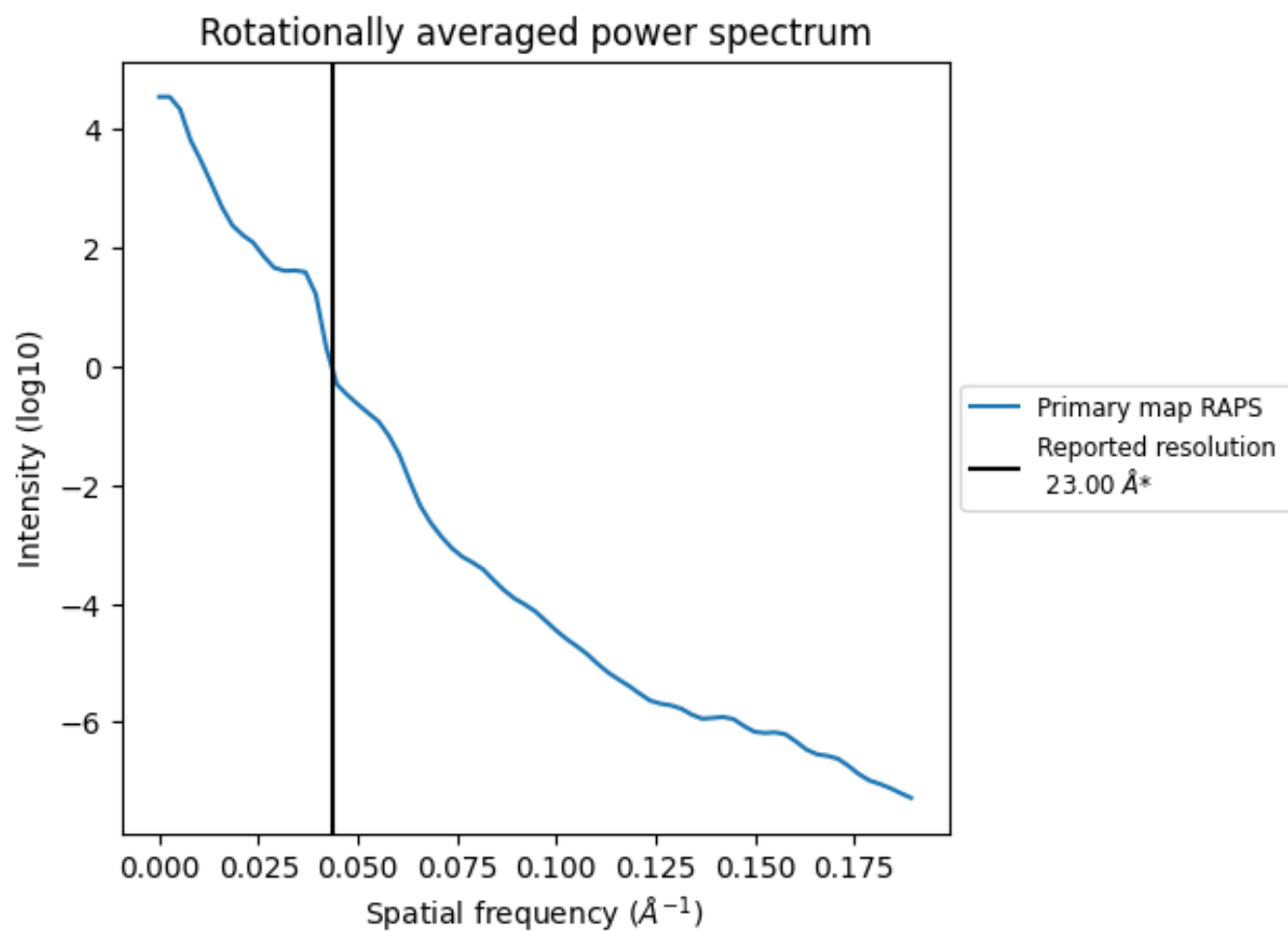
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 794 nm³; this corresponds to an approximate mass of 717 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 0.043 Å⁻¹

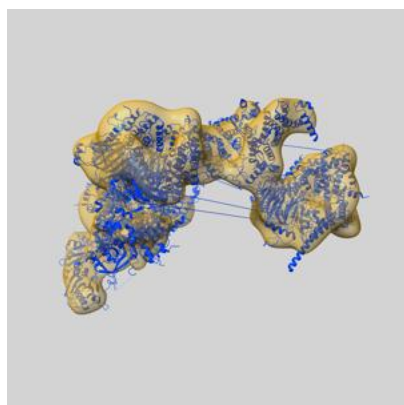
8 Fourier-Shell correlation

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

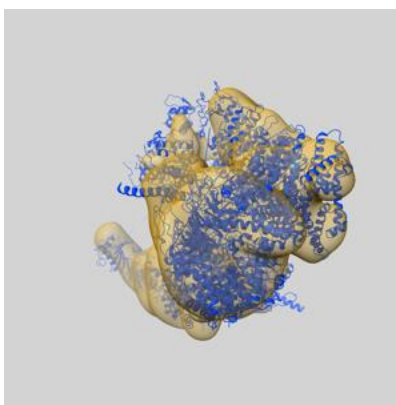
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9305 and PDB model 6MZL. Per-residue inclusion information can be found in section 3 on page 7.

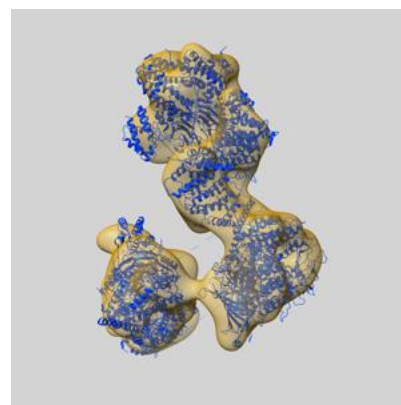
9.1 Map-model overlay [i](#)



X



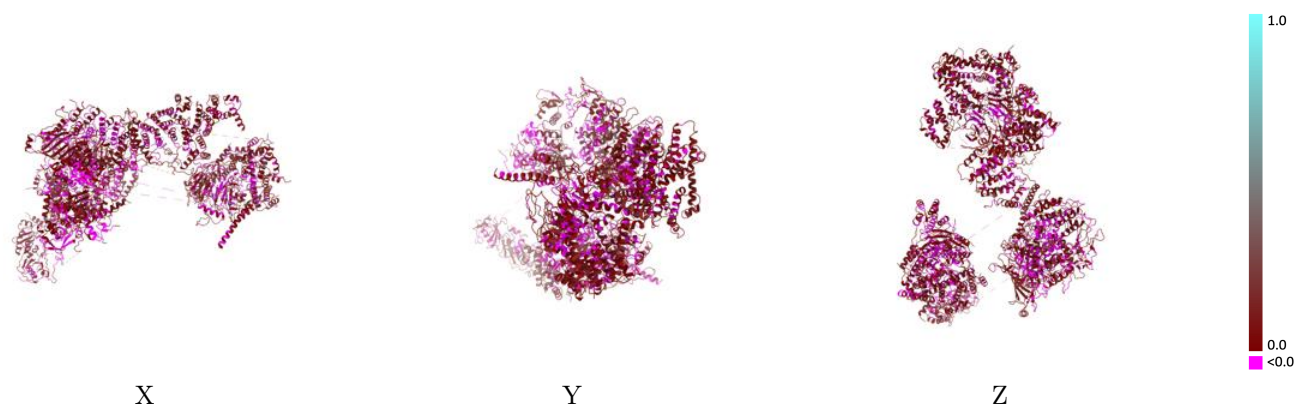
Y



Z

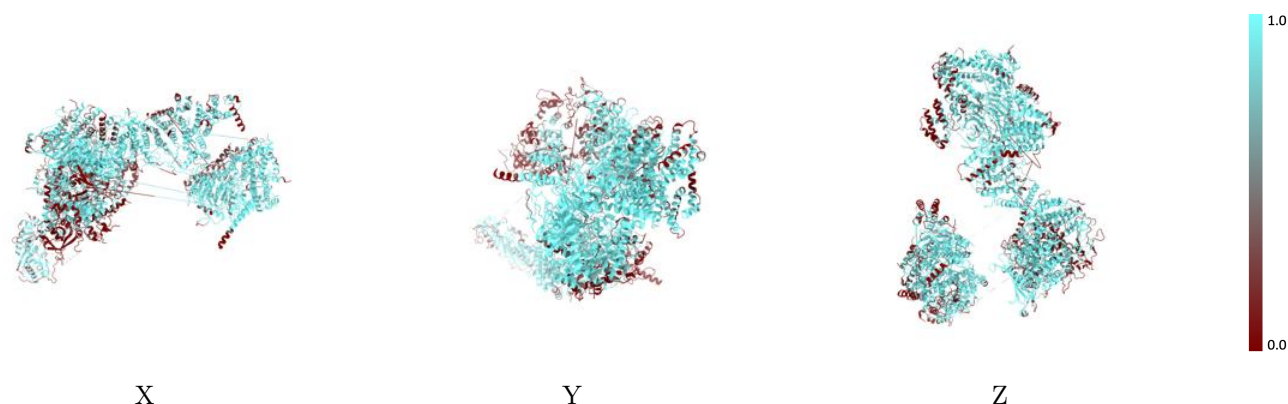
The images above show the 3D surface view of the map at the recommended contour level 0.026 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



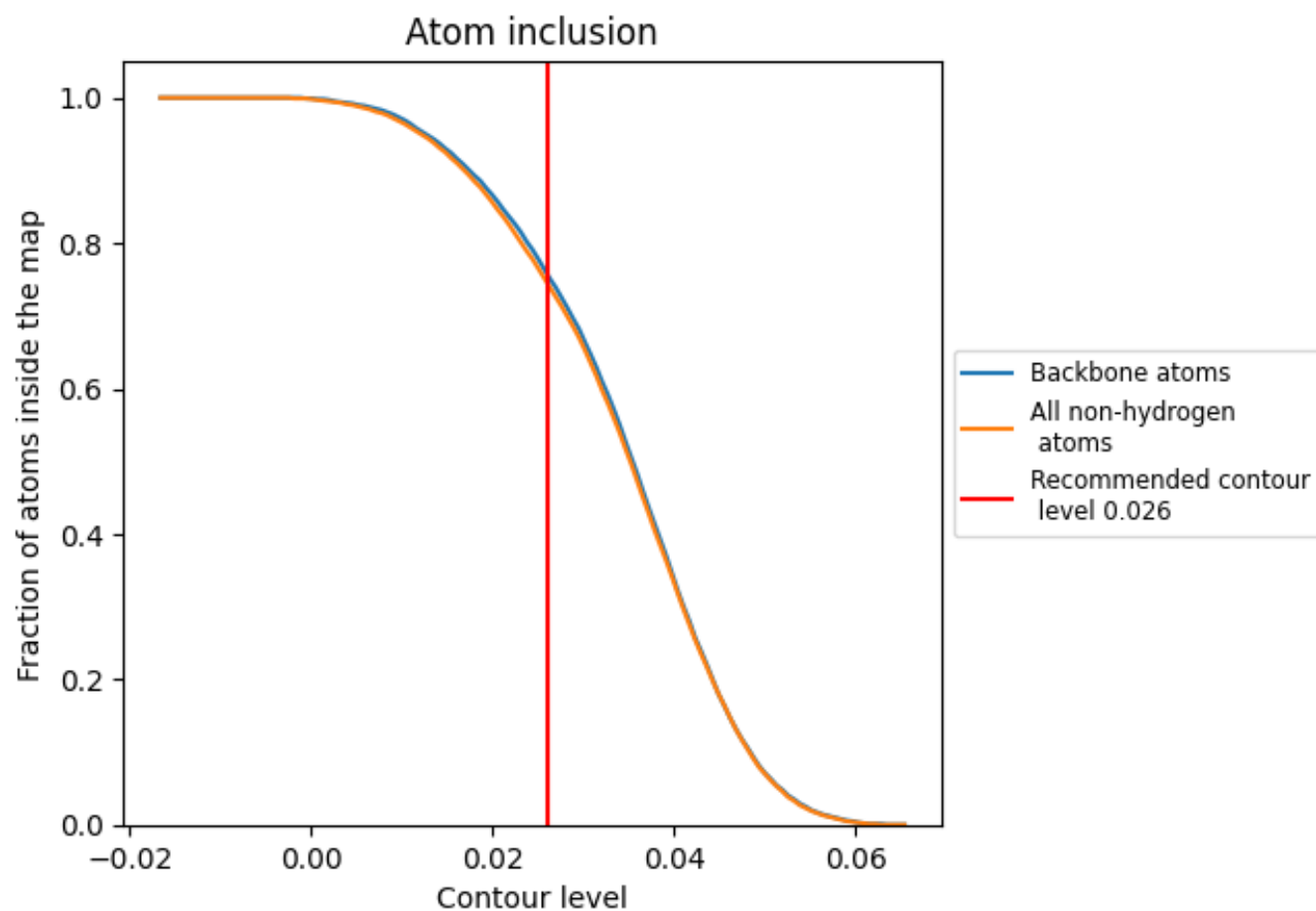
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.026).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 75% 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 (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7460	 0.0510
A	 0.4130	 0.0390
B	 0.7830	 0.0480
C	 0.9420	 0.0820
D	 0.6920	 0.0730
E	 0.7920	 0.0700
F	 0.7470	 0.0340
G	 0.8160	 0.0530
H	 0.8450	 0.0500
I	 0.8020	 0.0650
J	 0.2060	 0.0100
K	 0.9390	 0.0760
L	 0.9360	 0.0420
M	 0.7170	 0.0580
N	 0.8630	 0.0590
O	 0.9430	 0.0750
P	 0.6940	 0.0320
Q	 0.8170	 0.0450
R	 0.8400	 0.0710
S	 0.9670	 0.0990
T	 0.7180	 0.0690
Y	 0.4790	 0.0320
Z	 0.8570	 0.0550

