



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 12:41 AM EST

PDB ID : 6V92
EMDB ID : EMD-21114
Title : RSC-NCP
Authors : Patel, A.B.; Moore, C.M.; Greber, B.J.; Nogales, E.
Deposited on : 2019-12-13
Resolution : 20.00 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

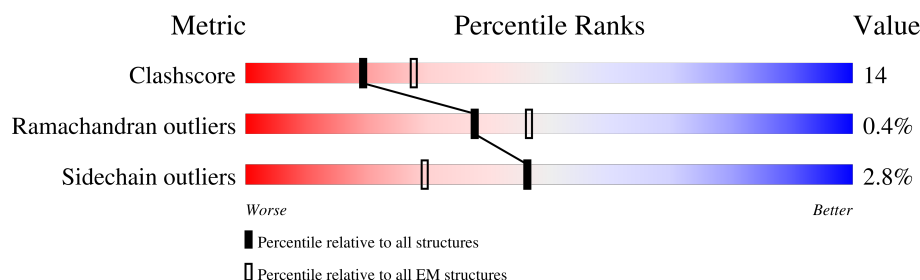
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 20.00 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.



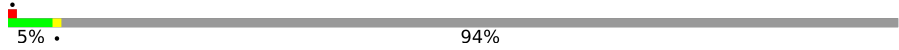

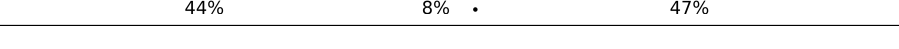
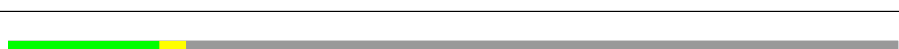
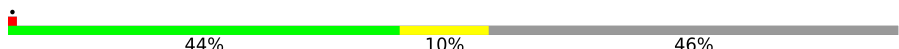


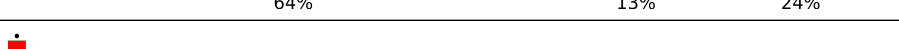
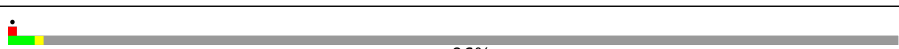
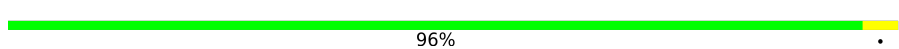
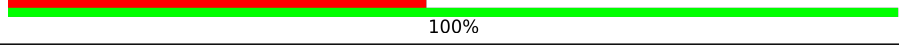
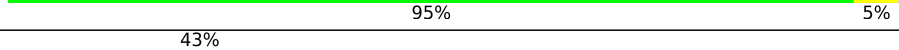
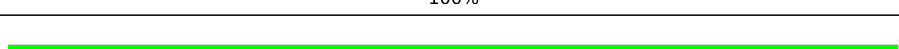
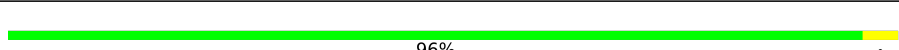
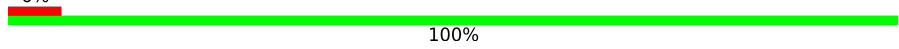
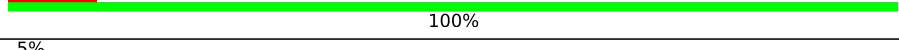
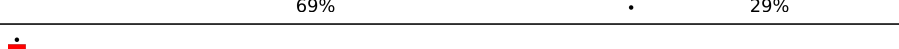







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	477	
2	R	1359	
3	B	467	
4	P	157	
5	C	78	
6	D	180	
7	E	435	
8	F	889	

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Mol	Chain	Length	Quality of chain
9	G	885	
10	H	625	
11	I	557	
11	J	557	
11	K	557	
11	L	557	
12	M	483	
13	N	581	
14	O	502	
15	Q	426	
16	S	883	
17	2	28	
18	3	19	
18	4	19	
19	5	14	
20	6	15	
21	7	49	
22	i	146	
22	j	146	
23	a	136	
23	e	136	
24	b	103	
24	f	103	
25	c	130	
25	g	130	

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Mol	Chain	Length	Quality of chain
26	d	126	<div> <div>10%</div> <div>71%</div> <div>5%</div> <div>24%</div> </div>
26	h	126	<div> <div>•</div> <div>69%</div> <div>6%</div> <div>25%</div> </div>

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 44583 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 Actin-related protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	399	Total	C	N	O	S	3	0
			3227	2081	528	603	15		

- Molecule 2 is a protein called Nuclear protein STH1/NPS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	325	Total	C	N	O	S	0	0
			2663	1668	487	504	4		

- Molecule 3 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	396	Total	C	N	O	S	1	0
			3198	2053	523	615	7		

- Molecule 4 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	54	Total	C	N	O	S	0	0
			490	313	84	92	1		

- Molecule 5 is a protein called High temperature lethal protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	60	Total	C	N	O	S	0	0
			493	301	92	96	4		

- Molecule 6 is a protein called Chromatin structure-remodeling complex protein RSC14.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	100	Total	C	N	O	S	0	0
			772	490	132	148	2		

- Molecule 7 is a protein called Chromatin structure-remodeling complex subunit RSC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	120	Total	C	N	O	S	0	0
			978	610	166	200	2		

- Molecule 8 is a protein called Chromatin structure-remodeling complex subunit RSC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	67	Total	C	N	O	S	0	0
			536	346	94	95	1		

- Molecule 9 is a protein called Chromatin structure-remodeling complex protein RSC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	53	Total	C	N	O	S	0	0
			422	270	71	79	2		

- Molecule 10 is a protein called Chromatin structure-remodeling complex subunit RSC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	131	Total	C	N	O	S	0	0
			1083	696	175	205	7		

- Molecule 11 is a protein called Chromatin structure-remodeling complex protein RSC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	293	Total	C	N	O	S	0	0
			2416	1537	423	448	8		
11	J	115	Total	C	N	O	S	0	0
			924	579	149	190	6		
11	K	109	Total	C	N	O	S	0	0
			878	554	139	179	6		
11	L	298	Total	C	N	O	S	0	0
			2445	1557	428	452	8		

- Molecule 12 is a protein called Chromatin structure-remodeling complex protein RSC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	310	Total	C	N	O	S	0	0
			2474	1558	414	496	6		

- Molecule 13 is a protein called Chromatin structure-remodeling complex subunit RSC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	412	Total	C	N	O	S	0	0
			3275	2105	540	612	18		

- Molecule 14 is a protein called Chromatin structure-remodeling complex protein RSC58.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	384	Total	C	N	O	S	0	0
			3145	2025	529	581	10		

- Molecule 15 is a protein called Chromatin structure-remodeling complex subunit SFH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	264	Total	C	N	O	S	0	0
			2137	1349	362	418	8		

- Molecule 16 is a protein called Chromatin structure-remodeling complex protein RSC30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	34	Total	C	N	O	S	0	0
			278	182	41	54	1		

- Molecule 17 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	2	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 18 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	3	19	Total	C	N	O	0	0
			95	57	19	19		
18	4	19	Total	C	N	O	0	0
			95	57	19	19		

- Molecule 19 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	5	14	Total	C	N	O	0	0
			70	42	14	14		

- Molecule 20 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	6	15	Total	C	N	O	0	0
			75	45	15	15		

- Molecule 21 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	7	49	Total	C	N	O	0	0
			245	147	49	49		

- Molecule 22 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	i	146	Total	C	N	O	P	0	0
			2990	1431	540	874	145		
22	j	146	Total	C	N	O	P	0	0
			2990	1431	540	874	145		

- Molecule 23 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	97	Total	C	N	O	S	0	0
			801	505	155	137	4		
23	e	99	Total	C	N	O	S	0	0
			816	514	158	140	4		

- Molecule 24 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	78	Total	C	N	O	S	0	0
			619	391	120	107	1		
24	f	85	Total	C	N	O	S	0	0
			683	430	136	116	1		

- Molecule 25 is a protein called Histone H2A type 1-B/E.

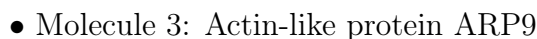
Mol	Chain	Residues	Atoms				AltConf	Trace
25	c	108	Total	C	N	O	0	0
			835	526	165	144		
25	g	104	Total	C	N	O	0	0
			805	508	157	140		

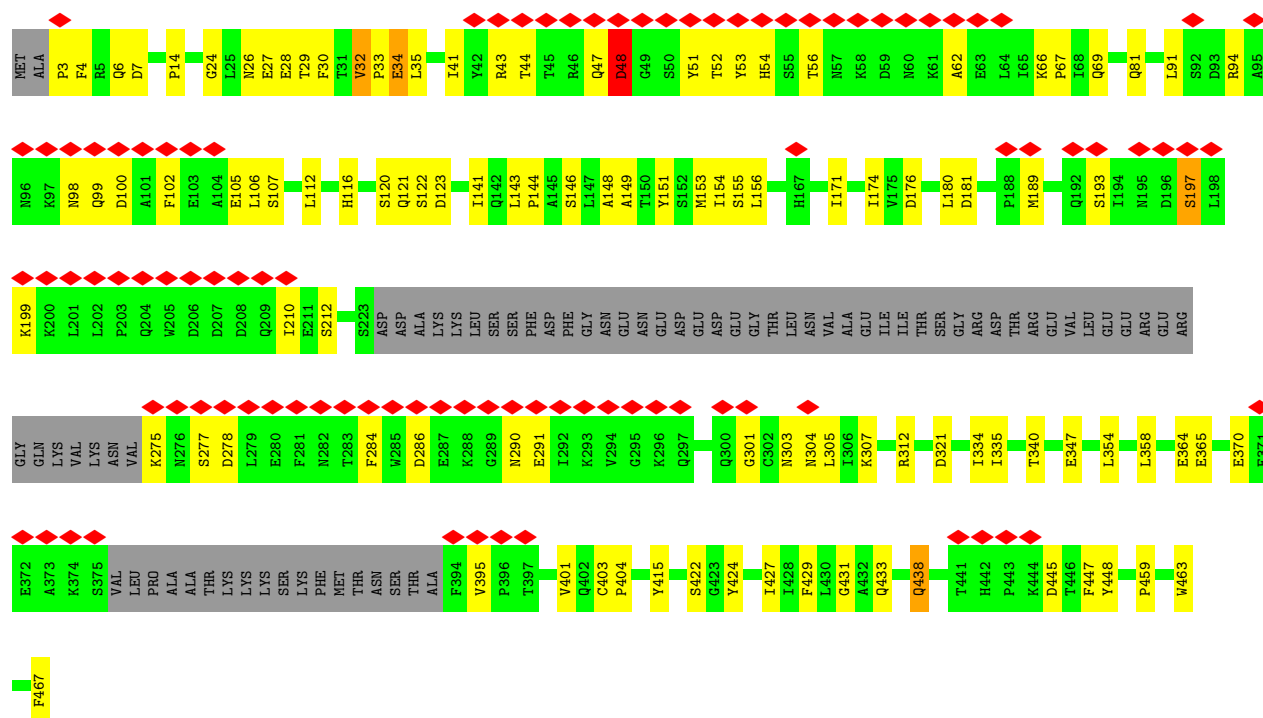
- Molecule 26 is a protein called Histone H2B type 1-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	96	Total	C	N	O	S	0	0
			754	473	138	141	2		
26	h	94	Total	C	N	O	S	0	0
			735	461	134	138	2		

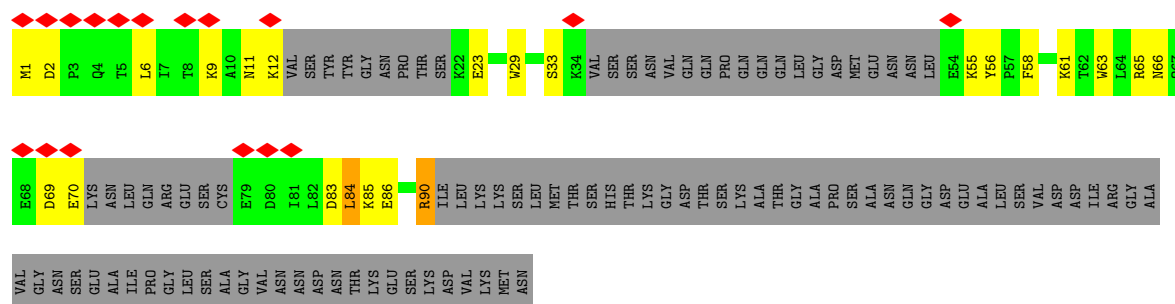
- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
27	I	1	Total	Zn	0
			1	1	





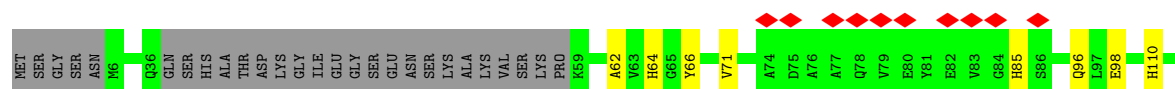
• Molecule 4: Regulator of Ty1 transposition protein 102

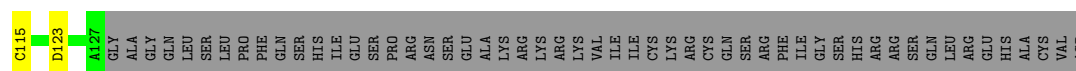


• Molecule 5: High temperature lethal protein 1

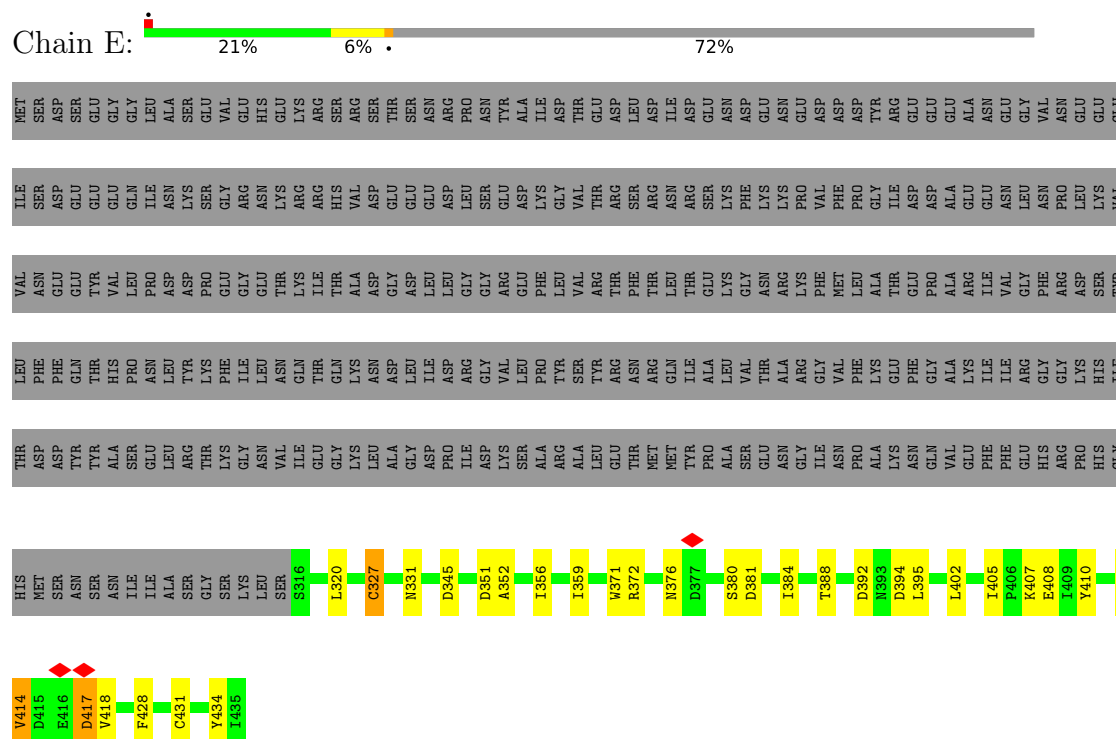


• Molecule 6: Chromatin structure-remodeling complex protein RSC14

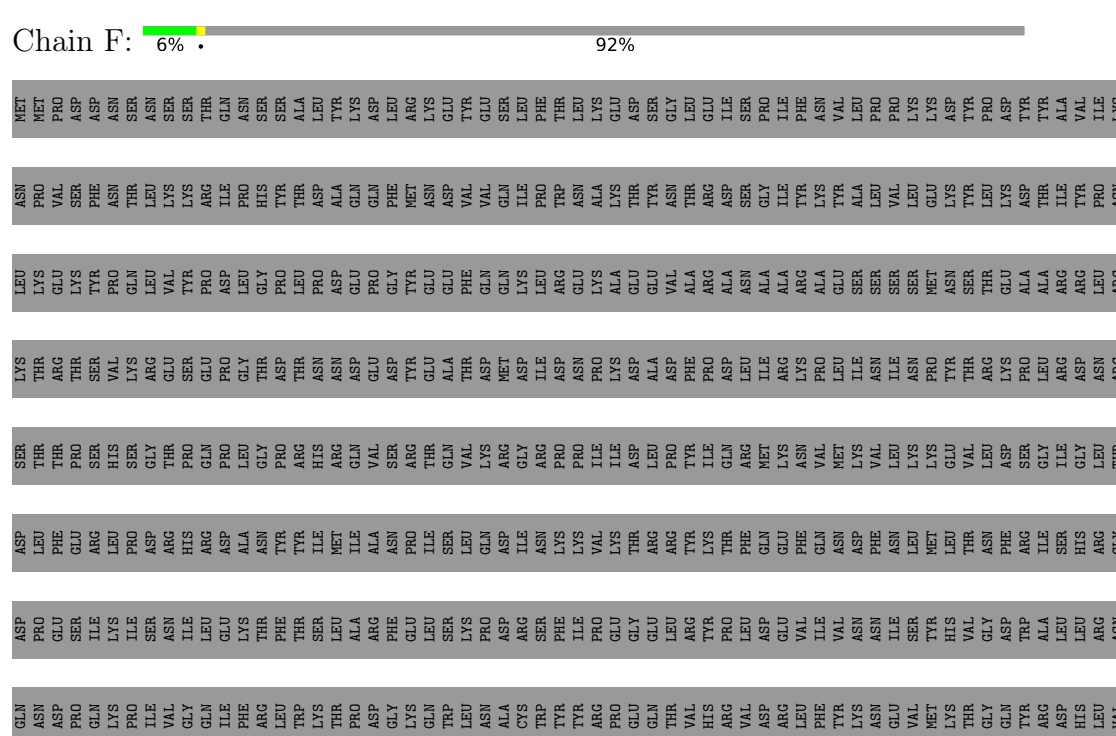




• Molecule 7: Chromatin structure-remodeling complex subunit RSC7



• Molecule 8: Chromatin structure-remodeling complex subunit RSC2





[illegible]

- Molecule 10: Chromatin structure-remodeling complex subunit RSC4

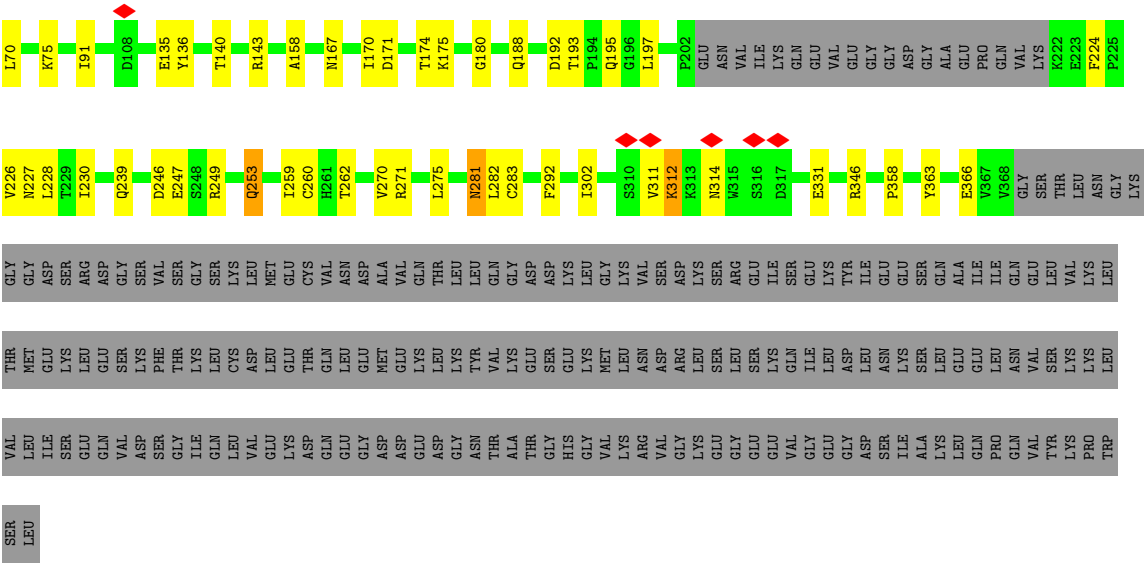
Chain H:  16% 5% 79%

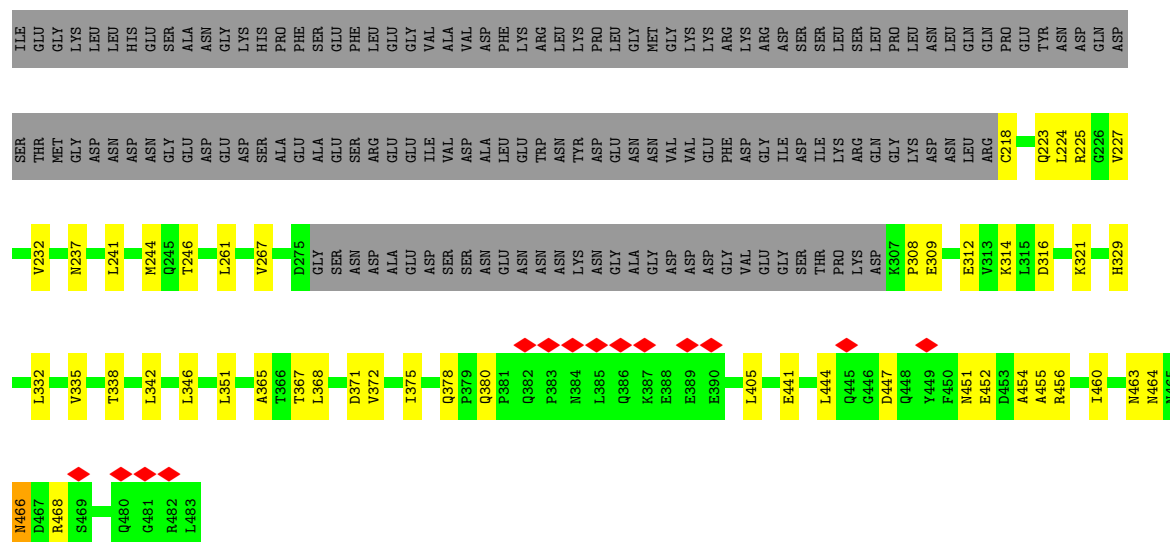
T588	L596	ILE	PHE	ASN	ASN	LYS	LEU
R605	T527	PRO	GLY	GLU	LEU	VAL	ASP
C606	I528	TYR	LEU	ARG	GLY	VAL	SER
D608	M529	ASN	GLY	GLY	ILE	ASP	THR
K609	P532	VAL	ASN	ILE	GLN	THR	LEU
I610	S535	ILE	GLY	ASN	GLY	GLU	ASP
F625	ARG	LYS	TYR	SER	TYR	LYS	LEU
	THR	MET	ASN	PHE	PHE	ALA	GLY
	SER	GLN	SER	ASP	ASP	ASN	ASP
	ASN	LYS	LEU	LYS	THR	GLN	ALA
	VAL	GLU	LEU	PHE	PHE	ALA	TYR
	ASN	MET	THR	GLU	ILE	LEU	ASN
	ASN	GLN	GLU	PHE	ILE	LEU	GLY
	ASN	SER	ASP	GLU	ILE	GLY	ASP
	LEU	LEU	TYR	ASN	MET	ALA	PHE
	SER	SER	LEU	TYR	LEU	SER	SER
	GLN	GLU	LEU	LEU	LEU	SER	LEU
	PRO	GLN	ASN	ALA	VAL	PRO	ILE
	GLN	HIS	PRO	ILE	LYS	VAL	ILE
	GLN	THR	ASN	GLY	ASN	LYS	LYS
	GLN	M443	ASN	GLY	ASN	LEU	ASN
	GLU	E444	PHE	GLY	ALA	SER	PRO
	ASN	Y445	LYS	GLY	HIS	ASP	LYS
	ASP		LYS	PRO	ILE	VAL	PRO
	VAL	Y448	LEU	ALA	PHE	VAL	ASN
	ILE	K449	ILE	ALA	ASN	LYS	VAL
	GLY		ALA	ALA	ASP	MET	MET
	ASN	Q453	LYS	GLY	PRO	LEU	LEU
	ASP		PRO	ALA	SER	GLU	ILE
	THR	F457	GLU	LEU	ALA	PRO	GLY
	LYS		THR	ILE	ALA	PHE	THR
	GLN	R474	VAL	ILE	ILE	GLU	TYR
	ASP		GLN	SER	TYR	VAL	LYS
	ILE	E483	SER	ALA	LYS	LEU	ILE
	GLU		GLU	LEU	ASP	LYS	GLN
	ASN	F486	VAL	ASN	ALA	ASP	ASP
	LEU	N487	LYS	ASN	THR	LYS	GLN
	THR	G488	ASN	ASP	THR	ASN	MET
	ILE	M489	GLY	ILE	THR	GLU	SER
	GLY	E490	ARG	GLU	THR	LEU	LEU
	GLY		SER	PRO	ASN	ARG	ASN
	GLY	Q493	THR	GLU	TYR	GLU	ASN
	ASN		THR	SER	PHE	TYR	ILE
	ASN	A497	SER	ASN	ASN	LEU	SER
	ASN		ASP	ARG	TYR	ILE	GLY
	ASP	L502	ILE	GLU	LEU	ASN	ASN
	ILE		GLU	ASP	ILE	VAL	SER
	VAL	L509	LYS	ILE	GLN	GLY	THR
	GLY	T510	THR	LEU	LYS	VAL	LYS
	ASN	L511	ASN	ASN	GLU	PRO	TYR
	ASP	G512	SER	GLN	PHE	MET	ALA
	ASN	S513	LEU	ALA	PHE	LYS	ASP
	ASP		GLU	ASP	PRO	LEU	GLY
	LYS	T516	SER	TYR	GLU	LEU	PRO
	ARG		HIS	ASP	LEU	HIS	LYS
	ASN	E523	GLY	PHE	GLN	VAL	ASN
	ASN	T524	LEU	ASN	THR	ASN	PHE
	THR	L525	LYS	HIS	THR	GLN	LEU

- Molecule 11: Chromatin structure-remodeling complex protein RSC8

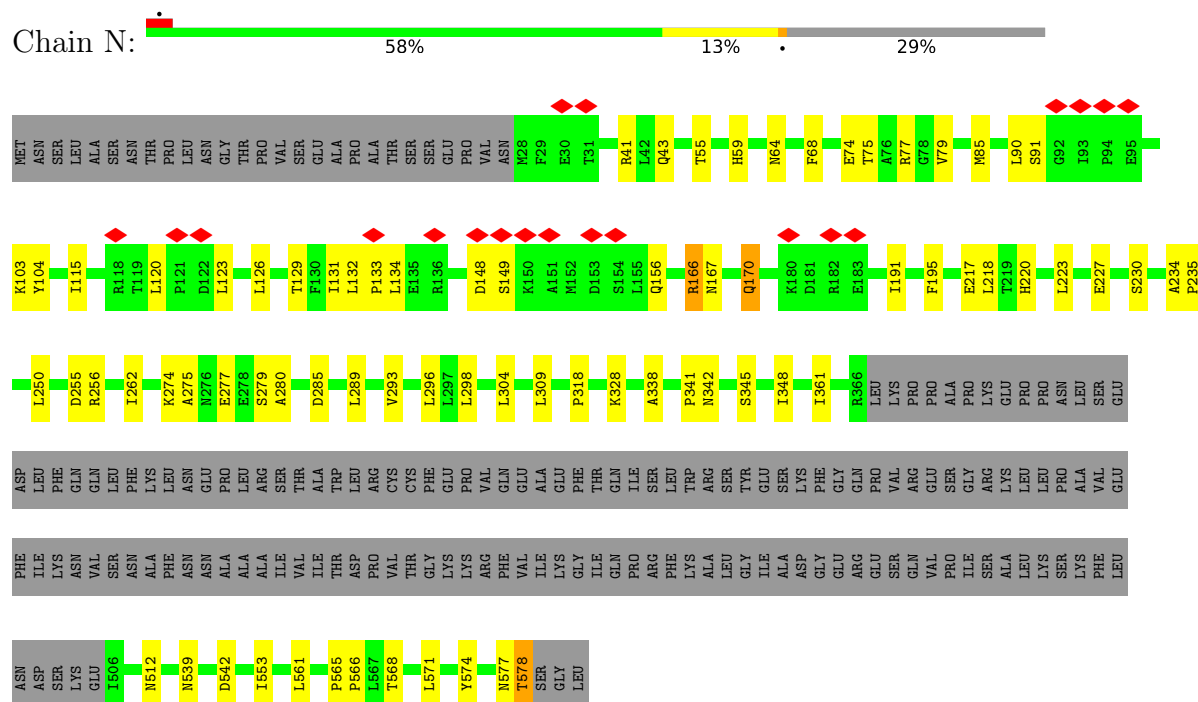
Chain I: 44% 8% 47%

MET	SER	ASP	THR	GLU	LYS	ASP	LYS	ASP	ASP	VAL	PRO	MET	VAL	ASP	SER	HIS	GLU	ALA	THR	GLU	GLU	PRO	PRO	THR	THR	SER	THR	THR	ASN	PRO	PRO	PHE	PRO	HIS	PRO	LEU	ALA	ALA	GLN	GLU	GLN	ALA	ALA	LYS	GLU	GLU	GLU	ALA	ALA	THR	THR	THR	SER	LYS	LYS	LYS	ILE	M57	Y58	E59
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

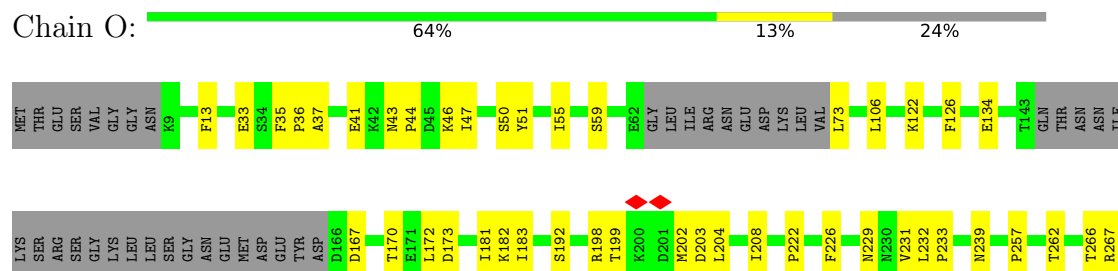


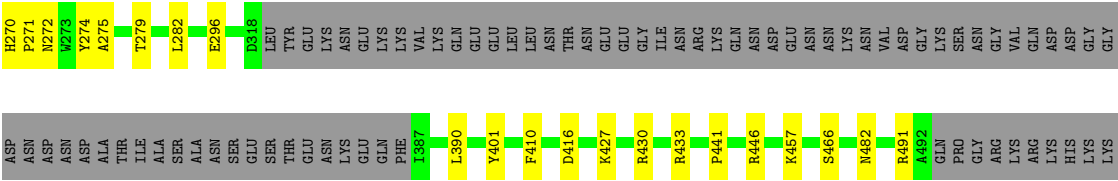


• Molecule 13: Chromatin structure-remodeling complex subunit RSC9

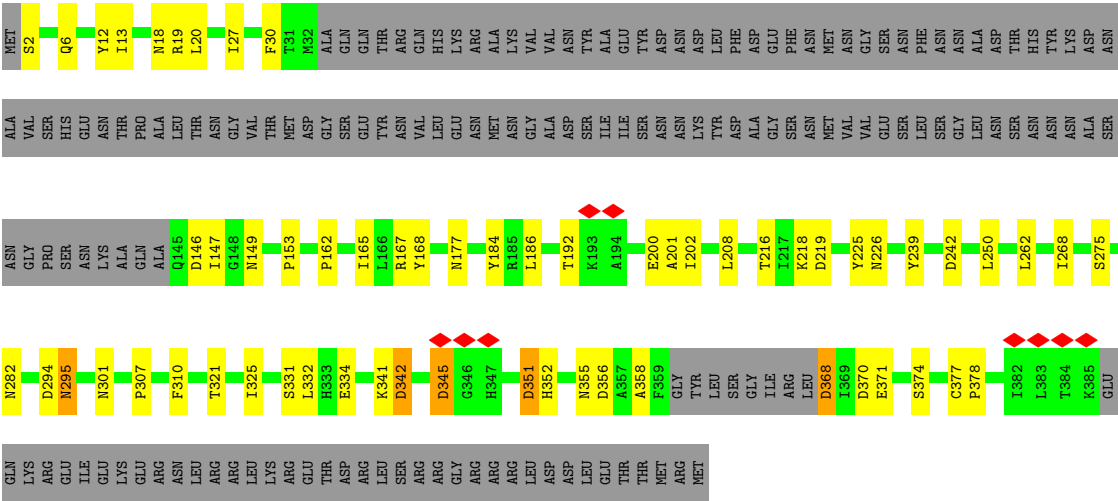


• Molecule 14: Chromatin structure-remodeling complex protein RSC58

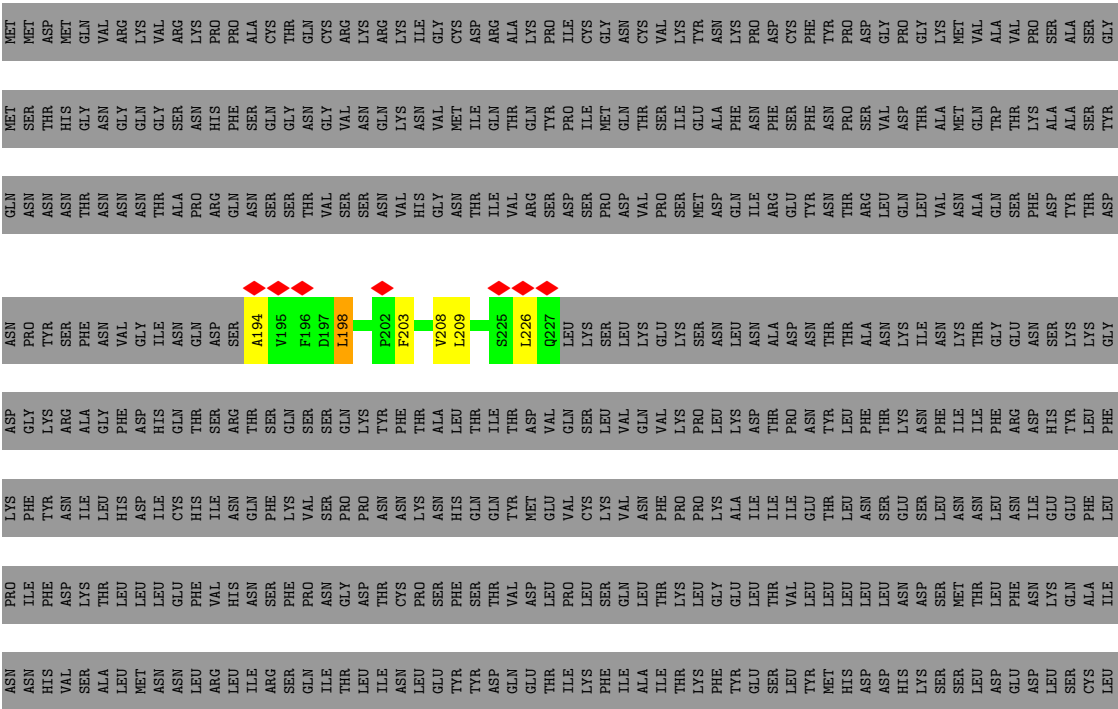




• Molecule 15: Chromatin structure-remodeling complex subunit SFH1



• Molecule 16: Chromatin structure-remodeling complex protein RSC30



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

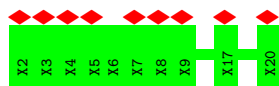
- Molecule 17: Unknown Protein

Chain 2: 96%



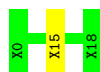
- Molecule 18: Unknown Protein

Chain 3:  47% 100%



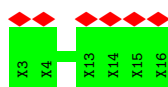
- Molecule 18: Unknown Protein

Chain 4: 95% 5%



- Molecule 19: Unknown Protein

Chain 5:  43% 100%



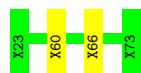
- Molecule 20: Unknown Protein

Chain 6: 100%

There are no outlier residues recorded for this chain.

- Molecule 21: Unknown Protein

Chain 7:  96%



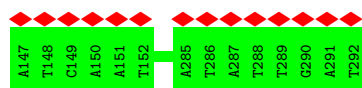
- Molecule 22: DNA (146-MER)

Chain i:  6% 100%



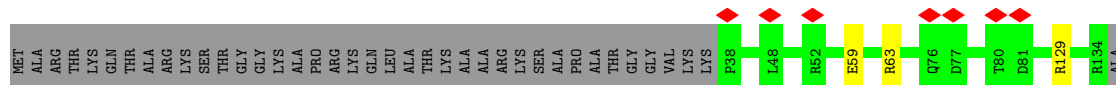
- Molecule 22: DNA (146-MER)

Chain j:  10% 100%



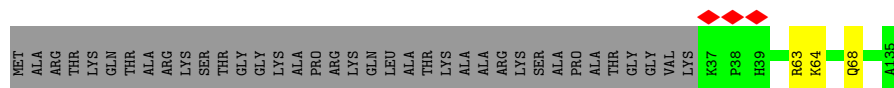
- Molecule 23: Histone H3.1

Chain a:  5% 69% 29%




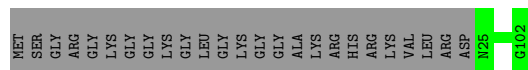
- Molecule 23: Histone H3.1

Chain e:  71% 27%




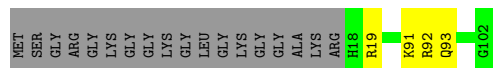
- Molecule 24: Histone H4

Chain b:  76% 24%




- Molecule 24: Histone H4

Chain f:  79% 17%




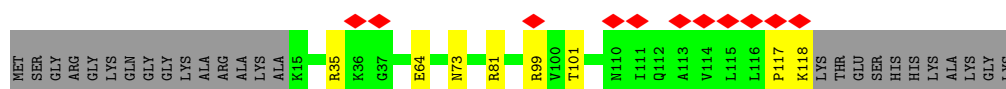
• Molecule 25: Histone H2A type 1-B/E

Chain c:  78% 5% 17%



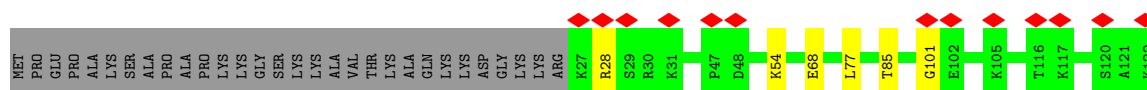
• Molecule 25: Histone H2A type 1-B/E

Chain g:  8% 74% 6% 20%



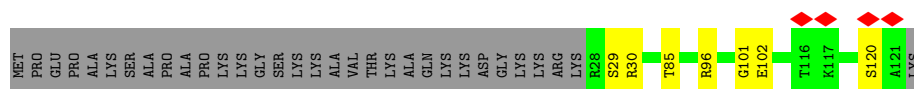
• Molecule 26: Histone H2B type 1-K

Chain d:  10% 71% 5% 24%



• Molecule 26: Histone H2B type 1-K

Chain h:  69% 6% 25%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13337	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.110	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	437.76, 437.76, 437.76	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	3.42, 3.42, 3.42	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/3303	0.60	1/4465 (0.0%)
2	R	0.36	2/2697 (0.1%)	0.49	3/3616 (0.1%)
3	B	0.45	0/3269	0.59	0/4432
4	P	0.41	0/501	0.57	0/669
5	C	0.24	0/495	0.36	0/662
6	D	0.27	0/786	0.38	0/1062
7	E	0.28	0/997	0.44	0/1356
8	F	0.27	0/551	0.41	0/748
9	G	0.26	0/431	0.43	0/584
10	H	0.29	0/1108	0.48	0/1497
11	I	0.32	0/2474	0.41	0/3343
11	J	0.30	0/926	0.40	0/1233
11	K	0.27	0/879	0.39	0/1172
11	L	0.29	0/2502	0.40	0/3376
12	M	0.28	0/2515	0.42	0/3423
13	N	0.30	0/3334	0.42	0/4515
14	O	0.30	0/3216	0.42	1/4358 (0.0%)
15	Q	0.28	0/2181	0.45	0/2964
16	S	0.26	0/281	0.35	0/378
22	i	0.38	0/3354	0.79	0/5175
22	j	0.36	0/3354	0.78	0/5175
23	a	0.40	0/813	0.59	0/1090
23	e	0.46	0/828	0.61	0/1109
24	b	0.38	0/626	0.62	0/837
24	f	0.44	0/691	0.63	0/923
25	c	0.39	0/845	0.60	0/1139
25	g	0.39	0/815	0.65	0/1100
26	d	0.41	0/765	0.63	0/1025
26	h	0.40	0/746	0.58	0/1003
All	All	0.35	2/45283 (0.0%)	0.55	5/62429 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	328	LYS	C-O	5.96	1.34	1.23
2	R	333	ILE	C-O	5.93	1.34	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	SER	C-N-CD	5.93	140.86	128.40
14	O	231	VAL	C-N-CA	5.36	135.09	121.70
2	R	333	ILE	CA-C-O	5.28	131.19	120.10
2	R	367	ASP	CB-CG-OD2	5.17	122.95	118.30
2	R	328	LYS	CA-C-O	5.10	130.81	120.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3227	0	3251	150	0
2	R	2663	0	2746	159	0
3	B	3198	0	3187	136	0
4	P	490	0	467	19	0
5	C	493	0	507	4	0
6	D	772	0	754	11	0
7	E	978	0	935	25	0
8	F	536	0	533	13	0
9	G	422	0	423	9	0
10	H	1083	0	1062	21	0
11	I	2416	0	2358	36	0
11	J	924	0	976	12	0
11	K	878	0	930	13	0
11	L	2445	0	2402	48	0
12	M	2474	0	2465	48	0
13	N	3275	0	3373	47	0
14	O	3145	0	3168	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	Q	2137	0	2069	42	0
16	S	278	0	287	6	0
17	2	140	0	34	1	0
18	3	95	0	21	0	0
18	4	95	0	21	1	0
19	5	70	0	16	0	0
20	6	75	0	17	0	0
21	7	245	0	63	2	0
22	i	2990	0	1652	0	0
22	j	2990	0	1652	0	0
23	a	801	0	839	0	0
23	e	816	0	856	0	0
24	b	619	0	659	0	0
24	f	683	0	729	0	0
25	c	835	0	897	0	0
25	g	805	0	861	0	0
26	d	754	0	782	0	0
26	h	735	0	756	0	0
27	I	1	0	0	0	0
All	All	44583	0	41748	652	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 14.

All (652) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:353:PHE:CZ	3:B:447:PHE:CE2	2.05	1.45
2:R:353:PHE:CZ	3:B:447:PHE:HE2	1.34	1.41
2:R:353:PHE:CE1	3:B:447:PHE:HE2	1.47	1.33
2:R:365:GLU:HG2	3:B:415:TYR:CD2	1.65	1.32
2:R:353:PHE:CE2	3:B:447:PHE:CE2	2.21	1.29
2:R:349:ARG:O	2:R:353:PHE:CD2	1.84	1.28
2:R:365:GLU:HG2	3:B:415:TYR:CE2	1.70	1.25
1:A:76:LEU:CD2	1:A:108:MET:CE	2.15	1.24
3:B:189:MET:HE1	3:B:305:LEU:CA	1.69	1.21
2:R:320:LYS:O	2:R:324:LEU:HG	1.34	1.20
2:R:353:PHE:CE2	3:B:447:PHE:CZ	2.31	1.19
2:R:365:GLU:OE2	3:B:415:TYR:CE2	1.96	1.18
2:R:353:PHE:CE1	3:B:447:PHE:CE2	2.30	1.17
1:A:76:LEU:CD2	1:A:108:MET:HE1	1.70	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:351:PHE:CE1	3:B:176:ASP:HB3	1.81	1.16
2:R:365:GLU:CG	3:B:415:TYR:CE2	2.28	1.14
1:A:343:SER:CB	1:A:344:ILE:HA	1.81	1.11
2:R:347:GLN:O	2:R:351:PHE:HD2	1.36	1.09
1:A:76:LEU:HD22	1:A:108:MET:HE1	1.13	1.08
1:A:150:GLY:HA2	2:R:336:ILE:HD11	1.31	1.08
1:A:343:SER:HB3	1:A:344:ILE:HA	1.09	1.07
1:A:114:LYS:HG3	1:A:115:PRO:HD3	1.37	1.06
2:R:336:ILE:HG22	2:R:339:ARG:NH2	1.70	1.06
3:B:189:MET:HE1	3:B:305:LEU:HA	1.06	1.05
2:R:320:LYS:O	2:R:324:LEU:CG	2.03	1.05
1:A:76:LEU:CD2	1:A:108:MET:HE3	1.86	1.04
2:R:353:PHE:CE2	3:B:447:PHE:HE2	1.69	1.04
2:R:365:GLU:CG	3:B:415:TYR:CZ	2.39	1.04
2:R:347:GLN:O	2:R:351:PHE:CD2	2.11	1.03
1:A:122:ARG:HH11	1:A:122:ARG:HG2	1.25	1.02
1:A:216:ARG:HG2	1:A:216:ARG:HH11	1.17	1.00
2:R:360:LEU:HD11	3:B:438:GLN:NE2	1.78	0.99
1:A:76:LEU:HD21	1:A:108:MET:HE3	1.41	0.99
1:A:442:THR:HB	2:R:339:ARG:HE	1.26	0.97
2:R:365:GLU:CD	3:B:415:TYR:CE2	2.37	0.97
2:R:360:LEU:CD1	3:B:438:GLN:HG2	1.94	0.97
2:R:320:LYS:HB3	2:R:324:LEU:HD11	1.46	0.96
2:R:336:ILE:HG22	2:R:339:ARG:HH22	1.29	0.96
3:B:189:MET:CE	3:B:305:LEU:HA	1.94	0.96
1:A:150:GLY:CA	2:R:336:ILE:HD11	1.96	0.96
1:A:343:SER:HB3	1:A:344:ILE:CA	1.95	0.96
2:R:364:MET:CE	3:B:30:PHE:HE1	1.79	0.95
2:R:351:PHE:CZ	3:B:176:ASP:HB3	2.00	0.95
2:R:365:GLU:HG2	3:B:415:TYR:CG	2.05	0.92
2:R:349:ARG:O	2:R:353:PHE:HD2	1.36	0.92
2:R:353:PHE:CD2	3:B:447:PHE:CE2	2.58	0.91
1:A:76:LEU:HD22	1:A:108:MET:CE	1.86	0.91
2:R:364:MET:HE2	3:B:30:PHE:HE1	1.36	0.91
2:R:365:GLU:OE2	3:B:415:TYR:HE2	1.52	0.90
1:A:84:GLU:OE2	1:A:88:ARG:NH1	2.05	0.88
2:R:353:PHE:CD1	3:B:447:PHE:HE2	1.91	0.87
1:A:148:SER:O	2:R:340:GLN:NE2	2.05	0.87
2:R:357:GLY:O	2:R:361:HIS:CD2	2.26	0.87
2:R:365:GLU:OE2	3:B:415:TYR:CZ	2.27	0.87
2:R:353:PHE:CE2	3:B:447:PHE:HZ	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:353:PHE:CD2	3:B:447:PHE:CZ	2.64	0.86
2:R:369:GLN:O	2:R:373:GLU:HG3	1.79	0.83
2:R:360:LEU:HD11	3:B:438:GLN:HE21	1.41	0.82
2:R:365:GLU:HG3	3:B:415:TYR:CZ	2.15	0.82
1:A:150:GLY:HA2	2:R:336:ILE:CD1	2.11	0.81
1:A:147:LEU:CD2	1:A:443:MET:SD	2.68	0.81
2:R:351:PHE:CE1	3:B:176:ASP:CB	2.62	0.80
2:R:329:ILE:O	2:R:332:ILE:HG22	1.80	0.80
2:R:353:PHE:CD1	3:B:447:PHE:CE2	2.66	0.80
3:B:189:MET:HE1	3:B:305:LEU:N	1.98	0.79
1:A:47:PHE:HB2	1:A:85:MET:HE2	1.65	0.79
3:B:459:PRO:HG2	4:P:63:TRP:CD2	2.18	0.79
2:R:360:LEU:HD11	3:B:438:GLN:CG	2.14	0.78
1:A:159:ILE:HD11	1:A:408:ILE:HD11	1.65	0.78
2:R:365:GLU:HG2	3:B:415:TYR:CZ	2.12	0.78
3:B:189:MET:CE	3:B:305:LEU:CA	2.59	0.78
2:R:360:LEU:HD13	3:B:438:GLN:HG2	1.63	0.77
1:A:114:LYS:HG3	1:A:115:PRO:CD	2.14	0.77
2:R:371:ARG:O	2:R:375:THR:HG23	1.84	0.77
2:R:320:LYS:HB3	2:R:324:LEU:CD1	2.15	0.76
2:R:360:LEU:CD1	3:B:438:GLN:CG	2.62	0.76
2:R:349:ARG:HB3	2:R:353:PHE:HE2	1.50	0.76
1:A:100:GLU:HG2	1:A:132:ASN:HB3	1.68	0.75
2:R:349:ARG:O	2:R:353:PHE:CE2	2.38	0.75
2:R:373:GLU:O	2:R:377:LYS:HG3	1.86	0.75
3:B:303:ASN:HD21	3:B:307:LYS:NZ	1.85	0.75
1:A:122:ARG:HH11	1:A:122:ARG:CG	1.99	0.75
15:Q:282:ASN:OD1	15:Q:295:ASN:ND2	2.20	0.74
1:A:147:LEU:HD22	1:A:443:MET:SD	2.28	0.74
2:R:360:LEU:CD1	3:B:438:GLN:HE21	2.00	0.74
2:R:287:ARG:NH1	13:N:217:GLU:OE1	2.21	0.73
1:A:216:ARG:HG2	1:A:216:ARG:NH1	1.94	0.73
4:P:84:LEU:O	4:P:85:LYS:HB2	1.89	0.73
2:R:348:GLU:O	2:R:352:GLN:HG3	1.88	0.72
3:B:14:PRO:O	3:B:116[B]:HIS:HE1	1.72	0.72
1:A:76:LEU:HD21	1:A:108:MET:CE	2.04	0.71
2:R:340:GLN:O	2:R:344:TRP:HD1	1.72	0.71
1:A:183:LYS:O	1:A:183:LYS:HG2	1.91	0.71
6:D:96:GLN:NE2	18:4:15:UNK:O	2.22	0.70
8:F:813:LEU:HD11	14:O:183:ILE:HD12	1.73	0.70
11:L:268:ILE:HD11	14:O:232:LEU:HD22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:353:PHE:CG	3:B:447:PHE:CE2	2.80	0.70
1:A:344:ILE:HG23	1:A:344:ILE:O	1.92	0.69
11:I:136:TYR:O	11:I:167:ASN:ND2	2.26	0.69
13:N:345:SER:HA	13:N:348:ILE:HD11	1.75	0.69
14:O:35:PHE:O	14:O:73:LEU:N	2.26	0.69
2:R:360:LEU:HD11	3:B:438:GLN:CD	2.12	0.69
3:B:98:ASN:O	3:B:99:GLN:HG2	1.93	0.69
5:C:20:THR:HG22	14:O:275:ALA:H	1.58	0.69
2:R:320:LYS:O	2:R:324:LEU:CB	2.41	0.69
2:R:364:MET:HE2	3:B:30:PHE:CE1	2.24	0.69
1:A:14:SER:HA	1:A:71:VAL:HB	1.74	0.68
2:R:364:MET:CE	3:B:30:PHE:CE1	2.72	0.68
2:R:364:MET:HE1	3:B:30:PHE:HE1	1.57	0.68
1:A:47:PHE:CD1	1:A:85:MET:HE1	2.28	0.68
11:I:135:GLU:OE2	15:Q:19:ARG:NH2	2.27	0.68
13:N:220:HIS:NE2	14:O:296:GLU:O	2.27	0.68
2:R:365:GLU:CG	3:B:415:TYR:CD2	2.58	0.68
11:L:178:LEU:HD21	15:Q:325:ILE:HD11	1.76	0.68
1:A:76:LEU:HD23	1:A:108:MET:CE	2.23	0.68
2:R:365:GLU:HG3	3:B:415:TYR:CE1	2.28	0.68
1:A:392:VAL:HB	1:A:423:THR:HG22	1.75	0.67
3:B:107:SER:O	4:P:11:ASN:HA	1.95	0.67
3:B:275:LYS:HB3	3:B:278:ASP:OD2	1.94	0.67
7:E:376:ASN:ND2	7:E:381:ASP:O	2.27	0.67
12:M:218:CYS:SG	21:7:60:UNK:N	2.68	0.67
1:A:311:GLU:OE2	1:A:407:ARG:NH2	2.28	0.67
3:B:303:ASN:ND2	3:B:307:LYS:NZ	2.43	0.67
2:R:231:SER:HB3	2:R:234:MET:HG2	1.75	0.67
2:R:226:THR:HG22	14:O:126:PHE:HB2	1.78	0.66
2:R:320:LYS:C	2:R:324:LEU:HG	2.14	0.66
2:R:353:PHE:CD2	3:B:447:PHE:HE2	2.08	0.66
10:H:527:THR:C	10:H:529:ASN:H	1.97	0.66
12:M:456:ARG:NH2	14:O:262:THR:O	2.28	0.66
3:B:303:ASN:HD21	3:B:307:LYS:HZ1	1.44	0.66
2:R:365:GLU:OE2	3:B:415:TYR:OH	2.14	0.66
13:N:55:THR:O	13:N:64:ASN:ND2	2.28	0.66
8:F:813:LEU:HD22	11:L:276:ARG:HH21	1.62	0.65
1:A:343:SER:CB	1:A:344:ILE:CA	2.66	0.65
2:R:365:GLU:CG	3:B:415:TYR:CE1	2.79	0.65
1:A:458:GLU:HG2	1:A:459:ASP:N	2.10	0.65
15:Q:18:ASN:ND2	15:Q:177:ASN:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:501:GLN:HG2	12:M:244:MET:HB3	1.79	0.65
1:A:180:VAL:HG11	1:A:332:LEU:HG	1.78	0.65
1:A:446:LEU:HD23	2:R:339:ARG:HH12	1.62	0.65
11:J:426:GLN:NE2	12:M:26:LYS:O	2.30	0.65
14:O:33:GLU:HG3	14:O:106:LEU:HD11	1.79	0.65
13:N:75:THR:HG1	15:Q:12:TYR:HH	1.42	0.64
2:R:351:PHE:HE1	3:B:176:ASP:HB3	1.57	0.64
2:R:116:ASN:ND2	11:L:363:TYR:OH	2.29	0.64
15:Q:184:TYR:OH	15:Q:242:ASP:OD1	2.15	0.64
14:O:41:GLU:OE2	14:O:50:SER:OG	2.16	0.64
1:A:150:GLY:CA	2:R:336:ILE:CD1	2.72	0.63
1:A:442:THR:HB	2:R:339:ARG:NE	2.05	0.63
1:A:446:LEU:HD11	2:R:332:ILE:HD11	1.80	0.63
1:A:108:MET:HE2	1:A:119:ILE:HG21	1.80	0.63
1:A:148:SER:HB2	1:A:442:THR:HG21	1.79	0.63
7:E:392:ASP:HB3	11:I:226:VAL:HB	1.80	0.63
1:A:121:GLU:O	1:A:125:GLU:HG3	1.98	0.63
2:R:221:CYS:HB3	8:F:875:THR:HG22	1.81	0.63
2:R:375:THR:O	2:R:379:ARG:HG3	1.98	0.63
2:R:365:GLU:CD	3:B:415:TYR:CZ	2.69	0.63
3:B:303:ASN:ND2	3:B:307:LYS:HZ2	1.96	0.62
1:A:446:LEU:CD2	2:R:332:ILE:HG13	2.29	0.62
1:A:153:SER:HA	1:A:169:ILE:O	1.99	0.62
1:A:149:MET:HA	2:R:340:GLN:HE22	1.64	0.62
3:B:47:GLN:O	3:B:48:ASP:HB3	2.00	0.62
2:R:48:LYS:NZ	14:O:401:TYR:OH	2.21	0.61
1:A:203:GLU:O	1:A:204:GLU:HB2	2.00	0.61
10:H:527:THR:O	10:H:529:ASN:N	2.33	0.61
10:H:449:LYS:O	10:H:516:THR:OG1	2.16	0.61
11:I:260:CYS:HB2	11:I:283:CYS:SG	2.40	0.61
1:A:256:ILE:O	1:A:260:GLN:HB2	2.00	0.61
1:A:108:MET:CE	1:A:119:ILE:HG21	2.31	0.61
3:B:14:PRO:O	3:B:116[B]:HIS:CE1	2.53	0.61
1:A:382:GLU:CD	1:A:382:GLU:H	2.03	0.61
11:I:282:LEU:HD21	11:I:292:PHE:HB3	1.83	0.61
11:I:312:LYS:H	11:I:312:LYS:HD3	1.66	0.60
12:M:463:ASN:HA	12:M:468:ARG:HH21	1.66	0.60
1:A:442:THR:O	2:R:339:ARG:CZ	2.49	0.60
2:R:351:PHE:HE1	3:B:176:ASP:CB	2.10	0.60
7:E:405:ILE:HD11	11:L:162:LYS:HD3	1.82	0.60
6:D:64:HIS:HD2	6:D:66:TYR:H	1.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:2:SER:N	15:Q:6:GLN:OE1	2.35	0.60
2:R:364:MET:HE1	3:B:30:PHE:CE1	2.35	0.60
3:B:53:TYR:CD1	3:B:81:GLN:HG3	2.37	0.60
1:A:389:LEU:HB3	1:A:421:LEU:HD23	1.84	0.60
2:R:353:PHE:CE1	3:B:447:PHE:CD2	2.90	0.60
3:B:44:THR:OG1	3:B:62:ALA:HB2	2.02	0.60
2:R:329:ILE:O	2:R:332:ILE:CG2	2.49	0.60
11:I:239:GLN:OE1	11:I:346:ARG:NH1	2.35	0.60
1:A:47:PHE:CB	1:A:85:MET:HE2	2.32	0.59
11:L:288:GLN:HB2	11:L:291:HIS:CE1	2.37	0.59
13:N:296:LEU:HD21	13:N:309:LEU:HG	1.83	0.59
1:A:399:SER:HA	1:A:404:MET:HG2	1.85	0.59
3:B:199:LYS:HD2	3:B:210:ILE:HD13	1.85	0.59
7:E:408:GLU:N	7:E:408:GLU:OE1	2.35	0.59
11:L:95:HIS:O	11:L:95:HIS:ND1	2.34	0.59
11:L:237:SER:OG	11:L:249:ARG:NH1	2.35	0.59
1:A:380:SER:O	1:A:383:GLN:HB2	2.03	0.59
3:B:35:LEU:HD11	4:P:84:LEU:HD13	1.84	0.59
1:A:334:ALA:HB2	1:A:415:ARG:HD3	1.85	0.58
12:M:378:GLN:OE1	12:M:380:GLN:NE2	2.36	0.58
1:A:418:GLN:HG3	1:A:418:GLN:O	2.03	0.58
1:A:159:ILE:HG23	1:A:164:CYS:SG	2.44	0.58
14:O:167:ASP:OD2	14:O:182:LYS:NZ	2.36	0.58
1:A:400:LEU:HD12	1:A:433:LYS:HE2	1.84	0.58
2:R:353:PHE:CG	3:B:447:PHE:HE2	2.19	0.58
14:O:170:THR:HG22	14:O:172:LEU:H	1.68	0.58
15:Q:351:ASP:OD1	15:Q:351:ASP:N	2.35	0.58
15:Q:368:ASP:OD1	15:Q:368:ASP:N	2.35	0.58
7:E:380:SER:HB2	12:M:464:ASN:HA	1.86	0.58
3:B:141:ILE:HG12	3:B:448:TYR:HB3	1.85	0.58
2:R:130:ASP:OD1	14:O:430:ARG:NH2	2.31	0.58
4:P:29:TRP:CD2	4:P:61:LYS:HD3	2.38	0.58
11:J:434:LYS:NZ	11:J:438:GLU:OE2	2.37	0.58
13:N:574:TYR:O	13:N:578:THR:OG1	2.21	0.57
1:A:241:LYS:NZ	1:A:245:GLU:HB3	2.19	0.57
2:R:340:GLN:O	2:R:344:TRP:CD1	2.54	0.57
1:A:44:GLU:O	1:A:44:GLU:HG2	2.05	0.57
8:F:852:ASP:OD1	8:F:853:VAL:N	2.36	0.57
11:I:57:ASN:N	11:I:59:GLU:OE1	2.38	0.57
11:I:271:ARG:HD2	11:I:281:ASN:HD22	1.68	0.57
2:R:287:ARG:NH2	13:N:156:GLN:OE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ARG:NE	1:A:216:ARG:HA	2.20	0.57
2:R:365:GLU:HG2	3:B:415:TYR:CD1	2.40	0.57
5:C:33:ARG:NH2	12:M:441:GLU:OE2	2.36	0.57
14:O:266:THR:HG23	14:O:267:ARG:HG3	1.87	0.56
1:A:381:PRO:HG2	1:A:382:GLU:OE2	2.04	0.56
1:A:72:ASP:OD1	1:A:74:GLN:HB2	2.05	0.56
1:A:426:ASN:O	1:A:432:ARG:NE	2.35	0.56
1:A:446:LEU:HD22	2:R:332:ILE:HG13	1.88	0.56
8:F:814:PRO:O	11:L:276:ARG:NH2	2.39	0.56
1:A:26:LEU:HB3	1:A:27:PRO:HD2	1.88	0.55
1:A:196:ARG:NH2	1:A:312:TYR:OH	2.39	0.55
15:Q:202:ILE:HG12	15:Q:226:ASN:HB2	1.87	0.55
11:L:268:ILE:HD12	14:O:233:PRO:HD2	1.88	0.55
1:A:194:HIS:NE2	1:A:203:GLU:OE1	2.39	0.55
1:A:426:ASN:HB3	1:A:432:ARG:HG2	1.88	0.55
10:H:513:SER:O	10:H:588:THR:HA	2.07	0.55
14:O:35:PHE:HB2	14:O:36:PRO:HD2	1.89	0.55
1:A:122:ARG:HG2	1:A:122:ARG:NH1	2.06	0.55
2:R:239:ILE:HG12	11:I:302:ILE:HD11	1.89	0.55
7:E:372:ARG:HB2	11:I:188:GLN:HB2	1.89	0.55
11:I:226:VAL:HG13	11:I:228:LEU:HG	1.88	0.55
11:L:179:ILE:HD11	15:Q:321:THR:HA	1.89	0.55
12:M:227:VAL:HG12	13:N:361:ILE:HD12	1.88	0.55
14:O:167:ASP:HB3	14:O:173:ASP:HB3	1.89	0.54
14:O:198:ARG:NH2	14:O:199:THR:O	2.41	0.54
4:P:69:ASP:O	4:P:70:GLU:HG3	2.06	0.54
12:M:351:LEU:HD11	12:M:368:LEU:HD11	1.90	0.54
15:Q:147:ILE:HD11	15:Q:167:ARG:HB3	1.90	0.54
2:R:105:ASP:OD1	2:R:106:LYS:N	2.40	0.54
10:H:489:ASN:O	10:H:490:GLU:HG2	2.06	0.54
12:M:225:ARG:HB3	21:7:66:UNK:HA	1.90	0.54
3:B:43:ARG:HG3	3:B:53:TYR:CE2	2.42	0.54
3:B:275:LYS:HE3	3:B:277:SER:H	1.73	0.54
2:R:295:VAL:HG12	13:N:170:GLN:HG3	1.90	0.54
11:L:191:LEU:HG	11:L:200:PHE:HB2	1.90	0.54
11:K:433:VAL:HG21	12:M:32:ASP:HB3	1.90	0.54
11:L:235:TYR:O	14:O:446:ARG:NH1	2.41	0.54
12:M:267:VAL:HG22	12:M:314:LYS:HE3	1.89	0.54
8:F:813:LEU:HD23	8:F:814:PRO:HD2	1.89	0.53
2:R:192:GLU:OE2	12:M:456:ARG:NH1	2.42	0.53
2:R:349:ARG:HB3	2:R:353:PHE:CE2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:57:GLN:NE2	11:L:251:SER:OG	2.41	0.53
3:B:189:MET:HG2	3:B:305:LEU:HD13	1.90	0.53
10:H:448:TYR:HA	10:H:493:GLN:HE21	1.73	0.53
1:A:25:GLU:OE1	2:R:346:ARG:NH1	2.42	0.53
7:E:431:CYS:HA	7:E:434:TYR:HD2	1.72	0.53
10:H:453:GLN:HA	10:H:486:PHE:O	2.09	0.53
12:M:451:ASN:OD1	12:M:451:ASN:N	2.42	0.53
14:O:491:ARG:HG2	17:2:358:UNK:HA	1.91	0.53
1:A:438:LEU:O	1:A:442:THR:HG23	2.08	0.53
13:N:285:ASP:OD1	13:N:285:ASP:N	2.36	0.53
11:L:80:VAL:HG21	11:L:130:ARG:HG2	1.91	0.53
1:A:261:GLN:HB2	1:A:262:GLU:OE1	2.09	0.53
2:R:253:LYS:HE3	2:R:257:ILE:HD11	1.89	0.53
6:D:66:TYR:OH	11:I:331:GLU:OE2	2.20	0.53
2:R:126:GLU:OE2	11:L:233:ASN:ND2	2.42	0.53
7:E:380:SER:OG	12:M:463:ASN:ND2	2.43	0.53
1:A:47:PHE:CD1	1:A:85:MET:CE	2.92	0.52
2:R:62:TYR:HB2	2:R:79:ILE:HG21	1.91	0.52
7:E:327:CYS:SG	11:L:145:ASN:ND2	2.82	0.52
11:I:363:TYR:HA	11:I:366:GLU:HG2	1.91	0.52
11:L:193:THR:OG1	11:L:196:GLY:O	2.26	0.52
2:R:361:HIS:CE1	3:B:151:TYR:O	2.62	0.52
15:Q:275:SER:O	15:Q:301:ASN:ND2	2.41	0.52
15:Q:345:ASP:OD1	15:Q:345:ASP:N	2.43	0.52
3:B:43:ARG:HD3	3:B:51:TYR:CD1	2.44	0.52
1:A:6:LYS:HE3	3:B:121:GLN:OE1	2.09	0.52
1:A:80:TRP:NE1	1:A:122:ARG:HD3	2.24	0.52
1:A:147:LEU:HD23	1:A:443:MET:SD	2.47	0.52
9:G:159:VAL:HG11	16:S:208:VAL:HG21	1.91	0.52
1:A:381:PRO:C	1:A:383:GLN:H	2.11	0.52
11:I:91:ILE:HD12	11:L:185:GLY:HA2	1.91	0.52
1:A:399:SER:OG	1:A:432:ARG:NH1	2.42	0.52
11:J:458:LYS:NZ	11:K:453:GLN:OE1	2.42	0.52
1:A:133:VAL:HG13	1:A:134:PRO:HD2	1.91	0.52
1:A:197:LEU:HD11	1:A:231:PHE:CZ	2.45	0.52
11:I:70:LEU:O	11:I:75:LYS:NZ	2.39	0.52
12:M:466:ASN:OD1	12:M:466:ASN:N	2.42	0.52
1:A:152:SER:OG	2:R:333:ILE:HD11	2.10	0.51
8:F:798:ILE:HD11	14:O:192:SER:HB2	1.91	0.51
9:G:175:ASP:OD1	9:G:175:ASP:N	2.43	0.51
11:J:467:LYS:NZ	12:M:62:THR:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:189:MET:CE	3:B:305:LEU:N	2.72	0.51
15:Q:342:ASP:N	15:Q:342:ASP:OD1	2.42	0.51
3:B:34:GLU:CD	3:B:34:GLU:H	2.13	0.51
11:I:249:ARG:NH2	11:I:253:GLN:HE21	2.09	0.51
11:J:430:GLN:NE2	11:K:425:SER:OG	2.41	0.51
11:L:348:GLU:HB3	14:O:457:LYS:HE3	1.92	0.51
13:N:227:GLU:O	13:N:230:SER:OG	2.15	0.51
10:H:497:ALA:HB3	14:O:229:ASN:HA	1.92	0.51
1:A:201:ILE:O	1:A:202:LYS:HB2	2.11	0.51
1:A:418:GLN:HG2	1:A:419:TYR:CE1	2.46	0.51
3:B:32:VAL:HG23	3:B:33:PRO:HD2	1.92	0.51
7:E:402:LEU:HD12	7:E:405:ILE:HD13	1.92	0.51
13:N:255:ASP:OD1	13:N:256:ARG:N	2.44	0.51
3:B:335:ILE:HG22	3:B:340:THR:HG21	1.93	0.51
2:R:111:ASP:OD1	2:R:111:ASP:N	2.38	0.50
2:R:365:GLU:HG2	3:B:415:TYR:CE1	2.44	0.50
4:P:85:LYS:O	4:P:90:ARG:NH1	2.44	0.50
11:L:147:ALA:HB1	15:Q:355:ASN:HD22	1.76	0.50
12:M:454:ALA:HB1	12:M:460:ILE:HG21	1.93	0.50
15:Q:30:PHE:HA	15:Q:216:THR:O	2.11	0.50
15:Q:358:ALA:H	15:Q:371:GLU:HB2	1.75	0.50
2:R:351:PHE:CZ	3:B:176:ASP:CB	2.83	0.50
3:B:171:ILE:HD13	3:B:312:ARG:CG	2.42	0.50
2:R:226:THR:HG21	14:O:122:LYS:HG3	1.93	0.50
10:H:511:LEU:HD23	10:H:525:LEU:HD11	1.94	0.50
12:M:60:THR:O	12:M:61:ASN:ND2	2.44	0.50
3:B:47:GLN:O	3:B:48:ASP:CB	2.59	0.50
15:Q:268:ILE:HD13	15:Q:341:LYS:HG2	1.93	0.50
3:B:102:PHE:HZ	4:P:6:LEU:CD2	2.25	0.50
13:N:250:LEU:HB2	13:N:262:ILE:HG21	1.92	0.50
1:A:460:TYR:CZ	1:A:464:LYS:HE3	2.47	0.50
7:E:417:ASP:N	7:E:417:ASP:OD1	2.42	0.50
1:A:22:SER:HA	1:A:441:LEU:CD1	2.42	0.49
14:O:270:HIS:HD2	14:O:272:ASN:HB2	1.77	0.49
15:Q:200:GLU:HG3	15:Q:201:ALA:H	1.76	0.49
3:B:153:MET:HG3	3:B:334:ILE:HD13	1.94	0.49
6:D:62:ALA:HB3	6:D:71:VAL:HG23	1.94	0.49
8:F:869:ARG:H	11:L:318:GLN:NE2	2.09	0.49
11:L:282:LEU:HD22	11:L:291:HIS:CD2	2.48	0.49
2:R:352:GLN:O	2:R:356:LEU:HG	2.13	0.49
7:E:345:ASP:O	15:Q:149:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:LEU:O	1:A:421:LEU:HA	2.13	0.49
1:A:407:ARG:O	1:A:411:GLU:HB2	2.12	0.49
7:E:331:ASN:HD21	11:L:137:LEU:HA	1.78	0.49
11:I:192:ASP:OD1	11:I:193:THR:N	2.45	0.49
15:Q:153:PRO:HB3	15:Q:168:TYR:CE2	2.47	0.49
11:K:440:LEU:HD13	12:M:39:MET:HE2	1.95	0.49
12:M:308:PRO:HB3	12:M:329:HIS:CD2	2.48	0.48
1:A:15:HIS:ND1	1:A:16[B]:ARG:HG2	2.28	0.48
1:A:241:LYS:O	1:A:242:ASP:C	2.52	0.48
9:G:163:ALA:HB1	16:S:194:ALA:HB1	1.94	0.48
13:N:341:PRO:HD3	13:N:553:ILE:HD11	1.95	0.48
1:A:141:GLU:HB3	1:A:142:PRO:HD3	1.94	0.48
11:L:236:ASP:OD2	11:L:239:GLN:NE2	2.45	0.48
1:A:170:ILE:O	1:A:173:ILE:HG22	2.13	0.48
1:A:183:LYS:O	1:A:183:LYS:CG	2.61	0.48
11:L:284:SER:HB2	14:O:181:ILE:HD11	1.95	0.48
13:N:126:LEU:O	13:N:129:THR:OG1	2.25	0.48
2:R:350:CYS:SG	3:B:467:PHE:C	2.92	0.48
3:B:189:MET:HE1	3:B:304:ASN:C	2.33	0.48
3:B:286:ASP:HB3	3:B:290:ASN:H	1.79	0.48
2:R:133:ASP:HA	14:O:427:LYS:HZ1	1.79	0.48
11:L:140:THR:HG22	11:L:143:ARG:HH22	1.79	0.48
13:N:191:ILE:HD12	13:N:218:LEU:HD21	1.96	0.48
2:R:215:THR:HG21	2:R:237:PHE:H	1.79	0.48
3:B:364:GLU:HG2	3:B:365:GLU:N	2.29	0.48
1:A:438:LEU:HD23	1:A:438:LEU:HA	1.67	0.47
15:Q:202:ILE:HB	15:Q:225:TYR:HB3	1.96	0.47
15:Q:294:ASP:OD1	15:Q:295:ASN:N	2.46	0.47
2:R:351:PHE:HE1	3:B:176:ASP:CG	2.18	0.47
2:R:372:ILE:O	2:R:375:THR:OG1	2.30	0.47
9:G:175:ASP:O	9:G:178:ILE:HG22	2.14	0.47
11:I:311:VAL:HB	11:I:314:ASN:HD22	1.79	0.47
15:Q:208:LEU:O	15:Q:218:LYS:HA	2.13	0.47
13:N:68:PHE:CZ	15:Q:13:ILE:HD11	2.49	0.47
15:Q:356:ASP:O	15:Q:374:SER:N	2.37	0.47
1:A:337:VAL:O	1:A:340:ALA:HB3	2.15	0.47
1:A:458:GLU:O	1:A:461:GLU:N	2.47	0.47
2:R:338:GLU:O	2:R:342:GLU:HG3	2.13	0.47
3:B:286:ASP:HB2	3:B:290:ASN:HB2	1.95	0.47
11:I:358:PRO:HB2	11:L:224:PHE:HB2	1.94	0.47
1:A:47:PHE:HB2	1:A:85:MET:CE	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:353:PHE:CD2	3:B:447:PHE:HZ	2.20	0.47
3:B:148:ALA:O	3:B:431:GLY:HA3	2.14	0.47
3:B:370:GLU:HG3	3:B:395:VAL:HG21	1.97	0.47
4:P:83:ASP:C	4:P:84:LEU:O	2.52	0.47
11:J:419:GLU:O	11:J:422:ILE:HG12	2.13	0.47
1:A:259:LYS:HD2	1:A:259:LYS:O	2.14	0.47
1:A:325:PRO:O	1:A:331:PRO:HG2	2.15	0.47
2:R:217:SER:OG	2:R:220:ASP:OD1	2.32	0.47
3:B:30:PHE:HB3	3:B:433:GLN:OE1	2.14	0.47
4:P:9:LYS:HD2	4:P:12:LYS:HE2	1.97	0.47
10:H:444:GLU:HG2	10:H:445:TYR:H	1.80	0.47
12:M:237:ASN:ND2	12:M:321:LYS:O	2.47	0.47
3:B:403:CYS:HB2	3:B:404:PRO:HA	1.97	0.47
10:H:524:THR:HG23	10:H:605:ARG:HB3	1.97	0.47
3:B:26:ASN:O	3:B:27:GLU:HB2	2.15	0.47
11:I:249:ARG:HH21	11:I:253:GLN:HE21	1.61	0.47
2:R:212:ASN:OD1	2:R:212:ASN:N	2.48	0.47
3:B:120:SER:HB2	3:B:123:ASP:H	1.79	0.47
11:K:472:ARG:NH2	11:K:503:ASP:OD2	2.37	0.47
13:N:279:SER:OG	13:N:280:ALA:N	2.48	0.47
14:O:198:ARG:HD3	14:O:203:ASP:OD1	2.14	0.47
7:E:372:ARG:HH12	11:I:227:ASN:HD21	1.62	0.46
15:Q:331:SER:O	15:Q:334:GLU:HB2	2.15	0.46
2:R:369:GLN:O	2:R:373:GLU:CG	2.59	0.46
12:M:23:PRO:HB2	12:M:26:LYS:HG2	1.97	0.46
1:A:447:PRO:HG3	2:R:335:PHE:CG	2.49	0.46
8:F:818:TRP:HA	11:L:287:PHE:CD1	2.51	0.46
13:N:115:ILE:HA	13:N:120:LEU:HD12	1.96	0.46
1:A:188:PHE:HZ	1:A:319:ILE:HD13	1.80	0.46
1:A:216:ARG:NH1	1:A:216:ARG:CG	2.69	0.46
3:B:189:MET:HG2	3:B:305:LEU:CD1	2.45	0.46
10:H:525:LEU:O	10:H:532:PRO:HD2	2.16	0.46
12:M:452:GLU:HA	12:M:455:ALA:HB3	1.98	0.46
10:H:490:GLU:HG3	11:L:264:GLY:O	2.15	0.46
12:M:309:GLU:N	12:M:312:GLU:OE1	2.47	0.46
7:E:331:ASN:ND2	11:L:137:LEU:HA	2.31	0.46
11:J:472:ARG:HH22	11:K:467:LYS:HB2	1.81	0.46
1:A:236:LEU:HD22	1:A:309:PHE:CD2	2.51	0.46
7:E:372:ARG:HH22	11:I:227:ASN:HD21	1.64	0.46
1:A:150:GLY:N	2:R:336:ILE:HD13	2.30	0.46
1:A:419:TYR:N	1:A:419:TYR:CD1	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:208:ARG:NH1	6:D:85:HIS:O	2.49	0.46
3:B:212:SER:HB3	3:B:284:PHE:HE2	1.81	0.46
4:P:56:TYR:HB3	4:P:58:PHE:CE2	2.51	0.46
6:D:64:HIS:CD2	6:D:66:TYR:H	2.30	0.46
7:E:388:THR:HG23	11:I:230:ILE:HB	1.98	0.46
1:A:6:LYS:HD2	1:A:23:ASN:ND2	2.30	0.46
15:Q:162:PRO:O	15:Q:165:ILE:HB	2.16	0.46
1:A:282:ASN:O	1:A:285:VAL:HG22	2.16	0.45
3:B:102:PHE:HZ	4:P:6:LEU:HD23	1.82	0.45
3:B:424:TYR:CD1	3:B:427:ILE:HD12	2.51	0.45
6:D:98:GLU:OE2	13:N:41:ARG:NH2	2.29	0.45
7:E:414:VAL:HG22	7:E:418:VAL:HB	1.98	0.45
12:M:372:VAL:HG12	12:M:375:ILE:HB	1.98	0.45
10:H:608:ASP:O	10:H:609:LYS:HG2	2.16	0.45
13:N:561:LEU:HD21	13:N:571:LEU:HD12	1.98	0.45
1:A:164:CYS:HB2	1:A:182:SER:HB3	1.98	0.45
1:A:232:LYS:HA	1:A:236:LEU:HG	1.99	0.45
1:A:320:SER:OG	1:A:322:LYS:N	2.38	0.45
9:G:192:LEU:HD11	16:S:209:LEU:HD22	1.97	0.45
11:J:482:LEU:HD11	11:K:507:GLN:HA	1.99	0.45
4:P:23:GLU:OE2	4:P:65:ARG:HD3	2.16	0.45
11:K:493:LYS:HE2	11:K:510:GLU:HG2	1.97	0.45
11:L:150:VAL:HG11	15:Q:310:PHE:CE1	2.51	0.45
15:Q:307:PRO:HB3	15:Q:332:LEU:HD23	1.97	0.45
3:B:143:LEU:HD12	3:B:144:PRO:HD2	1.98	0.45
11:L:298:SER:HB3	14:O:390:LEU:HG	1.98	0.45
3:B:3:PRO:HA	3:B:4:PHE:HA	1.67	0.45
4:P:33:SER:HB3	4:P:55:LYS:CD	2.46	0.45
9:G:157:ASN:ND2	16:S:203:PHE:O	2.46	0.45
11:L:147:ALA:HB3	15:Q:371:GLU:H	1.80	0.45
3:B:121:GLN:HG2	3:B:463:TRP:CH2	2.52	0.45
11:L:258:TYR:OH	14:O:173:ASP:OD1	2.33	0.45
1:A:412:LEU:HD12	1:A:412:LEU:HA	1.76	0.45
6:D:64:HIS:CD2	6:D:66:TYR:HB2	2.52	0.45
11:K:433:VAL:O	11:K:437:MET:HG2	2.17	0.45
13:N:77:ARG:NH1	16:S:198:LEU:H	2.15	0.45
1:A:344:ILE:O	1:A:344:ILE:CG2	2.64	0.44
3:B:197:SER:HB3	3:B:301:GLY:HA2	1.99	0.44
3:B:286:ASP:CB	3:B:290:ASN:H	2.29	0.44
6:D:64:HIS:HD2	6:D:66:TYR:HB2	1.81	0.44
10:H:487:ASN:ND2	10:H:490:GLU:OE2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:372:VAL:HG13	12:M:375:ILE:HD12	1.99	0.44
2:R:356:LEU:O	2:R:359:SER:OG	2.22	0.44
4:P:66:ASN:HB3	4:P:70:GLU:HB2	1.98	0.44
11:K:500:GLU:OE1	12:M:246:THR:OG1	2.33	0.44
12:M:447:ASP:HB3	14:O:270:HIS:CD2	2.52	0.44
15:Q:20:LEU:HA	15:Q:27:ILE:HD12	1.99	0.44
3:B:30:PHE:CD1	3:B:30:PHE:N	2.84	0.44
11:I:180:GLY:HA3	11:L:198:LYS:HE3	2.00	0.44
1:A:25:GLU:OE1	2:R:346:ARG:HD2	2.18	0.44
2:R:177:LYS:HG2	12:M:444:LEU:HD13	1.98	0.44
4:P:33:SER:HB3	4:P:55:LYS:HD3	1.98	0.44
6:D:123:ASP:OD2	10:H:474:ARG:NH2	2.50	0.44
2:R:157:LYS:HD3	5:C:44:GLU:HB2	1.98	0.44
2:R:248:LEU:O	14:O:257:PRO:HG2	2.18	0.44
2:R:351:PHE:CE1	3:B:176:ASP:CG	2.91	0.44
11:I:171:ASP:O	11:I:174:THR:HG22	2.17	0.44
11:I:281:ASN:OD1	11:I:281:ASN:N	2.50	0.44
3:B:180:LEU:HA	3:B:180:LEU:HD23	1.69	0.44
7:E:392:ASP:OD2	7:E:395:LEU:HD13	2.16	0.44
9:G:167:MET:HE1	9:G:177:ILE:HA	2.00	0.44
11:I:239:GLN:H	11:I:239:GLN:HG3	1.60	0.44
2:R:367:ASP:O	2:R:371:ARG:HG3	2.17	0.44
3:B:354:LEU:HD22	3:B:358:LEU:HD22	1.98	0.44
4:P:1:MET:HG2	4:P:2:ASP:N	2.33	0.44
1:A:145:ILE:O	1:A:149:MET:HG2	2.17	0.44
2:R:351:PHE:O	2:R:355:ARG:HG3	2.17	0.44
3:B:146:SER:HB2	3:B:174:ILE:HD11	1.99	0.44
11:I:246:ASP:OD1	11:I:247:GLU:N	2.49	0.44
14:O:202:MET:HG3	14:O:204:LEU:HD11	2.00	0.44
1:A:282:ASN:HA	1:A:283:PRO:HD2	1.90	0.44
1:A:149:MET:HA	2:R:340:GLN:NE2	2.33	0.43
1:A:458:GLU:O	1:A:459:ASP:C	2.57	0.43
13:N:234:ALA:HB3	13:N:235:PRO:HD3	1.99	0.43
1:A:320:SER:OG	1:A:321:ASP:N	2.49	0.43
1:A:334:ALA:CB	1:A:415:ARG:HD3	2.46	0.43
12:M:227:VAL:HG13	12:M:346:LEU:HD12	1.99	0.43
13:N:539:ASN:OD1	13:N:577:ASN:ND2	2.51	0.43
2:R:357:GLY:C	2:R:361:HIS:CD2	2.90	0.43
3:B:189:MET:HG3	3:B:193:SER:OG	2.19	0.43
1:A:76:LEU:HD23	1:A:108:MET:HE1	1.82	0.43
2:R:383:LEU:HB3	2:R:384:LYS:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:371:TRP:CD2	11:L:202:PRO:HG3	2.53	0.43
14:O:51:TYR:CE2	14:O:55:ILE:HD11	2.53	0.43
1:A:381:PRO:HG2	1:A:382:GLU:CD	2.39	0.43
1:A:381:PRO:C	1:A:383:GLN:N	2.72	0.43
1:A:446:LEU:CD1	2:R:332:ILE:CD1	2.97	0.43
2:R:112:GLU:OE2	14:O:466:SER:OG	2.29	0.43
12:M:10:VAL:HG22	12:M:11:THR:H	1.84	0.43
9:G:178:ILE:HD12	16:S:226:LEU:HD23	2.01	0.43
10:H:527:THR:C	10:H:529:ASN:N	2.68	0.43
14:O:173:ASP:OD1	14:O:173:ASP:N	2.48	0.43
1:A:431:ASP:O	1:A:435:GLN:HB2	2.19	0.43
9:G:158:TRP:CD1	13:N:74:GLU:HG3	2.54	0.43
12:M:335:VAL:O	12:M:338:THR:OG1	2.31	0.43
11:I:140:THR:HG23	11:I:143:ARG:HH21	1.83	0.43
13:N:59:HIS:O	13:N:59:HIS:ND1	2.49	0.43
13:N:75:THR:OG1	15:Q:12:TYR:OH	2.20	0.43
15:Q:20:LEU:HD23	15:Q:27:ILE:HG21	2.01	0.43
1:A:129:ASP:OD2	1:A:460:TYR:HE2	2.01	0.43
1:A:180:VAL:CG1	1:A:332:LEU:HG	2.48	0.43
12:M:378:GLN:HG2	12:M:380:GLN:HG3	2.00	0.43
13:N:132:LEU:N	13:N:133:PRO:HD2	2.33	0.43
15:Q:219:ASP:OD2	15:Q:239:TYR:OH	2.30	0.43
3:B:286:ASP:HB2	3:B:290:ASN:O	2.18	0.43
12:M:261:LEU:HD23	12:M:261:LEU:HA	1.88	0.43
13:N:542:ASP:OD1	13:N:542:ASP:N	2.50	0.43
1:A:80:TRP:CE2	1:A:122:ARG:HD3	2.53	0.42
1:A:147:LEU:HG	2:R:336:ILE:HG21	2.00	0.42
1:A:151:LYS:HE3	1:A:424:PHE:CE1	2.53	0.42
3:B:156:LEU:HD23	3:B:156:LEU:HA	1.76	0.42
8:F:808:ASP:OD1	8:F:809:PRO:HD2	2.19	0.42
14:O:55:ILE:O	14:O:59:SER:N	2.48	0.42
14:O:433:ARG:NH1	14:O:441:PRO:HB3	2.34	0.42
1:A:198:ALA:N	1:A:199:PRO:HD2	2.34	0.42
2:R:344:TRP:O	2:R:348:GLU:HG3	2.18	0.42
3:B:66:LYS:HA	3:B:67:PRO:HD3	1.78	0.42
7:E:394:ASP:HB2	7:E:428:PHE:HE1	1.84	0.42
13:N:166:ARG:HG3	13:N:167:ASN:N	2.34	0.42
13:N:223:LEU:HD23	13:N:223:LEU:HA	1.82	0.42
1:A:314:PHE:CZ	1:A:407:ARG:HG3	2.54	0.42
11:I:195:GLN:C	11:I:197:LEU:H	2.23	0.42
11:J:482:LEU:HD23	11:J:482:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:445:ASP:HA	3:B:448:TYR:CE1	2.55	0.42
4:P:83:ASP:O	4:P:86:GLU:HG3	2.18	0.42
12:M:371:ASP:OD1	12:M:371:ASP:N	2.53	0.42
1:A:122:ARG:CG	1:A:122:ARG:NH1	2.66	0.42
11:I:158:ALA:HB2	15:Q:186:LEU:HD12	2.01	0.42
11:J:479:ILE:HD11	11:K:475:LEU:HD21	2.01	0.42
13:N:85:MET:SD	13:N:103:LYS:HB3	2.59	0.42
15:Q:146:ASP:OD1	15:Q:147:ILE:N	2.52	0.42
11:L:121:THR:O	11:L:125:ILE:HG13	2.20	0.42
12:M:30:LEU:HA	12:M:30:LEU:HD23	1.86	0.42
13:N:148:ASP:OD1	13:N:149:SER:N	2.50	0.42
14:O:13:PHE:CE1	14:O:134:GLU:HB3	2.55	0.42
14:O:44:PRO:HA	14:O:47:ILE:HG13	2.00	0.42
3:B:275:LYS:HA	3:B:275:LYS:HD2	1.91	0.42
10:H:523:GLU:HG2	10:H:606:CYS:SG	2.59	0.42
11:I:135:GLU:HG2	11:I:136:TYR:H	1.84	0.42
11:L:90:ASP:HB3	11:L:93:LYS:HB2	2.02	0.42
11:L:119:LYS:HG3	11:L:122:ARG:NH2	2.34	0.42
15:Q:356:ASP:N	15:Q:374:SER:HA	2.35	0.42
1:A:197:LEU:HD11	1:A:231:PHE:CE1	2.55	0.42
7:E:320:LEU:HB3	11:L:73:LEU:HD11	2.02	0.42
8:F:818:TRP:HA	11:L:287:PHE:HD1	1.85	0.42
12:M:332:LEU:HD23	13:N:565:PRO:HB3	2.00	0.42
3:B:6:GLN:O	3:B:24:GLY:HA2	2.19	0.42
12:M:7:PRO:HB2	14:O:282:LEU:HB3	2.02	0.42
13:N:328:LYS:HE2	13:N:328:LYS:HB3	1.87	0.42
13:N:338:ALA:O	13:N:342:ASN:ND2	2.52	0.42
1:A:381:PRO:O	1:A:383:GLN:N	2.53	0.42
3:B:429:PHE:HE1	3:B:433:GLN:HE21	1.68	0.42
4:P:9:LYS:HD2	4:P:12:LYS:NZ	2.34	0.42
13:N:298:LEU:HD12	13:N:304:LEU:HD23	2.01	0.42
14:O:270:HIS:ND1	14:O:271:PRO:HD2	2.34	0.42
1:A:442:THR:O	2:R:339:ARG:NH2	2.53	0.41
1:A:451:LEU:HA	1:A:451:LEU:HD23	1.81	0.41
2:R:133:ASP:HA	14:O:427:LYS:NZ	2.34	0.41
11:K:493:LYS:HG3	11:K:510:GLU:HG2	2.02	0.41
13:N:274:LYS:HB2	13:N:277:GLU:HB3	2.02	0.41
1:A:150:GLY:N	2:R:336:ILE:CD1	2.83	0.41
2:R:63:ARG:HH21	11:L:287:PHE:HA	1.85	0.41
3:B:26:ASN:HB3	3:B:29:THR:O	2.20	0.41
11:I:260:CYS:SG	11:I:262:THR:OG1	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:222:PRO:HG2	14:O:226:PHE:CE2	2.55	0.41
1:A:235:MET:SD	3:B:401:VAL:HG21	2.61	0.41
2:R:248:LEU:HD23	2:R:248:LEU:HA	1.85	0.41
2:R:360:LEU:HD21	3:B:438:GLN:NE2	2.35	0.41
6:D:110:HIS:NE2	6:D:115:CYS:SG	2.93	0.41
11:J:443:LYS:NZ	12:M:44:ASP:OD1	2.51	0.41
11:J:447:LEU:HD23	11:J:447:LEU:HA	1.91	0.41
13:N:90:LEU:HD23	13:N:90:LEU:HA	1.93	0.41
14:O:239:ASN:ND2	14:O:482:ASN:O	2.53	0.41
1:A:446:LEU:HD11	2:R:332:ILE:CD1	2.47	0.41
2:R:184:THR:HG21	12:M:451:ASN:O	2.21	0.41
10:H:457:PHE:HB3	10:H:483:GLU:HG3	2.03	0.41
2:R:136:LEU:C	2:R:139:PRO:HD2	2.40	0.41
7:E:407:LYS:HA	7:E:410:TYR:CZ	2.55	0.41
8:F:807:GLY:O	11:L:316:SER:HB2	2.21	0.41
3:B:91:LEU:CD2	3:B:106:LEU:HD22	2.50	0.41
11:I:259:ILE:HD12	13:N:43:GLN:HG2	2.02	0.41
13:N:361:ILE:HA	13:N:512:ASN:HD21	1.86	0.41
1:A:139:VAL:HG11	1:A:443:MET:HG3	2.03	0.41
3:B:112:LEU:HD12	3:B:141:ILE:HD12	2.02	0.41
5:C:61:SER:O	5:C:65:MET:HG2	2.20	0.41
12:M:223:GLN:HG3	12:M:224:LEU:H	1.85	0.41
13:N:561:LEU:HD22	13:N:568:THR:HA	2.03	0.41
2:R:62:TYR:O	2:R:66:GLN:HG3	2.21	0.41
11:L:312:LYS:N	11:L:345:LYS:HZ2	2.19	0.41
14:O:37:ALA:HB3	14:O:73:LEU:HB2	2.02	0.41
14:O:43:ASN:HD21	14:O:46:LYS:HD2	1.86	0.41
14:O:416:ASP:N	14:O:416:ASP:OD1	2.54	0.41
1:A:418:GLN:HG2	1:A:419:TYR:CD1	2.55	0.41
2:R:360:LEU:HD21	3:B:438:GLN:HE21	1.86	0.41
2:R:365:GLU:O	2:R:369:GLN:HG3	2.21	0.41
3:B:154:ILE:HG22	3:B:154:ILE:O	2.21	0.41
7:E:352:ALA:O	15:Q:19:ARG:HD2	2.21	0.41
8:F:862:GLY:HA3	8:F:864:PHE:CE2	2.56	0.41
12:M:316:ASP:N	12:M:316:ASP:OD1	2.53	0.41
12:M:338:THR:O	12:M:342:LEU:HG	2.21	0.41
12:M:365:ALA:O	12:M:367:THR:HG23	2.21	0.41
13:N:275:ALA:HB2	13:N:318:PRO:O	2.20	0.41
15:Q:377:CYS:HB2	15:Q:378:PRO:HD2	2.03	0.41
1:A:442:THR:CB	2:R:339:ARG:HH21	2.34	0.41
1:A:458:GLU:O	1:A:460:TYR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:405:LEU:HD12	12:M:405:LEU:HA	1.92	0.41
1:A:153:SER:HG	1:A:171:ASP:H	1.66	0.40
1:A:241:LYS:HZ2	1:A:245:GLU:HB3	1.86	0.40
1:A:108:MET:SD	1:A:123:TYR:HE2	2.43	0.40
2:R:360:LEU:CD2	3:B:438:GLN:HE21	2.34	0.40
3:B:312:ARG:HA	3:B:312:ARG:HD3	1.79	0.40
10:H:502:LEU:HD11	10:H:509:LEU:HD11	2.03	0.40
11:L:166:ILE:HG22	11:L:167:ASN:CG	2.42	0.40
13:N:565:PRO:N	13:N:566:PRO:HD2	2.36	0.40
15:Q:358:ALA:H	15:Q:371:GLU:CB	2.32	0.40
1:A:389:LEU:HD22	1:A:421:LEU:CD2	2.52	0.40
2:R:365:GLU:CG	3:B:415:TYR:CD1	3.03	0.40
13:N:131:ILE:O	13:N:134:LEU:HB3	2.21	0.40
14:O:170:THR:HG22	14:O:172:LEU:N	2.36	0.40
3:B:146:SER:O	3:B:149:ALA:HB3	2.21	0.40
11:I:175:LYS:HE2	11:L:192:ASP:OD1	2.21	0.40
13:N:289:LEU:O	13:N:293:VAL:HG23	2.21	0.40
1:A:381:PRO:HG2	1:A:382:GLU:H	1.86	0.40
2:R:104:ILE:HG23	14:O:410:PHE:HD1	1.87	0.40
2:R:371:ARG:HH12	3:B:28:GLU:C	2.19	0.40
7:E:331:ASN:HD22	11:L:137:LEU:HD12	1.87	0.40
10:H:489:ASN:OD1	10:H:489:ASN:N	2.54	0.40
12:M:50:ARG:HA	12:M:50:ARG:HD3	1.78	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	392/477 (82%)	369 (94%)	18 (5%)	5 (1%)	12 48
2	R	319/1359 (24%)	296 (93%)	23 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	391/467 (84%)	368 (94%)	21 (5%)	2 (0%)	29	69
4	P	46/157 (29%)	43 (94%)	2 (4%)	1 (2%)	6	35
5	C	58/78 (74%)	56 (97%)	2 (3%)	0	100	100
6	D	96/180 (53%)	90 (94%)	6 (6%)	0	100	100
7	E	118/435 (27%)	108 (92%)	10 (8%)	0	100	100
8	F	63/889 (7%)	56 (89%)	7 (11%)	0	100	100
9	G	51/885 (6%)	49 (96%)	2 (4%)	0	100	100
10	H	127/625 (20%)	114 (90%)	10 (8%)	3 (2%)	6	33
11	I	289/557 (52%)	274 (95%)	15 (5%)	0	100	100
11	J	113/557 (20%)	109 (96%)	4 (4%)	0	100	100
11	K	105/557 (19%)	101 (96%)	4 (4%)	0	100	100
11	L	292/557 (52%)	277 (95%)	15 (5%)	0	100	100
12	M	302/483 (62%)	281 (93%)	21 (7%)	0	100	100
13	N	408/581 (70%)	380 (93%)	28 (7%)	0	100	100
14	O	376/502 (75%)	352 (94%)	24 (6%)	0	100	100
15	Q	258/426 (61%)	224 (87%)	34 (13%)	0	100	100
16	S	32/883 (4%)	32 (100%)	0	0	100	100
23	a	95/136 (70%)	92 (97%)	3 (3%)	0	100	100
23	e	97/136 (71%)	95 (98%)	2 (2%)	0	100	100
24	b	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
24	f	83/103 (81%)	80 (96%)	3 (4%)	0	100	100
25	c	106/130 (82%)	101 (95%)	5 (5%)	0	100	100
25	g	102/130 (78%)	98 (96%)	3 (3%)	1 (1%)	15	55
26	d	94/126 (75%)	89 (95%)	4 (4%)	1 (1%)	14	52
26	h	92/126 (73%)	88 (96%)	0	4 (4%)	2	22
All	All	4581/11645 (39%)	4297 (94%)	267 (6%)	17 (0%)	38	72

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	48	ASP
10	H	528	ILE
26	h	120	SER

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Mol	Chain	Res	Type
1	A	343	SER
26	d	101	GLY
26	h	29	SER
26	h	30	ARG
26	h	101	GLY
1	A	382	GLU
1	A	459	ASP
4	P	84	LEU
10	H	529	ASN
1	A	431	ASP
1	A	458	GLU
3	B	155	SER
10	H	527	THR
25	g	117	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	357/420 (85%)	338 (95%)	19 (5%)	22	47
2	R	297/1228 (24%)	294 (99%)	3 (1%)	76	86
3	B	363/423 (86%)	343 (94%)	20 (6%)	21	47
4	P	53/140 (38%)	52 (98%)	1 (2%)	57	75
5	C	58/75 (77%)	58 (100%)	0	100	100
6	D	82/151 (54%)	82 (100%)	0	100	100
7	E	113/388 (29%)	105 (93%)	8 (7%)	14	39
8	F	60/810 (7%)	60 (100%)	0	100	100
9	G	48/832 (6%)	47 (98%)	1 (2%)	53	72
10	H	126/578 (22%)	124 (98%)	2 (2%)	62	79
11	I	268/500 (54%)	261 (97%)	7 (3%)	46	66
11	J	111/500 (22%)	110 (99%)	1 (1%)	78	87
11	K	106/500 (21%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L	270/500 (54%)	270 (100%)	0	100	100
12	M	286/435 (66%)	281 (98%)	5 (2%)	60	78
13	N	374/521 (72%)	366 (98%)	8 (2%)	53	72
14	O	358/462 (78%)	355 (99%)	3 (1%)	81	89
15	Q	243/384 (63%)	233 (96%)	10 (4%)	30	55
16	S	33/824 (4%)	32 (97%)	1 (3%)	41	63
23	a	85/111 (77%)	82 (96%)	3 (4%)	36	59
23	e	86/111 (78%)	83 (96%)	3 (4%)	36	59
24	b	63/79 (80%)	63 (100%)	0	100	100
24	f	70/79 (89%)	66 (94%)	4 (6%)	20	45
25	c	85/100 (85%)	79 (93%)	6 (7%)	14	39
25	g	83/100 (83%)	76 (92%)	7 (8%)	11	33
26	d	82/105 (78%)	77 (94%)	5 (6%)	18	44
26	h	80/105 (76%)	77 (96%)	3 (4%)	33	57
All	All	4240/10461 (40%)	4120 (97%)	120 (3%)	46	65

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	79	ASN
1	A	88	ARG
1	A	122	ARG
1	A	216	ARG
1	A	230	GLN
1	A	246	LEU
1	A	251	LYS
1	A	293	LYS
1	A	301	LEU
1	A	319	ILE
1	A	321	ASP
1	A	343	SER
1	A	380	SER
1	A	386	SER
1	A	397	SER
1	A	432	ARG
1	A	442	THR

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Mol	Chain	Res	Type
1	A	462	THR
2	R	215	THR
2	R	265	VAL
2	R	297	VAL
3	B	7	ASP
3	B	32	VAL
3	B	34	GLU
3	B	41	ILE
3	B	48	ASP
3	B	52	THR
3	B	54	HIS
3	B	56	THR
3	B	69	GLN
3	B	94	ARG
3	B	100	ASP
3	B	105	GLU
3	B	122	SER
3	B	181	ASP
3	B	197	SER
3	B	291	GLU
3	B	321	ASP
3	B	347	GLU
3	B	422	SER
3	B	438	GLN
4	P	90	ARG
7	E	327	CYS
7	E	351	ASP
7	E	356	ILE
7	E	359	ILE
7	E	384	ILE
7	E	413	VAL
7	E	414	VAL
7	E	417	ASP
9	G	175	ASP
10	H	510	THR
10	H	527	THR
11	I	170	ILE
11	I	224	PHE
11	I	253	GLN
11	I	270	VAL
11	I	275	LEU
11	I	281	ASN

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Mol	Chain	Res	Type
11	I	312	LYS
11	J	459	LEU
12	M	58	LEU
12	M	62	THR
12	M	232	VAL
12	M	241	LEU
12	M	466	ASN
13	N	79	VAL
13	N	91	SER
13	N	104	TYR
13	N	123	LEU
13	N	166	ARG
13	N	170	GLN
13	N	195	PHE
13	N	578	THR
14	O	208	ILE
14	O	274	TYR
14	O	279	THR
15	Q	192	THR
15	Q	250	LEU
15	Q	262	LEU
15	Q	295	ASN
15	Q	342	ASP
15	Q	345	ASP
15	Q	351	ASP
15	Q	352	HIS
15	Q	368	ASP
15	Q	370	ASP
16	S	198	LEU
23	a	59	GLU
23	a	63	ARG
23	a	129	ARG
25	c	29	ARG
25	c	59	THR
25	c	71	ARG
25	c	81	ARG
25	c	84	GLN
25	c	101	THR
26	d	28	ARG
26	d	54	LYS
26	d	68	GLU
26	d	77	LEU

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Mol	Chain	Res	Type
26	d	85	THR
23	e	63	ARG
23	e	64	LYS
23	e	68	GLN
24	f	19	ARG
24	f	91	LYS
24	f	92	ARG
24	f	93	GLN
25	g	35	ARG
25	g	64	GLU
25	g	73	ASN
25	g	81	ARG
25	g	99	ARG
25	g	101	THR
25	g	118	LYS
26	h	85	THR
26	h	96	ARG
26	h	102	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
2	R	57	GLN
2	R	72	ASN
2	R	116	ASN
2	R	123	GLN
2	R	270	HIS
2	R	290	GLN
2	R	340	GLN
2	R	361	HIS
3	B	303	ASN
3	B	304	ASN
3	B	438	GLN
6	D	64	HIS
6	D	108	HIS
7	E	331	ASN
7	E	432	ASN
9	G	180	HIS
10	H	493	GLN
10	H	506	GLN
10	H	601	HIS
11	I	60	GLN

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Mol	Chain	Res	Type
11	I	63	GLN
11	I	227	ASN
11	I	314	ASN
11	K	426	GLN
11	K	501	GLN
11	L	145	ASN
11	L	291	HIS
11	L	318	GLN
12	M	61	ASN
12	M	233	GLN
12	M	340	ASN
12	M	378	GLN
12	M	380	GLN
13	N	43	GLN
13	N	512	ASN
13	N	559	HIS
13	N	577	ASN
14	O	18	GLN
14	O	22	ASN
14	O	97	HIS
14	O	270	HIS
14	O	484	ASN
15	Q	3	HIS
15	Q	15	ASN
15	Q	158	GLN
15	Q	164	ASN
15	Q	261	GLN
23	a	76	GLN
23	a	85	GLN
24	b	75	HIS
25	c	31	HIS
25	c	38	ASN
25	c	73	ASN
25	c	84	GLN
26	d	60	ASN
26	d	92	GLN
24	f	75	HIS
24	f	93	GLN
25	g	31	HIS
25	g	73	ASN
26	h	79	HIS
26	h	92	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
21	7	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	7	57:UNK	C	60:UNK	N	4.98

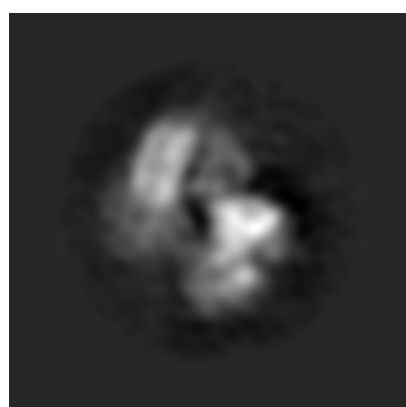
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21114. 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

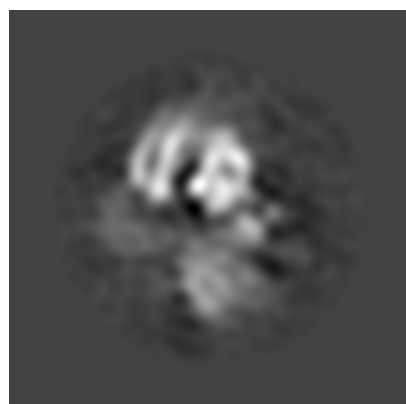


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 64



Y Index: 64



Z Index: 64

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

6.3 Largest variance slices [i](#)

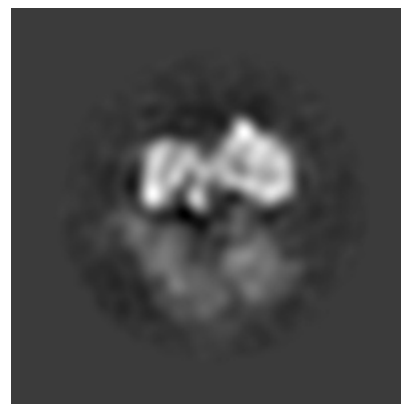
6.3.1 Primary map



X Index: 68



Y Index: 71



Z Index: 59

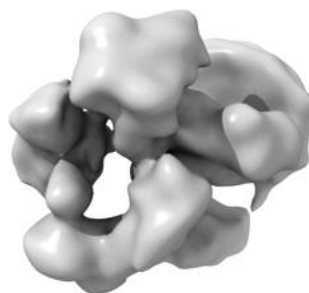
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

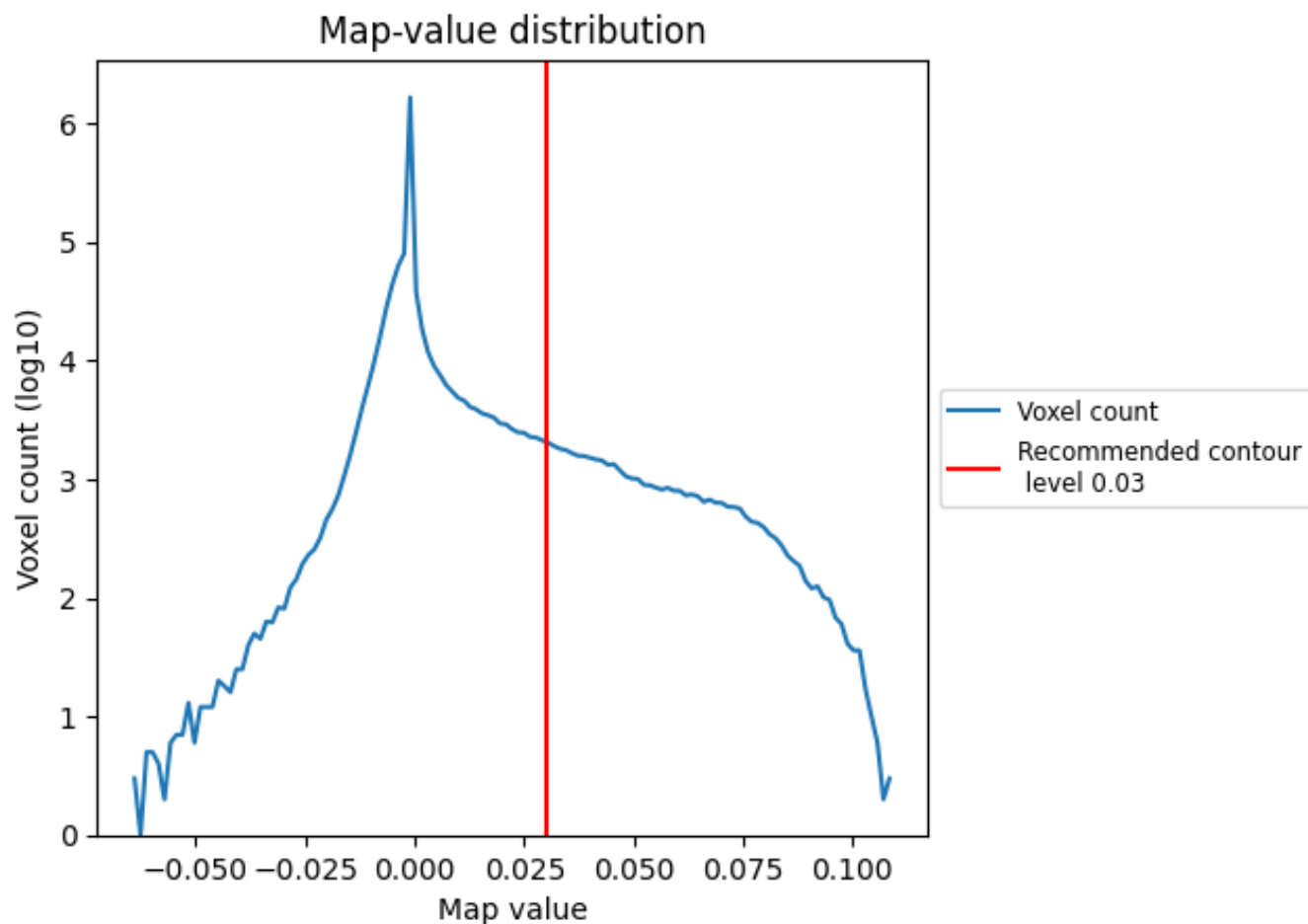
6.5 Mask visualisation

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

7 Map analysis [i](#)

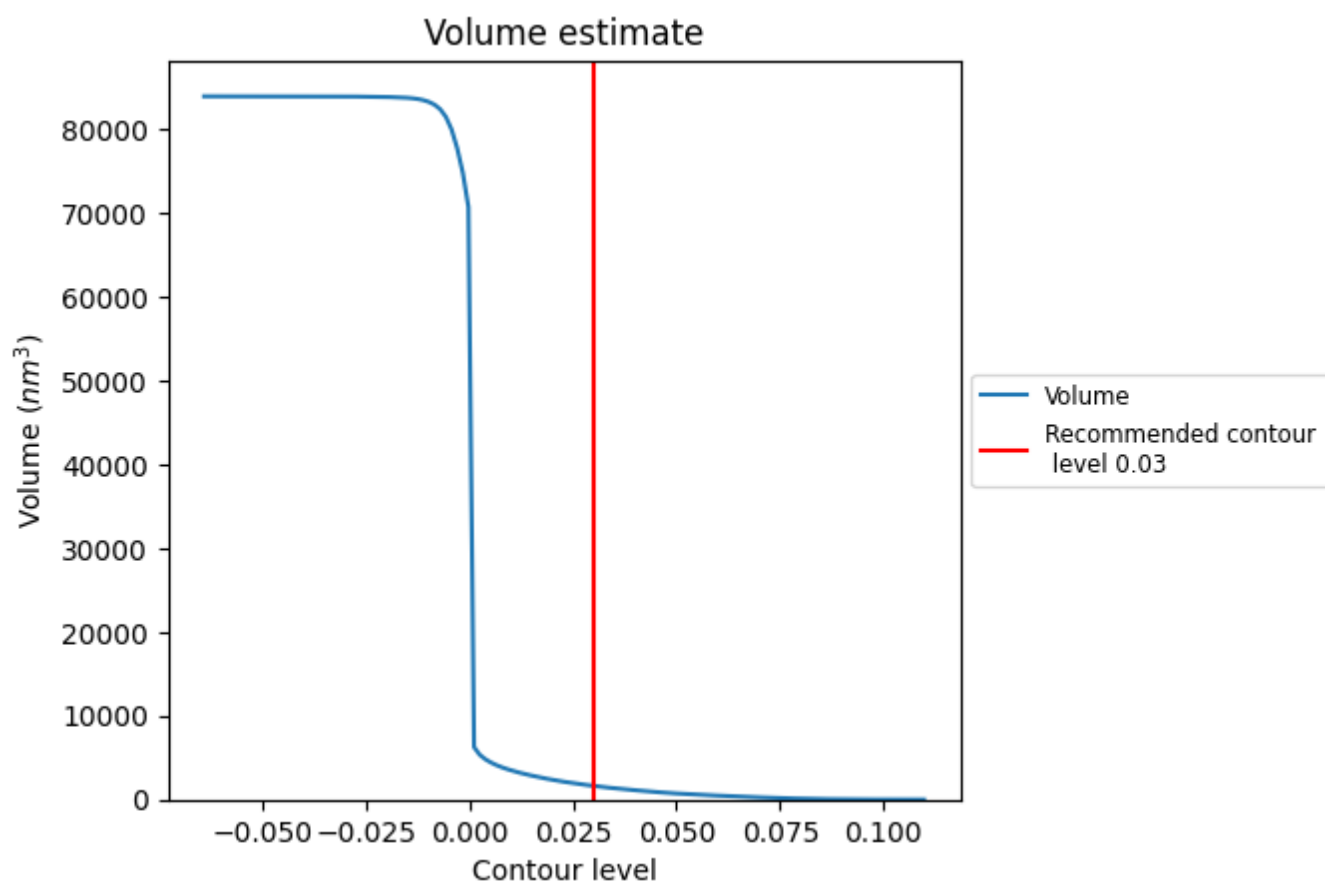
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

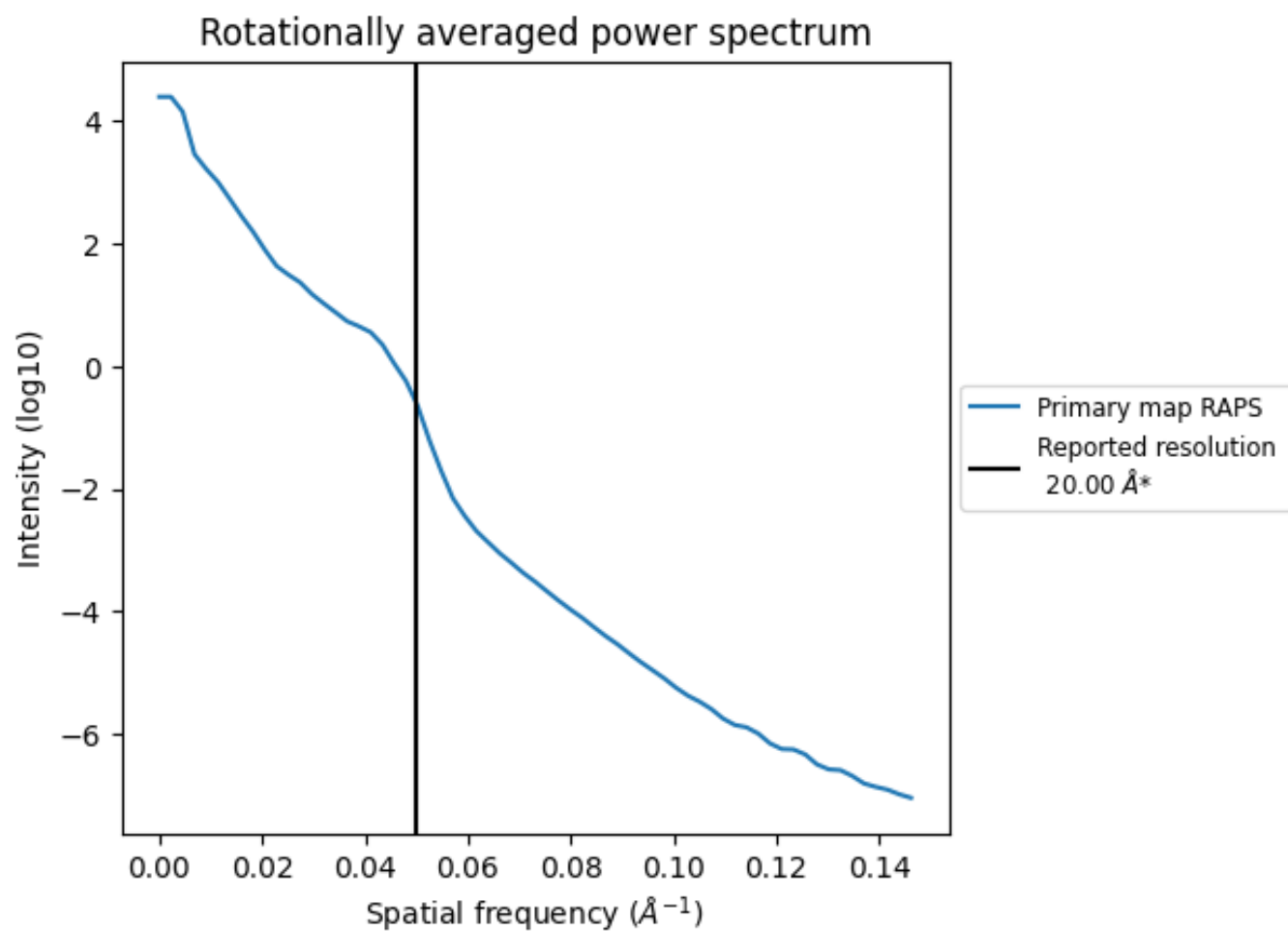
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1633 nm^3 ; this corresponds to an approximate mass of 1475 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 0.050 Å⁻¹

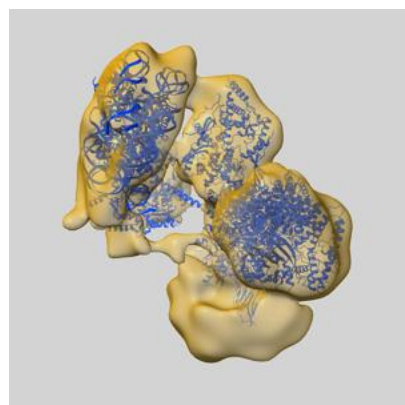
8 Fourier-Shell correlation ⓘ

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

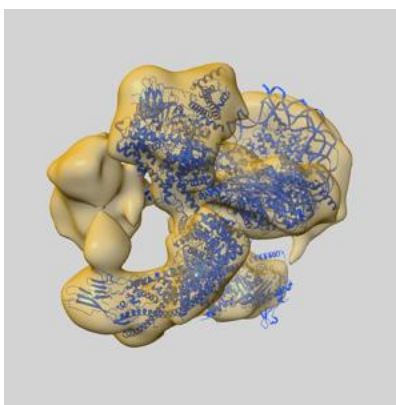
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21114 and PDB model 6V92. Per-residue inclusion information can be found in section [3](#) on page [10](#).

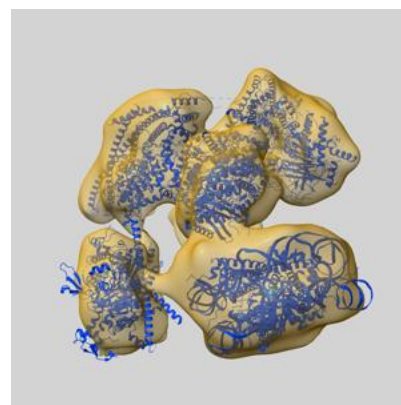
9.1 Map-model overlay [i](#)



X



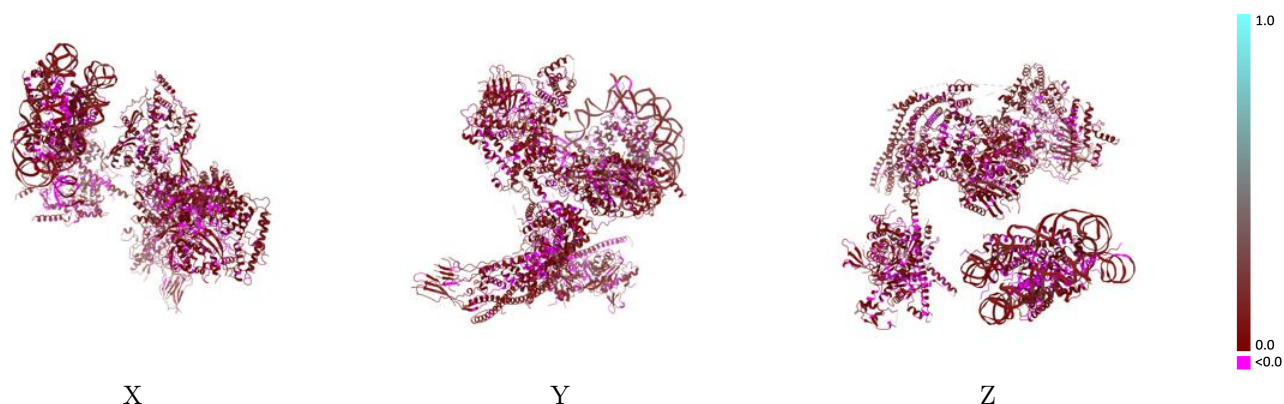
Y



Z

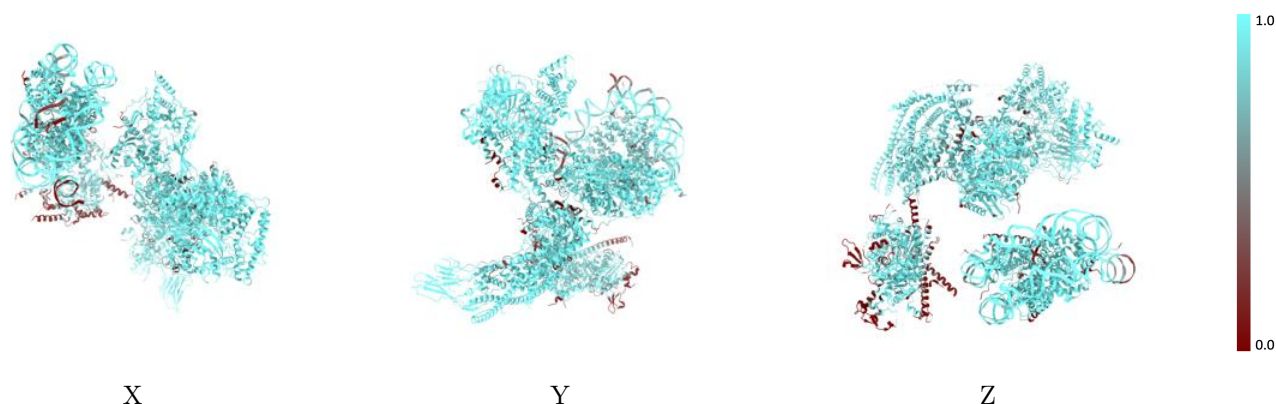
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



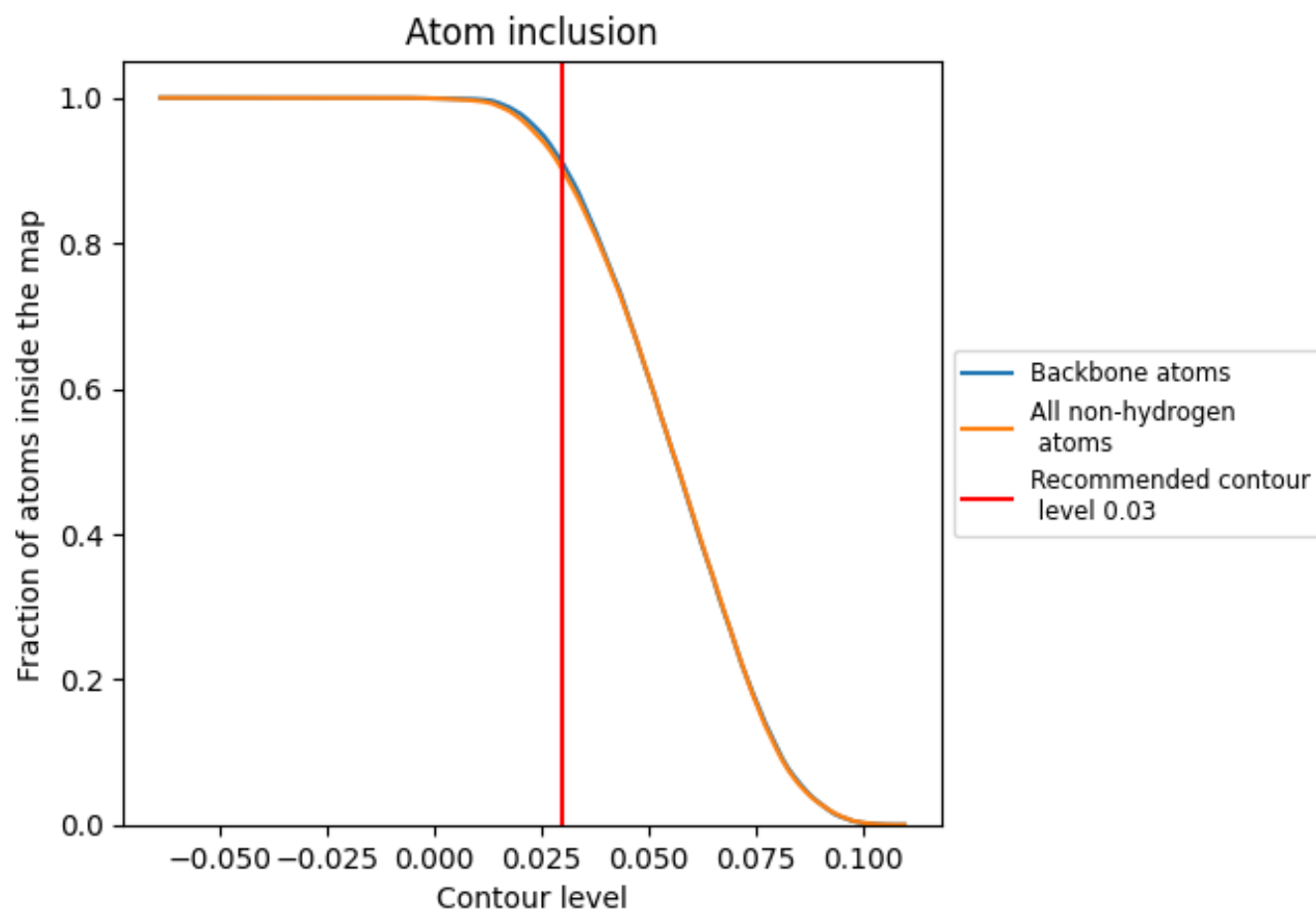
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 90% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8997	 0.0530
2	 1.0000	 0.0480
3	 0.5789	 0.0250
4	 0.9895	 0.0570
5	 0.5714	 0.0050
6	 1.0000	 0.0500
7	 0.9878	 0.0500
A	 0.6959	 0.0330
B	 0.7389	 0.0370
C	 0.9917	 0.0650
D	 0.8765	 0.0380
E	 0.9687	 0.0740
F	 1.0000	 0.0290
G	 0.8230	 0.0470
H	 0.9570	 0.0530
I	 0.9709	 0.0510
J	 0.9717	 0.0800
K	 0.9691	 0.0810
L	 0.9720	 0.0510
M	 0.9429	 0.0480
N	 0.9367	 0.0490
O	 0.9942	 0.0650
P	 0.6977	 0.0590
Q	 0.9560	 0.0660
R	 0.8229	 0.0410
S	 0.7626	 0.0680
a	 0.9364	 0.0280
b	 0.9899	 0.0440
c	 0.9579	 0.0380
d	 0.8558	 0.0200
e	 0.9554	 0.0430
f	 0.9954	 0.0050
g	 0.8833	 0.0110
h	 0.9372	 0.0120
i	 0.8987	 0.0860
j	 0.8970	 0.0930

