



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 10:24 PM UTC

PDB ID : 6KW4 / pdb_00006kw4
EMDB ID : EMD-0778
Title : The ClassB RSC-Nucleosome Complex
Authors : Ye, Y.P.; Wu, H.; Chen, K.J.; Verma, N.; Cairns, B.; Gao, N.; Chen, Z.C.
Deposited on : 2019-09-06
Resolution : 7.55 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

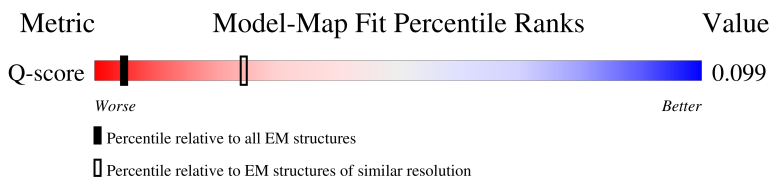
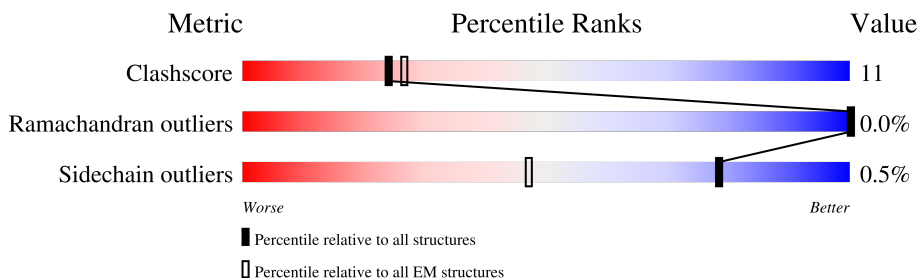
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.55 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.



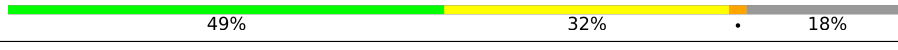
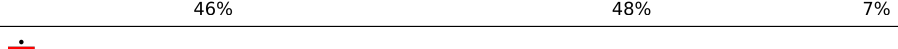
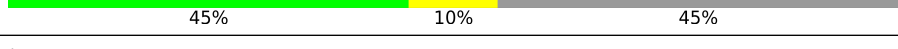
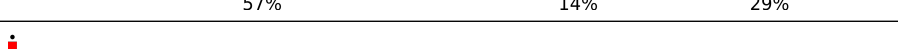
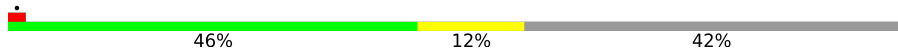
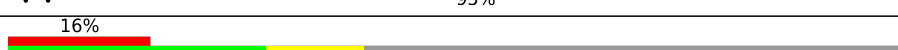
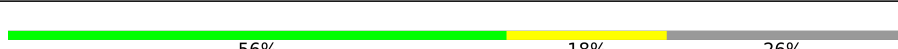
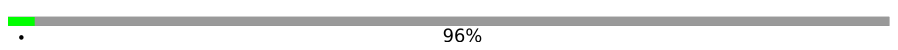
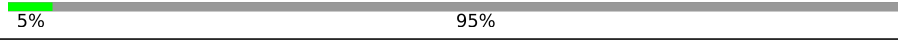
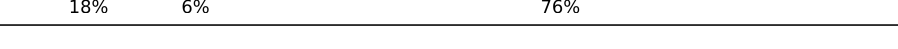
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	373 (7.06 - 8.04)

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	N	136	
1	Q	136	
2	B	103	
2	R	103	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	O	130	
3	S	130	
4	U	167	
5	W	167	
6	f	477	
7	h	157	
8	F	435	
9	D	557	
9	H	557	
10	M	581	
11	I	483	
12	G	426	
13	A	502	
14	J	1359	
14	V	1359	
14	Y	1359	
15	E	78	
16	C	883	
17	K	885	
18	X	625	
19	L	889	
20	P	126	
20	T	126	
21	g	467	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 45924 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 Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	98	Total	C	N	O	S	0	0
			810	511	157	139	3		
1	Q	95	Total	C	N	O	S	0	0
			784	494	151	136	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	82	Total	C	N	O	S	0	0
			657	416	128	112	1		
2	R	87	Total	C	N	O	S	0	0
			703	443	142	117	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	O	107	Total	C	N	O	0	0
			823	519	161	143		
3	S	107	Total	C	N	O	0	0
			823	519	161	143		

- Molecule 4 is a DNA chain called DNA 167.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	156	Total	C	N	O	P	0	0
			3183	1512	579	936	156		

- Molecule 5 is a DNA chain called DNA 167.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	156	Total	C	N	O	P	0	0
			3213	1522	599	936	156		

- Molecule 6 is a protein called Actin-related protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	398	Total	C	N	O	S	3	0
			3219	2075	527	602	15		

- Molecule 7 is a protein called Regulator of Ty1 transposition protein 102.

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

- Molecule 8 is a protein called Chromatin structure-remodeling complex subunit RSC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	118	Total	C	N	O	S	0	0
			964	601	164	197	2		

- Molecule 9 is a protein called Chromatin structure-remodeling complex protein RSC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	393	Total	C	N	O	S	0	0
			3215	2036	552	613	14		
9	D	305	Total	C	N	O	S	0	0
			2510	1613	416	471	10		

- Molecule 10 is a protein called Chromatin structure-remodeling complex subunit RSC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	384	Total	C	N	O	S	0	0
			3058	1970	497	574	17		

- Molecule 11 is a protein called Chromatin structure-remodeling complex protein RSC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	244	Total	C	N	O	S	0	0
			1944	1234	328	377	5		

- Molecule 12 is a protein called Chromatin structure-remodeling complex subunit SFH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	246	Total	C	N	O	S	0	0
			1996	1271	337	380	8		

- Molecule 13 is a protein called Chromatin structure-remodeling complex protein RSC58.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	365	Total	C	N	O	S	0	0
			3007	1942	509	547	9		

- Molecule 14 is a protein called Nuclear protein STH1/NPS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	235	Total	C	N	O	S	0	0
			1814	1136	327	349	2		
14	V	69	Total	C	N	O	S	0	0
			592	364	121	105	2		
14	Y	548	Total	C	N	O	S	0	0
			4503	2873	780	832	18		

- Molecule 15 is a protein called High temperature lethal protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	58	Total	C	N	O	S	0	0
			477	295	86	92	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	C	33	Total	C	N	O	S	0	0
			269	177	39	52	1		

- Molecule 17 is a protein called Chromatin structure-remodeling complex protein RSC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	42	Total	C	N	O	S	0	0
			347	225	57	63	2		

- Molecule 18 is a protein called Chromatin structure-remodeling complex subunit RSC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	147	Total	C	N	O	S	0	0
			1220	776	202	234	8		

- Molecule 19 is a protein called Chromatin structure-remodeling complex subunit RSC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	85	Total	C	N	O	S	0	0
			669	428	120	119	2		

- Molecule 20 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	93	Total	C	N	O	S	0	0
			717	450	128	137	2		
20	T	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

- Molecule 21 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	395	Total	C	N	O	S	1	0
			3191	2048	522	614	7		

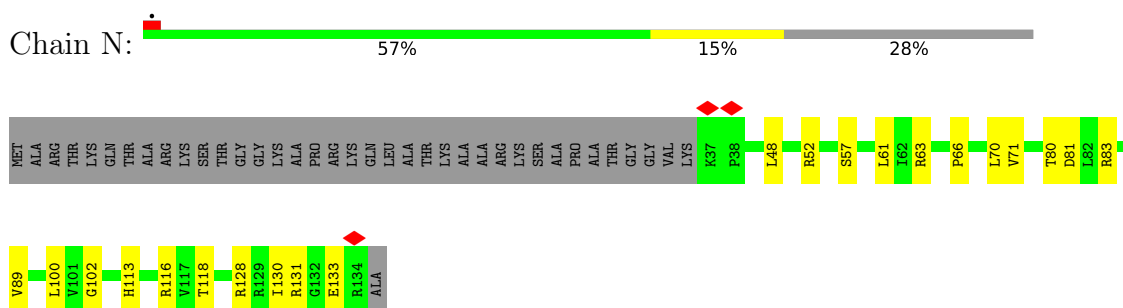
- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
22	H	1	Total	Zn	0
			1	1	

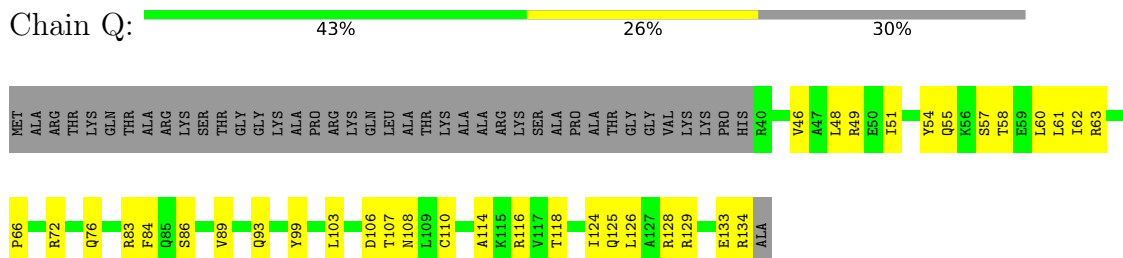
3 Residue-property plots [i](#)

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.

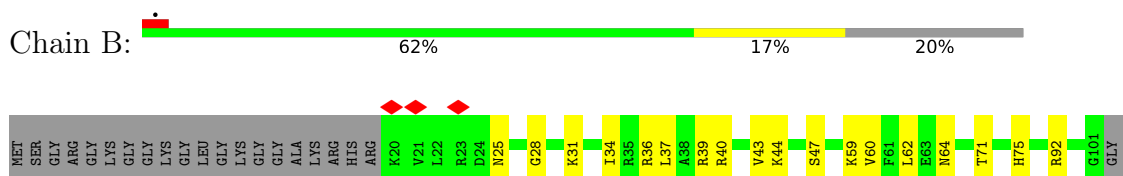
• Molecule 1: Histone H3.2



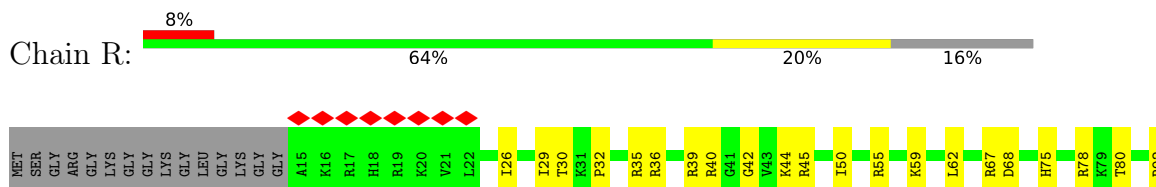
• Molecule 1: Histone H3.2



• Molecule 2: Histone H4



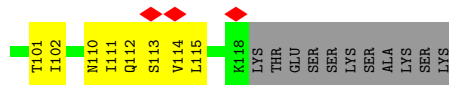
• Molecule 2: Histone H4





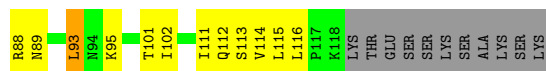
- Molecule 3: Histone H2A

Chain O: 52% 28% 18%



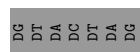
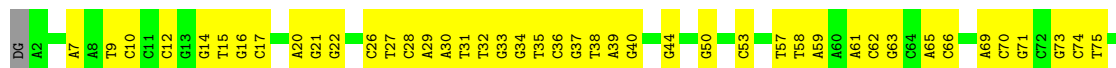
- Molecule 3: Histone H2A

Chain S: 49% 32% 18%



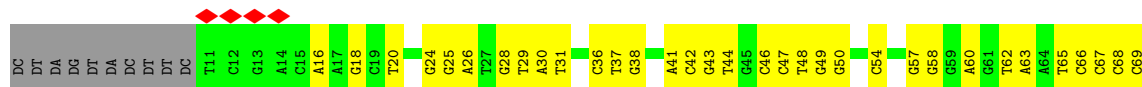
- Molecule 4: DNA 167

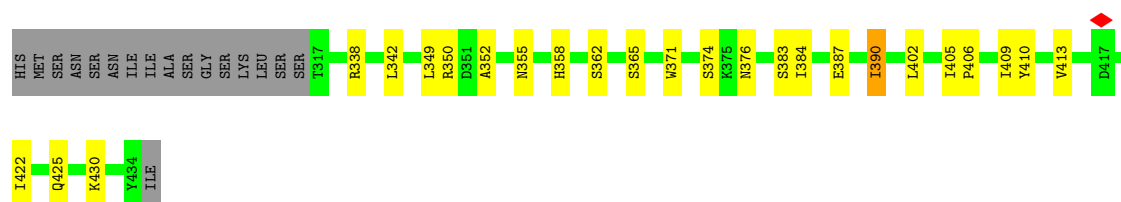
Chain U: 46% 48% 7%



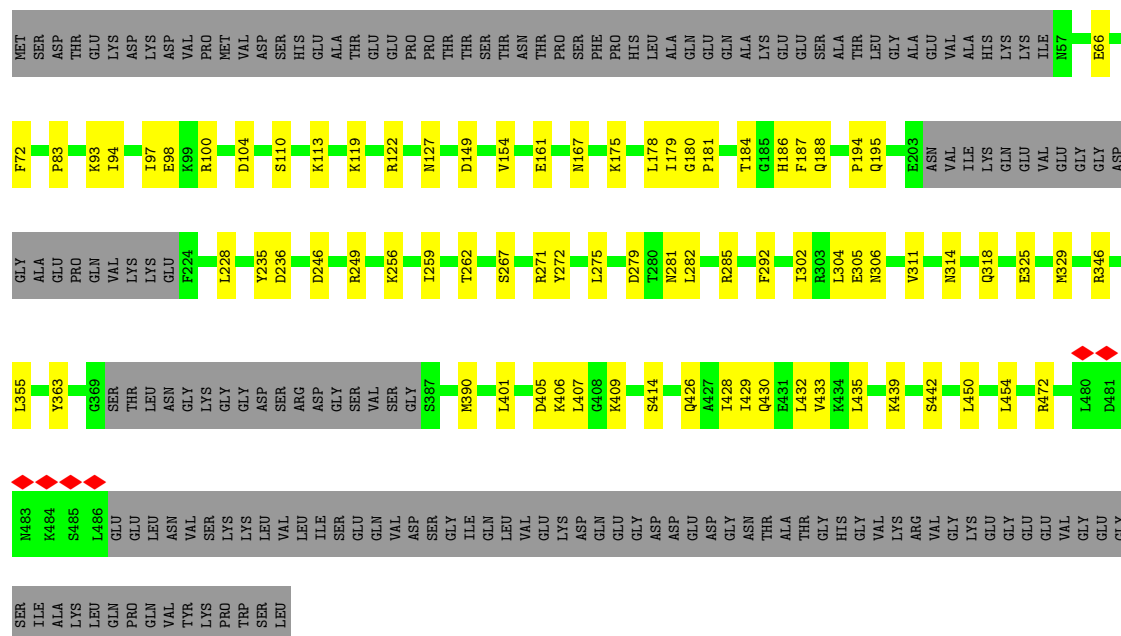
- Molecule 5: DNA 167

Chain W: 47% 46% 7%

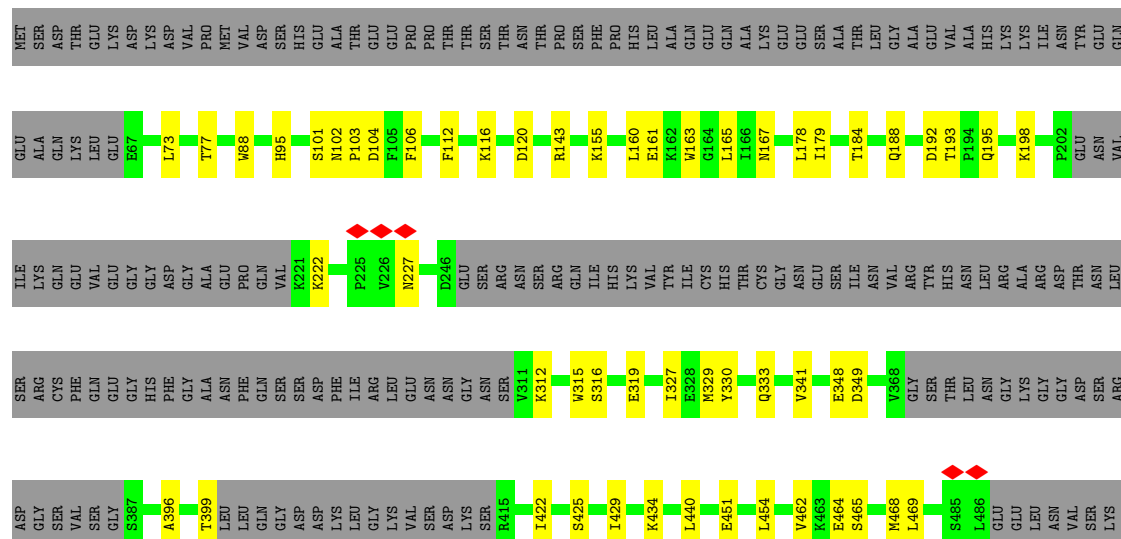




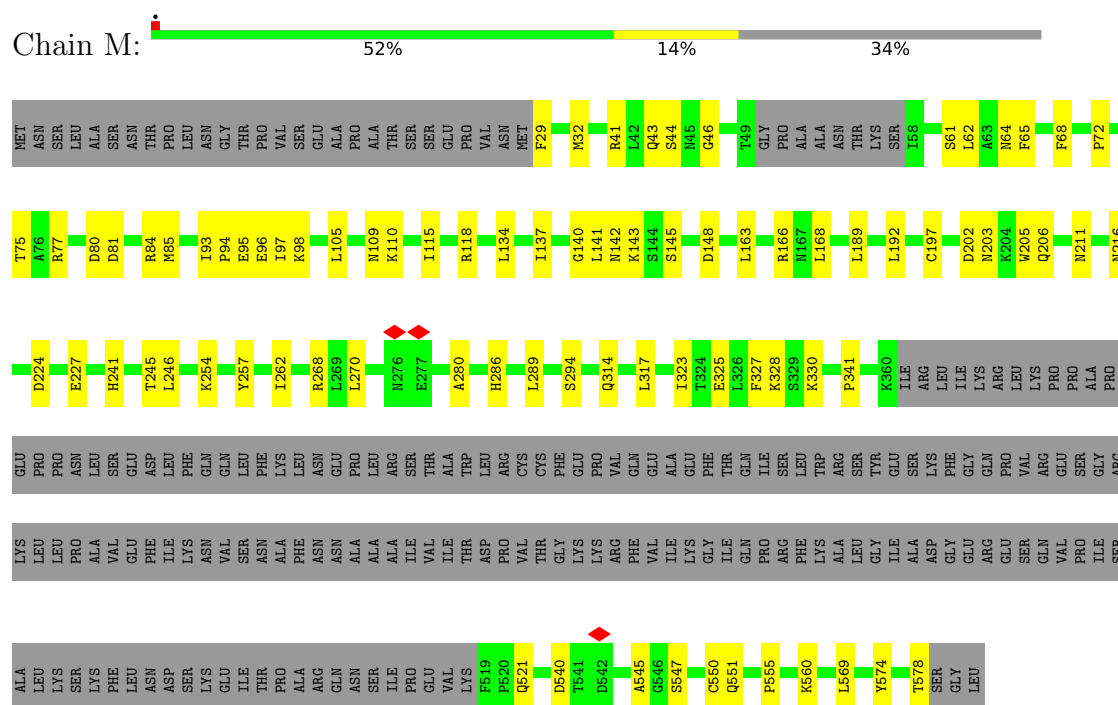
• Molecule 9: Chromatin structure-remodeling complex protein RSC8



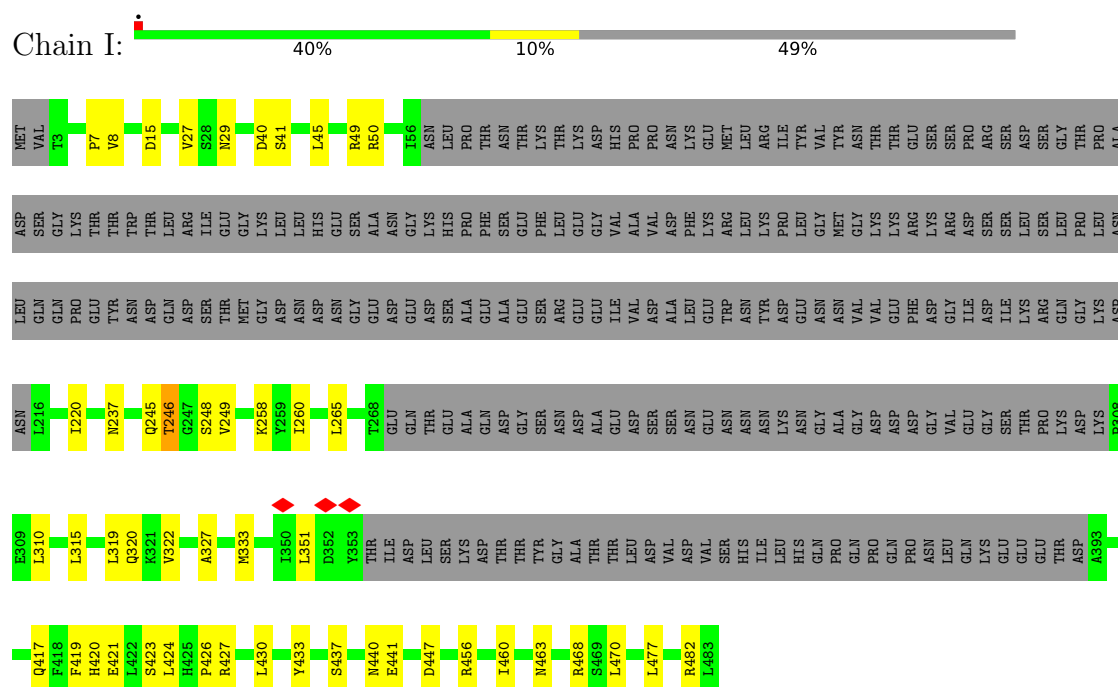
• Molecule 9: Chromatin structure-remodeling complex protein RSC8



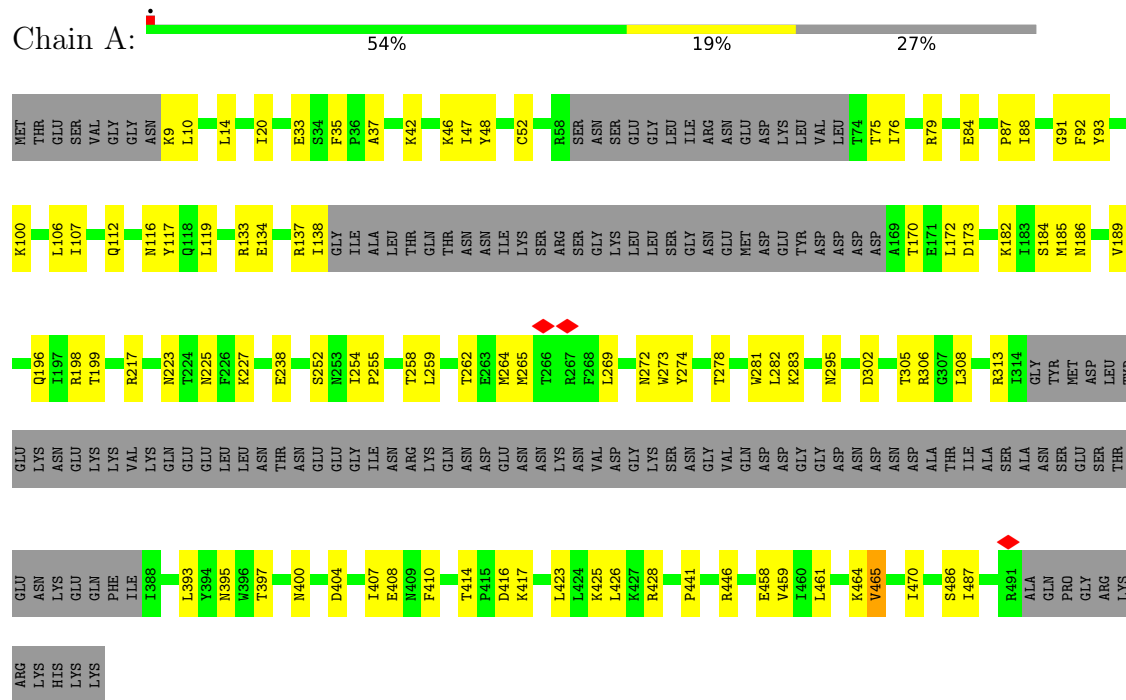
- Molecule 10: Chromatin structure-remodeling complex subunit RSC9



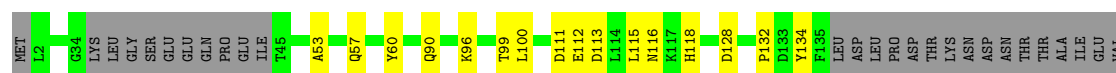
- Molecule 11: Chromatin structure-remodeling complex protein RSC6



- Molecule 12: Chromatin structure-remodeling complex subunit SFH1



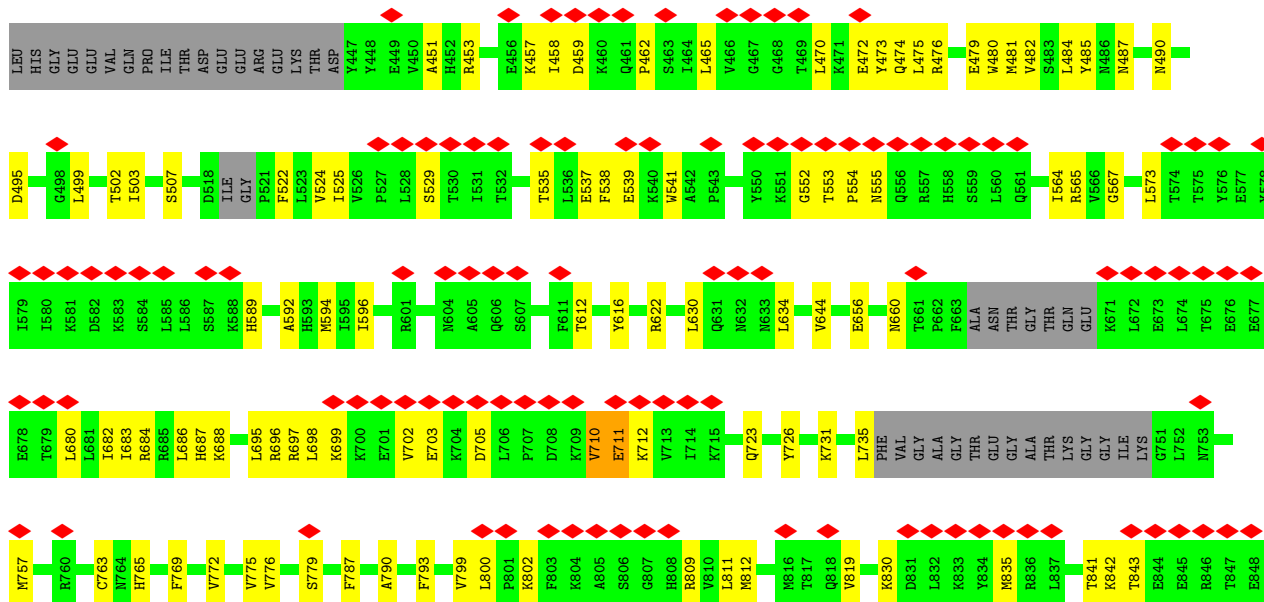
Chain J: 15% 83%

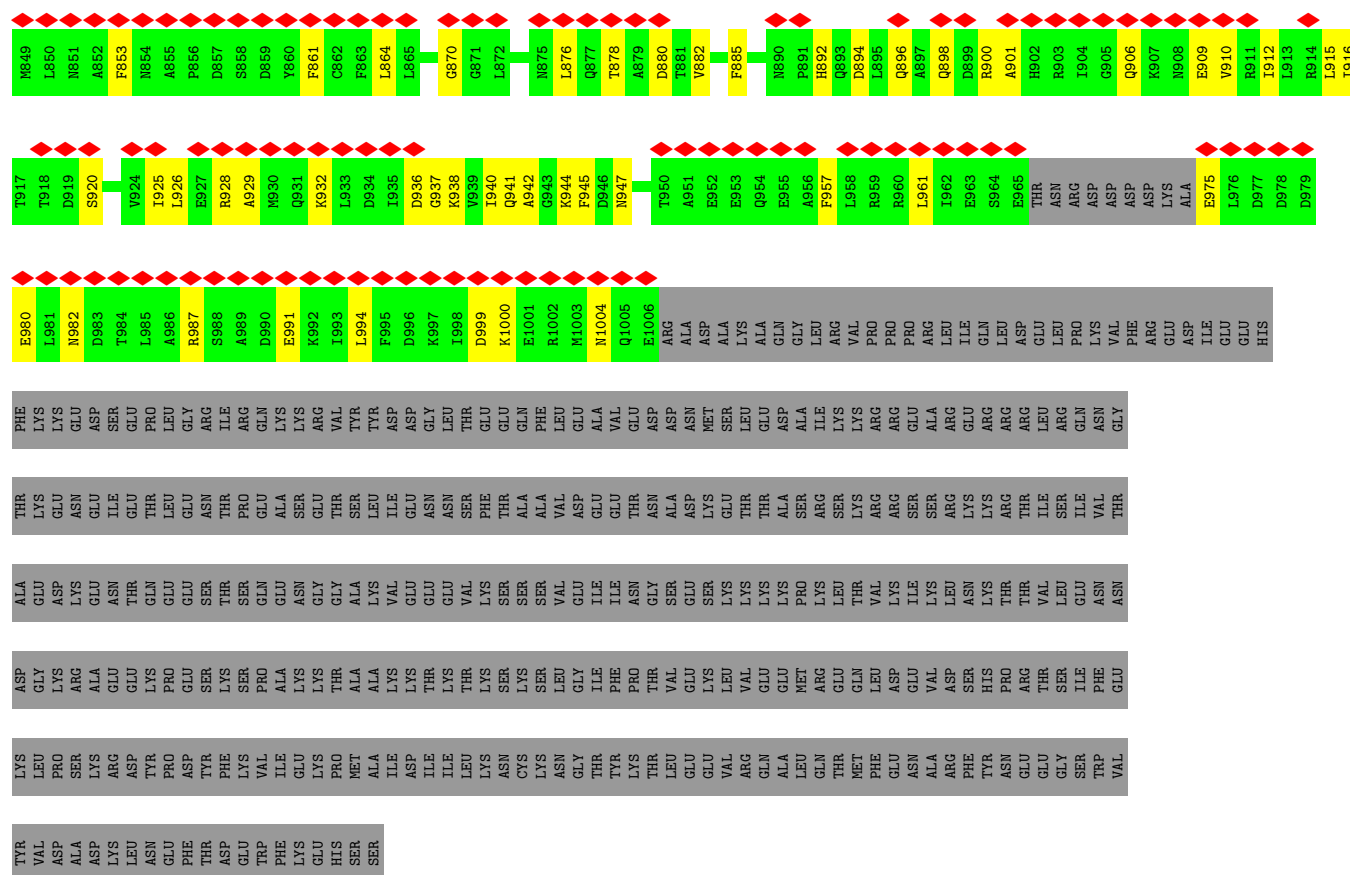


- Molecule 14: Nuclear protein STH1/NPS1

95%







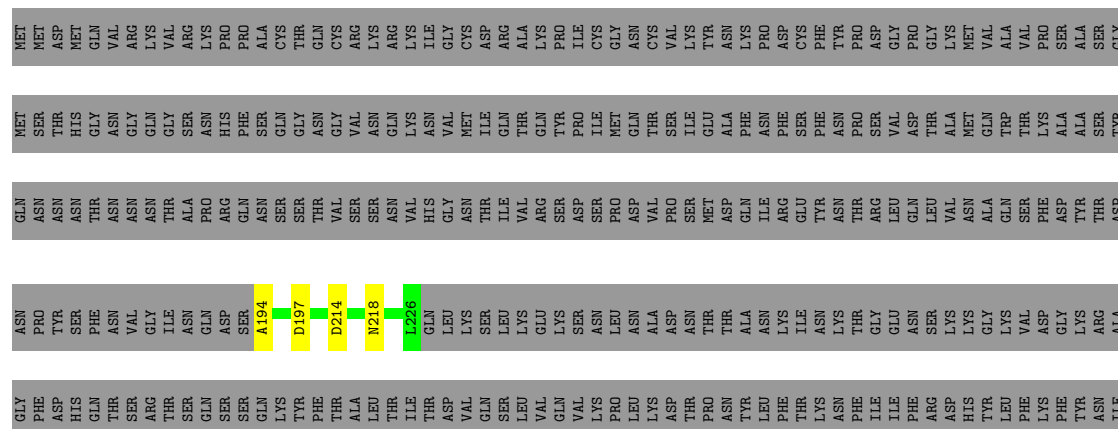
- Molecule 15: High temperature lethal protein 1

Chain E: 56% 18% 26%



- Molecule 16: Chromatin structure-remodeling complex protein RSC30

Chain C: 96%





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

- Molecule 18: Chromatin structure-remodeling complex subunit RSC4

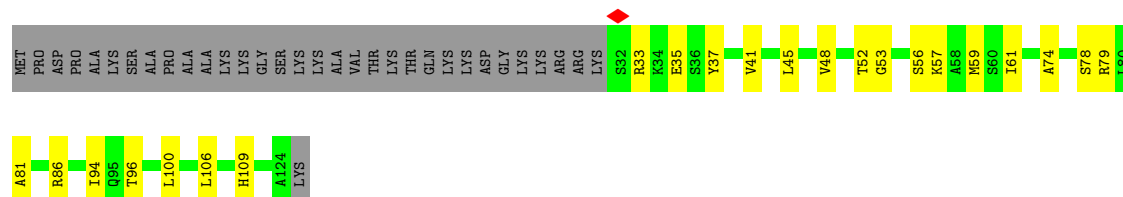
[illegible]

- Molecule 19: Chromatin structure-remodeling complex subunit RSC2

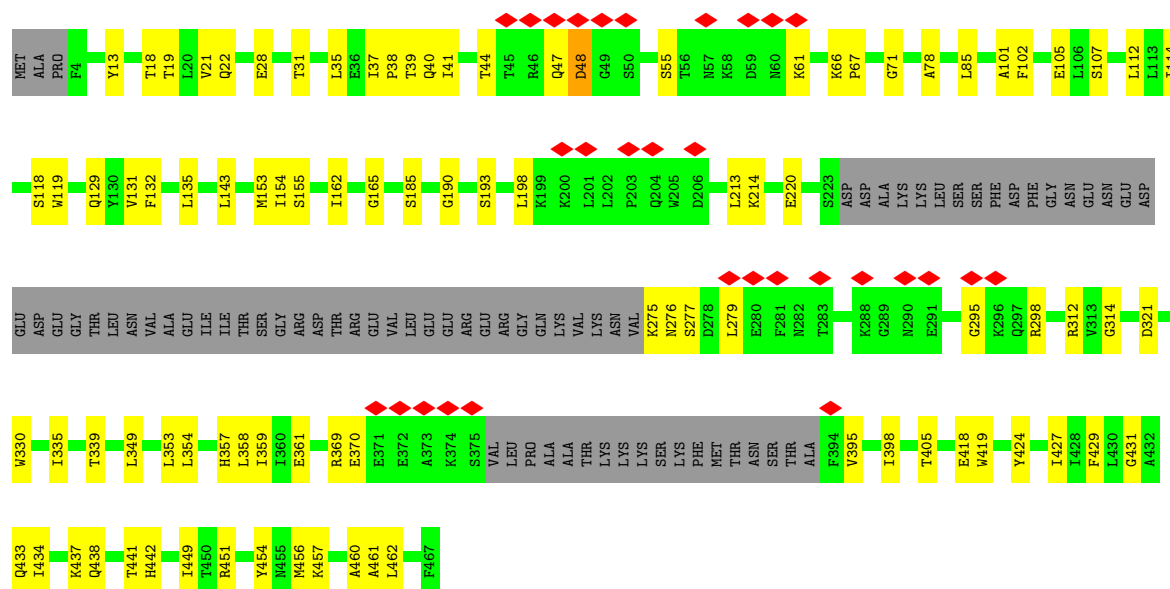
- Molecule 20: Histone H4

A77	S78	R79	L80	A81	R86	I89	T90	S91	R92	E93	T96	L100	A110	E113	K116	A117	A124	Lys
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	-----

Chain T:



Chain g:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45256	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.104	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	385.2, 385.2, 385.2	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.14, 2.14, 2.14	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	N	0.25	0/822	0.57	0/1102
1	Q	0.23	0/794	0.55	0/1064
2	B	0.25	0/664	0.60	0/889
2	R	0.25	0/711	0.57	0/950
3	O	0.27	0/833	0.58	0/1124
3	S	0.27	0/833	0.58	0/1124
4	U	0.48	0/3567	0.67	0/5499
5	W	0.51	0/3607	0.66	0/5569
6	f	0.19	0/3295	0.44	0/4454
7	h	0.17	0/501	0.45	0/669
8	F	0.21	0/983	0.51	0/1337
9	D	0.17	0/2557	0.44	0/3442
9	H	0.18	0/3275	0.46	0/4409
10	M	0.21	0/3113	0.55	0/4215
11	I	0.18	0/1976	0.44	0/2685
12	G	0.20	0/2039	0.55	0/2769
13	A	0.18	0/3077	0.49	0/4169
14	J	0.19	0/1836	0.49	0/2480
14	V	0.15	0/598	0.40	0/789
14	Y	0.22	0/4580	0.57	1/6167 (0.0%)
15	E	0.19	0/480	0.48	0/643
16	C	0.11	0/272	0.31	0/366
17	K	0.17	0/356	0.42	0/483
18	X	0.21	0/1243	0.57	0/1672
19	L	0.21	0/681	0.54	0/921
20	P	0.21	0/728	0.53	0/983
20	T	0.22	0/736	0.51	0/991
21	g	0.19	0/3261	0.48	1/4421 (0.0%)
All	All	0.27	0/47418	0.54	2/65386 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	g	48	ASP	CB-CA-C	8.76	118.50	109.83
14	Y	710	VAL	N-CA-C	5.28	116.00	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	810	0	851	18	0
1	Q	784	0	824	30	0
2	B	657	0	706	16	0
2	R	703	0	757	23	0
3	O	823	0	882	33	0
3	S	823	0	882	32	0
4	U	3183	0	1752	75	0
5	W	3213	0	1752	67	0
6	f	3219	0	3240	52	0
7	h	490	0	467	14	0
8	F	964	0	919	24	0
9	D	2510	0	2542	50	0
9	H	3215	0	3196	76	0
10	M	3058	0	3127	55	0
11	I	1944	0	1964	43	0
12	G	1996	0	1948	36	0
13	A	3007	0	3045	71	0
14	J	1814	0	1777	27	0
14	V	592	0	610	13	0
14	Y	4503	0	4573	99	0
15	E	477	0	491	15	0
16	C	269	0	279	3	0
17	K	347	0	342	3	0
18	X	1220	0	1192	24	0
19	L	669	0	693	14	0
20	P	717	0	723	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	T	725	0	745	21	0
21	g	3191	0	3179	61	0
22	H	1	0	0	0	0
All	All	45924	0	43458	792	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 11.

All (792) 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)
14:Y:710:VAL:CG2	14:Y:912:ILE:H	1.60	1.15
14:Y:710:VAL:HG21	14:Y:912:ILE:H	1.17	1.05
14:Y:710:VAL:HG21	14:Y:912:ILE:N	1.74	1.02
21:g:47:GLN:OE1	21:g:47:GLN:N	2.08	0.86
14:Y:710:VAL:O	14:Y:712:LYS:HG2	1.77	0.85
14:Y:710:VAL:O	14:Y:712:LYS:N	2.10	0.85
14:Y:710:VAL:O	14:Y:711:GLU:C	2.21	0.80
2:B:44:LYS:HB2	3:S:115:LEU:HD22	1.74	0.70
4:U:107:DC:N3	5:W:60:DA:N6	2.39	0.70
4:U:113:DA:N6	5:W:54:DC:N3	2.38	0.69
2:R:75:HIS:HD1	20:P:96:THR:HG1	1.38	0.69
3:O:29:ARG:HH22	20:T:37:TYR:HE1	1.41	0.69
4:U:79:DC:O2	5:W:90:DG:N2	2.26	0.68
4:U:27:DT:O2	5:W:142:DG:N2	2.26	0.68
4:U:82:DC:O2	5:W:87:DG:N2	2.26	0.68
14:Y:880:ASP:HB2	14:Y:910:VAL:HA	1.76	0.68
4:U:44:DG:N2	5:W:125:DT:O2	2.27	0.67
8:F:387:GLU:HG3	9:H:188:GLN:HB3	1.76	0.67
12:G:295:ASN:HB2	12:G:376:TRP:HB2	1.75	0.67
8:F:376:ASN:H	9:H:184:THR:HB	1.59	0.67
9:H:83:PRO:HA	9:D:192:ASP:HB3	1.77	0.67
13:A:404:ASP:H	14:J:96:LYS:HD3	1.59	0.67
4:U:50:DG:N2	5:W:119:DT:O2	2.28	0.66
4:U:124:DA:H2''	4:U:125:DC:H2'	1.76	0.66
5:W:36:DC:H4'	5:W:37:DT:H5'	1.77	0.66
10:M:521:GLN:HE21	11:I:333:MET:HE2	1.60	0.66
4:U:7:DA:N6	5:W:160:DT:O4	2.29	0.66
14:Y:710:VAL:HA	14:Y:712:LYS:HE2	1.77	0.65
14:Y:763:CYS:HG	14:Y:920:SER:HG	1.42	0.65
11:I:447:ASP:HB2	13:A:272:ASN:HD22	1.62	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:186:ASN:HB3	18:X:433:GLU:HB3	1.78	0.65
3:O:88:ARG:HH22	3:O:101:THR:HA	1.62	0.64
3:S:88:ARG:HH22	3:S:101:THR:HA	1.62	0.64
4:U:144:DC:O2	5:W:25:DG:N2	2.30	0.64
2:B:60:VAL:O	2:B:64:ASN:ND2	2.31	0.64
9:H:175:LYS:HG2	10:M:77:ARG:HH21	1.63	0.64
13:A:258:THR:HG23	14:J:196:SER:HB2	1.80	0.63
14:Y:710:VAL:CG2	14:Y:912:ILE:N	2.40	0.63
8:F:384:ILE:HB	9:H:235:TYR:HB2	1.80	0.63
2:R:75:HIS:HB2	20:P:96:THR:HG21	1.81	0.62
9:H:433:VAL:HG11	9:D:429:ILE:HG23	1.80	0.62
14:Y:799:VAL:HA	14:Y:802:LYS:HD2	1.81	0.62
18:X:493:GLN:NE2	18:X:614:THR:O	2.32	0.62
2:R:26:ILE:HA	2:R:29:ILE:HD12	1.81	0.62
21:g:437:LYS:HD3	14:V:358:LEU:HD11	1.81	0.62
14:Y:809:ARG:HA	14:Y:861:PHE:HB3	1.80	0.62
14:Y:702:VAL:HG12	14:Y:703:GLU:HG3	1.82	0.61
9:H:272:TYR:HB2	9:H:282:LEU:HB2	1.82	0.61
9:H:275:LEU:HD11	9:H:302:ILE:HG13	1.82	0.61
14:Y:479:GLU:HA	14:Y:482:VAL:HB	1.81	0.61
3:O:83:LEU:HB3	3:O:102:ILE:HD13	1.82	0.61
8:F:413:VAL:HG13	9:D:88:TRP:HB3	1.83	0.61
14:Y:474:GLN:NE2	14:Y:499:LEU:O	2.34	0.61
11:I:27:VAL:HG12	11:I:29:ASN:H	1.64	0.61
1:N:52:ARG:HG3	3:S:111:ILE:HD11	1.83	0.60
2:R:39:ARG:NH1	2:R:44:LYS:O	2.33	0.60
9:H:279:ASP:HB2	10:M:41:ARG:HH11	1.66	0.60
3:S:83:LEU:HB3	3:S:102:ILE:HD13	1.82	0.60
14:Y:812:MET:HB2	14:Y:864:LEU:HA	1.82	0.60
2:B:71:THR:HG22	20:T:96:THR:HG23	1.82	0.60
2:B:39:ARG:NH1	2:B:43:VAL:O	2.34	0.60
6:f:76:LEU:HD22	6:f:119:ILE:HG13	1.83	0.60
4:U:36:DC:H4'	4:U:37:DG:H5'	1.84	0.60
21:g:295:GLY:O	21:g:298:ARG:NH1	2.35	0.60
4:U:40:DG:N2	5:W:129:DT:O2	2.34	0.60
4:U:80:DC:O2	5:W:89:DG:N2	2.35	0.60
3:S:85:LEU:O	3:S:89:ASN:ND2	2.35	0.59
9:H:426:GLN:HB2	9:D:422:ILE:HD11	1.84	0.59
13:A:9:LYS:HE2	13:A:138:ILE:HG12	1.83	0.59
14:Y:802:LYS:HE3	14:Y:982:ASN:HD21	1.66	0.59
3:S:87:VAL:HB	3:S:93:LEU:HD23	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:132:DG:N2	5:W:37:DT:O2	2.33	0.59
8:F:338:ARG:NH1	12:G:317:ASP:OD1	2.35	0.59
1:N:57:SER:OG	2:B:40:ARG:NH2	2.36	0.59
15:E:20:THR:H	15:E:23:ASN:HB2	1.68	0.59
3:O:87:VAL:HB	3:O:93:LEU:HD23	1.85	0.59
5:W:65:DT:H4'	5:W:66:DC:H5'	1.85	0.59
6:f:242:ASP:OD1	6:f:407:ARG:NH2	2.36	0.59
13:A:254:ILE:HG21	14:J:250:LEU:HD23	1.85	0.59
3:O:85:LEU:O	3:O:89:ASN:ND2	2.35	0.59
10:M:294:SER:HB2	11:I:45:LEU:HD11	1.84	0.58
13:A:112:GLN:HE21	13:A:217:ARG:HD2	1.68	0.58
18:X:604:PHE:HB3	18:X:617:MET:HB2	1.84	0.58
4:U:29:DA:H4'	4:U:30:DA:H5'	1.84	0.58
4:U:101:DG:N2	5:W:68:DC:O2	2.36	0.58
14:Y:710:VAL:O	14:Y:712:LYS:CG	2.49	0.58
4:U:73:DG:H1'	4:U:74:DC:H5'	1.86	0.58
9:H:94:ILE:HD11	9:H:119:LYS:HB2	1.85	0.58
14:J:115:LEU:HA	14:J:118:HIS:HB2	1.85	0.58
3:O:42:ARG:HH22	5:W:58:DG:H21	1.52	0.57
6:f:326:GLU:HA	6:f:331:PRO:HB2	1.86	0.57
21:g:437:LYS:NZ	14:V:362:MET:SD	2.74	0.57
9:D:327:ILE:HG23	13:A:470:ILE:HD13	1.85	0.57
6:f:66:GLU:HG2	6:f:215:LYS:HA	1.86	0.57
8:F:365:SER:H	9:H:194:PRO:HB3	1.69	0.57
12:G:315:VAL:HG13	12:G:320:LEU:HB2	1.87	0.57
13:A:33:GLU:HG3	13:A:106:LEU:HD11	1.86	0.57
21:g:28:GLU:O	14:V:369:ARG:NH1	2.37	0.57
4:U:151:DT:O2	5:W:18:DG:N2	2.38	0.57
6:f:290:PHE:HB3	6:f:299:LEU:HB2	1.86	0.57
14:Y:683:ILE:HA	14:Y:686:LEU:HB2	1.87	0.57
1:N:48:LEU:HD21	3:S:116:LEU:HA	1.86	0.57
18:X:375:GLU:HB2	18:X:514:HIS:HB2	1.87	0.57
8:F:376:ASN:ND2	8:F:383:SER:O	2.38	0.57
14:Y:459:ASP:HB3	14:Y:475:LEU:HD13	1.85	0.57
12:G:337:LEU:HA	12:G:340:LYS:HB2	1.86	0.57
13:A:264:MET:HA	14:J:259:GLN:HE21	1.70	0.57
1:Q:108:ASN:ND2	2:R:42:GLY:O	2.38	0.56
6:f:88:ARG:NH2	6:f:130:LYS:O	2.38	0.56
9:D:178:LEU:HB2	12:G:316:GLN:HE21	1.70	0.56
9:D:451:GLU:OE2	11:I:49:ARG:NH2	2.37	0.56
10:M:216:ASN:ND2	13:A:302:ASP:OD1	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:10:LEU:HB3	13:A:87:PRO:HB3	1.87	0.56
13:A:404:ASP:HB3	13:A:407:ILE:HG22	1.86	0.56
14:Y:763:CYS:SG	14:Y:920:SER:OG	2.59	0.56
2:R:67:ARG:HH22	20:P:100:LEU:HA	1.69	0.56
6:f:35:TYR:OH	6:f:79:ASN:ND2	2.39	0.56
13:A:35:PHE:HB3	13:A:75:THR:HA	1.88	0.56
13:A:185:MET:HG2	19:L:860:LEU:HD22	1.86	0.56
13:A:410:PHE:HZ	13:A:417:LYS:HB3	1.71	0.56
14:Y:1000:LYS:HA	14:Y:1004:ASN:HD22	1.69	0.56
10:M:227:GLU:O	10:M:268:ARG:NH1	2.38	0.56
14:Y:476:ARG:O	14:Y:480:TRP:N	2.38	0.56
9:D:143:ARG:HH12	12:G:314:ILE:HD11	1.70	0.56
13:A:88:ILE:HG13	13:A:91:GLY:H	1.70	0.56
14:Y:790:ALA:HB3	14:Y:793:PHE:HB2	1.88	0.56
10:M:325:GLU:HA	10:M:328:LYS:HE2	1.86	0.56
4:U:21:DG:N2	5:W:148:DT:O2	2.39	0.56
21:g:437:LYS:HB3	14:V:358:LEU:HD21	1.88	0.56
14:Y:687:HIS:HE1	14:Y:942:ALA:HB1	1.71	0.56
4:U:22:DG:N2	5:W:147:DC:O2	2.39	0.56
10:M:166:ARG:NH1	14:J:292:ARG:O	2.37	0.56
13:A:414:THR:OG1	13:A:416:ASP:OD1	2.24	0.55
20:P:68:ASP:OD2	20:P:72:ARG:NH2	2.39	0.55
14:Y:470:LEU:HD13	14:Y:475:LEU:HD21	1.88	0.55
14:Y:975:GLU:HG2	14:Y:980:GLU:HG3	1.89	0.55
8:F:402:LEU:HA	8:F:405:ILE:HD12	1.88	0.55
9:H:282:LEU:HD11	9:H:292:PHE:HB3	1.88	0.55
6:f:411:GLU:O	6:f:415:ARG:NH1	2.36	0.55
2:R:67:ARG:NH2	2:R:68:ASP:OD1	2.40	0.55
4:U:57:DT:O2	5:W:112:DG:N2	2.39	0.55
5:W:67:DC:H4'	5:W:68:DC:H5'	1.89	0.55
18:X:511:LEU:HB2	18:X:591:PHE:HB2	1.89	0.55
4:U:145:DT:O2	5:W:24:DG:N2	2.40	0.55
5:W:46:DC:H4'	5:W:47:DC:H5'	1.88	0.55
10:M:110:LYS:HG3	17:K:164:ILE:HG23	1.87	0.55
14:Y:565:ARG:O	14:Y:589:HIS:NE2	2.40	0.55
5:W:94:DG:H1'	5:W:95:DC:H5'	1.89	0.55
1:Q:72:ARG:O	1:Q:76:GLN:NE2	2.40	0.55
21:g:431:GLY:HA2	21:g:434:ILE:HD12	1.88	0.55
10:M:551:GLN:NE2	10:M:578:THR:O	2.40	0.55
1:Q:48:LEU:HD23	1:Q:51:ILE:HD12	1.88	0.55
7:h:25:TRP:NE1	21:g:454:TYR:O	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:435:LEU:O	11:I:398:LYS:NZ	2.38	0.55
13:A:185:MET:HE2	18:X:432:LYS:HD2	1.88	0.55
13:A:282:LEU:HD11	13:A:295:ASN:HB2	1.88	0.55
4:U:14:DG:N2	5:W:155:DC:O2	2.40	0.54
9:H:472:ARG:NH2	9:D:464:GLU:O	2.40	0.54
2:R:26:ILE:HG23	2:R:55:ARG:HD3	1.89	0.54
4:U:112:DT:O2	5:W:57:DG:N2	2.41	0.54
6:f:18:VAL:HG22	6:f:30:ILE:HG23	1.90	0.54
9:H:271:ARG:NH1	9:H:305:GLU:O	2.40	0.54
14:J:215:THR:OG1	14:J:233:ARG:O	2.24	0.54
3:O:35:ARG:HA	3:O:43:VAL:HG21	1.90	0.54
9:H:236:ASP:OD1	9:H:236:ASP:N	2.39	0.54
11:I:477:LEU:HD22	11:I:482:ARG:HD2	1.88	0.54
5:W:37:DT:H4'	5:W:38:DG:H5'	1.89	0.54
9:H:267:SER:OG	9:H:306:ASN:ND2	2.41	0.54
1:N:71:VAL:HG11	1:N:89:VAL:HG22	1.90	0.54
3:S:35:ARG:HA	3:S:43:VAL:HG21	1.90	0.54
4:U:65:DA:H1'	4:U:66:DC:H5'	1.89	0.54
9:D:120:ASP:OD2	12:G:366:ARG:NH1	2.41	0.54
9:D:160:LEU:HD22	9:D:165:LEU:HD22	1.90	0.54
3:O:63:LEU:HD11	20:T:41:VAL:HG13	1.90	0.54
9:H:355:LEU:O	14:J:258:ARG:NH1	2.38	0.54
9:H:429:ILE:HA	9:H:432:LEU:HD12	1.89	0.54
12:G:294:ASP:HB3	12:G:378:PRO:HB3	1.88	0.54
13:A:133:ARG:NH2	19:L:870:PRO:O	2.41	0.54
20:P:77:ALA:HA	20:P:80:LEU:HB2	1.89	0.54
1:Q:57:SER:OG	2:R:40:ARG:NH2	2.40	0.54
4:U:78:DC:H4'	4:U:79:DC:H5'	1.89	0.54
3:O:58:LEU:HA	3:O:61:GLU:HB3	1.90	0.53
2:R:75:HIS:HA	20:P:92:ARG:HH21	1.73	0.53
4:U:106:DA:H1'	4:U:107:DC:H5'	1.90	0.53
9:H:127:ASN:ND2	9:D:184:THR:OG1	2.41	0.53
9:D:222:LYS:H	11:I:463:ASN:HD21	1.56	0.53
3:O:29:ARG:HG2	3:O:32:ARG:HH21	1.74	0.53
8:F:349:LEU:HB2	8:F:358:HIS:HB2	1.91	0.53
8:F:350:ARG:NH1	8:F:355:ASN:OD1	2.40	0.53
14:Y:941:GLN:HA	14:Y:944:LYS:HE3	1.90	0.53
6:f:426:ASN:ND2	6:f:435:GLN:OE1	2.38	0.53
7:h:88:ASP:HB3	7:h:90:ARG:HH21	1.73	0.53
21:g:457:LYS:HB2	21:g:461:ALA:HB2	1.91	0.53
11:I:456:ARG:NH1	13:A:262:THR:O	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:149:ASP:N	9:H:149:ASP:OD1	2.42	0.53
9:H:439:LYS:NZ	11:I:40:ASP:OD2	2.37	0.53
14:V:351:PHE:HA	14:V:354:LEU:HB2	1.89	0.53
6:f:145:ILE:HD13	6:f:395:THR:HG21	1.91	0.53
9:H:178:LEU:HD11	9:D:195:GLN:HG3	1.91	0.53
14:Y:397:LYS:HE2	14:Y:688:LYS:HB2	1.91	0.53
3:O:80:PRO:HG2	20:T:57:LYS:HG3	1.89	0.53
11:I:441:GLU:HG3	15:E:29:LEU:HD21	1.89	0.53
18:X:524:THR:OG1	18:X:589:GLU:OE1	2.27	0.53
21:g:31:THR:HG22	21:g:418:GLU:HG3	1.89	0.53
21:g:155:SER:HB3	14:V:356:ALA:HB2	1.90	0.53
2:R:78:ARG:NH1	2:R:80:THR:O	2.41	0.53
12:G:17:HIS:HA	12:G:20:LEU:HD12	1.91	0.53
12:G:358:ALA:HB1	12:G:365:ILE:H	1.73	0.53
13:A:461:LEU:O	13:A:464:LYS:NZ	2.39	0.53
1:Q:61:LEU:HB3	2:R:36:ARG:HE	1.73	0.52
6:f:242:ASP:O	6:f:246:LEU:N	2.42	0.52
9:H:406:LYS:NZ	9:D:396:ALA:O	2.31	0.52
3:O:32:ARG:NH2	20:T:35:GLU:OE2	2.42	0.52
13:A:116:ASN:HA	13:A:119:LEU:HB2	1.90	0.52
14:Y:656:GLU:O	14:Y:660:ASN:ND2	2.43	0.52
1:Q:61:LEU:O	2:R:36:ARG:NH2	2.39	0.52
3:S:58:LEU:HA	3:S:61:GLU:HB3	1.90	0.52
6:f:70:LEU:HD23	6:f:79:ASN:HB3	1.91	0.52
6:f:217:SER:HA	6:f:220:VAL:HB	1.92	0.52
21:g:47:GLN:H	21:g:47:GLN:CD	2.12	0.52
14:Y:999:ASP:O	14:Y:1004:ASN:ND2	2.42	0.52
3:O:67:GLY:HA2	20:T:52:THR:HG21	1.92	0.52
6:f:18:VAL:HG13	6:f:30:ILE:HG12	1.91	0.52
6:f:36:ILE:HG13	6:f:54:MET:HE3	1.91	0.52
6:f:96:LYS:NZ	21:g:118:SER:O	2.42	0.52
12:G:294:ASP:N	12:G:294:ASP:OD1	2.42	0.52
14:Y:481:MET:O	14:Y:485:TYR:N	2.40	0.52
12:G:12:TYR:HB3	12:G:180:VAL:HG13	1.92	0.52
21:g:55:SER:HB2	21:g:85:LEU:HD11	1.92	0.52
2:B:75:HIS:HD1	20:T:96:THR:HG1	1.53	0.52
4:U:34:DG:H3'	4:U:35:DT:H71	1.92	0.52
10:M:143:LYS:O	10:M:211:ASN:ND2	2.39	0.52
9:H:271:ARG:HB2	9:H:281:ASN:HB3	1.91	0.52
12:G:228:ASP:OD1	12:G:228:ASP:N	2.43	0.52
13:A:79:ARG:HD2	13:A:84:GLU:HG3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:63:LEU:HD22	20:T:45:LEU:HD13	1.91	0.51
5:W:98:DG:H4'	5:W:99:DT:H5'	1.92	0.51
6:f:98:SER:HB2	6:f:101:GLU:HG3	1.91	0.51
10:M:323:ILE:HG22	10:M:545:ALA:HB3	1.92	0.51
19:L:867:GLY:O	19:L:869:ARG:NH1	2.43	0.51
3:O:112:GLN:HB2	3:O:115:LEU:HG	1.92	0.51
3:S:29:ARG:HG2	3:S:32:ARG:HH21	1.74	0.51
3:S:42:ARG:HB3	5:W:132:DG:H5''	1.91	0.51
9:H:285:ARG:HE	19:L:763:GLN:HB2	1.75	0.51
12:G:165:ILE:HG12	12:G:171:ILE:HG21	1.92	0.51
14:Y:775:VAL:HG23	14:Y:776:VAL:HG13	1.92	0.51
14:Y:787:PHE:HA	14:Y:793:PHE:HB3	1.92	0.51
9:D:161:GLU:HG3	9:D:167:ASN:HB2	1.92	0.51
10:M:197:CYS:O	10:M:202:ASP:N	2.43	0.51
16:C:214:ASP:O	16:C:218:ASN:ND2	2.44	0.51
7:h:25:TRP:O	21:g:129:GLN:NE2	2.44	0.51
8:F:390:ILE:HD12	9:H:228:LEU:HB2	1.93	0.51
9:D:315:TRP:NE1	9:D:349:ASP:OD2	2.43	0.51
9:D:469:LEU:HD22	11:I:258:LYS:HD3	1.93	0.51
3:S:43:VAL:HA	20:P:89:ILE:HG13	1.91	0.51
5:W:75:DG:H2''	5:W:76:DG:H2'	1.92	0.51
6:f:200:LEU:HB3	6:f:299:LEU:HD22	1.92	0.51
9:H:256:LYS:NZ	10:M:46:GLY:O	2.39	0.51
21:g:18:THR:HA	21:g:38:PRO:HA	1.91	0.51
14:Y:481:MET:HA	14:Y:484:LEU:HB2	1.91	0.51
4:U:90:DA:H2	5:W:79:DA:H2	1.57	0.51
9:H:235:TYR:OH	9:D:188:GLN:NE2	2.36	0.51
9:H:259:ILE:HD12	10:M:43:GLN:HB3	1.93	0.51
4:U:86:DT:O4	5:W:81:DA:N6	2.44	0.51
9:H:97:ILE:HG12	9:H:100:ARG:HH21	1.76	0.51
14:J:112:GLU:O	14:J:116:ASN:N	2.37	0.51
13:A:425:LYS:HG2	13:A:428:ARG:HH12	1.75	0.51
14:Y:680:LEU:HD22	14:Y:684:ARG:HG3	1.93	0.51
2:R:30:THR:HG21	4:U:61:DA:H5''	1.93	0.51
6:f:154:ALA:HA	6:f:391:ASN:HB3	1.93	0.51
9:H:311:VAL:O	9:H:314:ASN:ND2	2.44	0.51
18:X:378:LEU:HB2	18:X:484:TYR:HB2	1.93	0.51
14:Y:552:GLY:HA2	14:Y:843:THR:HG21	1.93	0.51
1:N:66:PRO:HB3	2:B:28:GLY:HA3	1.93	0.50
3:O:80:PRO:HA	3:O:83:LEU:HB2	1.93	0.50
6:f:148:SER:O	14:V:338:GLN:NE2	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:224:ALA:HA	6:f:228:ILE:HB	1.92	0.50
9:H:98:GLU:OE1	9:H:122:ARG:NH1	2.44	0.50
20:P:67:ASN:HA	20:P:70:PHE:HB3	1.93	0.50
20:T:81:ALA:O	20:T:86:ARG:N	2.42	0.50
14:Y:800:LEU:HD13	14:Y:830:LYS:HD3	1.92	0.50
14:Y:809:ARG:HH22	14:Y:853:PHE:HA	1.77	0.50
6:f:449:TRP:HB2	7:h:56:TYR:CZ	2.47	0.50
13:A:172:LEU:HB2	18:X:379:LEU:HD12	1.93	0.50
2:B:47:SER:HA	4:U:81:DC:H5''	1.93	0.50
3:S:40:ALA:HB3	20:P:89:ILE:HG12	1.92	0.50
5:W:43:DG:H3'	5:W:44:DT:H71	1.92	0.50
12:G:19:ARG:HA	12:G:22:ASN:HB2	1.92	0.50
1:N:128:ARG:HB3	1:N:133:GLU:HB2	1.93	0.50
3:S:80:PRO:HA	3:S:83:LEU:HB2	1.93	0.50
10:M:327:PHE:HB2	10:M:545:ALA:HB1	1.94	0.50
11:I:417:GLN:HA	11:I:420:HIS:HB3	1.94	0.50
12:G:279:VAL:HG21	12:G:339:ILE:HD13	1.92	0.50
21:g:13:TYR:HB2	21:g:114:ILE:HD12	1.92	0.50
11:I:220:ILE:HB	11:I:351:LEU:HB3	1.94	0.50
14:J:111:ASP:OD1	14:J:111:ASP:N	2.43	0.50
20:T:106:LEU:HA	20:T:109:HIS:HB2	1.93	0.50
4:U:29:DA:H2	5:W:140:DG:H22	1.59	0.50
4:U:90:DA:N6	5:W:78:DT:O4	2.45	0.50
6:f:428:VAL:HB	6:f:431:ASP:HB2	1.94	0.50
12:G:205:PRO:HA	12:G:222:LEU:HA	1.93	0.50
1:N:116:ARG:NH1	1:N:118:THR:O	2.45	0.50
3:S:112:GLN:HB2	3:S:115:LEU:HG	1.92	0.50
6:f:53:ASN:ND2	6:f:89:TYR:OH	2.44	0.50
9:H:355:LEU:HD22	14:J:258:ARG:HG3	1.94	0.50
14:Y:495:ASP:OD2	14:Y:697:ARG:NH2	2.45	0.50
14:Y:630:LEU:O	14:Y:892:HIS:NE2	2.45	0.50
9:H:325:GLU:HB3	9:H:329:MET:HE3	1.92	0.50
3:S:77:ARG:HE	4:U:20:DA:H4'	1.76	0.49
14:Y:525:ILE:HB	14:Y:596:ILE:HA	1.93	0.49
14:Y:535:THR:HA	14:Y:538:PHE:HB2	1.93	0.49
4:U:124:DA:H5'	20:T:33:ARG:HA	1.93	0.49
10:M:551:GLN:NE2	10:M:578:THR:OG1	2.39	0.49
11:I:8:VAL:O	13:A:283:LYS:N	2.45	0.49
12:G:374:SER:OG	12:G:375:ASN:N	2.46	0.49
3:S:43:VAL:N	5:W:133:DA:OP1	2.45	0.49
3:O:110:ASN:O	1:Q:55:GLN:NE2	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:110:SER:HB3	12:G:201:ALA:H	1.77	0.49
13:A:42:LYS:O	13:A:93:TYR:OH	2.28	0.49
18:X:433:GLU:HG3	18:X:444:GLU:HB3	1.95	0.49
4:U:151:DT:O4	5:W:16:DA:N6	2.45	0.49
9:H:181:PRO:O	11:I:468:ARG:NH1	2.45	0.49
21:g:449:ILE:HD11	21:g:462:LEU:HA	1.93	0.49
1:Q:110:CYS:O	1:Q:114:ALA:N	2.45	0.49
3:S:67:GLY:O	3:S:71:ARG:NE	2.42	0.49
4:U:101:DG:H4'	4:U:102:DG:H5'	1.95	0.49
21:g:19:THR:N	21:g:37:ILE:O	2.45	0.49
3:S:43:VAL:HG22	20:P:89:ILE:HD11	1.95	0.49
4:U:122:DG:H4'	4:U:123:DC:H5'	1.95	0.49
13:A:305:THR:HA	13:A:308:LEU:HB2	1.94	0.49
21:g:370:GLU:HG2	21:g:395:VAL:HG21	1.93	0.49
14:Y:876:LEU:HD23	14:Y:901:ALA:HA	1.94	0.49
4:U:30:DA:H1'	4:U:31:DT:H5'	1.95	0.49
6:f:145:ILE:HG12	6:f:435:GLN:HG3	1.93	0.49
21:g:112:LEU:HD21	21:g:143:LEU:HD23	1.94	0.49
1:Q:124:ILE:HD11	2:R:50:ILE:HD12	1.95	0.49
9:H:259:ILE:HB	10:M:44:SER:HA	1.95	0.49
11:I:315:LEU:HB3	11:I:320:GLN:HG3	1.95	0.49
21:g:354:LEU:HA	21:g:358:LEU:HB2	1.93	0.49
9:H:405:ASP:O	9:H:409:LYS:NZ	2.46	0.48
9:D:348:GLU:HG3	13:A:461:LEU:HD11	1.95	0.48
21:g:185:SER:HB2	21:g:312:ARG:HH11	1.78	0.48
4:U:89:DT:H4'	4:U:90:DA:H5'	1.95	0.48
12:G:307:PRO:HB3	12:G:332:LEU:HD22	1.95	0.48
14:Y:765:HIS:HD2	14:Y:819:VAL:HB	1.78	0.48
14:Y:885:PHE:HE1	14:Y:915:LEU:HB2	1.77	0.48
8:F:410:TYR:HB3	9:D:163:TRP:HH2	1.78	0.48
9:D:116:LYS:NZ	9:D:120:ASP:OD1	2.46	0.48
12:G:15:ASN:HD22	12:G:174:THR:HG22	1.79	0.48
13:A:397:THR:H	13:A:400:ASN:HD21	1.59	0.48
11:I:260:ILE:HG23	11:I:265:LEU:HD12	1.96	0.48
19:L:874:PHE:O	19:L:878:ARG:N	2.44	0.48
21:g:434:ILE:HD13	14:V:359:HIS:CE1	2.49	0.48
3:S:21:ALA:HB1	20:P:117:ALA:HB1	1.96	0.48
13:A:182:LYS:HD2	18:X:431:GLN:HG3	1.95	0.48
13:A:196:GLN:N	13:A:227:LYS:O	2.43	0.48
14:Y:451:ALA:O	14:Y:487:ASN:ND2	2.46	0.48
10:M:115:ILE:HG13	10:M:168:LEU:HD21	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:158:GLN:O	12:G:164:ASN:ND2	2.44	0.48
14:Y:408:THR:HG22	14:Y:487:ASN:HB3	1.95	0.48
1:N:70:LEU:HD13	2:B:25:ASN:HB2	1.96	0.48
1:Q:99:TYR:O	1:Q:103:LEU:N	2.46	0.48
4:U:28:DC:H4'	4:U:29:DA:H5'	1.94	0.48
20:P:56:SER:HA	20:P:59:MET:HB3	1.96	0.48
21:g:438:GLN:O	21:g:442:HIS:ND1	2.46	0.48
14:Y:524:VAL:HB	14:Y:573:LEU:HD23	1.96	0.48
14:Y:594:MET:HB2	14:Y:622:ARG:HA	1.95	0.48
8:F:352:ALA:HB1	12:G:25:ASP:HB3	1.96	0.48
10:M:141:LEU:HB3	10:M:205:TRP:HZ2	1.78	0.48
14:J:260:LYS:O	14:J:264:ASN:ND2	2.47	0.48
20:P:51:ASP:OD1	20:P:51:ASP:N	2.47	0.48
21:g:190:GLY:O	21:g:193:SER:OG	2.29	0.48
14:Y:529:SER:OG	14:Y:870:GLY:O	2.29	0.48
1:N:130:ILE:HG23	1:Q:106:ASP:HB3	1.95	0.48
8:F:374:SER:HB2	9:H:186:HIS:H	1.79	0.48
10:M:94:PRO:HA	10:M:97:ILE:HB	1.95	0.48
13:A:107:ILE:HG23	13:A:117:TYR:HE1	1.78	0.48
13:A:458:GLU:HA	13:A:461:LEU:HB2	1.95	0.48
1:Q:116:ARG:HD3	4:U:71:DG:H3'	1.96	0.47
9:D:425:SER:HA	15:E:62:LEU:HD13	1.96	0.47
10:M:550:CYS:HB3	10:M:574:TYR:HE1	1.79	0.47
13:A:223:ASN:HD21	13:A:225:ASN:HB2	1.78	0.47
3:O:73:ASN:HB2	3:O:82:HIS:HE2	1.79	0.47
12:G:27:ILE:HG22	12:G:29:ILE:H	1.80	0.47
13:A:133:ARG:NH2	13:A:134:GLU:OE2	2.47	0.47
14:J:225:ILE:HG23	14:J:229:ASP:HB3	1.96	0.47
5:W:130:DA:H4'	5:W:131:DC:H5'	1.96	0.47
9:D:462:VAL:HG11	10:M:555:PRO:HB3	1.95	0.47
4:U:9:DT:H4'	4:U:10:DC:H5'	1.96	0.47
14:J:128:ASP:OD2	14:J:198:ARG:NH2	2.47	0.47
15:E:59:ARG:NH1	15:E:63:GLU:OE2	2.47	0.47
21:g:21:VAL:HB	21:g:35:LEU:HB2	1.96	0.47
3:O:67:GLY:O	3:O:71:ARG:NE	2.42	0.47
4:U:62:DC:H2''	4:U:63:DG:C8	2.50	0.47
10:M:192:LEU:HB3	10:M:245:THR:HG21	1.95	0.47
10:M:314:GLN:HA	10:M:317:LEU:HD23	1.95	0.47
10:M:569:LEU:HD13	11:I:310:LEU:HB2	1.96	0.47
21:g:22:GLN:OE1	21:g:433:GLN:NE2	2.38	0.47
1:Q:83:ARG:HE	4:U:50:DG:H4'	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:178:ALA:HA	6:f:339:LYS:HE3	1.96	0.47
6:f:392:VAL:HB	6:f:423:THR:HA	1.97	0.47
20:P:58:ALA:HA	20:P:61:ILE:HD12	1.97	0.47
20:T:56:SER:HA	20:T:59:MET:HB3	1.96	0.47
21:g:321:ASP:OD1	21:g:321:ASP:N	2.45	0.47
14:Y:457:LYS:HA	14:Y:479:GLU:HG2	1.96	0.47
14:Y:945:PHE:HE1	14:Y:957:PHE:HB2	1.79	0.47
3:S:39:TYR:HB2	20:P:89:ILE:HD13	1.95	0.47
4:U:85:DG:N1	5:W:83:DC:O2	2.36	0.47
6:f:87:TRP:HE3	6:f:131:LEU:HD11	1.79	0.47
7:h:65:ARG:NH2	21:g:456:MET:O	2.48	0.47
9:H:414:SER:HB3	15:E:39:LEU:HD21	1.96	0.47
10:M:80:ASP:OD1	10:M:80:ASP:N	2.46	0.47
18:X:378:LEU:HD22	18:X:509:LEU:HD13	1.97	0.47
14:Y:695:LEU:HD12	14:Y:947:ASN:HB3	1.97	0.47
1:N:61:LEU:HB3	2:B:36:ARG:HB3	1.97	0.47
1:N:83:ARG:HD3	5:W:70:DT:H4'	1.97	0.47
9:H:262:THR:O	19:L:748:SER:OG	2.28	0.47
21:g:330:TRP:HZ3	21:g:353:LEU:HD22	1.79	0.47
8:F:406:PRO:HG2	8:F:409:ILE:HG12	1.97	0.47
14:Y:811:LEU:HB2	14:Y:882:VAL:HG22	1.95	0.47
14:Y:909:GLU:HB3	14:Y:987:ARG:HD2	1.97	0.47
3:O:62:ILE:HD12	3:O:65:LEU:HB2	1.96	0.46
4:U:53:DC:H5''	14:Y:757:MET:HE3	1.97	0.46
20:P:81:ALA:O	20:P:86:ARG:N	2.37	0.46
21:g:153:MET:O	14:V:359:HIS:NE2	2.48	0.46
14:Y:564:ILE:O	14:Y:567:GLY:N	2.42	0.46
1:N:80:THR:OG1	1:N:81:ASP:N	2.49	0.46
3:S:73:ASN:HB2	3:S:82:HIS:HE2	1.79	0.46
5:W:85:DC:H1'	5:W:86:DG:C5	2.51	0.46
6:f:180:VAL:HG11	6:f:332:LEU:HD11	1.97	0.46
10:M:224:ASP:OD1	10:M:257:TYR:OH	2.30	0.46
11:I:440:ASN:HB2	15:E:29:LEU:HD13	1.96	0.46
14:Y:535:THR:O	14:Y:539:GLU:N	2.47	0.46
14:Y:876:LEU:O	14:Y:906:GLN:NE2	2.48	0.46
3:S:62:ILE:HD12	3:S:65:LEU:HB2	1.96	0.46
6:f:241:LYS:HD2	6:f:410:LYS:HG2	1.98	0.46
9:D:101:SER:OG	9:D:102:ASN:N	2.49	0.46
18:X:528:ILE:HA	18:X:602:LEU:HD12	1.97	0.46
21:g:437:LYS:O	21:g:441:THR:OG1	2.29	0.46
3:S:12:ALA:HB3	4:U:32:DT:H4'	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:134:LEU:HD12	10:M:137:ILE:HD12	1.95	0.46
21:g:279:LEU:O	21:g:298:ARG:NH2	2.48	0.46
6:f:442:THR:HB	14:V:334:ILE:HG12	1.97	0.46
7:h:6:LEU:HD23	21:g:102:PHE:HZ	1.81	0.46
9:H:180:GLY:HA3	9:D:198:LYS:HE2	1.96	0.46
12:G:276:ASP:OD1	12:G:301:ASN:ND2	2.42	0.46
13:A:14:LEU:HD13	13:A:92:PHE:HE1	1.79	0.46
20:P:110:ALA:HA	20:P:113:GLU:HB2	1.97	0.46
9:H:430:GLN:HG2	9:D:429:ILE:HD11	1.98	0.46
14:Y:809:ARG:HG2	14:Y:861:PHE:HD1	1.80	0.46
3:S:76:THR:O	20:P:53:GLY:N	2.49	0.46
4:U:33:DG:H1'	4:U:34:DG:C8	2.50	0.46
6:f:80:TRP:HZ2	6:f:119:ILE:HD12	1.81	0.46
8:F:342:LEU:HD22	9:D:179:ILE:HD13	1.98	0.46
9:H:390:MET:HG3	15:E:33:ARG:HD2	1.97	0.46
9:H:454:LEU:HB3	9:D:454:LEU:HD11	1.97	0.46
9:D:193:THR:HG22	9:D:195:GLN:H	1.81	0.46
10:M:93:ILE:HB	10:M:96:GLU:HB2	1.98	0.46
13:A:486:SER:O	18:X:622:ASN:ND2	2.49	0.46
3:O:43:VAL:N	4:U:113:DA:OP1	2.49	0.46
10:M:95:GLU:HA	10:M:98:LYS:HB2	1.98	0.46
10:M:547:SER:HA	10:M:550:CYS:HB2	1.98	0.46
11:I:260:ILE:HG12	11:I:319:LEU:HD21	1.97	0.46
1:Q:86:SER:HA	1:Q:89:VAL:HB	1.97	0.46
2:R:32:PRO:O	2:R:36:ARG:N	2.45	0.46
19:L:745:ALA:HB1	19:L:793:ARG:HH22	1.81	0.46
19:L:874:PHE:HA	19:L:877:HIS:HB3	1.98	0.46
21:g:41:ILE:HG21	21:g:78:ALA:HB1	1.98	0.46
14:Y:731:LYS:HA	14:Y:735:LEU:HD12	1.98	0.46
7:h:26:ARG:NH1	7:h:70:GLU:OE1	2.49	0.45
10:M:72:PRO:HB2	10:M:75:THR:HG22	1.98	0.45
1:N:48:LEU:HG	3:S:111:ILE:HG21	1.98	0.45
4:U:16:DG:H1'	4:U:17:DC:H5'	1.97	0.45
4:U:149:DG:N2	5:W:20:DT:O2	2.49	0.45
6:f:105:VAL:HG22	6:f:137:GLN:HB3	1.98	0.45
9:H:66:GLU:HB2	9:H:228:LEU:HD13	1.98	0.45
1:Q:63:ARG:HB2	1:Q:66:PRO:HD2	1.99	0.45
6:f:247:GLU:HG2	6:f:284:LEU:HD11	1.99	0.45
11:I:430:LEU:HA	11:I:433:TYR:HB3	1.97	0.45
12:G:355:ASN:N	12:G:355:ASN:OD1	2.48	0.45
13:A:170:THR:HG22	13:A:173:ASP:H	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Y:490:ASN:ND2	14:Y:644:VAL:O	2.49	0.45
14:Y:769:PHE:HB2	14:Y:772:VAL:HG23	1.98	0.45
2:B:59:LYS:HA	2:B:62:LEU:HD12	1.99	0.45
13:A:37:ALA:O	13:A:79:ARG:NH2	2.45	0.45
20:P:86:ARG:HA	20:P:86:ARG:HD3	1.78	0.45
14:Y:916:ILE:HG13	14:Y:926:LEU:HD22	1.98	0.45
14:Y:925:ILE:HA	14:Y:928:ARG:HB2	1.98	0.45
6:f:56:ASP:OD2	21:g:312:ARG:NH2	2.48	0.45
9:H:414:SER:OG	11:I:423:SER:OG	2.30	0.45
9:D:434:LYS:HE3	9:D:434:LYS:HB2	1.71	0.45
13:A:47:ILE:HD13	13:A:100:LYS:HB3	1.97	0.45
13:A:134:GLU:HA	13:A:137:ARG:HD3	1.99	0.45
18:X:434:MET:O	18:X:443:MET:N	2.46	0.45
14:Y:991:GLU:HA	14:Y:994:LEU:HB3	1.99	0.45
9:H:161:GLU:HG3	9:H:167:ASN:HB2	1.99	0.45
9:H:178:LEU:HB2	9:D:198:LYS:HB3	1.99	0.45
13:A:423:LEU:HD23	13:A:426:LEU:HD12	1.98	0.45
18:X:443:MET:HE2	18:X:443:MET:HB3	1.79	0.45
21:g:165:GLY:O	21:g:339:THR:OG1	2.33	0.45
14:Y:929:ALA:HA	14:Y:932:LYS:HE2	1.98	0.45
21:g:39:THR:HG22	21:g:67:PRO:HD2	1.97	0.45
2:B:31:LYS:HA	2:B:34:ILE:HD12	1.98	0.45
3:O:102:ILE:HG23	20:T:61:ILE:HD12	1.98	0.45
1:Q:125:GLN:HA	1:Q:128:ARG:HB2	1.98	0.45
8:F:371:TRP:HZ3	9:H:187:PHE:HB3	1.81	0.45
9:D:73:LEU:O	9:D:77:THR:OG1	2.30	0.45
10:M:140:GLY:O	10:M:145:SER:OG	2.30	0.45
14:Y:612:THR:O	14:Y:616:TYR:N	2.45	0.45
2:B:92:ARG:HG3	20:T:79:ARG:HH22	1.82	0.45
1:Q:116:ARG:NH1	1:Q:118:THR:O	2.50	0.45
4:U:37:DG:H4'	4:U:38:DT:H5'	1.99	0.45
6:f:410:LYS:HD2	6:f:410:LYS:HA	1.72	0.45
9:D:227:ASN:HD21	14:J:240:LYS:HE2	1.82	0.45
13:A:255:PRO:HB2	13:A:259:LEU:HD22	1.99	0.45
15:E:62:LEU:O	15:E:66:LYS:N	2.48	0.45
18:X:374:THR:O	18:X:488:GLY:N	2.50	0.45
14:Y:462:PRO:HG2	14:Y:465:LEU:HG	1.99	0.45
4:U:12:DC:O2	5:W:157:DG:N2	2.50	0.44
9:H:426:GLN:HA	9:H:429:ILE:HD12	2.00	0.44
13:A:252:SER:HB3	13:A:254:ILE:HG12	1.98	0.44
19:L:878:ARG:HA	19:L:881:MET:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:g:101:ALA:HB1	21:g:105:GLU:HB2	1.99	0.44
1:Q:62:ILE:HG23	2:R:29:ILE:HG12	1.98	0.44
6:f:155:PHE:HB3	6:f:392:VAL:HA	1.97	0.44
9:D:330:TYR:O	9:D:333:GLN:NE2	2.50	0.44
11:I:27:VAL:O	11:I:29:ASN:ND2	2.50	0.44
13:A:393:LEU:O	14:J:60:TYR:OH	2.35	0.44
18:X:377:TYR:HB2	18:X:512:GLN:HB3	1.99	0.44
14:Y:465:LEU:HD22	14:Y:541:TRP:HE3	1.83	0.44
14:Y:696:ARG:O	14:Y:947:ASN:ND2	2.48	0.44
3:O:81:ARG:HD3	1:Q:58:THR:HB	1.98	0.44
1:Q:125:GLN:O	1:Q:129:ARG:N	2.49	0.44
4:U:109:DC:H1'	4:U:110:DC:C2	2.52	0.44
7:h:34:LYS:HG2	7:h:56:TYR:CZ	2.52	0.44
21:g:44:THR:HB	21:g:61:LYS:HZ1	1.81	0.44
1:N:102:GLY:O	1:N:131:ARG:NH2	2.44	0.44
8:F:384:ILE:O	9:H:235:TYR:N	2.46	0.44
20:P:90:THR:OG1	20:P:93:GLU:OE1	2.29	0.44
21:g:131:VAL:HA	21:g:135:LEU:HB2	1.98	0.44
21:g:198:LEU:HD13	21:g:213:LEU:HD23	1.99	0.44
2:R:59:LYS:HA	2:R:62:LEU:HD12	1.99	0.44
4:U:102:DG:N2	5:W:67:DC:O2	2.51	0.44
9:H:401:LEU:HD22	11:I:427:ARG:HD2	1.99	0.44
13:A:408:GLU:OE2	14:J:99:THR:OG1	2.33	0.44
1:Q:46:VAL:HG12	1:Q:49:ARG:HH12	1.83	0.44
4:U:87:DT:H6	4:U:87:DT:H2'	1.68	0.44
1:Q:128:ARG:HB3	1:Q:133:GLU:HB2	1.99	0.44
9:H:450:LEU:HD13	11:I:50:ARG:HG2	2.00	0.44
21:g:214:LYS:HB3	21:g:214:LYS:HE2	1.84	0.44
21:g:361:GLU:OE1	21:g:369:ARG:NH2	2.50	0.44
14:Y:553:THR:HG22	14:Y:555:ASN:H	1.83	0.44
4:U:26:DC:H2''	4:U:27:DT:C5	2.51	0.44
9:H:401:LEU:O	11:I:427:ARG:NH2	2.51	0.44
9:D:329:MET:HE2	19:L:874:PHE:HB2	2.00	0.44
11:I:237:ASN:HB3	11:I:322:VAL:HG12	2.00	0.44
1:N:113:HIS:ND1	1:Q:126:LEU:HD13	2.32	0.44
5:W:25:DG:H2''	5:W:26:DA:C8	2.53	0.44
5:W:102:DG:H1'	5:W:103:DT:H5'	2.00	0.44
7:h:2:ASP:HB3	7:h:5:THR:HG22	2.00	0.44
7:h:22:LYS:HA	21:g:451:ARG:HH21	1.83	0.44
13:A:269:LEU:HG	13:A:274:TYR:HE1	1.83	0.44
1:N:100:LEU:HD12	2:B:37:LEU:HD22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:88:DT:H2''	4:U:89:DT:C6	2.53	0.43
10:M:105:LEU:HD21	10:M:163:LEU:HD23	2.00	0.43
13:A:281:TRP:CH2	13:A:306:ARG:HG3	2.53	0.43
21:g:419:TRP:HH2	21:g:429:PHE:HB3	1.83	0.43
21:g:424:TYR:HB3	21:g:427:ILE:HD12	2.00	0.43
14:Y:896:GLN:HG3	14:Y:900:ARG:HH22	1.83	0.43
3:S:30:VAL:O	3:S:34:LEU:N	2.50	0.43
4:U:58:DT:H4'	4:U:59:DA:H5'	1.98	0.43
6:f:89:TYR:O	6:f:93:THR:OG1	2.29	0.43
13:A:313:ARG:HD3	15:E:16:TYR:HB3	2.00	0.43
14:Y:937:GLY:HA2	14:Y:941:GLN:HB2	1.99	0.43
1:Q:118:THR:HA	2:R:45:ARG:HB3	1.99	0.43
5:W:48:DT:H4'	5:W:49:DG:H5'	2.00	0.43
5:W:139:DT:H2''	5:W:140:DG:C5	2.54	0.43
13:A:459:VAL:O	13:A:464:LYS:N	2.50	0.43
20:T:94:ILE:H	20:T:94:ILE:HG13	1.66	0.43
14:Y:938:LYS:HG2	14:Y:961:LEU:HD21	2.01	0.43
7:h:12:LYS:N	21:g:107:SER:O	2.51	0.43
9:H:472:ARG:HH21	9:D:468:MET:HG2	1.82	0.43
14:V:350:GLN:O	14:V:354:LEU:N	2.43	0.43
14:Y:472:GLU:HA	14:Y:475:LEU:HB2	2.01	0.43
3:O:30:VAL:O	3:O:34:LEU:N	2.50	0.43
2:R:35:ARG:HH21	2:R:39:ARG:HH21	1.66	0.43
6:f:333:MET:HB3	6:f:412:LEU:HD13	2.00	0.43
8:F:358:HIS:HB3	9:D:179:ILE:HG13	1.99	0.43
9:H:93:LYS:HB3	9:H:93:LYS:HE2	1.82	0.43
10:M:203:ASN:HD22	10:M:206:GLN:HE21	1.67	0.43
21:g:47:GLN:N	21:g:47:GLN:CD	2.73	0.43
4:U:127:DT:H2''	4:U:128:DG:C8	2.53	0.43
12:G:208:LEU:HD11	12:G:254:ILE:HG12	2.01	0.43
14:Y:473:TYR:O	14:Y:697:ARG:NH1	2.51	0.43
8:F:402:LEU:HD12	8:F:425:GLN:HB3	2.01	0.43
9:H:249:ARG:HH22	9:H:346:ARG:HD2	1.83	0.43
14:Y:835:MET:SD	14:Y:835:MET:N	2.92	0.43
9:H:407:LEU:HD22	11:I:426:PRO:HB2	2.00	0.43
9:D:319:GLU:HB3	9:D:341:VAL:HG13	2.01	0.43
10:M:29:PHE:HA	10:M:32:MET:HE3	2.01	0.43
10:M:341:PRO:O	10:M:560:LYS:NZ	2.51	0.43
18:X:502:LEU:HD23	18:X:502:LEU:HA	1.91	0.43
3:S:65:LEU:HD23	3:S:68:ASN:HD22	1.84	0.43
5:W:46:DC:H1'	5:W:47:DC:C2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:129:DT:H2''	5:W:130:DA:C5	2.53	0.43
8:F:402:LEU:HD13	8:F:422:ILE:HG23	2.01	0.43
12:G:20:LEU:HD23	12:G:27:ILE:HG21	2.01	0.43
13:A:20:ILE:HD11	19:L:875:THR:HB	2.01	0.43
20:P:46:LYS:HA	20:P:46:LYS:HD3	1.84	0.43
21:g:71:GLY:O	21:g:119:TRP:NE1	2.48	0.43
21:g:220:GLU:HG2	21:g:276:ASN:HD22	1.84	0.43
14:Y:699:LYS:NZ	14:Y:705:ASP:OD1	2.52	0.43
4:U:117:DT:H2''	4:U:118:DC:H2'	2.01	0.43
5:W:28:DG:H1'	5:W:29:DT:H5'	2.01	0.43
10:M:109:ASN:HA	14:J:292:ARG:HD3	2.01	0.43
10:M:254:LYS:NZ	11:I:15:ASP:OD2	2.44	0.43
14:Y:682:ILE:O	14:Y:686:LEU:N	2.49	0.43
7:h:31:GLN:HG2	7:h:55:LYS:HE3	2.00	0.42
9:H:401:LEU:HD23	9:H:407:LEU:HD21	2.01	0.42
14:Y:876:LEU:HD12	14:Y:878:THR:H	1.83	0.42
5:W:93:DA:H2''	5:W:94:DG:H8	1.84	0.42
7:h:85:LYS:HE3	7:h:85:LYS:HB2	1.83	0.42
9:D:316:SER:HB2	19:L:807:GLY:HA3	2.01	0.42
18:X:447:PRO:HB3	18:X:480:ASN:HD22	1.83	0.42
14:Y:698:LEU:HD21	14:Y:944:LYS:HD3	2.01	0.42
3:O:83:LEU:HD13	20:T:61:ILE:HG21	2.01	0.42
10:M:286:HIS:HA	10:M:289:LEU:HB3	2.02	0.42
14:J:268:GLN:HB3	14:J:271:HIS:HD2	1.84	0.42
20:P:116:LYS:HB3	20:P:116:LYS:HE2	1.83	0.42
21:g:132:PHE:O	21:g:451:ARG:NH1	2.42	0.42
21:g:335:ILE:HD13	21:g:349:LEU:HD23	2.01	0.42
3:O:42:ARG:HH22	5:W:58:DG:N2	2.16	0.42
3:O:76:THR:O	20:T:53:GLY:N	2.53	0.42
1:Q:54:TYR:HB3	2:R:40:ARG:HE	1.83	0.42
4:U:59:DA:H2	5:W:110:DA:H2	1.67	0.42
9:D:116:LYS:HD2	9:D:116:LYS:HA	1.81	0.42
13:A:487:ILE:HG21	19:L:747:SER:HB2	2.01	0.42
18:X:435:GLN:HA	18:X:442:THR:HA	2.01	0.42
14:Y:630:LEU:HB2	14:Y:634:LEU:HD12	2.01	0.42
3:O:65:LEU:HD23	3:O:68:ASN:HD22	1.84	0.42
4:U:69:DA:H4'	4:U:70:DC:H5'	2.02	0.42
5:W:149:DC:H2''	5:W:150:DG:N7	2.35	0.42
11:I:419:PHE:O	11:I:423:SER:N	2.47	0.42
18:X:376:ASP:O	18:X:486:PHE:N	2.49	0.42
14:Y:522:PHE:HE1	14:Y:592:ALA:HB3	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:39:DA:H2	5:W:130:DA:H2	1.66	0.42
6:f:422:THR:O	6:f:422:THR:OG1	2.37	0.42
7:h:85:LYS:HA	7:h:88:ASP:HB2	2.00	0.42
13:A:273:TRP:HA	15:E:20:THR:HB	2.01	0.42
16:C:194:ALA:N	17:K:164:ILE:O	2.52	0.42
21:g:457:LYS:HB3	21:g:460:ALA:HB3	2.01	0.42
14:Y:499:LEU:HD22	14:Y:702:VAL:HG11	2.01	0.42
6:f:161:ALA:HA	6:f:186:GLY:H	1.84	0.42
10:M:323:ILE:HD13	10:M:540:ASP:HB2	2.02	0.42
21:g:40:GLN:HB3	21:g:66:LYS:HG2	2.00	0.42
14:Y:475:LEU:HD23	14:Y:475:LEU:HA	1.89	0.42
14:Y:503:ILE:O	14:Y:507:SER:OG	2.34	0.42
4:U:123:DC:O2	20:T:33:ARG:NH1	2.53	0.42
6:f:453:LYS:NZ	6:f:459:ASP:OD2	2.52	0.42
9:H:179:ILE:HG22	11:I:468:ARG:HH12	1.85	0.42
9:H:428:ILE:HD13	9:H:428:ILE:HA	1.90	0.42
20:P:71:GLU:HA	20:P:74:ALA:HB3	2.01	0.42
14:Y:453:ARG:H	14:Y:453:ARG:HG2	1.62	0.42
12:G:211:GLU:HA	12:G:216:THR:HA	2.02	0.42
13:A:48:TYR:O	13:A:52:CYS:N	2.40	0.42
4:U:15:DT:H2'	4:U:16:DG:C8	2.55	0.42
11:I:41:SER:O	11:I:45:LEU:N	2.52	0.42
14:Y:894:ASP:O	14:Y:898:GLN:N	2.51	0.42
11:I:245:GLN:HG2	11:I:246:THR:HG22	2.02	0.41
13:A:198:ARG:HD2	13:A:198:ARG:HA	1.87	0.41
13:A:278:THR:HB	13:A:306:ARG:HG2	2.01	0.41
16:C:197:ASP:O	17:K:160:GLN:NE2	2.53	0.41
14:Y:779:SER:O	14:Y:779:SER:OG	2.38	0.41
4:U:95:DC:N4	5:W:72:DG:O6	2.53	0.41
15:E:54:ASN:HB3	15:E:57:ARG:HE	1.84	0.41
1:N:63:ARG:HH11	5:W:81:DA:H5''	1.86	0.41
1:Q:103:LEU:O	1:Q:107:THR:OG1	2.30	0.41
1:Q:134:ARG:O	3:S:95:LYS:NZ	2.48	0.41
3:S:34:LEU:HA	3:S:39:TYR:HE2	1.85	0.41
6:f:196:ARG:NH2	6:f:312:TYR:OH	2.53	0.41
8:F:430:LYS:HA	8:F:430:LYS:HD2	1.83	0.41
9:H:363:TYR:HB3	14:J:195:ILE:HG23	2.01	0.41
9:H:426:GLN:HG2	11:I:27:VAL:HA	2.03	0.41
10:M:64:ASN:OD1	10:M:64:ASN:N	2.52	0.41
10:M:330:LYS:HB2	10:M:330:LYS:HE2	1.83	0.41
11:I:220:ILE:HD12	11:I:351:LEU:HD22	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:248:SER:OG	11:I:249:VAL:N	2.53	0.41
13:A:395:ASN:O	14:J:90:GLN:NE2	2.53	0.41
20:P:54:ILE:HD13	20:P:59:MET:HE2	2.01	0.41
3:O:111:ILE:HG23	1:Q:51:ILE:HG21	2.03	0.41
2:R:75:HIS:ND1	20:P:96:THR:OG1	2.41	0.41
4:U:75:DT:H6	4:U:75:DT:H2'	1.63	0.41
5:W:41:DA:H1'	5:W:42:DC:H5'	2.02	0.41
6:f:69:THR:OG1	6:f:78:TYR:OH	2.35	0.41
6:f:198:ALA:HA	6:f:201:ILE:HG12	2.02	0.41
8:F:362:SER:OG	9:H:195:GLN:O	2.31	0.41
14:J:53:ALA:HB1	14:J:57:GLN:HG2	2.02	0.41
14:J:132:PRO:HG2	14:J:134:TYR:HE1	1.86	0.41
20:P:36:SER:OG	20:P:37:TYR:N	2.54	0.41
14:V:334:ILE:O	14:V:338:GLN:N	2.49	0.41
4:U:113:DA:H2''	4:U:114:DG:H8	1.84	0.41
5:W:30:DA:H2'	5:W:31:DT:C2	2.55	0.41
5:W:155:DC:H6	5:W:155:DC:H2'	1.61	0.41
8:F:350:ARG:NH2	12:G:25:ASP:OD1	2.42	0.41
9:H:414:SER:HB2	11:I:419:PHE:HB3	2.03	0.41
10:M:81:ASP:HB3	10:M:85:MET:HE3	2.02	0.41
13:A:238:GLU:OE1	14:J:212:ASN:ND2	2.53	0.41
14:V:337:ARG:HA	14:V:340:GLU:HB2	2.02	0.41
2:B:71:THR:HG21	20:T:100:LEU:HD21	2.03	0.41
3:O:63:LEU:HB3	20:T:48:VAL:HG21	2.03	0.41
4:U:118:DC:O2	5:W:50:DG:N1	2.47	0.41
10:M:61:SER:O	10:M:61:SER:OG	2.38	0.41
13:A:265:MET:HE1	14:J:262:ILE:HG21	2.01	0.41
14:Y:485:TYR:OH	14:Y:622:ARG:O	2.36	0.41
5:W:69:DC:H1'	5:W:70:DT:C2	2.55	0.41
11:I:421:GLU:HA	11:I:424:LEU:HB2	2.01	0.41
18:X:602:LEU:HB3	18:X:619:PHE:HB2	2.02	0.41
20:T:74:ALA:O	20:T:78:SER:OG	2.33	0.41
14:Y:723:GLN:HA	14:Y:726:TYR:HD2	1.86	0.41
3:O:62:ILE:O	3:O:66:ALA:N	2.48	0.41
2:R:92:ARG:HD3	20:P:79:ARG:HH22	1.86	0.41
3:S:62:ILE:O	3:S:66:ALA:N	2.48	0.41
6:f:236:LEU:HD23	6:f:236:LEU:HA	1.85	0.41
9:H:246:ASP:OD2	12:G:160:HIS:NE2	2.53	0.41
9:H:409:LYS:HB3	9:D:399:THR:HA	2.03	0.41
9:D:112:PHE:HB3	12:G:361:TYR:CG	2.56	0.41
9:D:312:LYS:HD3	9:D:312:LYS:HA	1.91	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:76:ILE:HA	13:A:79:ARG:HG2	2.02	0.41
21:g:162:ILE:HD12	21:g:335:ILE:HG12	2.02	0.41
21:g:275:LYS:HG3	21:g:277:SER:H	1.86	0.41
21:g:369:ARG:NH1	21:g:398:ILE:HG12	2.36	0.41
14:Y:502:THR:OG1	14:Y:537:GLU:OE1	2.27	0.41
14:Y:841:THR:OG1	14:Y:842:LYS:N	2.51	0.41
1:N:128:ARG:HH22	2:B:60:VAL:HG21	1.85	0.41
3:S:75:LYS:HA	3:S:75:LYS:HD3	1.85	0.41
4:U:109:DC:H6	4:U:109:DC:H2'	1.76	0.41
4:U:114:DG:H1'	4:U:115:DT:H5'	2.03	0.41
5:W:79:DA:H2''	5:W:80:DA:C8	2.56	0.41
6:f:38:ARG:HB3	6:f:46:GLU:HB3	2.03	0.41
9:H:104:ASP:HB3	9:H:113:LYS:HD3	2.03	0.41
9:D:155:LYS:HE2	9:D:155:LYS:HB3	1.76	0.41
9:D:192:ASP:O	10:M:84:ARG:NH2	2.52	0.41
9:D:465:SER:HA	9:D:468:MET:HB2	2.03	0.41
10:M:118:ARG:HD2	10:M:118:ARG:HA	1.91	0.41
11:I:7:PRO:HB2	13:A:282:LEU:HB3	2.03	0.41
13:A:273:TRP:HE1	15:E:22:LYS:HD2	1.86	0.41
21:g:359:ILE:HB	21:g:405:THR:HA	2.02	0.41
14:Y:936:ASP:HB3	14:Y:940:ILE:HG23	2.02	0.41
5:W:62:DT:H2''	5:W:63:DA:N7	2.36	0.41
9:H:390:MET:HE2	15:E:33:ARG:HB3	2.03	0.41
9:D:103:PRO:HA	9:D:106:PHE:HD2	1.86	0.41
12:G:20:LEU:HB3	12:G:30:PHE:HD2	1.86	0.41
14:J:113:ASP:HA	14:J:116:ASN:HB2	2.03	0.41
21:g:314:GLY:HA3	21:g:357:HIS:CE1	2.56	0.41
1:Q:72:ARG:HG2	1:Q:84:PHE:CD2	2.56	0.40
6:f:292:PHE:HD2	6:f:295:LEU:HB2	1.86	0.40
9:H:439:LYS:O	9:H:442:SER:OG	2.31	0.40
9:D:88:TRP:O	9:D:95:HIS:NE2	2.54	0.40
10:M:189:LEU:HD11	10:M:241:HIS:HB3	2.03	0.40
10:M:270:LEU:HD13	10:M:280:ALA:HB2	2.03	0.40
11:I:320:GLN:NE2	11:I:327:ALA:O	2.51	0.40
15:E:66:LYS:HB2	15:E:66:LYS:HE3	1.86	0.40
18:X:602:LEU:HD22	18:X:621:ILE:HD11	2.02	0.40
14:Y:495:ASP:OD1	14:Y:697:ARG:N	2.49	0.40
1:Q:60:LEU:HD13	1:Q:93:GLN:HG2	2.03	0.40
9:H:304:LEU:HD22	9:H:318:GLN:HG3	2.02	0.40
10:M:246:LEU:HG	10:M:262:ILE:HD12	2.03	0.40
13:A:119:LEU:HD23	13:A:119:LEU:HA	1.94	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:34:LEU:HD12	3:O:34:LEU:HA	1.96	0.40
5:W:136:DA:N7	5:W:137:DA:N6	2.69	0.40
5:W:164:DC:H2"	5:W:165:DA:C8	2.56	0.40
6:f:159:ILE:HG22	6:f:398:THR:HB	2.04	0.40
10:M:148:ASP:OD1	10:M:148:ASP:N	2.53	0.40
11:I:433:TYR:O	11:I:437:SER:OG	2.32	0.40
11:I:460:ILE:HG23	11:I:470:LEU:HD21	2.04	0.40
13:A:46:LYS:HA	13:A:46:LYS:HD3	1.90	0.40
13:A:459:VAL:HG12	13:A:465:VAL:HG22	2.02	0.40
3:O:34:LEU:HA	3:O:39:TYR:HE2	1.85	0.40
4:U:138:DT:H2"	4:U:139:DA:C8	2.56	0.40
6:f:5:ARG:NH2	6:f:444:ALA:O	2.55	0.40
6:f:241:LYS:H	6:f:246:LEU:HD13	1.85	0.40
9:H:72:PHE:HA	12:G:155:LEU:HD22	2.03	0.40
9:H:154:VAL:HG11	12:G:230:ILE:HD12	2.02	0.40
9:D:104:ASP:OD2	9:D:155:LYS:NZ	2.52	0.40
10:M:62:LEU:HD11	12:G:163:PHE:HD1	1.86	0.40
13:A:184:SER:HB2	19:L:857:LYS:HG2	2.03	0.40
13:A:407:ILE:HG23	14:J:100:LEU:HD13	2.03	0.40
13:A:441:PRO:HG2	13:A:446:ARG:HH21	1.85	0.40
14:Y:553:THR:HA	14:Y:554:PRO:HD3	1.94	0.40
10:M:65:PHE:HB2	10:M:68:PHE:HD2	1.86	0.40
10:M:142:ASN:OD1	10:M:142:ASN:N	2.54	0.40
15:E:57:ARG:O	15:E:61:SER:N	2.44	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	N	96/136 (71%)	95 (99%)	1 (1%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	93/136 (68%)	90 (97%)	3 (3%)	0	100	100
2	B	80/103 (78%)	78 (98%)	2 (2%)	0	100	100
2	R	85/103 (82%)	81 (95%)	4 (5%)	0	100	100
3	O	105/130 (81%)	98 (93%)	7 (7%)	0	100	100
3	S	105/130 (81%)	98 (93%)	7 (7%)	0	100	100
6	f	391/477 (82%)	382 (98%)	9 (2%)	0	100	100
7	h	46/157 (29%)	44 (96%)	2 (4%)	0	100	100
8	F	116/435 (27%)	104 (90%)	12 (10%)	0	100	100
9	D	295/557 (53%)	282 (96%)	13 (4%)	0	100	100
9	H	387/557 (70%)	360 (93%)	27 (7%)	0	100	100
10	M	378/581 (65%)	349 (92%)	29 (8%)	0	100	100
11	I	236/483 (49%)	220 (93%)	16 (7%)	0	100	100
12	G	238/426 (56%)	221 (93%)	17 (7%)	0	100	100
13	A	357/502 (71%)	332 (93%)	25 (7%)	0	100	100
14	J	229/1359 (17%)	203 (89%)	26 (11%)	0	100	100
14	V	67/1359 (5%)	67 (100%)	0	0	100	100
14	Y	536/1359 (39%)	483 (90%)	52 (10%)	1 (0%)	43	78
15	E	56/78 (72%)	54 (96%)	2 (4%)	0	100	100
16	C	31/883 (4%)	31 (100%)	0	0	100	100
17	K	40/885 (4%)	37 (92%)	3 (8%)	0	100	100
18	X	139/625 (22%)	124 (89%)	15 (11%)	0	100	100
19	L	79/889 (9%)	68 (86%)	11 (14%)	0	100	100
20	P	91/126 (72%)	90 (99%)	1 (1%)	0	100	100
20	T	91/126 (72%)	90 (99%)	1 (1%)	0	100	100
21	g	390/467 (84%)	377 (97%)	13 (3%)	0	100	100
All	All	4757/13069 (36%)	4458 (94%)	298 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	Y	711	GLU

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	N	86/111 (78%)	86 (100%)	0	100	100
1	Q	83/111 (75%)	83 (100%)	0	100	100
2	B	68/79 (86%)	68 (100%)	0	100	100
2	R	72/79 (91%)	72 (100%)	0	100	100
3	O	84/102 (82%)	77 (92%)	7 (8%)	10	30
3	S	84/102 (82%)	77 (92%)	7 (8%)	10	30
6	f	356/420 (85%)	356 (100%)	0	100	100
7	h	53/140 (38%)	53 (100%)	0	100	100
8	F	111/388 (29%)	110 (99%)	1 (1%)	70	79
9	D	285/500 (57%)	284 (100%)	1 (0%)	84	84
9	H	363/500 (73%)	363 (100%)	0	100	100
10	M	349/521 (67%)	349 (100%)	0	100	100
11	I	223/435 (51%)	222 (100%)	1 (0%)	84	84
12	G	226/384 (59%)	226 (100%)	0	100	100
13	A	343/462 (74%)	340 (99%)	3 (1%)	70	79
14	J	187/1228 (15%)	186 (100%)	1 (0%)	81	83
14	V	63/1228 (5%)	63 (100%)	0	100	100
14	Y	502/1228 (41%)	501 (100%)	1 (0%)	87	87
15	E	56/75 (75%)	56 (100%)	0	100	100
16	C	32/824 (4%)	32 (100%)	0	100	100
17	K	39/832 (5%)	39 (100%)	0	100	100
18	X	141/578 (24%)	141 (100%)	0	100	100
19	L	77/810 (10%)	77 (100%)	0	100	100
20	P	77/105 (73%)	77 (100%)	0	100	100
20	T	79/105 (75%)	79 (100%)	0	100	100
21	g	362/423 (86%)	360 (99%)	2 (1%)	78	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4401/11770 (37%)	4377 (100%)	24 (0%)	78 83

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	O	13	LYS
3	O	18	SER
3	O	19	SER
3	O	87	VAL
3	O	93	LEU
3	O	113	SER
3	O	114	VAL
3	S	13	LYS
3	S	18	SER
3	S	19	SER
3	S	87	VAL
3	S	93	LEU
3	S	113	SER
3	S	114	VAL
8	F	390	ILE
9	D	440	LEU
11	I	246	THR
13	A	189	VAL
13	A	199	THR
13	A	465	VAL
14	J	226	THR
21	g	48	ASP
21	g	154	ILE
14	Y	458	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	68	GLN
3	O	110	ASN
3	O	112	GLN
1	Q	125	GLN
2	R	18	HIS
3	S	104	GLN
3	S	110	ASN
3	S	112	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	f	12	ASN
6	f	28	GLN
6	f	53	ASN
6	f	63	ASN
6	f	79	ASN
6	f	229	GLN
6	f	230	GLN
6	f	237	GLN
6	f	253	GLN
6	f	406	GLN
8	F	396	ASN
8	F	425	GLN
9	H	63	GLN
9	H	123	ASN
9	H	127	ASN
9	H	167	ASN
9	H	169	GLN
9	H	186	HIS
9	H	242	ASN
9	H	250	ASN
9	H	281	ASN
9	H	307	ASN
9	H	314	ASN
9	D	76	GLN
9	D	107	ASN
9	D	188	GLN
9	D	227	ASN
9	D	242	ASN
9	D	318	GLN
9	D	340	HIS
9	D	344	HIS
9	D	394	ASN
9	D	483	ASN
10	M	69	GLN
10	M	203	ASN
10	M	251	ASN
10	M	283	ASN
10	M	314	GLN
10	M	521	GLN
10	M	551	GLN
11	I	6	ASN
11	I	29	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	I	264	ASN
11	I	410	ASN
11	I	417	GLN
11	I	473	ASN
11	I	480	GLN
12	G	10	GLN
12	G	177	ASN
12	G	220	GLN
12	G	295	ASN
12	G	316	GLN
12	G	330	GLN
12	G	347	HIS
12	G	352	HIS
13	A	22	ASN
13	A	112	GLN
13	A	272	ASN
13	A	288	ASN
13	A	400	ASN
13	A	412	ASN
13	A	484	ASN
14	J	66	GLN
14	J	109	GLN
14	J	201	ASN
14	J	204	ASN
14	J	259	GLN
14	J	263	ASN
14	J	271	HIS
15	E	35	ASN
16	C	218	ASN
17	K	160	GLN
17	K	183	ASN
18	X	480	ASN
18	X	512	GLN
19	L	800	ASN
19	L	805	ASN
20	T	84	ASN
21	g	192	GLN
21	g	324	ASN
21	g	438	GLN
14	V	328	ASN
14	V	360	ASN
14	Y	487	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	Y	488	HIS
14	Y	558	HIS
14	Y	568	ASN
14	Y	600	HIS
14	Y	621	ASN
14	Y	660	ASN
14	Y	758	GLN
14	Y	931	GLN
14	Y	982	ASN
14	Y	1004	ASN
14	Y	1005	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

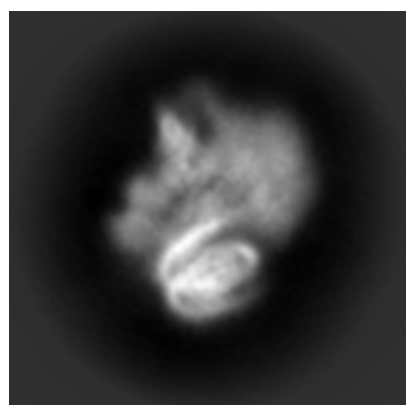
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0778. These allow visual inspection of the internal detail of the map and identification of artifacts.

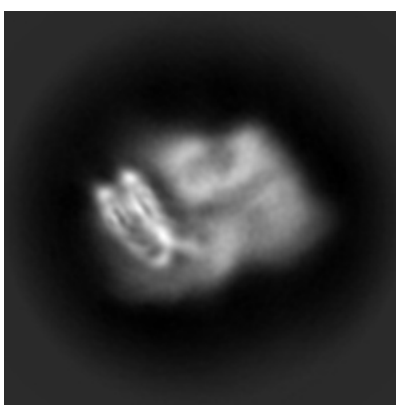
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

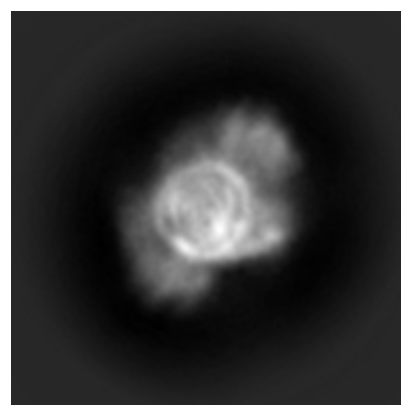
6.1.1 Primary map



X



Y

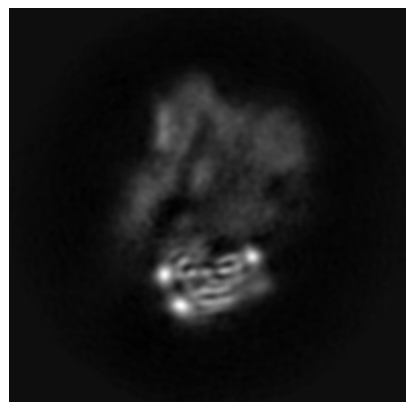


Z

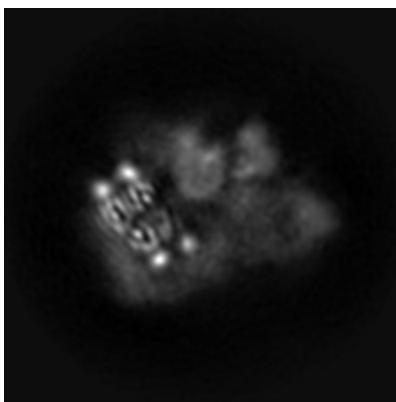
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

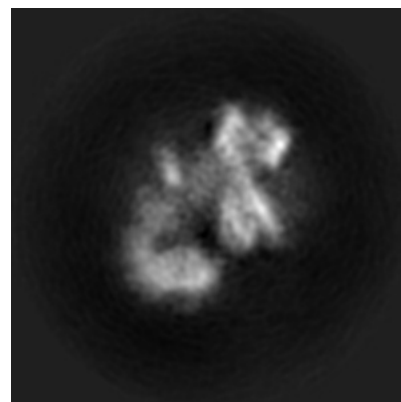
6.2.1 Primary map



X Index: 90



Y Index: 90

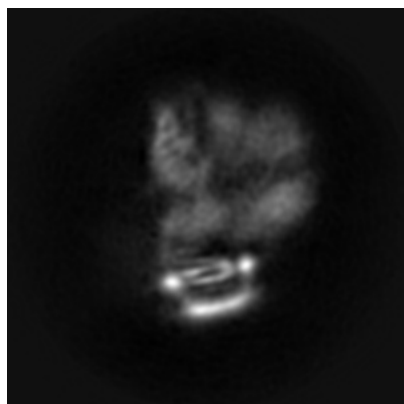


Z Index: 90

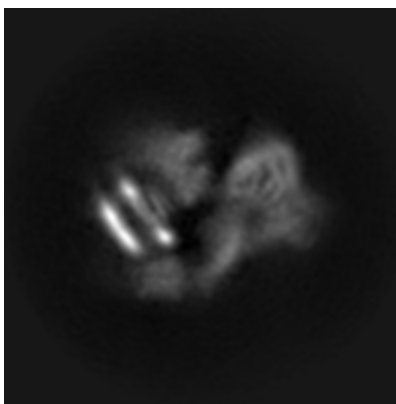
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

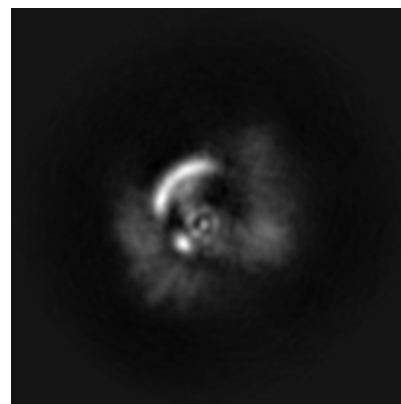
6.3.1 Primary map



X Index: 97



Y Index: 74



Z Index: 71

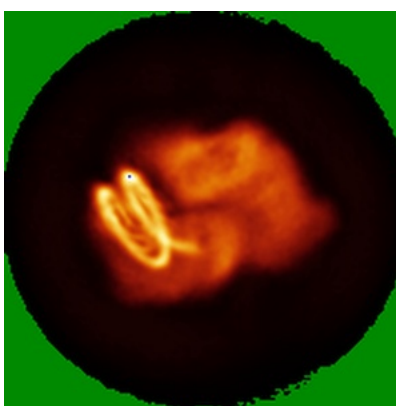
The images above show the largest variance slices of the map in three orthogonal directions.

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

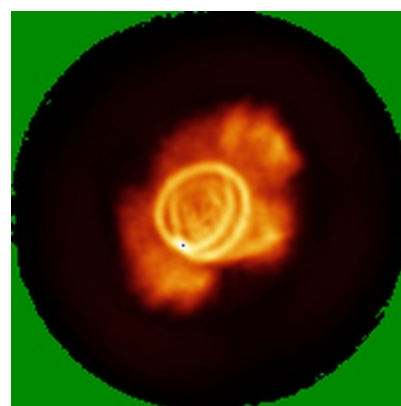
6.4.1 Primary map



X



Y

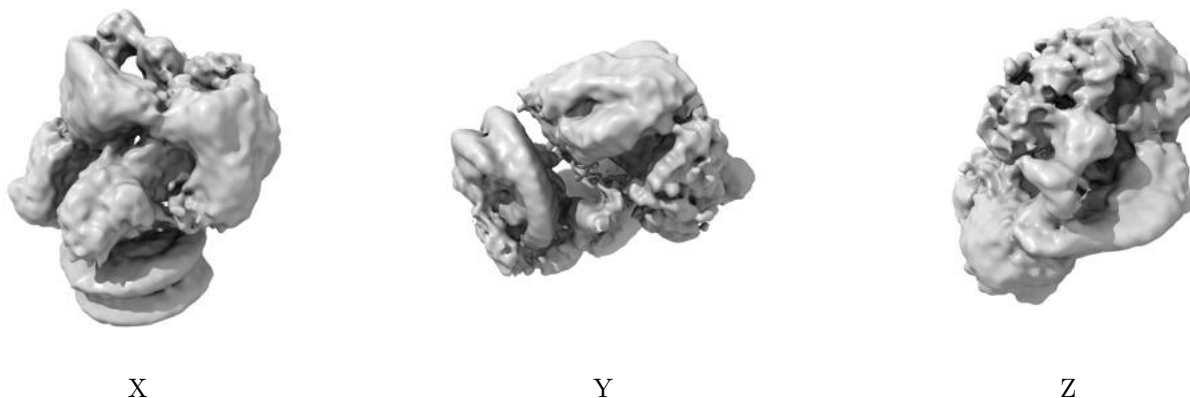


Z

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 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

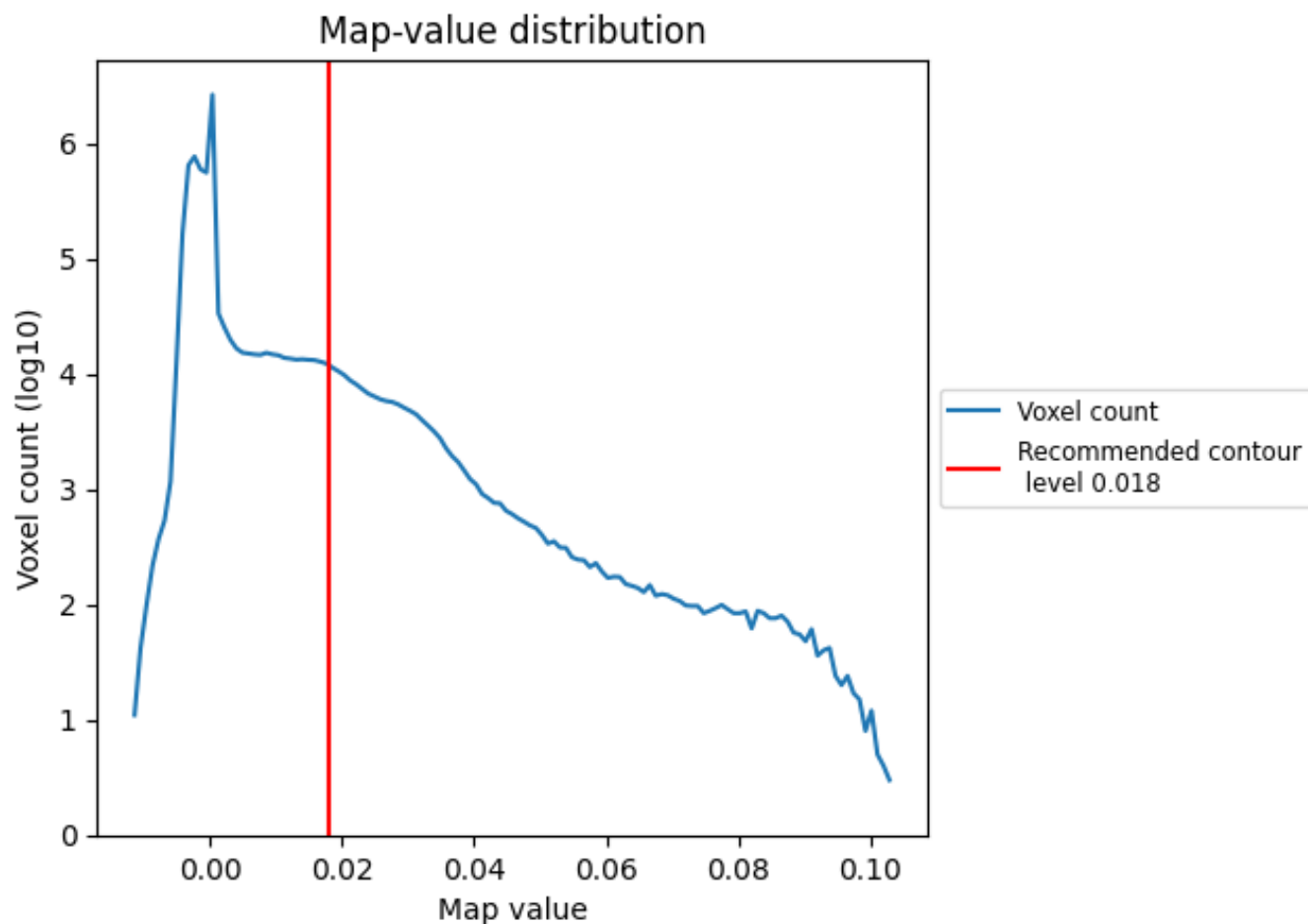
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

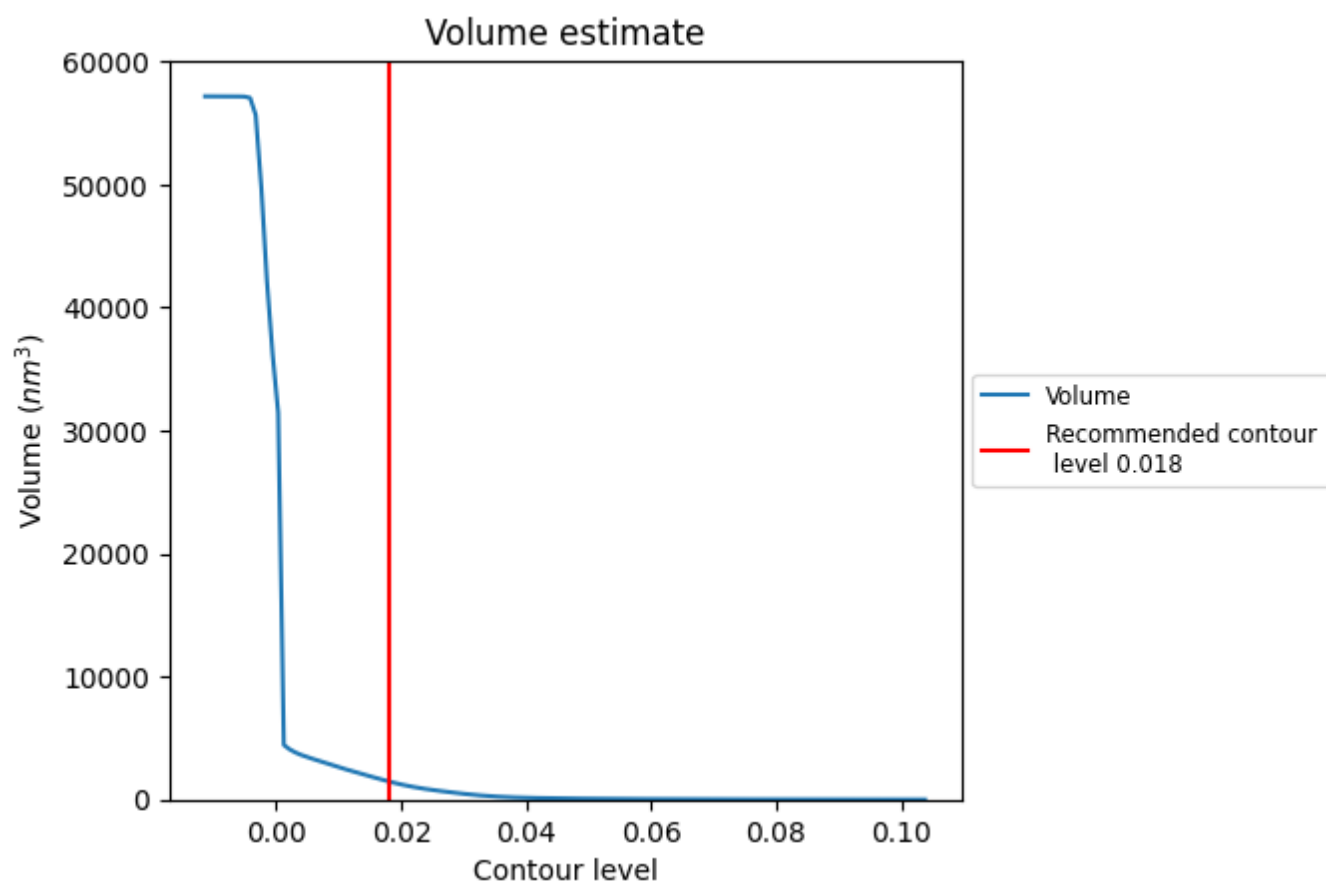
This section contains the results of statistical analysis of the map.

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.

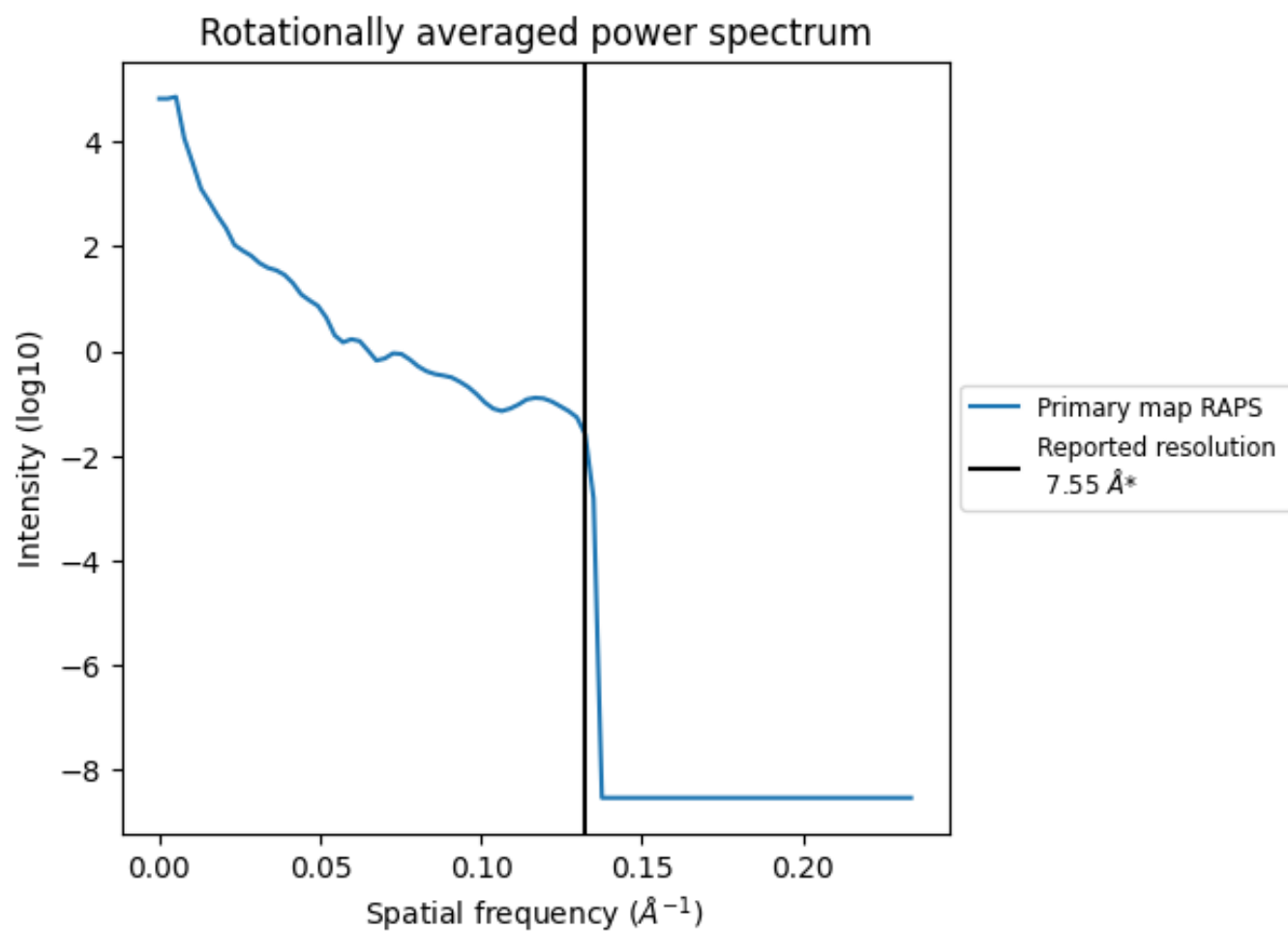
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1474 nm³; this corresponds to an approximate mass of 1331 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 0.132 Å⁻¹

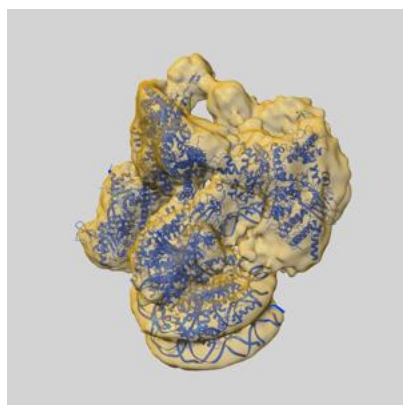
8 Fourier-Shell correlation

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

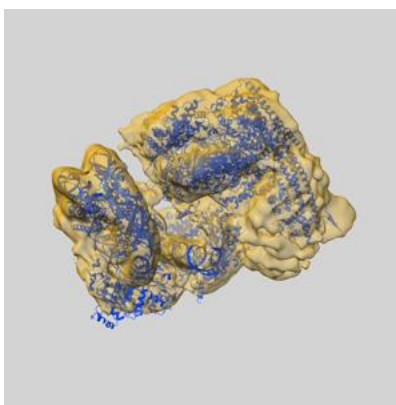
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0778 and PDB model 6KW4. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

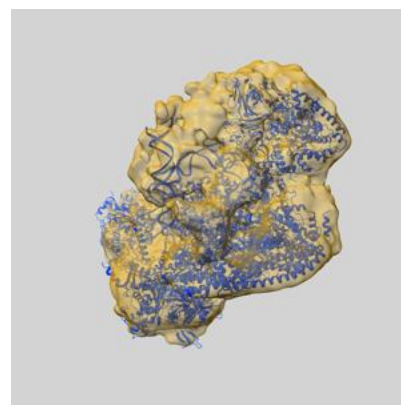
9.1 Map-model overlay [i](#)



X



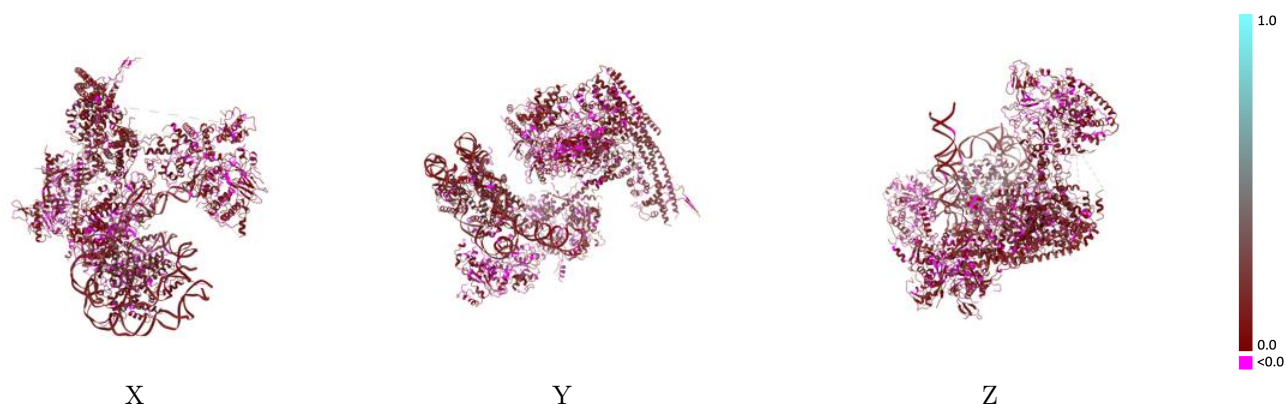
Y



Z

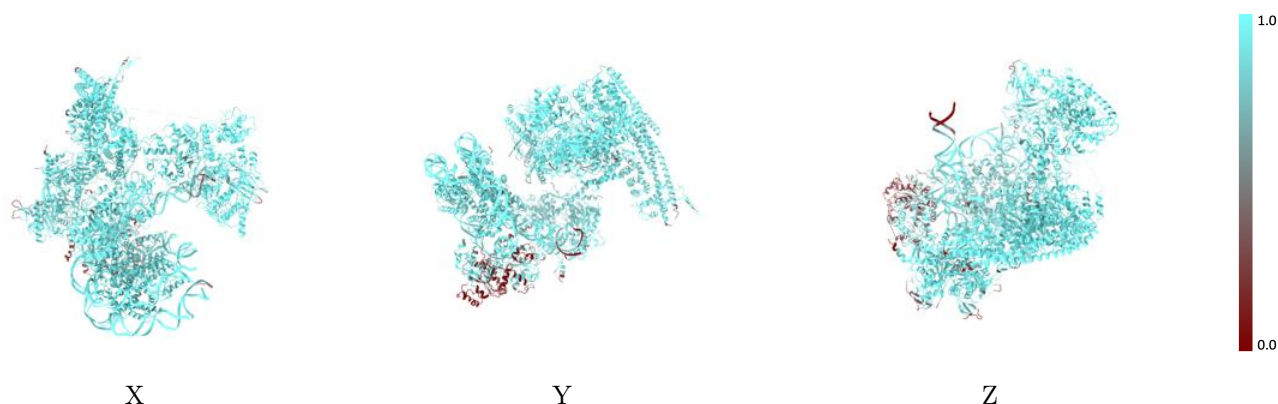
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



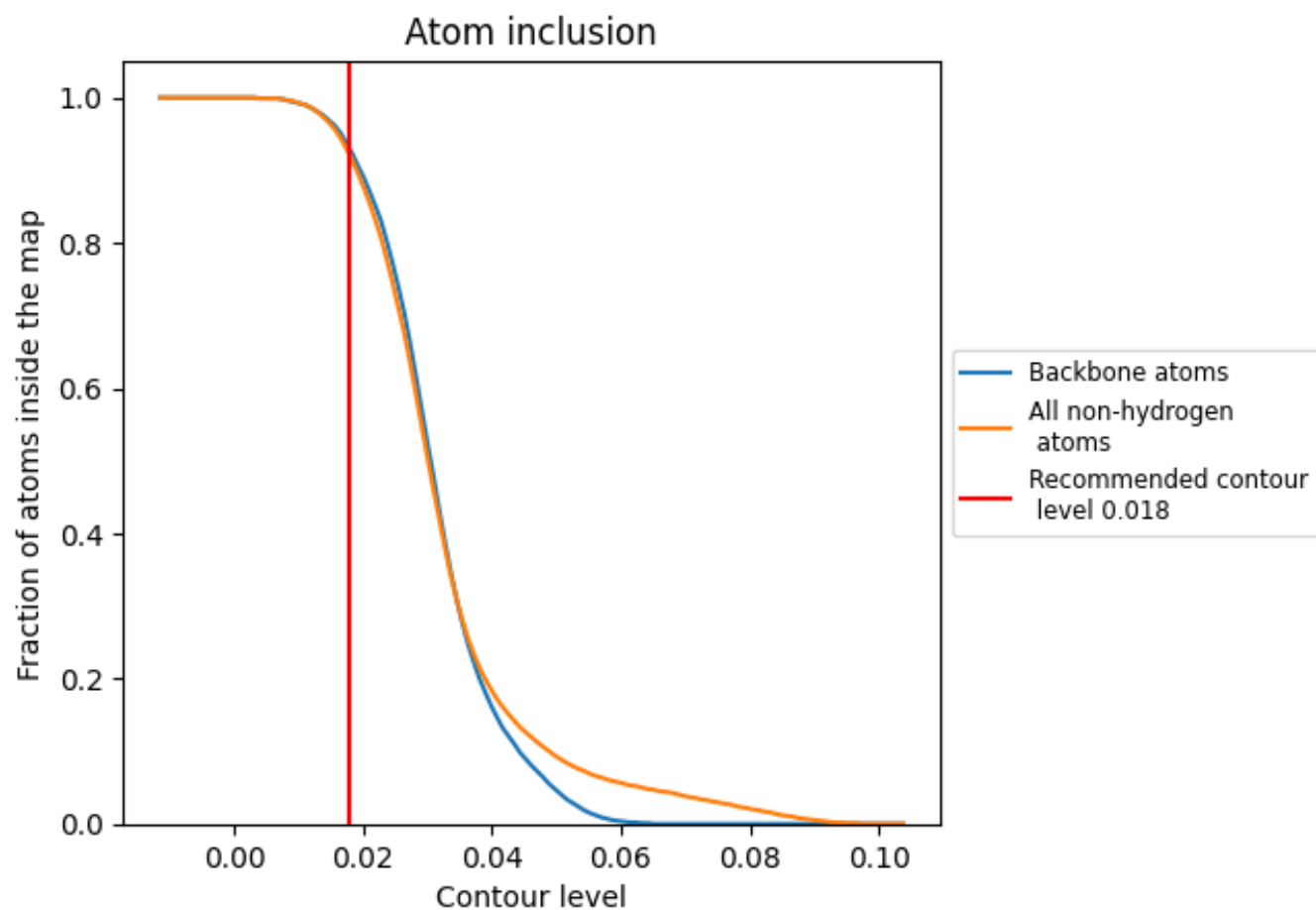
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9210	 0.0990
A	 0.9840	 0.0990
B	 0.9590	 0.1370
C	 0.9700	 0.1140
D	 0.9770	 0.1080
E	 0.9960	 0.1150
F	 0.9730	 0.0990
G	 0.9510	 0.0870
H	 0.9780	 0.1040
I	 0.9730	 0.1180
J	 0.9750	 0.0830
K	 0.9070	 0.1210
L	 0.9470	 0.0440
M	 0.9790	 0.1170
N	 0.9650	 0.1300
O	 0.9360	 0.1150
P	 0.9930	 0.1580
Q	 0.9910	 0.1440
R	 0.9140	 0.1290
S	 0.9960	 0.1360
T	 0.9660	 0.1490
U	 0.9570	 0.1270
V	 0.7440	 0.0870
W	 0.9450	 0.1230
X	 0.9320	 0.0820
Y	 0.5680	 0.0540
f	 0.9770	 0.0780
g	 0.9040	 0.0540
h	 0.9370	 0.0660

