



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 06:39 AM UTC

PDB ID : 6KW5 / pdb_00006kw5
EMDB ID : EMD-0779
Title : The ClassC 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 : 10.13 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

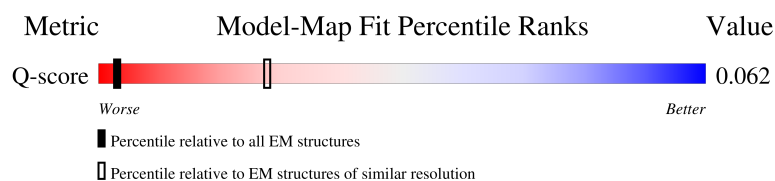
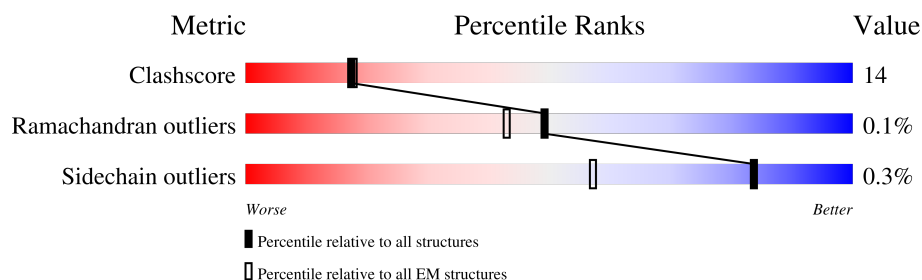
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

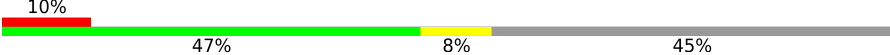
The reported resolution of this entry is 10.13 Å.

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	116 (9.68 - 10.60)

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	F	435	
2	D	557	
2	H	557	
3	M	581	

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Mol	Chain	Length	Quality of chain
4	I	483	
5	G	426	
6	A	502	
7	J	1359	
7	P	1359	
7	Q	1359	
8	E	78	
9	C	883	
10	K	885	
11	X	625	
12	L	889	
13	S	103	
13	W	103	
14	f	477	
15	h	157	
16	R	136	
16	V	136	
17	O	130	
17	T	130	
18	U	126	
18	Y	126	
19	g	467	
20	B	167	
21	N	167	

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 45484 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 Chromatin structure-remodeling complex subunit RSC7.

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

- Molecule 2 is a protein called Chromatin structure-remodeling complex protein RSC8.

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

- Molecule 3 is a protein called Chromatin structure-remodeling complex subunit RSC9.

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

- Molecule 4 is a protein called Chromatin structure-remodeling complex protein RSC6.

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

- Molecule 5 is a protein called Chromatin structure-remodeling complex subunit SFH1.

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

- Molecule 6 is a protein called Chromatin structure-remodeling complex protein RSC58.

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

- Molecule 7 is a protein called Nuclear protein STH1/NPS1.

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

- Molecule 8 is a protein called High temperature lethal protein 1.

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

- Molecule 9 is a protein called Chromatin structure-remodeling complex protein RSC30.

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

- Molecule 10 is a protein called Chromatin structure-remodeling complex protein RSC3.

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

- Molecule 11 is a protein called Chromatin structure-remodeling complex subunit RSC4.

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

- Molecule 12 is a protein called Chromatin structure-remodeling complex subunit RSC2.

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

- Molecule 13 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	88	Total	C	N	O	S	0	0
			708	445	143	119	1		
13	S	82	Total	C	N	O	S	0	0
			657	416	128	112	1		

- Molecule 14 is a protein called Actin-related protein 7.

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

- Molecule 15 is a protein called Regulator of Ty1 transposition protein 102.

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

- Molecule 16 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	96	Total	C	N	O	S	0	0
			794	500	154	137	3		
16	V	95	Total	C	N	O	S	0	0
			784	494	151	136	3		

- Molecule 17 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	104	Total	C	N	O	S	0	0
			804	507	157	140			
17	O	107	Total	C	N	O	S	0	0
			823	519	161	143			

- Molecule 18 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	93	Total	C	N	O	S	0	0
			725	456	130	137	2		
18	Y	93	Total	C	N	O	S	0	0
			717	450	128	137	2		

- Molecule 19 is a protein called Actin-like protein ARP9.

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

- Molecule 20 is a DNA chain called DNA 167.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B	146	Total	C	N	O	P	0	0
			2977	1414	542	875	146		

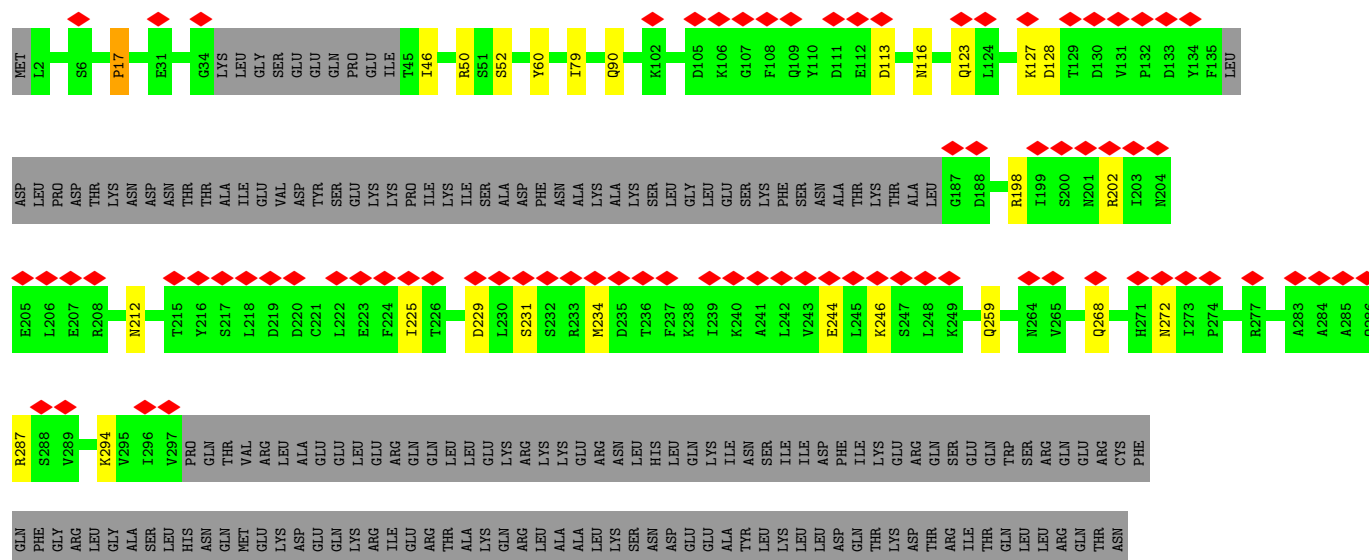
- Molecule 21 is a DNA chain called DNA 167.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	146	Total	C	N	O	P	0	0
			3009	1425	561	877	146		

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

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

Chain A:



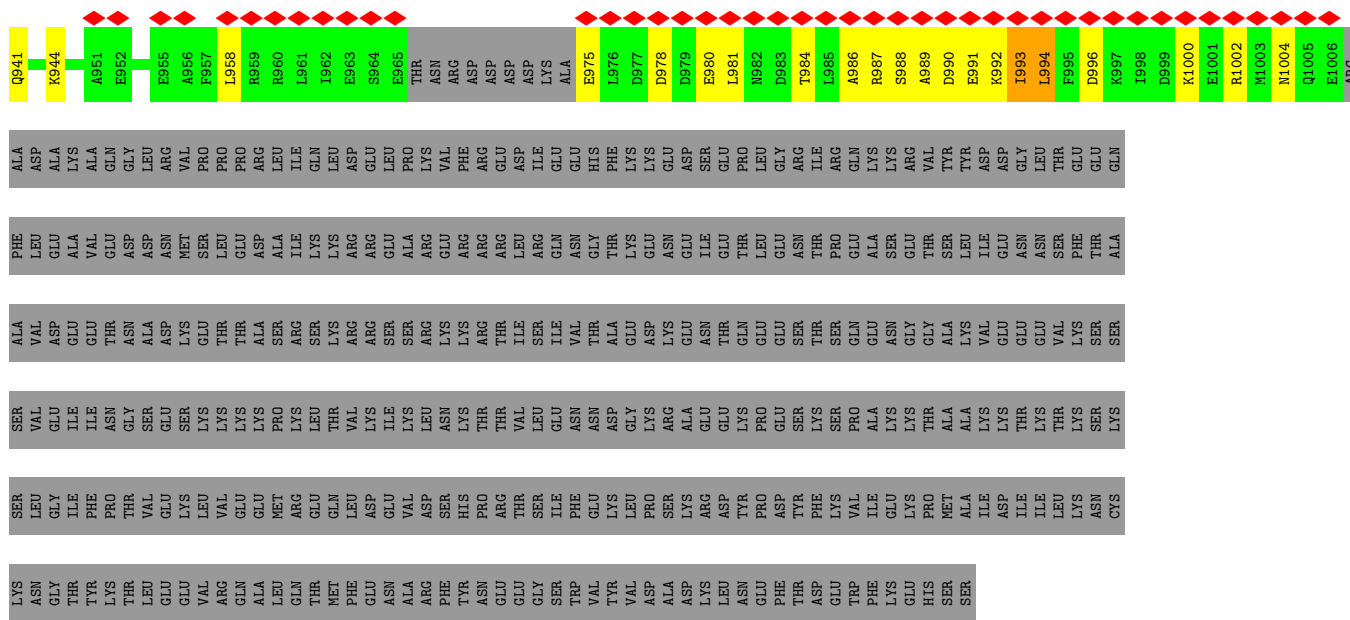


WORLD WIDE
PDB
PROTEIN DATA BANK

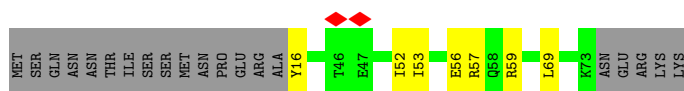


Chain Q:

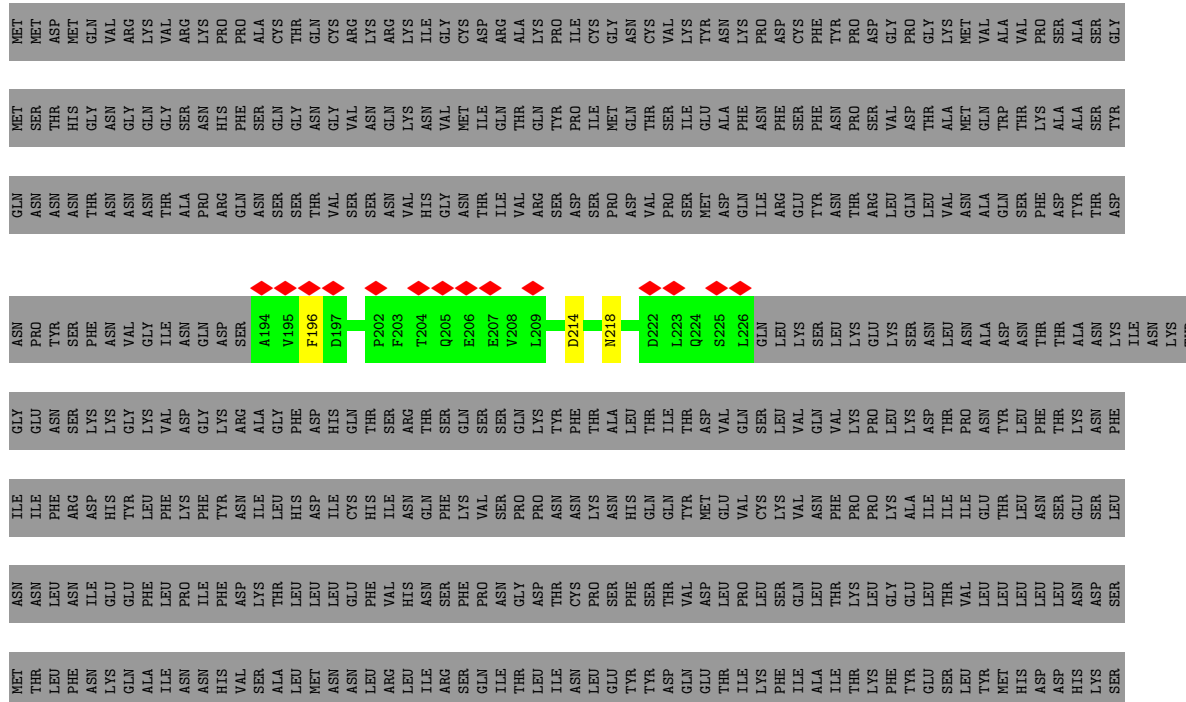




- Molecule 8: High temperature lethal protein 1



- Molecule 9: Chromatin structure-remodeling complex protein RSC30



[illegible]

- Molecule 10: Chromatin structure-remodeling complex protein RSC3

Chain K: 5% 95%

LEU	LEU	CYS	GLU	GLY	ASN	TYR	LYS	ALA	THR	MET
ILE	LYS	TRP	THR	PHE	LYS	LEU	PRO	ASN	ARG	ASP
LEU	LEU	HIS	LEU	ILE	TYR	ILE	ILE	ASN	GLN	ILE
LEU	LEU	LEU	PHE	THR	LEU	GLU	PRO	ALA	VAL	ARG
LYS	LYS	PHE	ILE	CYS	THR	ASP	GLU	THR	ALA	GLY
ASN	ASN	LEU	SER	LEU	ILE	PRO	GLU	ASN	LYS	ASN
LYS	LYS	GLY	LEU	LEU	THR	PHE	ARG	GLN	PRO	MET
ASN	ASN	GLN	TRP	ILE	GLU	LEU	ARG	GLN	TYR	LYS
ILE	ILE	LEU	LYS	ILE	THR	PHE	PRO	HIS	LEU	LYS
GLU	GLU	PRO	TYR	PHE	ASN	LEU	PRO	THR	ASN	PRO
VAL	VAL	LEU	TYR	GLU	SER	PHE	HIS	GLN	SER	PRO
SER	SER	LEU	GLN	SER	ILE	PHE	ASN	TYR	ALA	ALA
GLN	GLN	MET	PHE	LEU	LEU	ASN	GLY	ILE	TYR	CYS
SER	SER	SER	VAL	ASN	PRO	ASP	PHE	PRO	ALA	VAL
CYS	CYS	GLU	MET	SER	ILE	LEU	LYS	LYS	SER	GLN
LEU	LEU	PRO	ASP	THR	LEU	ASN	ASP	SER	SER	CYS
THR	THR	PHE	THR	VAL	LYS	ILE	LEU	VAL	ARG	LYS
THR	THR	THR	SER	VAL	PRO	LEU	ASP	PRO	VAL	ARG
PRO	PRO	ASN	SER	ILE	LYS	ILE	PRO	PRO	LYS	ARG
SER	SER	SER	SER	ILE	ARG	GLU	GLN	SER	LYS	ILE
ILE	ILE	THR	SER	LEU	LEU	THR	PHE	THR	GLU	GLY
ILE	ILE	PRO	SER	ARG	LEU	GLN	LEU	SER	THR	ASN
ASN	ASN	ILE	PHE	ASP	LEU	THR	ASN	VAL	LEU	ARG
ASN	ASN	ILE	VAL	ASP	ILE	GLY	LYS	VAL	ASP	ARG
ILE	ILE	ASP	ILE	GLU	VAL	GLY	ASN	VAL	LEU	VAL
MET	MET	PRO	ASP	HIS	GLU	PRO	ASN	THR	ASP	VAL
ASP	ASP	LEU	TYR	LEU	GLN	LEU	VAL	SER	LEU	LYS
SER	SER	LEU	ASP	GLN	LEU	HIS	PHE	ALA	ALA	PRO
LEU	LEU	ASN	GLU	LEU	PHE	LEU	ASN	SER	LYS	ASN
ILE	ILE	ASN	GLU	PHE	PRO	ASP	ASN	ALA	ASN	ILE
TYR	TYR	ASN	ASP	PHE	ASN	LEU	VAL	GLU	PRO	CYS
ARG	ARG	PHE	HIS	ASN	SER	ALA	ASN	SER	GLY	ASN
ASN	ASN	GLU	ALA	LEU	THR	SER	SER	THR	ALA	CYS
SER	SER	LEU	LEU	PHE	ILE	ARG	ALA	SER	SER	LYS
MET	MET	ILE	CYS	ASN	ASN	ASN	ILE	THR	LEU	MET
LEU	LEU	ASP	LEU	TYR	LYS	SER	SER	GLU	GLU	LYS
TYR	TYR	PHE	LEU	LEU	PRO	ILE	GLU	ASN	GLN	HIS
LEU	LEU	GLU	SER	PRO	ASN	ARG	ASN	ILE	ILE	LYS
ASN	ASN	VAL	LEU	LEU	SER	GLU	GLY	ARG	ARG	LYS
PHE	PHE	ASN	ASN	LEU	LYS	ASN	ARG	ASN	GLU	MET
LEU	LEU	MET	HIS	LYS	ASP	SER	ASN	CYS	TYR	ASP
LEU	LEU	LEU	THR	SER	PHE	GLY	ARG	GLN	TYR	PHE
LEU	LEU	LYS	GLN	ASN	LEU	ILE	LEU	LEU	ARG	PRO
PHE	PHE	GLN	ASN	THR	PHE	GLN	LEU	ILE	LEU	ASP
GLU	GLU	SER	SER	LEU	GLN	LEU	PRO	LYS	LEU	VAL
THR	THR	LYS	HIS	ARG	VAL	LEU	LYS	LYS	LEU	PRO
LYS	LYS	ASP	ILE	PHE	PHE	LEU	ASN	ARG	GLN	VAL
ASN	ASN	GLN	THR	GLU	SER	PRO	ASN	ALA	ALA	TYR
PRO	PRO	LEU	TRP	GLY	THR	GLN	LYS	ASN	GLN	VAL
ALA	ALA	SER	ASN	LYS	ASN	ILE	LYS	ASN	ASN	PRO
PHE	PHE	ILE	PHE	ARG	ASN	ILE	GLU	GLU	GLN	SER
ASN	ASN	ASP	ILE	SER	GLN	THR	ILE	ASP	LEU	SER
THR	THR	THR	THR	THR	GLN	THR	GLY	E176	ASN	SER
GLU	GLU	ILE	ASN	CYS	LEU	THR	VAL	E177	ASN	SER
ILE	ILE	ILE	LYS	ASN	ASN	LEU	ILE	I178	ARG	SER
LEU	LEU	GLN	TYR	ILE	LEU	ILE	THR	I179	SER	SER
								H180	ASP	ASN

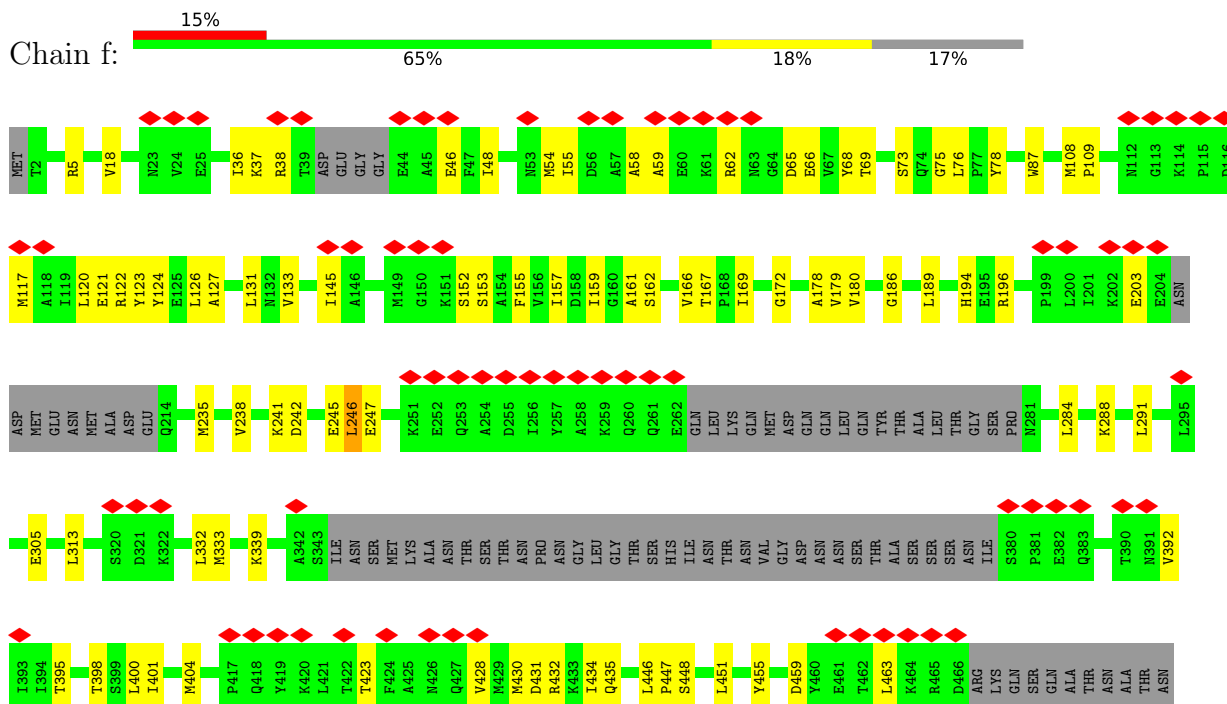
[illegible]

- Molecule 11: Chromatin structure-remodeling complex subunit RSC4

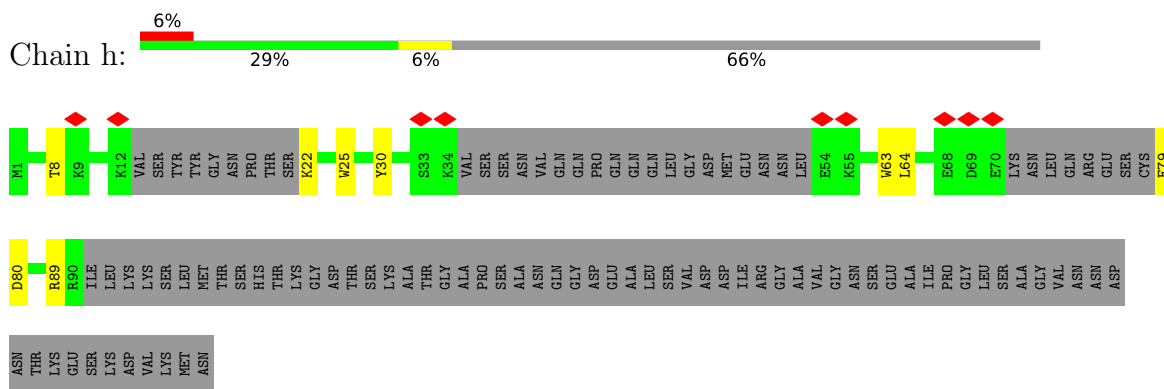
[illegible]

- Molecule 12: Chromatin structure-remodeling complex subunit RSC2

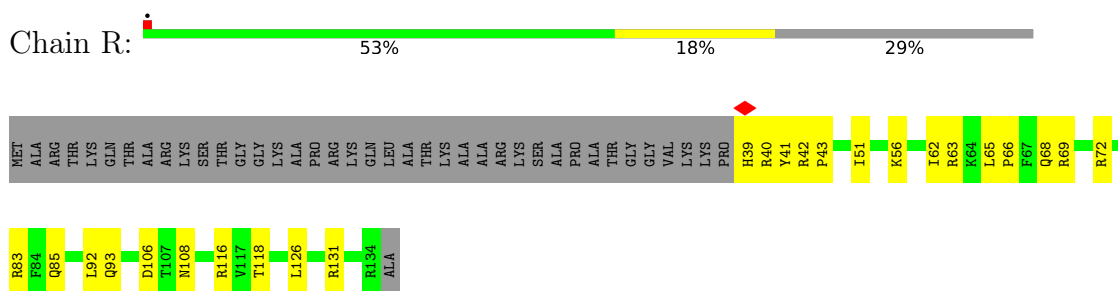
[illegible]



- Molecule 15: Regulator of Ty1 transposition protein 102

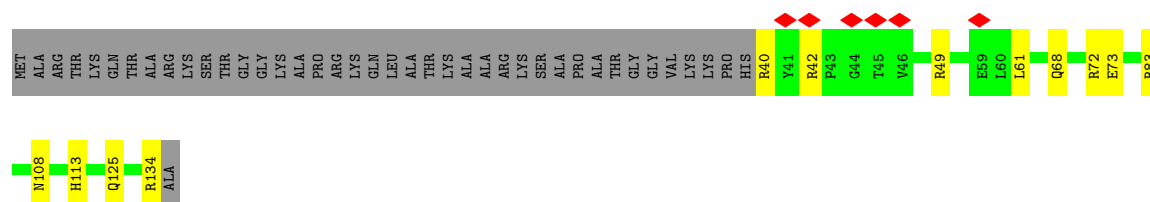


- Molecule 16: Histone H3.2

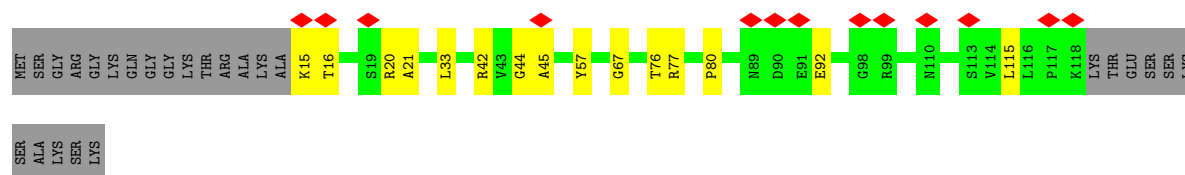


- Molecule 16: Histone H3.2

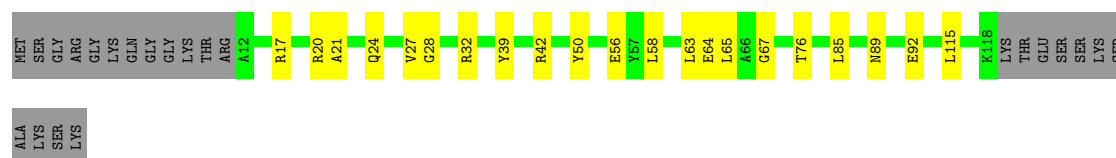




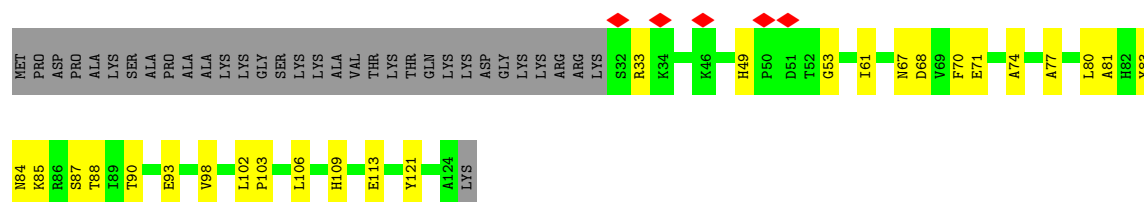
- Molecule 17: Histone H2A



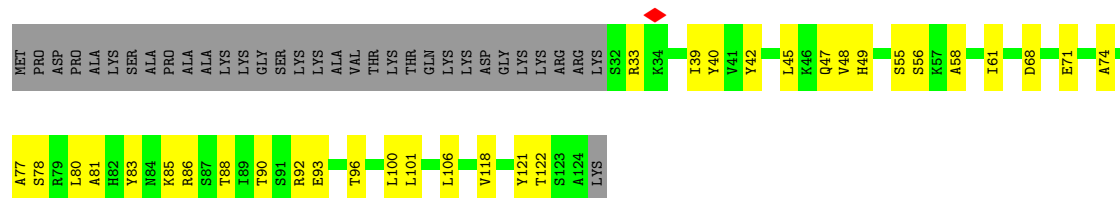
- Molecule 17: Histone H2A



- Molecule 18: Histone H4

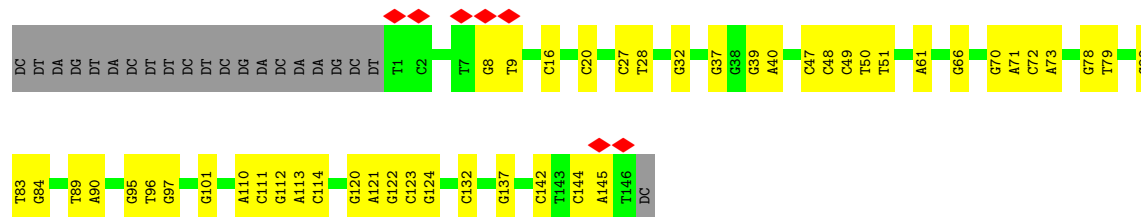


- Molecule 18: Histone H4



- Molecule 19: Actin-like protein ARP9





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24146	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	0.099	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.022	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	F	0.21	0/983	0.58	0/1337
2	D	0.22	0/2557	0.50	0/3442
2	H	0.24	0/3275	0.54	2/4409 (0.0%)
3	M	0.26	0/3113	0.58	1/4215 (0.0%)
4	I	0.23	0/1976	0.54	0/2685
5	G	0.23	0/2039	0.60	1/2769 (0.0%)
6	A	0.26	0/3077	0.61	0/4169
7	J	0.25	0/1836	0.62	1/2480 (0.0%)
7	P	0.27	0/598	0.63	0/789
7	Q	0.34	0/4580	0.77	6/6167 (0.1%)
8	E	0.21	0/480	0.52	0/643
9	C	0.16	0/272	0.38	0/366
10	K	0.19	0/356	0.50	0/483
11	X	0.28	0/1243	0.59	0/1672
12	L	0.25	0/681	0.61	0/921
13	S	0.45	0/664	0.63	0/889
13	W	0.45	0/716	0.63	0/955
14	f	0.21	0/3295	0.52	1/4454 (0.0%)
15	h	0.19	0/501	0.44	0/669
16	R	0.47	0/805	0.65	0/1079
16	V	0.43	0/794	0.54	0/1064
17	O	0.45	0/833	0.67	1/1124 (0.1%)
17	T	0.41	0/814	0.55	0/1099
18	U	0.46	0/736	0.64	0/991
18	Y	0.47	0/728	0.70	0/983
19	g	0.23	0/3261	0.60	4/4421 (0.1%)
20	B	0.54	0/3336	0.52	0/5142
21	N	0.54	0/3378	0.54	0/5216
All	All	0.34	0/46927	0.59	17/64633 (0.0%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	g	48	ASP	CB-CA-C	9.60	119.34	109.83
7	Q	993	ILE	N-CA-C	-6.71	103.78	110.62
7	J	17	PRO	N-CA-CB	6.68	110.26	103.25
5	G	338	LYS	N-CA-C	-6.58	102.56	112.04
3	M	553	ILE	N-CA-C	-6.14	107.51	113.53
17	O	27	VAL	N-CA-C	-6.10	106.29	113.42
7	Q	564	ILE	N-CA-C	5.79	117.06	111.91
7	Q	531	ILE	N-CA-C	-5.53	107.47	112.12
7	Q	860	TYR	CA-CB-CG	-5.53	103.94	113.90
14	f	246	LEU	CA-CB-CG	5.52	135.63	116.30
2	H	261	HIS	CA-C-N	5.36	131.78	121.54
2	H	261	HIS	C-N-CA	5.36	131.78	121.54
19	g	48	ASP	N-CA-C	-5.32	105.43	113.51
7	Q	702	VAL	N-CA-C	5.24	116.01	110.72
19	g	98	ASN	CA-C-N	5.23	131.53	121.54
19	g	98	ASN	C-N-CA	5.23	131.53	121.54
7	Q	990	ASP	N-CA-C	-5.15	105.58	111.14

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	F	964	0	919	5	0
2	D	2510	0	2542	34	0
2	H	3215	0	3195	42	0
3	M	3058	0	3127	26	0
4	I	1944	0	1964	25	0
5	G	1996	0	1948	32	0
6	A	3007	0	3045	50	0
7	J	1814	0	1777	23	0
7	P	592	0	610	19	0
7	Q	4503	0	4567	248	0
8	E	477	0	491	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	269	0	279	2	0
10	K	347	0	342	2	0
11	X	1220	0	1192	29	0
12	L	669	0	693	19	0
13	S	657	0	706	36	0
13	W	708	0	758	32	0
14	f	3219	0	3240	114	0
15	h	490	0	467	10	0
16	R	794	0	830	52	0
16	V	784	0	823	31	0
17	O	823	0	881	75	0
17	T	804	0	859	52	0
18	U	725	0	744	69	0
18	Y	717	0	723	86	0
19	g	3191	0	3179	86	0
20	B	2977	0	1639	169	0
21	N	3009	0	1640	158	0
22	H	1	0	0	0	0
All	All	45484	0	43180	1047	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 (1047) 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:f:238:VAL:HG21	14:f:404:MET:SD	1.19	1.76
14:f:76:LEU:CD2	14:f:108:MET:HE1	1.23	1.67
7:Q:473:TYR:CZ	7:Q:702:VAL:HA	1.27	1.58
14:f:36:ILE:HG13	14:f:54:MET:CE	1.28	1.56
14:f:76:LEU:CD2	14:f:108:MET:CE	1.85	1.55
7:Q:883:ILE:CG2	7:Q:885:PHE:CE2	1.94	1.51
14:f:36:ILE:CB	14:f:54:MET:HE1	1.42	1.49
16:V:42:ARG:CZ	20:B:144:DC:H3'	1.41	1.49
20:B:56:DC:C5'	7:Q:528:LEU:HD12	1.44	1.47
14:f:36:ILE:CG1	14:f:54:MET:CE	1.93	1.46
11:X:439:GLU:OE1	11:X:490:GLU:CG	1.64	1.45
18:U:33:ARG:NH1	21:N:28:DT:H5''	1.20	1.42
7:Q:883:ILE:HG22	7:Q:885:PHE:CE2	1.53	1.42
7:Q:986:ALA:CB	7:Q:992:LYS:HG2	1.50	1.38
13:S:78:ARG:CB	20:B:102:DG:OP1	1.72	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:33:ARG:NE	21:N:124:DG:H5'	1.35	1.38
18:U:33:ARG:NH1	21:N:28:DT:C5'	1.88	1.37
20:B:54:DC:C4'	7:Q:868:ARG:HG2	1.54	1.34
14:f:238:VAL:CG2	14:f:404:MET:SD	2.11	1.34
18:Y:33:ARG:HE	21:N:124:DG:C5'	1.42	1.32
14:f:157:ILE:CD1	14:f:333:MET:HE2	1.57	1.32
20:B:54:DC:H4'	7:Q:868:ARG:CG	1.58	1.32
7:Q:548:ILE:CD1	7:Q:572:LEU:HD23	1.61	1.30
14:f:155:PHE:CE2	14:f:333:MET:HE3	1.68	1.28
16:R:85:GLN:HG2	21:N:50:DT:OP1	1.15	1.26
20:B:58:DT:OP2	7:Q:554:PRO:HD3	1.29	1.26
17:O:32:ARG:NE	20:B:30:DA:OP2	1.68	1.25
14:f:36:ILE:CG1	14:f:54:MET:HE3	1.57	1.24
19:g:359:ILE:HD12	19:g:402:GLN:OE1	1.07	1.24
14:f:76:LEU:HD21	14:f:108:MET:CE	1.57	1.23
16:R:83:ARG:HG2	21:N:51:DT:C5'	1.67	1.23
6:A:238:GLU:OE2	7:J:212:ASN:ND2	1.71	1.22
18:U:88:THR:OG1	21:N:40:DA:OP1	1.58	1.22
17:O:42:ARG:HB3	21:N:113:DA:OP1	1.37	1.21
7:Q:548:ILE:HD12	7:Q:572:LEU:CD2	1.71	1.21
21:N:95:DG:OP2	7:Q:608:LYS:CB	1.87	1.20
7:Q:478:LEU:HD21	7:Q:507:SER:OG	1.37	1.20
20:B:56:DC:H5''	7:Q:528:LEU:CD1	1.72	1.20
14:f:36:ILE:CG1	14:f:54:MET:HE1	1.62	1.20
18:Y:55:SER:HA	20:B:20:DA:OP1	1.38	1.20
7:Q:473:TYR:CZ	7:Q:702:VAL:CA	2.24	1.20
21:N:95:DG:OP2	7:Q:608:LYS:HB2	1.03	1.19
13:W:98:TYR:OH	18:U:68:ASP:OD2	1.54	1.19
17:O:42:ARG:CG	21:N:113:DA:H5''	1.73	1.18
12:L:765:THR:HG22	12:L:790:LEU:HD21	1.23	1.18
17:O:42:ARG:HG2	21:N:113:DA:H5''	1.24	1.16
20:B:58:DT:OP2	7:Q:554:PRO:CD	1.92	1.16
20:B:58:DT:OP1	7:Q:554:PRO:HG2	1.45	1.16
17:O:42:ARG:HG2	21:N:113:DA:C5'	1.76	1.16
20:B:56:DC:C5'	7:Q:528:LEU:CD1	2.23	1.16
18:U:33:ARG:HH12	21:N:28:DT:C5'	1.53	1.15
7:Q:883:ILE:HG21	7:Q:885:PHE:CE2	1.71	1.15
3:M:272:ARG:CD	7:P:314:GLU:OE2	1.95	1.13
14:f:157:ILE:HD11	14:f:333:MET:CE	1.79	1.13
19:g:359:ILE:CD1	19:g:402:GLN:OE1	1.96	1.13
18:Y:33:ARG:CD	21:N:124:DG:H5'	1.78	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:f:76:LEU:HD21	14:f:108:MET:HE3	1.13	1.12
7:Q:473:TYR:OH	7:Q:702:VAL:HA	1.50	1.12
13:S:78:ARG:CA	20:B:102:DG:OP1	1.97	1.12
16:R:63:ARG:CZ	20:B:91:DA:H5''	1.77	1.11
13:S:78:ARG:HB3	20:B:102:DG:OP1	1.39	1.11
7:Q:473:TYR:CE2	7:Q:702:VAL:HA	1.83	1.11
18:Y:42:TYR:OH	20:B:21:DG:P	2.10	1.10
13:S:88:TYR:CZ	18:U:83:TYR:CE1	2.39	1.10
14:f:157:ILE:CD1	14:f:333:MET:CE	2.29	1.09
20:B:55:DG:P	7:Q:839:GLY:HA3	1.92	1.09
16:R:63:ARG:HD2	20:B:91:DA:H4'	1.13	1.09
14:f:36:ILE:CA	14:f:54:MET:HE1	1.82	1.09
20:B:55:DG:H2''	7:Q:840:SER:HB3	1.36	1.08
13:S:88:TYR:CE1	18:U:83:TYR:CE1	2.42	1.07
16:V:42:ARG:CZ	20:B:144:DC:C3'	2.31	1.07
13:S:91:LYS:NZ	18:Y:71:GLU:OE1	1.86	1.07
7:Q:986:ALA:HB1	7:Q:992:LYS:HG2	1.10	1.07
14:f:155:PHE:CE2	14:f:333:MET:CE	2.38	1.06
14:f:157:ILE:CG1	14:f:333:MET:HE1	1.83	1.06
16:R:83:ARG:CG	21:N:51:DT:H5''	1.84	1.06
11:X:439:GLU:OE1	11:X:490:GLU:HG2	0.91	1.06
14:f:157:ILE:HG12	14:f:333:MET:HE1	1.36	1.06
7:Q:883:ILE:HG21	7:Q:885:PHE:CZ	1.91	1.06
14:f:157:ILE:HG12	14:f:333:MET:CE	1.85	1.05
7:Q:909:GLU:OE1	7:Q:987:ARG:HD2	1.56	1.05
13:S:88:TYR:CD1	18:U:83:TYR:CZ	2.44	1.05
16:R:40:ARG:O	21:N:145:DA:OP2	1.75	1.04
21:N:96:DT:OP1	7:Q:607:SER:HB3	1.55	1.04
14:f:36:ILE:CD1	14:f:54:MET:HE3	1.87	1.04
14:f:157:ILE:HD11	14:f:333:MET:HE2	1.07	1.04
17:T:45:ALA:N	20:B:112:DT:OP1	1.91	1.04
14:f:157:ILE:CG1	14:f:333:MET:CE	2.36	1.04
14:f:36:ILE:HB	14:f:54:MET:HE1	1.40	1.03
17:O:17:ARG:HG3	20:B:31:DT:P	1.98	1.03
17:O:17:ARG:NE	20:B:31:DT:OP2	1.90	1.03
16:V:42:ARG:NE	20:B:144:DC:H3'	1.71	1.03
19:g:323:ILE:HG13	19:g:403:CYS:HB3	1.39	1.03
17:O:32:ARG:CZ	20:B:30:DA:OP2	2.06	1.03
7:Q:473:TYR:CD1	7:Q:702:VAL:HG12	1.95	1.02
7:Q:815:GLN:N	7:Q:886:ASP:OD2	1.91	1.02
13:W:88:TYR:CE1	18:Y:83:TYR:CE1	2.47	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:f:76:LEU:HD22	14:f:108:MET:CE	1.64	1.02
13:S:78:ARG:HG2	20:B:102:DG:P	2.00	1.02
14:f:36:ILE:CB	14:f:54:MET:CE	2.28	1.02
17:O:21:ALA:HB2	18:Y:121:TYR:HB2	1.41	1.02
17:O:42:ARG:NE	21:N:113:DA:C5'	2.22	1.02
6:A:187:TYR:OH	6:A:235:THR:HG21	1.57	1.02
12:L:750:VAL:HG11	12:L:788:GLU:OE1	1.59	1.02
21:N:96:DT:H3'	7:Q:604:ASN:ND2	1.73	1.02
7:Q:812:MET:HE1	7:Q:885:PHE:CE2	1.95	1.02
18:Y:42:TYR:OH	20:B:21:DG:O5'	1.78	1.01
18:Y:86:ARG:HD2	20:B:40:DG:OP1	1.60	1.01
6:A:238:GLU:CD	7:J:212:ASN:ND2	2.18	1.01
16:R:56:LYS:NZ	20:B:10:DC:OP2	1.93	1.01
16:R:85:GLN:CG	21:N:50:DT:OP1	2.08	1.01
7:Q:564:ILE:HG12	7:Q:569:PHE:CE2	1.95	1.01
7:Q:986:ALA:HB1	7:Q:992:LYS:CG	1.91	1.01
17:O:28:GLY:HA3	20:B:30:DA:H5''	1.40	1.00
14:f:36:ILE:N	14:f:54:MET:HE1	1.75	1.00
14:f:155:PHE:CZ	14:f:333:MET:HE3	1.95	1.00
7:Q:883:ILE:CG2	7:Q:885:PHE:CZ	2.42	1.00
17:O:42:ARG:CB	21:N:113:DA:OP1	2.09	1.00
6:A:190:PRO:HB3	11:X:437:LEU:CD2	1.91	1.00
21:N:96:DT:H3'	7:Q:604:ASN:HD21	1.16	1.00
14:f:36:ILE:HG13	14:f:54:MET:HE3	1.00	0.99
7:Q:548:ILE:CD1	7:Q:572:LEU:CD2	2.32	0.99
18:Y:33:ARG:NE	21:N:124:DG:C5'	2.08	0.99
18:Y:42:TYR:CE1	20:B:21:DG:OP2	2.14	0.99
20:B:56:DC:O5'	7:Q:528:LEU:CD1	2.11	0.99
13:S:88:TYR:CE1	18:U:83:TYR:CZ	2.52	0.98
6:A:190:PRO:HB3	11:X:437:LEU:HD22	1.43	0.97
18:Y:33:ARG:HD3	21:N:124:DG:P	2.04	0.97
13:W:88:TYR:CD1	18:Y:83:TYR:CZ	2.52	0.97
12:L:765:THR:HG22	12:L:790:LEU:CD2	1.94	0.96
21:N:95:DG:P	7:Q:608:LYS:HB2	2.04	0.96
17:O:32:ARG:NH2	20:B:29:DA:H2''	1.80	0.96
11:X:439:GLU:OE1	11:X:490:GLU:CD	2.09	0.96
16:V:40:ARG:NH1	21:N:83:DT:O2	1.99	0.95
17:T:42:ARG:NH1	21:N:39:DG:C4'	2.30	0.95
16:V:40:ARG:NH2	21:N:83:DT:O4'	1.98	0.95
17:O:42:ARG:NE	21:N:113:DA:H5''	1.80	0.95
16:V:42:ARG:NH2	20:B:144:DC:H3'	1.81	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:f:36:ILE:N	14:f:54:MET:CE	2.30	0.94
14:f:108:MET:SD	14:f:123:TYR:OH	2.23	0.94
17:O:42:ARG:CD	21:N:113:DA:C5'	2.46	0.94
17:T:42:ARG:NH1	21:N:39:DG:H4'	1.82	0.93
20:B:55:DG:C2'	7:Q:840:SER:HB3	1.98	0.93
16:V:42:ARG:HD3	20:B:144:DC:O5'	1.69	0.93
7:Q:986:ALA:HB3	7:Q:992:LYS:HG2	1.47	0.93
7:P:372:ARG:O	7:P:376:GLN:HG3	1.69	0.93
17:O:42:ARG:CD	21:N:113:DA:H5''	1.99	0.93
20:B:58:DT:OP1	7:Q:554:PRO:CG	2.15	0.93
19:g:359:ILE:HG12	19:g:404:PRO:HG2	1.52	0.92
17:O:20:ARG:NH1	20:B:32:DT:OP1	2.01	0.92
14:f:155:PHE:HE2	14:f:333:MET:HE3	1.34	0.92
16:R:40:ARG:O	21:N:145:DA:P	2.28	0.92
17:T:42:ARG:CD	21:N:39:DG:H4'	2.00	0.92
17:O:42:ARG:CG	21:N:113:DA:C5'	2.42	0.92
13:S:78:ARG:HA	20:B:102:DG:OP1	1.69	0.91
7:Q:986:ALA:CB	7:Q:992:LYS:CG	2.45	0.91
7:Q:989:ALA:HA	7:Q:992:LYS:CG	2.00	0.91
16:V:42:ARG:HD3	20:B:144:DC:P	2.11	0.91
19:g:323:ILE:CG1	19:g:403:CYS:HB3	2.00	0.91
17:O:17:ARG:CD	20:B:31:DT:OP2	2.19	0.91
7:Q:991:GLU:O	7:Q:994:LEU:N	2.02	0.90
13:W:88:TYR:CZ	18:Y:83:TYR:CE1	2.59	0.90
16:R:65:LEU:HB2	20:B:92:DC:OP2	1.71	0.90
18:Y:55:SER:CA	20:B:20:DA:OP1	2.19	0.90
16:V:42:ARG:NH2	20:B:144:DC:C3'	2.35	0.90
7:Q:883:ILE:CG2	7:Q:885:PHE:HE2	1.60	0.90
7:Q:991:GLU:O	7:Q:994:LEU:HB2	1.71	0.90
17:T:42:ARG:HD3	21:N:39:DG:H4'	1.54	0.89
21:N:96:DT:OP1	7:Q:607:SER:CB	2.20	0.89
16:R:83:ARG:HG2	21:N:51:DT:H5''	0.91	0.89
18:Y:42:TYR:HE1	20:B:21:DG:OP2	1.54	0.89
7:Q:473:TYR:OH	7:Q:701:GLU:O	1.90	0.89
18:U:33:ARG:NH1	21:N:28:DT:H5'	1.88	0.89
13:S:88:TYR:CD1	18:U:83:TYR:OH	2.26	0.89
14:f:36:ILE:H	14:f:54:MET:CE	1.86	0.88
20:B:56:DC:H5''	7:Q:528:LEU:HD12	0.90	0.88
20:B:56:DC:O5'	7:Q:528:LEU:HD12	1.68	0.88
7:Q:814:PHE:C	7:Q:886:ASP:OD2	2.16	0.88
20:B:57:DT:H4'	7:Q:581:LYS:NZ	1.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:42:ARG:CZ	21:N:39:DG:H4'	2.05	0.87
18:Y:33:ARG:HD3	21:N:124:DG:H5'	1.56	0.87
3:M:272:ARG:HD2	7:P:314:GLU:OE2	1.74	0.87
13:S:78:ARG:CG	20:B:102:DG:OP1	2.23	0.87
17:O:39:TYR:CE1	18:Y:74:ALA:HB1	2.08	0.87
20:B:55:DG:OP1	7:Q:839:GLY:HA3	1.74	0.87
18:Y:33:ARG:CD	21:N:124:DG:C5'	2.49	0.87
14:f:48:ILE:O	14:f:54:MET:SD	2.33	0.86
17:O:64:GLU:HG2	18:Y:48:VAL:HG11	1.57	0.86
17:O:76:THR:N	21:N:132:DC:OP1	2.08	0.86
5:G:279:VAL:HG21	5:G:339:ILE:HD13	1.57	0.86
12:L:765:THR:CG2	12:L:790:LEU:HD21	2.04	0.86
19:g:189:MET:HE3	19:g:193:SER:OG	1.74	0.86
20:B:58:DT:P	7:Q:554:PRO:CG	2.62	0.86
18:U:33:ARG:HH11	21:N:28:DT:H5''	1.36	0.86
17:O:42:ARG:NE	21:N:113:DA:H5'	1.90	0.85
17:T:57:TYR:CZ	18:U:109:HIS:HB3	2.11	0.85
17:O:64:GLU:HG2	18:Y:48:VAL:CG1	2.06	0.85
7:Q:815:GLN:H	7:Q:886:ASP:CG	1.84	0.85
13:W:88:TYR:CE1	18:Y:83:TYR:CZ	2.65	0.84
16:R:69:ARG:NH2	20:B:91:DA:OP1	2.10	0.84
13:W:88:TYR:CD1	18:Y:83:TYR:OH	2.31	0.84
7:Q:989:ALA:HA	7:Q:992:LYS:CD	2.06	0.84
14:f:166:VAL:CG2	14:f:333:MET:SD	2.66	0.84
16:R:66:PRO:HG3	20:B:91:DA:OP1	1.76	0.84
13:W:92:ARG:NH2	18:Y:100:LEU:O	2.11	0.84
16:R:83:ARG:HH11	21:N:51:DT:H5'	1.41	0.83
20:B:57:DT:OP1	7:Q:578:TYR:CE2	2.30	0.83
17:T:76:THR:O	18:U:53:GLY:N	2.10	0.83
20:B:55:DG:H2''	7:Q:840:SER:CB	2.07	0.83
7:Q:473:TYR:OH	7:Q:702:VAL:CA	2.22	0.83
19:g:189:MET:CE	19:g:193:SER:OG	2.26	0.83
16:R:63:ARG:HD2	20:B:91:DA:C4'	2.03	0.83
19:g:358:LEU:HD11	19:g:405:THR:O	1.78	0.83
4:I:476:LEU:HD21	4:I:480:GLN:NE2	1.94	0.82
17:T:42:ARG:O	18:U:88:THR:HG23	1.78	0.82
7:Q:909:GLU:CD	7:Q:987:ARG:HD2	2.04	0.82
7:Q:815:GLN:N	7:Q:886:ASP:CG	2.37	0.82
18:U:33:ARG:CZ	21:N:28:DT:H5'	2.09	0.82
20:B:58:DT:P	7:Q:554:PRO:HG2	2.19	0.82
7:Q:883:ILE:HG22	7:Q:885:PHE:CD2	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:f:291:LEU:HB3	19:g:402:GLN:NE2	1.94	0.82
15:h:89:ARG:NH2	19:g:33:PRO:O	2.11	0.82
18:Y:56:SER:CB	20:B:20:DA:OP2	2.28	0.82
19:g:457:LYS:NZ	19:g:464:ASP:OD2	2.11	0.82
7:P:373:THR:O	7:P:377:ARG:HG3	1.79	0.82
18:Y:42:TYR:OH	20:B:21:DG:OP2	1.96	0.82
14:f:235:MET:SD	19:g:401:VAL:HG21	2.20	0.82
20:B:54:DC:C5'	7:Q:868:ARG:HG2	2.09	0.82
7:Q:473:TYR:CE2	7:Q:702:VAL:CA	2.58	0.82
17:O:28:GLY:CA	20:B:30:DA:H5''	2.10	0.81
17:O:42:ARG:HG2	21:N:113:DA:O5'	1.79	0.81
14:f:117:MET:O	14:f:120:LEU:HB3	1.79	0.81
6:A:187:TYR:HH	6:A:235:THR:HG21	1.45	0.81
7:Q:989:ALA:HA	7:Q:992:LYS:HG3	1.61	0.81
19:g:359:ILE:HG13	19:g:404:PRO:HD2	1.63	0.80
4:I:476:LEU:CD2	4:I:480:GLN:NE2	2.45	0.80
7:Q:989:ALA:HA	7:Q:992:LYS:HD2	1.61	0.80
6:A:218:PRO:HA	11:X:364:LEU:HD23	1.62	0.80
17:O:64:GLU:HA	18:Y:48:VAL:HG11	1.64	0.80
17:O:39:TYR:CD1	18:Y:74:ALA:HB1	2.17	0.79
17:O:63:LEU:HD21	18:Y:45:LEU:HA	1.64	0.79
3:M:272:ARG:NE	7:P:314:GLU:OE2	2.16	0.79
16:R:40:ARG:O	21:N:144:DC:O3'	2.00	0.79
17:O:42:ARG:HE	21:N:113:DA:H5''	1.43	0.79
18:U:88:THR:CB	21:N:40:DA:OP1	2.30	0.79
20:B:56:DC:O5'	7:Q:528:LEU:HD13	1.80	0.79
13:S:78:ARG:CG	20:B:102:DG:P	2.69	0.79
18:Y:86:ARG:CD	20:B:40:DG:OP1	2.31	0.78
18:U:33:ARG:CZ	21:N:28:DT:C5'	2.61	0.78
7:Q:473:TYR:CE1	7:Q:702:VAL:HG12	2.18	0.78
17:T:45:ALA:HB2	20:B:112:DT:OP2	1.83	0.78
5:G:273:ILE:HD11	5:G:340:LYS:HG2	1.65	0.78
18:Y:42:TYR:CZ	20:B:21:DG:OP2	2.36	0.78
5:G:344:VAL:O	5:G:347:HIS:CE1	2.37	0.77
11:X:377:TYR:O	11:X:511:LEU:HA	1.84	0.77
16:R:63:ARG:NH2	20:B:91:DA:H5''	1.98	0.77
18:U:88:THR:N	21:N:40:DA:OP1	2.16	0.77
14:f:48:ILE:HG22	14:f:54:MET:SD	2.23	0.77
17:T:15:LYS:HD2	21:N:32:DG:P	2.24	0.77
17:T:15:LYS:HD2	21:N:32:DG:OP1	1.85	0.77
17:O:67:GLY:HA3	18:Y:49:HIS:CD2	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:272:ARG:HD3	7:P:314:GLU:OE2	1.84	0.77
17:T:57:TYR:CD1	18:U:113:GLU:HG3	2.20	0.77
18:Y:33:ARG:HD3	21:N:124:DG:OP1	1.85	0.77
19:g:295:GLY:O	19:g:298:ARG:NH1	2.18	0.77
7:Q:548:ILE:HD12	7:Q:572:LEU:HD23	0.82	0.76
17:T:57:TYR:OH	18:U:109:HIS:HB3	1.85	0.76
11:X:366:ASN:O	11:X:369:ASN:CG	2.28	0.76
17:O:76:THR:OG1	21:N:132:DC:P	2.43	0.76
13:W:72:TYR:CE1	18:Y:80:LEU:HD21	2.20	0.76
17:O:21:ALA:CB	18:Y:121:TYR:HB2	2.14	0.76
14:f:166:VAL:HG22	14:f:333:MET:SD	2.26	0.76
13:S:91:LYS:HZ1	18:Y:71:GLU:CD	1.91	0.76
7:Q:991:GLU:O	7:Q:994:LEU:CB	2.33	0.76
2:H:254:ILE:HG22	2:H:254:ILE:O	1.84	0.76
20:B:54:DC:OP1	7:Q:815:GLN:O	2.02	0.76
21:N:95:DG:OP2	7:Q:608:LYS:HD2	1.85	0.75
16:R:42:ARG:H	21:N:144:DC:H5'	1.49	0.75
16:R:83:ARG:NH1	21:N:50:DT:H1'	2.01	0.75
17:O:42:ARG:CD	21:N:113:DA:H5'	2.15	0.75
16:R:63:ARG:CD	20:B:91:DA:H4'	2.05	0.74
19:g:403:CYS:SG	19:g:404:PRO:HD3	2.27	0.74
14:f:48:ILE:HB	14:f:54:MET:SD	2.27	0.74
16:R:83:ARG:NH1	21:N:51:DT:H5'	2.03	0.74
7:P:333:PHE:HB3	7:P:337:ARG:HH12	1.52	0.74
18:Y:56:SER:HB2	20:B:20:DA:OP2	1.87	0.74
21:N:97:DG:OP1	7:Q:631:GLN:NE2	2.20	0.74
18:Y:33:ARG:HE	21:N:124:DG:C4'	2.00	0.73
17:O:32:ARG:CG	20:B:30:DA:OP2	2.36	0.73
7:Q:473:TYR:CG	7:Q:702:VAL:HG12	2.23	0.73
18:Y:33:ARG:HD3	21:N:124:DG:C5'	2.14	0.72
20:B:56:DC:H4'	7:Q:577:GLU:OE1	1.90	0.72
16:R:39:HIS:N	21:N:145:DA:OP1	2.23	0.72
12:L:765:THR:CG2	12:L:790:LEU:CD2	2.63	0.72
16:R:83:ARG:HH11	21:N:50:DT:H1'	1.54	0.72
17:T:42:ARG:HH11	21:N:39:DG:C4'	2.00	0.72
18:Y:33:ARG:HD3	21:N:123:DC:O3'	1.88	0.72
18:Y:33:ARG:CB	21:N:124:DG:H5''	2.20	0.72
7:Q:993:ILE:O	7:Q:996:ASP:N	2.14	0.72
21:N:97:DG:P	7:Q:631:GLN:NE2	2.63	0.71
21:N:96:DT:P	7:Q:607:SER:HB3	2.30	0.71
18:U:87:SER:C	21:N:40:DA:OP1	2.33	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:33:ARG:HH12	21:N:28:DT:H5''	1.14	0.71
6:A:238:GLU:OE1	7:J:212:ASN:ND2	2.23	0.71
14:f:166:VAL:HG21	14:f:333:MET:SD	2.29	0.71
4:I:476:LEU:HD21	4:I:480:GLN:HE22	1.53	0.71
16:V:83:ARG:NH2	21:N:101:DG:OP1	2.24	0.71
19:g:359:ILE:CG1	19:g:404:PRO:HG2	2.20	0.71
20:B:79:DC:O2	21:N:70:DG:N2	2.23	0.71
15:h:80:ASP:OD2	19:g:54:HIS:ND1	2.20	0.70
20:B:57:DT:H4'	7:Q:581:LYS:HZ2	1.55	0.70
17:O:32:ARG:HH22	20:B:29:DA:H2''	1.55	0.70
14:f:76:LEU:HD22	14:f:108:MET:HE1	0.71	0.70
17:O:42:ARG:HE	21:N:113:DA:C5'	1.98	0.70
5:G:15:ASN:HD22	5:G:174:THR:HA	1.56	0.70
20:B:6:DG:H1	21:N:142:DC:H42	1.40	0.70
14:f:238:VAL:HG21	14:f:404:MET:CG	2.20	0.70
15:h:79:GLU:OE1	19:g:84:ARG:NH1	2.25	0.70
16:V:40:ARG:HA	21:N:84:DG:OP1	1.91	0.70
16:R:65:LEU:N	20:B:92:DC:OP2	2.25	0.70
16:R:83:ARG:NH1	21:N:51:DT:C5'	2.55	0.70
17:T:92:GLU:OE1	18:U:106:LEU:HG	1.92	0.69
20:B:56:DC:OP2	7:Q:840:SER:CB	2.39	0.69
7:Q:991:GLU:HB3	7:Q:994:LEU:HD12	1.75	0.69
14:f:76:LEU:HD23	14:f:108:MET:CE	2.16	0.69
19:g:323:ILE:CD1	19:g:403:CYS:HB3	2.22	0.69
13:W:91:LYS:NZ	18:U:71:GLU:OE1	2.26	0.69
14:f:155:PHE:HE2	14:f:333:MET:CE	1.96	0.69
16:R:65:LEU:CB	20:B:92:DC:OP2	2.39	0.69
16:R:83:ARG:CG	21:N:51:DT:C5'	2.58	0.69
17:O:17:ARG:HG3	20:B:31:DT:OP1	1.91	0.69
20:B:57:DT:OP1	7:Q:578:TYR:CZ	2.42	0.69
14:f:48:ILE:CG2	14:f:54:MET:SD	2.81	0.69
13:S:78:ARG:HG2	20:B:102:DG:OP2	1.91	0.69
17:T:42:ARG:HH11	21:N:39:DG:H4'	1.58	0.69
17:T:42:ARG:HD3	21:N:39:DG:C4'	2.24	0.68
18:Y:39:ILE:HD11	21:N:123:DC:OP2	1.92	0.68
7:Q:473:TYR:HD1	7:Q:697:ARG:HD2	1.59	0.68
17:T:45:ALA:HB2	20:B:112:DT:P	2.34	0.68
6:A:218:PRO:HA	11:X:364:LEU:CD2	2.24	0.68
7:Q:809:ARG:HA	7:Q:861:PHE:HB3	1.75	0.68
14:f:36:ILE:HB	14:f:54:MET:CE	2.10	0.68
18:U:88:THR:OG1	21:N:40:DA:P	2.52	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:88:TYR:CZ	18:U:83:TYR:CD1	2.83	0.67
7:Q:880:ASP:HB2	7:Q:910:VAL:HA	1.76	0.67
13:W:91:LYS:HZ1	18:U:71:GLU:CD	2.03	0.67
14:f:157:ILE:HD13	14:f:333:MET:HE2	1.71	0.67
14:f:291:LEU:O	19:g:402:GLN:NE2	2.27	0.67
14:f:430:MET:SD	19:g:321:ASP:OD1	2.53	0.67
14:f:76:LEU:CD2	14:f:108:MET:HE3	1.81	0.67
16:R:83:ARG:HB3	21:N:50:DT:O3'	1.94	0.67
16:R:83:ARG:NH1	21:N:51:DT:O4'	2.27	0.67
19:g:323:ILE:HG13	19:g:403:CYS:CB	2.21	0.67
16:R:63:ARG:NE	20:B:91:DA:H5''	2.10	0.67
2:H:279:ASP:OD1	2:H:329:MET:HE1	1.94	0.66
17:T:42:ARG:NE	21:N:39:DG:H4'	2.09	0.66
7:Q:473:TYR:OH	7:Q:701:GLU:C	2.38	0.66
7:Q:473:TYR:HE2	7:Q:702:VAL:O	1.78	0.66
6:A:238:GLU:CD	7:J:212:ASN:HD22	2.00	0.66
14:f:36:ILE:HD12	14:f:54:MET:HE3	1.77	0.66
17:T:57:TYR:OH	18:U:109:HIS:CB	2.43	0.66
17:O:32:ARG:CD	20:B:30:DA:OP2	2.42	0.66
5:G:273:ILE:CD1	5:G:340:LYS:HG2	2.26	0.66
17:O:32:ARG:NH2	20:B:29:DA:C2'	2.57	0.66
7:Q:699:LYS:HA	7:Q:702:VAL:HG22	1.77	0.66
14:f:108:MET:SD	14:f:123:TYR:CE2	2.89	0.66
3:M:272:ARG:NE	7:P:314:GLU:CD	2.54	0.65
19:g:369:ARG:NH1	19:g:398:ILE:HG12	2.11	0.65
7:Q:698:LEU:HB2	7:Q:701:GLU:HG3	1.77	0.65
16:V:42:ARG:CD	20:B:144:DC:O5'	2.43	0.65
20:B:58:DT:OP2	7:Q:554:PRO:CG	2.43	0.65
14:f:48:ILE:CB	14:f:54:MET:SD	2.85	0.65
21:N:95:DG:OP2	7:Q:608:LYS:CG	2.45	0.65
2:H:304:LEU:HD22	2:H:318:GLN:HG3	1.78	0.65
20:B:54:DC:H4'	7:Q:868:ARG:HG2	0.72	0.65
7:Q:473:TYR:CE2	7:Q:702:VAL:O	2.50	0.65
17:O:28:GLY:HA3	20:B:30:DA:C5'	2.21	0.65
18:Y:56:SER:HB3	20:B:20:DA:OP2	1.96	0.64
19:g:359:ILE:HG21	19:g:402:GLN:HB2	1.79	0.64
17:T:42:ARG:HH11	21:N:39:DG:C5'	2.09	0.64
18:U:33:ARG:NH2	21:N:28:DT:H5'	2.12	0.64
14:f:36:ILE:HG13	14:f:54:MET:HE2	1.64	0.64
17:O:76:THR:HG1	21:N:132:DC:P	2.21	0.64
7:Q:809:ARG:HH22	7:Q:853:PHE:HA	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:170:THR:HG23	11:X:379:LEU:HD22	1.80	0.64
21:N:95:DG:OP2	7:Q:608:LYS:CD	2.46	0.64
17:O:39:TYR:CE1	18:Y:74:ALA:CB	2.79	0.64
13:W:88:TYR:CZ	18:Y:83:TYR:CD1	2.86	0.63
21:N:95:DG:OP1	7:Q:609:LEU:HG	1.97	0.63
7:Q:812:MET:HE1	7:Q:885:PHE:HE2	1.57	0.63
7:Q:500:GLY:H	7:Q:903:ARG:HH11	1.46	0.63
6:A:190:PRO:HB3	11:X:437:LEU:HD23	1.76	0.63
17:T:77:ARG:HA	18:U:53:GLY:O	1.97	0.63
18:Y:56:SER:H	20:B:20:DA:P	2.21	0.63
20:B:55:DG:P	7:Q:839:GLY:CA	2.80	0.63
13:W:42:GLY:O	16:V:108:ASN:ND2	2.31	0.63
13:S:98:TYR:OH	18:Y:68:ASP:OD2	2.14	0.63
16:R:68:GLN:HE21	16:R:72:ARG:HH21	1.46	0.63
6:A:264:MET:HA	7:J:259:GLN:HE21	1.63	0.62
7:Q:497:MET:SD	7:Q:896:GLN:NE2	2.72	0.62
2:H:439:LYS:NZ	4:I:40:ASP:OD2	2.32	0.62
3:M:272:ARG:CD	7:P:314:GLU:CD	2.72	0.62
7:Q:728:GLN:HE21	7:Q:730:LEU:HD12	1.64	0.62
14:f:121:GLU:O	14:f:124:TYR:HB2	1.99	0.62
14:f:157:ILE:HG12	14:f:333:MET:SD	2.38	0.62
17:T:67:GLY:HA3	18:U:49:HIS:CD2	2.34	0.62
17:T:80:PRO:HB3	18:U:61:ILE:CD1	2.28	0.62
19:g:358:LEU:CD1	19:g:405:THR:O	2.47	0.62
13:S:79:LYS:HD2	20:B:101:DG:O5'	1.98	0.62
7:Q:840:SER:HA	7:Q:846:ARG:HH21	1.64	0.62
20:B:56:DC:OP2	7:Q:840:SER:HB2	1.98	0.62
21:N:96:DT:C3'	7:Q:604:ASN:HD21	2.02	0.62
6:A:238:GLU:O	6:A:238:GLU:HG3	1.99	0.61
7:Q:594:MET:HB2	7:Q:622:ARG:HA	1.82	0.61
13:W:72:TYR:HE1	18:Y:80:LEU:HD21	1.62	0.61
13:S:88:TYR:CE1	18:U:83:TYR:OH	2.51	0.61
17:O:64:GLU:CG	18:Y:48:VAL:HG11	2.29	0.61
17:O:24:GLN:HE22	18:Y:47:GLN:HE22	1.48	0.61
17:O:92:GLU:OE1	18:Y:106:LEU:HG	2.01	0.61
16:R:108:ASN:ND2	13:S:42:GLY:O	2.34	0.61
17:T:15:LYS:CD	21:N:32:DG:OP2	2.49	0.61
19:g:369:ARG:HH12	19:g:398:ILE:HG12	1.65	0.61
20:B:55:DG:OP1	7:Q:839:GLY:CA	2.48	0.61
21:N:96:DT:P	7:Q:607:SER:CB	2.88	0.60
7:Q:564:ILE:HG22	7:Q:564:ILE:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:56:DC:OP2	7:Q:840:SER:HB3	2.00	0.60
6:A:88:ILE:HG13	6:A:91:GLY:H	1.66	0.60
7:P:372:ARG:O	7:P:376:GLN:CG	2.48	0.60
4:I:237:ASN:HB3	4:I:322:VAL:HG12	1.83	0.60
17:T:44:GLY:C	20:B:112:DT:OP1	2.44	0.60
20:B:110:DC:O2	21:N:39:DG:N2	2.35	0.60
6:A:222:PRO:HG3	12:L:758:ASN:HB2	1.84	0.60
14:f:108:MET:SD	14:f:123:TYR:CZ	2.95	0.60
2:H:83:PRO:HA	2:D:192:ASP:HB3	1.82	0.60
18:Y:40:TYR:OH	21:N:122:DG:P	2.59	0.60
7:P:333:PHE:HB3	7:P:337:ARG:NH1	2.16	0.60
11:X:437:LEU:HD23	11:X:437:LEU:O	2.01	0.59
13:W:68:ASP:OD1	18:Y:100:LEU:HD22	2.02	0.59
18:Y:33:ARG:HE	21:N:124:DG:H5''	1.59	0.59
6:A:189:VAL:O	11:X:437:LEU:N	2.27	0.59
19:g:370:GLU:HG2	19:g:395:VAL:HG21	1.84	0.59
7:Q:407:GLN:HA	7:Q:411:PHE:HB2	1.85	0.59
17:O:17:ARG:CG	20:B:31:DT:P	2.85	0.59
7:Q:528:LEU:O	7:Q:846:ARG:NH1	2.36	0.59
17:O:42:ARG:HD3	21:N:112:DG:O3'	2.02	0.59
20:B:55:DG:OP2	7:Q:839:GLY:HA3	2.01	0.59
14:f:36:ILE:CD1	14:f:54:MET:CE	2.63	0.59
16:V:42:ARG:HD3	20:B:144:DC:OP1	2.03	0.59
7:Q:722:GLN:HE22	7:Q:766:PRO:HB3	1.68	0.59
14:f:36:ILE:N	14:f:54:MET:HE2	2.14	0.58
7:Q:638:TRP:HD1	7:Q:648:ILE:HD12	1.67	0.58
7:Q:909:GLU:CD	7:Q:987:ARG:CD	2.75	0.58
16:V:42:ARG:HB2	20:B:144:DC:OP1	2.02	0.58
7:Q:473:TYR:CD1	7:Q:697:ARG:HD2	2.38	0.58
7:Q:767:PHE:CE2	7:Q:786:LEU:CD2	2.87	0.58
15:h:25:TRP:O	19:g:129:GLN:NE2	2.35	0.58
11:X:375:GLU:HB2	11:X:514:HIS:HB2	1.85	0.58
5:G:344:VAL:O	5:G:347:HIS:NE2	2.36	0.58
13:W:98:TYR:CZ	18:U:68:ASP:OD2	2.53	0.58
17:T:42:ARG:NH1	21:N:39:DG:O4'	2.35	0.58
17:O:42:ARG:CA	21:N:113:DA:OP1	2.52	0.58
7:Q:644:VAL:HG12	7:Q:645:LEU:HG	1.86	0.58
14:f:48:ILE:C	14:f:54:MET:SD	2.86	0.58
20:B:128:DG:H1	21:N:20:DC:H42	1.51	0.58
7:Q:478:LEU:HD11	7:Q:507:SER:HB2	1.85	0.58
7:Q:909:GLU:OE2	7:Q:911:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:279:ASP:OD1	2:H:329:MET:CE	2.51	0.58
2:H:464:GLU:O	2:H:467:LYS:HB3	2.04	0.58
11:X:438:SER:HB3	11:X:441:HIS:HE1	1.68	0.58
14:f:241:LYS:HE3	14:f:245:GLU:HB3	1.86	0.58
17:T:15:LYS:HE3	21:N:32:DG:OP2	2.04	0.58
7:Q:784:ASP:O	7:Q:785:LEU:HB2	2.04	0.58
18:Y:56:SER:N	20:B:20:DA:OP1	2.37	0.57
19:g:438:GLN:O	19:g:442:HIS:ND1	2.37	0.57
7:Q:896:GLN:O	7:Q:900:ARG:NH2	2.37	0.57
16:R:42:ARG:HG3	21:N:144:DC:C5'	2.35	0.57
17:O:32:ARG:CG	20:B:30:DA:P	2.93	0.57
18:Y:33:ARG:HB2	21:N:124:DG:H5''	1.87	0.57
20:B:11:DC:H42	21:N:137:DG:H1	1.52	0.57
7:Q:564:ILE:HG23	7:Q:569:PHE:HD2	1.70	0.57
5:G:273:ILE:HD12	5:G:340:LYS:HE2	1.87	0.57
6:A:195:TYR:H	6:A:206:SER:HB3	1.70	0.57
13:S:88:TYR:CE2	18:U:83:TYR:CD1	2.92	0.57
7:Q:476:ARG:O	7:Q:480:TRP:N	2.36	0.57
2:H:311:VAL:O	2:H:314:ASN:ND2	2.38	0.57
3:M:521:GLN:HE21	4:I:333:MET:HE2	1.69	0.57
5:G:338:LYS:O	5:G:341:LYS:HB3	2.05	0.57
13:S:30:THR:HG21	21:N:61:DA:H5''	1.85	0.57
20:B:54:DC:H5''	7:Q:868:ARG:HE	1.69	0.57
7:Q:473:TYR:HH	7:Q:701:GLU:C	2.12	0.57
6:A:395:ASN:O	7:J:90:GLN:NE2	2.38	0.57
20:B:54:DC:H5''	7:Q:868:ARG:HG2	1.86	0.57
13:W:77:LYS:HE3	18:Y:92:ARG:HH12	1.68	0.57
7:Q:989:ALA:CA	7:Q:992:LYS:HG3	2.31	0.57
2:H:310:SER:OG	2:H:314:ASN:ND2	2.38	0.56
13:W:44:LYS:HE2	17:T:115:LEU:HG	1.87	0.56
15:h:22:LYS:HA	19:g:451:ARG:HH21	1.69	0.56
17:T:42:ARG:HG3	18:U:88:THR:OG1	2.03	0.56
19:g:39:THR:HG22	19:g:67:PRO:HD2	1.87	0.56
3:M:272:ARG:NE	7:P:314:GLU:OE1	2.39	0.56
2:H:246:ASP:OD2	5:G:160:HIS:NE2	2.39	0.56
2:H:446:LYS:NZ	6:A:287:TYR:OH	2.39	0.56
12:L:805:ASN:ND2	12:L:808:ASP:OD2	2.39	0.56
17:T:80:PRO:HG3	18:U:61:ILE:HD12	1.88	0.56
19:g:153:MET:HE1	19:g:411:LYS:O	2.04	0.56
20:B:122:DG:N2	21:N:27:DC:O2	2.39	0.56
7:P:382:LYS:HG3	7:P:382:LYS:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:325:GLU:OE2	7:J:246:LYS:NZ	2.34	0.56
2:H:435:LEU:O	4:I:398:LYS:NZ	2.38	0.56
14:f:430:MET:SD	19:g:321:ASP:CG	2.89	0.56
7:J:128:ASP:OD2	7:J:198:ARG:NH2	2.39	0.56
20:B:27:DT:O2	21:N:122:DG:N2	2.39	0.56
4:I:267:VAL:HG21	4:I:309:GLU:HB2	1.87	0.55
6:A:209:ILE:HG22	6:A:211:LYS:H	1.71	0.55
13:S:78:ARG:HG2	20:B:102:DG:OP1	1.95	0.55
17:T:15:LYS:CD	21:N:32:DG:P	2.93	0.55
16:V:42:ARG:NH2	20:B:144:DC:C2'	2.69	0.55
18:Y:33:ARG:HB3	21:N:124:DG:H5''	1.87	0.55
7:Q:911:ARG:NH2	7:Q:987:ARG:HG2	2.21	0.55
14:f:196:ARG:NH1	14:f:305:GLU:OE1	2.40	0.55
7:Q:482:VAL:O	7:Q:486:ASN:N	2.35	0.55
7:Q:815:GLN:N	7:Q:886:ASP:OD1	2.30	0.55
3:M:257:TYR:OH	7:J:294:LYS:NZ	2.40	0.55
17:T:21:ALA:HB2	18:U:121:TYR:HB2	1.87	0.55
17:O:17:ARG:CG	20:B:31:DT:OP2	2.55	0.55
14:f:108:MET:SD	14:f:123:TYR:HE2	2.29	0.55
18:Y:39:ILE:CD1	21:N:123:DC:OP2	2.54	0.55
7:Q:986:ALA:HB3	7:Q:992:LYS:CG	2.27	0.55
7:Q:991:GLU:O	7:Q:994:LEU:CA	2.55	0.55
19:g:327:LYS:HE2	19:g:403:CYS:HA	1.88	0.55
7:Q:991:GLU:CB	7:Q:994:LEU:HD12	2.36	0.55
6:A:238:GLU:HB3	12:L:804:ILE:HD11	1.89	0.55
6:A:484:ASN:HD22	11:X:624:LEU:HD13	1.72	0.55
16:V:83:ARG:CZ	21:N:101:DG:OP1	2.54	0.55
19:g:427:ILE:O	19:g:430:LEU:HB3	2.07	0.55
11:X:520:LYS:NZ	11:X:611:SER:OG	2.39	0.55
21:N:47:DC:H4'	21:N:48:DC:H5'	1.89	0.55
14:f:38:ARG:HB3	14:f:46:GLU:HB3	1.88	0.55
7:Q:815:GLN:HG3	7:Q:886:ASP:OD2	2.07	0.54
5:G:279:VAL:HG21	5:G:339:ILE:CD1	2.35	0.54
2:H:127:ASN:ND2	2:D:184:THR:OG1	2.40	0.54
17:T:80:PRO:HG3	18:U:61:ILE:CD1	2.37	0.54
3:M:272:ARG:HD3	7:P:314:GLU:CD	2.33	0.54
11:X:366:ASN:O	11:X:369:ASN:ND2	2.41	0.54
14:f:37:LYS:O	14:f:65:ASP:HA	2.07	0.54
14:f:189:LEU:HD11	14:f:313:LEU:HD11	1.87	0.54
19:g:457:LYS:HB2	19:g:461:ALA:HB2	1.88	0.54
7:Q:481:MET:O	7:Q:485:TYR:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:W:98:TYR:OH	18:U:68:ASP:CG	2.43	0.54
17:T:20:ARG:O	18:U:121:TYR:HA	2.08	0.54
7:Q:459:ASP:HB3	7:Q:475:LEU:HD13	1.89	0.54
14:f:242:ASP:O	14:f:246:LEU:N	2.37	0.54
12:L:765:THR:HG22	12:L:790:LEU:CG	2.38	0.54
4:I:476:LEU:HD23	4:I:480:GLN:NE2	2.21	0.53
19:g:189:MET:HE1	19:g:193:SER:OG	2.05	0.53
17:O:64:GLU:CA	18:Y:48:VAL:HG11	2.35	0.53
20:B:33:DG:H2''	20:B:34:DG:H5''	1.90	0.53
2:H:272:TYR:OH	2:H:303:ARG:NH1	2.41	0.53
17:O:17:ARG:HG3	20:B:31:DT:OP2	2.09	0.53
18:U:77:ALA:HA	18:U:80:LEU:HD12	1.91	0.53
19:g:153:MET:HE1	19:g:411:LYS:C	2.34	0.53
14:f:447:PRO:HD3	7:P:337:ARG:HH22	1.74	0.53
2:H:475:LEU:HD21	2:D:475:LEU:HD11	1.91	0.53
13:S:88:TYR:CG	18:U:83:TYR:CZ	2.95	0.53
17:T:15:LYS:HD2	21:N:32:DG:OP2	2.09	0.53
16:V:42:ARG:NH1	20:B:144:DC:O5'	2.42	0.53
18:Y:90:THR:OG1	18:Y:93:GLU:OE1	2.24	0.53
7:Q:612:THR:O	7:Q:616:TYR:N	2.40	0.53
2:H:271:ARG:NH1	2:H:305:GLU:O	2.42	0.53
3:M:264:ARG:NH2	3:M:303:GLU:OE2	2.40	0.53
20:B:55:DG:C3'	7:Q:840:SER:HB3	2.39	0.53
3:M:551:GLN:NE2	3:M:578:THR:O	2.42	0.53
5:G:158:GLN:O	5:G:164:ASN:ND2	2.42	0.53
11:X:366:ASN:O	11:X:369:ASN:OD1	2.26	0.53
16:V:42:ARG:HH11	20:B:144:DC:P	2.31	0.53
19:g:28:GLU:C	7:P:369:ARG:HH12	2.13	0.53
2:H:446:LYS:O	2:H:449:ASP:HB2	2.08	0.53
14:f:54:MET:O	14:f:58:ALA:N	2.40	0.53
16:R:66:PRO:HD3	20:B:91:DA:O5'	2.09	0.53
7:Q:471:LYS:NZ	7:Q:703:GLU:OE2	2.41	0.53
7:Q:473:TYR:CE1	7:Q:702:VAL:CG1	2.91	0.52
2:H:421:TYR:O	2:H:424:GLU:HB3	2.08	0.52
2:D:227:ASN:ND2	7:J:244:GLU:OE2	2.38	0.52
12:L:750:VAL:HG11	12:L:788:GLU:CD	2.32	0.52
16:R:63:ARG:NH2	20:B:91:DA:C5'	2.70	0.52
17:O:85:LEU:O	17:O:89:ASN:ND2	2.42	0.52
19:g:437:LYS:O	19:g:441:THR:OG1	2.23	0.52
7:Q:941:GLN:HA	7:Q:944:LYS:HE3	1.91	0.52
16:R:66:PRO:HD3	20:B:91:DA:H3'	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:178:LEU:HD11	2:D:195:GLN:HG3	1.90	0.52
6:A:313:ARG:NH1	8:E:16:TYR:O	2.41	0.52
17:O:20:ARG:CZ	20:B:32:DT:OP1	2.56	0.52
18:U:98:VAL:HG13	18:U:102:LEU:HD12	1.90	0.52
4:I:482:ARG:O	4:I:483:LEU:CB	2.56	0.52
2:H:406:LYS:NZ	2:D:396:ALA:O	2.38	0.52
2:D:125:ILE:HG12	2:D:142:VAL:HG21	1.90	0.52
13:W:72:TYR:HE1	18:Y:80:LEU:CD2	2.21	0.52
7:Q:465:LEU:HD22	7:Q:541:TRP:HE3	1.73	0.52
7:Q:485:TYR:OH	7:Q:622:ARG:O	2.28	0.52
7:Q:684:ARG:HA	7:Q:687:HIS:HD2	1.72	0.52
16:R:83:ARG:NH1	21:N:51:DT:C4'	2.73	0.52
7:Q:603:LYS:HE2	7:Q:630:LEU:HA	1.91	0.52
14:f:291:LEU:HB3	19:g:402:GLN:CD	2.35	0.52
7:Q:813:PHE:HB3	7:Q:867:THR:HG22	1.91	0.52
12:L:765:THR:O	12:L:766:ASP:HB2	2.09	0.52
14:f:155:PHE:CZ	14:f:333:MET:CE	2.78	0.52
7:Q:511:TYR:O	7:Q:515:VAL:N	2.37	0.52
6:A:129:GLU:OE2	12:L:869:ARG:NE	2.42	0.51
11:X:431:GLN:HG2	11:X:446:LYS:HB3	1.91	0.51
2:H:453:GLN:O	2:H:456:MET:HB3	2.10	0.51
17:T:57:TYR:OH	18:U:109:HIS:CG	2.63	0.51
17:T:92:GLU:OE1	18:U:106:LEU:CG	2.58	0.51
20:B:57:DT:OP1	7:Q:578:TYR:HE2	1.91	0.51
21:N:113:DA:H2''	21:N:114:DC:H5''	1.91	0.51
2:D:158:ALA:O	2:D:162:LYS:HB2	2.10	0.51
14:f:5:ARG:NH2	14:f:446:LEU:O	2.43	0.51
19:g:18:THR:HA	19:g:38:PRO:HA	1.92	0.51
7:Q:896:GLN:HG3	7:Q:900:ARG:HH12	1.73	0.51
19:g:359:ILE:HG12	19:g:404:PRO:CG	2.34	0.51
7:Q:551:LYS:NZ	7:Q:844:GLU:OE2	2.36	0.51
7:Q:894:ASP:O	7:Q:898:GLN:N	2.44	0.51
16:R:42:ARG:HG3	21:N:144:DC:H5'	1.91	0.51
7:Q:679:THR:HB	7:Q:683:ILE:HD12	1.92	0.51
7:Q:790:ALA:HB3	7:Q:793:PHE:HB2	1.92	0.51
7:Q:875:ASN:OD1	7:Q:903:ARG:NE	2.43	0.51
7:Q:883:ILE:HG21	7:Q:885:PHE:HE2	1.33	0.51
2:D:143:ARG:HH12	5:G:314:ILE:HD11	1.75	0.51
13:W:88:TYR:CG	18:Y:83:TYR:CZ	2.99	0.51
15:h:63:TRP:NE1	19:g:125:GLU:OE1	2.40	0.51
7:Q:841:THR:OG1	7:Q:842:LYS:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:18:GLN:OE1	6:A:22:ASN:ND2	2.44	0.51
17:O:32:ARG:HG2	20:B:30:DA:P	2.50	0.51
2:D:469:LEU:HD22	4:I:258:LYS:HD3	1.92	0.51
4:I:220:ILE:HD12	4:I:351:LEU:HD22	1.92	0.51
7:Q:811:LEU:HB2	7:Q:882:VAL:HG13	1.92	0.51
6:A:398:PRO:HD3	7:J:52:SER:HA	1.93	0.51
14:f:235:MET:SD	19:g:401:VAL:CG2	2.97	0.51
3:M:82:LEU:HD21	3:M:120:LEU:HD21	1.93	0.50
6:A:445:GLU:O	6:A:449:TYR:N	2.44	0.50
15:h:79:GLU:N	19:g:84:ARG:HH12	2.09	0.50
17:O:32:ARG:HH22	20:B:29:DA:C2'	2.20	0.50
20:B:54:DC:H5''	7:Q:868:ARG:CG	2.41	0.50
7:Q:978:ASP:HA	7:Q:981:LEU:HB2	1.93	0.50
2:H:271:ARG:NH1	2:H:306:ASN:OD1	2.40	0.50
18:Y:58:ALA:HA	18:Y:61:ILE:HD12	1.93	0.50
2:H:426:GLN:HB2	2:D:422:ILE:HD11	1.93	0.50
7:J:268:GLN:OE1	7:J:272:ASN:ND2	2.43	0.50
14:f:161:ALA:HA	14:f:186:GLY:H	1.76	0.50
19:g:149:ALA:HB2	19:g:428:ILE:HG12	1.94	0.50
21:N:97:DG:P	7:Q:631:GLN:HE22	2.34	0.50
7:Q:451:ALA:O	7:Q:487:ASN:ND2	2.44	0.50
6:A:112:GLN:HE21	6:A:217:ARG:HD2	1.77	0.50
11:X:438:SER:HB3	11:X:441:HIS:CE1	2.46	0.50
11:X:439:GLU:CD	11:X:490:GLU:CD	2.78	0.50
13:S:88:TYR:CG	18:U:83:TYR:CE2	3.00	0.50
17:O:20:ARG:NH2	20:B:32:DT:OP1	2.45	0.50
20:B:58:DT:H4'	20:B:59:DA:H5'	1.94	0.50
2:H:454:LEU:HB3	2:D:454:LEU:HD11	1.94	0.50
14:f:36:ILE:H	14:f:54:MET:HE1	1.52	0.50
14:f:145:ILE:HG21	14:f:395:THR:HG21	1.94	0.50
16:R:106:ASP:OD2	16:R:131:ARG:NH2	2.37	0.50
17:T:15:LYS:NZ	17:T:16:THR:O	2.42	0.50
19:g:28:GLU:O	7:P:369:ARG:NH1	2.25	0.50
19:g:144:PRO:HG2	19:g:147:LEU:HD12	1.94	0.50
7:Q:630:LEU:O	7:Q:892:HIS:NE2	2.45	0.50
7:Q:731:LYS:HA	7:Q:735:LEU:HD12	1.94	0.50
7:Q:909:GLU:HB3	7:Q:987:ARG:CD	2.42	0.50
11:X:447:PRO:HB3	11:X:480:ASN:HD22	1.77	0.50
17:T:42:ARG:HH11	21:N:39:DG:H5'	1.75	0.50
17:O:32:ARG:CZ	20:B:29:DA:C2'	2.90	0.50
7:Q:760:ARG:O	7:Q:764:ASN:ND2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:196:PHE:HB3	10:K:160:GLN:HE21	1.76	0.49
13:W:75:HIS:HB2	18:Y:96:THR:HG21	1.93	0.49
13:W:77:LYS:HE3	18:Y:92:ARG:NH1	2.26	0.49
13:S:75:HIS:CE1	18:U:93:GLU:HG3	2.47	0.49
7:Q:478:LEU:CD2	7:Q:507:SER:OG	2.32	0.49
7:Q:988:SER:O	7:Q:989:ALA:HB3	2.12	0.49
17:O:42:ARG:HD3	21:N:113:DA:H5'	1.93	0.49
7:Q:809:ARG:HB2	7:Q:879:ALA:HB2	1.94	0.49
3:M:519:PHE:HB2	4:I:333:MET:HE1	1.94	0.49
17:O:64:GLU:HG2	18:Y:48:VAL:HG13	1.94	0.49
13:W:64:ASN:O	13:W:93:GLN:NE2	2.45	0.49
17:O:76:THR:OG1	21:N:132:DC:OP1	2.31	0.49
5:G:285:CYS:HB2	5:G:292:PHE:HB3	1.95	0.49
19:g:13:TYR:HB2	19:g:114:ILE:HD12	1.94	0.49
19:g:323:ILE:HD11	19:g:403:CYS:HB3	1.92	0.49
14:f:400:LEU:HD23	14:f:432:ARG:HH11	1.77	0.49
14:f:401:ILE:O	14:f:404:MET:HG2	2.12	0.49
16:V:68:GLN:HE21	16:V:72:ARG:HH21	1.59	0.49
14:f:455:TYR:HA	14:f:459:ASP:OD2	2.13	0.49
13:S:75:HIS:HD2	18:U:84:ASN:ND2	2.11	0.49
18:Y:40:TYR:OH	21:N:122:DG:O5'	2.30	0.49
20:B:96:DC:H2''	20:B:97:DA:C8	2.47	0.49
7:Q:565:ARG:O	7:Q:589:HIS:NE2	2.46	0.49
5:G:315:VAL:HG13	5:G:320:LEU:HB2	1.95	0.49
3:M:192:LEU:HB3	3:M:245:THR:HG21	1.95	0.49
6:A:190:PRO:CB	11:X:437:LEU:HD22	2.30	0.49
11:X:377:TYR:HB2	11:X:512:GLN:HB3	1.94	0.49
7:Q:767:PHE:CE2	7:Q:786:LEU:HD23	2.48	0.49
17:O:17:ARG:HD2	20:B:31:DT:OP2	2.08	0.48
19:g:132:PHE:HB3	19:g:451:ARG:NH1	2.28	0.48
20:B:55:DG:C2'	7:Q:840:SER:CB	2.78	0.48
7:Q:473:TYR:HD1	7:Q:697:ARG:CD	2.23	0.48
7:Q:797:ASP:HB3	7:Q:1002:ARG:HH22	1.78	0.48
7:Q:988:SER:OG	7:Q:991:GLU:HG3	2.13	0.48
1:F:351:ASP:HB2	1:F:358:HIS:CD2	2.47	0.48
5:G:374:SER:OG	5:G:375:ASN:N	2.46	0.48
19:g:12:ILE:HG22	19:g:14:PRO:HD3	1.95	0.48
19:g:19:THR:OG1	19:g:39:THR:OG1	2.29	0.48
16:R:42:ARG:HG3	21:N:144:DC:H5''	1.96	0.48
19:g:102:PHE:HA	19:g:106:LEU:HB2	1.95	0.48
7:P:376:GLN:C	7:P:378:LEU:N	2.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:f:62:ARG:HB2	14:f:65:ASP:OD2	2.13	0.48
17:T:42:ARG:CZ	21:N:39:DG:C4'	2.82	0.48
20:B:56:DC:C4'	7:Q:577:GLU:OE1	2.61	0.48
7:Q:522:PHE:HE1	7:Q:592:ALA:HB3	1.77	0.48
15:h:8:THR:HA	19:g:136:GLU:OE1	2.14	0.48
7:Q:564:ILE:HG23	7:Q:569:PHE:CD2	2.47	0.48
2:D:231:LYS:HG2	7:J:202:ARG:HH22	1.79	0.48
2:D:460:LYS:HA	2:D:463:LYS:HG2	1.96	0.48
19:g:22:GLN:OE1	19:g:433:GLN:NE2	2.39	0.48
20:B:99:DG:N2	21:N:49:DC:N3	2.59	0.48
7:J:46:ILE:HD13	7:J:79:ILE:HG12	1.95	0.48
7:J:225:ILE:HG23	7:J:229:ASP:HB3	1.95	0.48
13:W:20:LYS:HB2	7:Q:770:ASP:OD2	2.13	0.48
20:B:57:DT:H4'	7:Q:581:LYS:HZ1	1.76	0.48
20:B:97:DA:H2'	20:B:98:DA:C8	2.49	0.48
7:Q:525:ILE:HB	7:Q:596:ILE:HA	1.95	0.48
6:A:393:LEU:O	7:J:60:TYR:OH	2.32	0.48
3:M:341:PRO:HG3	3:M:553:ILE:HG23	1.95	0.48
14:f:167:THR:HG23	14:f:179:VAL:HG22	1.95	0.48
2:H:433:VAL:HG11	2:D:429:ILE:HG23	1.95	0.47
3:M:324:THR:O	3:M:328:LYS:HB2	2.14	0.47
11:X:374:THR:OG1	11:X:514:HIS:O	2.30	0.47
19:g:147:LEU:HA	19:g:150:THR:HG22	1.95	0.47
2:H:450:LEU:HD13	4:I:50:ARG:HG2	1.95	0.47
2:H:259:ILE:HB	3:M:44:SER:HA	1.95	0.47
15:h:89:ARG:HH22	19:g:32:VAL:HG22	1.79	0.47
7:Q:911:ARG:NH1	7:Q:984:THR:O	2.44	0.47
16:R:83:ARG:NH1	21:N:50:DT:O2	2.45	0.47
17:T:80:PRO:CG	18:U:61:ILE:CD1	2.93	0.47
7:Q:800:LEU:HD13	7:Q:830:LYS:HD3	1.96	0.47
7:Q:815:GLN:HG3	7:Q:886:ASP:CG	2.39	0.47
7:Q:986:ALA:HB3	7:Q:992:LYS:HE2	1.96	0.47
16:R:66:PRO:HG3	20:B:91:DA:P	2.53	0.47
17:O:50:TYR:HD1	18:Y:118:VAL:HG21	1.80	0.47
6:A:487:ILE:HD13	12:L:747:SER:HB2	1.96	0.47
16:R:63:ARG:HG3	16:R:66:PRO:HD2	1.95	0.47
13:S:79:LYS:HD2	20:B:101:DG:C5'	2.45	0.47
17:T:80:PRO:CG	18:U:61:ILE:HD11	2.45	0.47
18:Y:74:ALA:O	18:Y:78:SER:N	2.46	0.47
1:F:371:TRP:O	1:F:434:TYR:OH	2.32	0.47
1:F:410:TYR:CE2	1:F:422:ILE:HG21	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:W:72:TYR:CE1	18:Y:80:LEU:CD2	2.94	0.47
17:O:32:ARG:HG3	20:B:30:DA:P	2.55	0.47
19:g:303:ASN:OD1	19:g:307:LYS:NZ	2.45	0.47
20:B:99:DG:H1	21:N:49:DC:H42	1.61	0.47
21:N:89:DT:H2''	21:N:90:DA:C8	2.50	0.47
21:N:97:DG:OP2	7:Q:604:ASN:ND2	2.46	0.47
19:g:359:ILE:CG1	19:g:404:PRO:HD2	2.40	0.47
7:J:123:GLN:OE1	7:J:127:LYS:NZ	2.44	0.47
13:S:47:SER:OG	13:S:48:GLY:N	2.48	0.47
7:Q:812:MET:HE1	7:Q:885:PHE:CD2	2.47	0.47
7:Q:844:GLU:O	7:Q:847:THR:OG1	2.29	0.47
14:f:127:ALA:HB1	14:f:133:VAL:HB	1.97	0.47
14:f:392:VAL:HB	14:f:423:THR:HG22	1.96	0.47
16:V:40:ARG:NH2	21:N:83:DT:C1'	2.77	0.47
19:g:327:LYS:HE2	19:g:403:CYS:O	2.14	0.47
2:H:401:LEU:HD22	4:I:427:ARG:HD2	1.97	0.46
19:g:337:GLY:O	19:g:340:THR:OG1	2.29	0.46
20:B:81:DC:N4	21:N:66:DG:O6	2.48	0.46
1:F:384:ILE:HB	2:H:235:TYR:HB2	1.97	0.46
2:D:418:SER:O	2:D:422:ILE:HB	2.15	0.46
3:M:341:PRO:O	3:M:560:LYS:NZ	2.47	0.46
14:f:247:GLU:HG2	14:f:284:LEU:HD11	1.97	0.46
6:A:194:THR:OG1	6:A:229:ASN:OD1	2.26	0.46
13:W:25:ASN:ND2	16:V:73:GLU:OE1	2.48	0.46
7:Q:812:MET:HB2	7:Q:864:LEU:HA	1.98	0.46
16:R:116:ARG:NH1	16:R:118:THR:O	2.49	0.46
18:U:67:ASN:HA	18:U:70:PHE:HB3	1.96	0.46
2:D:148:MET:HE1	2:D:156:ILE:HD12	1.98	0.46
18:U:81:ALA:O	18:U:85:LYS:N	2.49	0.46
7:Q:1000:LYS:HA	7:Q:1004:ASN:HD22	1.80	0.46
7:Q:470:LEU:HB3	7:Q:475:LEU:HD21	1.98	0.46
6:A:235:THR:OG1	12:L:800:ASN:ND2	2.48	0.46
14:f:448:SER:HB3	14:f:451:LEU:HG	1.97	0.46
18:Y:33:ARG:NE	21:N:124:DG:H5''	2.17	0.46
20:B:141:DA:N3	21:N:8:DG:N2	2.64	0.46
21:N:96:DT:H6	21:N:96:DT:H2'	1.54	0.46
17:T:80:PRO:HB3	18:U:61:ILE:HD13	1.97	0.46
17:O:28:GLY:O	20:B:30:DA:OP1	2.34	0.46
6:A:278:THR:OG1	6:A:306:ARG:NH2	2.48	0.46
7:J:234:MET:HE1	12:L:803:ILE:HD11	1.98	0.46
18:Y:86:ARG:CD	20:B:40:DG:P	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:680:LEU:HD22	7:Q:684:ARG:HG3	1.98	0.46
7:Q:842:LYS:HD2	7:Q:845:GLU:HB2	1.97	0.46
2:H:195:GLN:HE22	2:D:175:LYS:HD3	1.81	0.45
5:G:205:PRO:HD2	5:G:337:LEU:HD21	1.98	0.45
16:R:42:ARG:HB3	16:R:43:PRO:CD	2.46	0.45
17:O:24:GLN:N	17:O:56:GLU:OE2	2.48	0.45
3:M:137:ILE:HG21	3:M:155:LEU:HD13	1.99	0.45
14:f:194:HIS:NE2	14:f:203:GLU:OE1	2.49	0.45
17:O:32:ARG:CZ	20:B:29:DA:H2''	2.45	0.45
5:G:358:ALA:HB1	5:G:365:ILE:H	1.81	0.45
6:A:112:GLN:NE2	6:A:215:ASP:OD2	2.50	0.45
6:A:206:SER:OG	6:A:207:SER:N	2.50	0.45
14:f:122:ARG:O	14:f:126:LEU:N	2.49	0.45
16:R:51:ILE:HD12	13:S:42:GLY:HA2	1.98	0.45
13:S:44:LYS:HB2	17:O:115:LEU:HD13	1.97	0.45
2:H:334:TRP:HE1	4:I:483:LEU:HD21	1.81	0.45
5:G:27:ILE:HG22	5:G:29:ILE:H	1.81	0.45
19:g:361:GLU:OE1	19:g:369:ARG:NH2	2.49	0.45
12:L:867:GLY:O	12:L:869:ARG:NH1	2.49	0.45
14:f:153:SER:HA	14:f:169:ILE:O	2.17	0.45
14:f:428:VAL:HB	14:f:431:ASP:HB2	1.98	0.45
14:f:18:VAL:HG21	14:f:434:ILE:HG22	1.98	0.45
16:V:49:ARG:HD2	21:N:9:DT:OP1	2.17	0.45
7:Q:524:VAL:HB	7:Q:573:LEU:HD23	1.98	0.45
7:Q:783:SER:OG	7:Q:784:ASP:N	2.46	0.45
7:Q:851:ASN:O	7:Q:855:ALA:N	2.50	0.45
2:H:454:LEU:HD11	4:I:50:ARG:HD3	1.99	0.45
13:W:91:LYS:NZ	18:U:71:GLU:CD	2.73	0.45
14:f:145:ILE:HD13	14:f:395:THR:HG21	1.98	0.45
7:Q:495:ASP:OD1	7:Q:697:ARG:N	2.40	0.45
7:Q:761:LYS:O	7:Q:765:HIS:N	2.42	0.45
5:G:165:ILE:HG12	5:G:171:ILE:HG21	1.99	0.45
16:R:41:TYR:HA	21:N:144:DC:H4'	1.99	0.45
2:D:315:TRP:NE1	2:D:349:ASP:OD2	2.45	0.45
12:L:745:ALA:HB1	12:L:793:ARG:HH22	1.82	0.45
19:g:359:ILE:HG13	19:g:404:PRO:CD	2.42	0.45
7:Q:684:ARG:HA	7:Q:687:HIS:CD2	2.51	0.45
3:M:215:PHE:O	3:M:218:LEU:HB3	2.17	0.45
4:I:27:VAL:HG12	4:I:29:ASN:H	1.82	0.45
19:g:336:VAL:HG21	19:g:428:ILE:HD11	1.98	0.45
7:Q:896:GLN:HG3	7:Q:900:ARG:HH22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:135:GLU:OE2	5:G:19:ARG:NH2	2.50	0.44
14:f:159:ILE:HG22	14:f:398:THR:HB	1.98	0.44
16:V:42:ARG:CZ	20:B:144:DC:C2'	2.95	0.44
7:Q:593:HIS:CE1	7:Q:621:ASN:HD22	2.35	0.44
19:g:91:LEU:HD23	19:g:106:LEU:HD22	1.99	0.44
7:Q:866:SER:HB3	7:Q:869:ALA:HB3	2.00	0.44
7:Q:809:ARG:HG2	7:Q:861:PHE:HD1	1.83	0.44
13:W:88:TYR:CG	18:Y:83:TYR:CE2	3.05	0.44
15:h:30:TYR:HB2	15:h:64:LEU:HD11	1.99	0.44
17:O:42:ARG:CB	18:Y:88:THR:HG23	2.47	0.44
7:Q:399:THR:O	7:Q:402:THR:OG1	2.32	0.44
2:D:432:LEU:HD13	8:E:69:LEU:HD22	2.00	0.44
5:G:17:HIS:HA	5:G:20:LEU:HD12	1.98	0.44
6:A:31:VAL:HG12	6:A:77:ASN:HB2	2.00	0.44
7:J:113:ASP:HA	7:J:116:ASN:HD22	1.82	0.44
17:T:92:GLU:OE1	18:U:106:LEU:CD2	2.66	0.44
7:P:376:GLN:C	7:P:378:LEU:H	2.25	0.44
1:F:318:ASN:OD1	2:D:71:ARG:NH2	2.48	0.44
3:M:217:GLU:OE2	7:J:287:ARG:NH2	2.43	0.44
13:S:88:TYR:CE2	18:U:83:TYR:CE1	2.98	0.44
20:B:125:DC:H2''	20:B:126:DG:H5''	1.98	0.44
6:A:235:THR:HG22	6:A:235:THR:O	2.18	0.44
13:W:20:LYS:HB2	7:Q:770:ASP:CG	2.42	0.44
2:D:321:LEU:HD23	6:A:476:PHE:HE1	1.83	0.44
17:T:15:LYS:CE	21:N:32:DG:OP2	2.65	0.44
18:U:88:THR:HG1	21:N:40:DA:P	2.18	0.44
20:B:58:DT:OP1	7:Q:554:PRO:HG3	2.11	0.44
7:Q:975:GLU:HA	7:Q:980:GLU:HB2	2.00	0.44
18:Y:56:SER:N	20:B:20:DA:P	2.91	0.44
2:H:72:PHE:HA	5:G:155:LEU:HD22	2.00	0.43
14:f:291:LEU:HB3	19:g:402:GLN:HE22	1.75	0.43
19:g:172:ILE:HG12	19:g:184:VAL:HG13	1.99	0.43
21:N:72:DC:H2''	21:N:73:DA:C8	2.53	0.43
7:Q:473:TYR:CE2	7:Q:702:VAL:C	2.95	0.43
14:f:180:VAL:HG11	14:f:332:LEU:HD11	2.00	0.43
13:S:78:ARG:HD2	20:B:102:DG:O5'	2.17	0.43
20:B:57:DT:P	7:Q:578:TYR:CE2	3.10	0.43
7:Q:497:MET:HG3	7:Q:899:ASP:HB2	2.00	0.43
7:Q:556:GLN:O	7:Q:559:SER:OG	2.35	0.43
7:Q:632:ASN:ND2	7:Q:932:LYS:HB3	2.32	0.43
2:D:143:ARG:HH21	5:G:378:PRO:HD3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:335:VAL:O	4:I:338:THR:OG1	2.35	0.43
7:Q:484:LEU:O	7:Q:489:LEU:N	2.49	0.43
7:Q:809:ARG:NH1	7:Q:853:PHE:O	2.45	0.43
7:Q:989:ALA:CA	7:Q:992:LYS:HD2	2.40	0.43
2:D:316:SER:OG	2:D:319:GLU:OE1	2.23	0.43
2:D:325:GLU:OE2	12:L:871:SER:OG	2.28	0.43
20:B:140:DC:H2''	20:B:141:DA:N7	2.33	0.43
7:Q:473:TYR:CE1	7:Q:702:VAL:HA	2.22	0.43
7:Q:564:ILE:HG12	7:Q:569:PHE:HE2	1.73	0.43
7:Q:812:MET:CE	7:Q:885:PHE:CE2	2.84	0.43
7:Q:986:ALA:O	7:Q:992:LYS:HE2	2.18	0.43
5:G:20:LEU:HB3	5:G:30:PHE:HD2	1.83	0.43
6:A:191:ILE:HD12	6:A:230:ASN:HB3	2.01	0.43
16:V:40:ARG:CZ	21:N:83:DT:O2	2.64	0.43
16:V:125:GLN:HB3	16:V:134:ARG:HH22	1.82	0.43
21:N:96:DT:P	7:Q:607:SER:HB2	2.59	0.43
7:Q:638:TRP:HZ2	7:Q:655:PHE:H	1.66	0.43
2:H:426:GLN:NE2	4:I:26:LYS:O	2.52	0.43
9:C:214:ASP:O	9:C:218:ASN:ND2	2.52	0.43
14:f:145:ILE:HG12	14:f:435:GLN:HG3	2.00	0.43
2:D:161:GLU:HG3	2:D:167:ASN:HB2	2.01	0.43
5:G:306:THR:HG22	5:G:308:GLU:H	1.83	0.43
13:W:24:ASP:OD1	13:W:24:ASP:N	2.51	0.43
13:W:68:ASP:OD1	18:Y:100:LEU:CD2	2.66	0.43
19:g:354:LEU:HD22	19:g:358:LEU:HD22	2.01	0.43
20:B:111:DC:H42	21:N:37:DG:H1	1.66	0.43
21:N:16:DC:H6	21:N:16:DC:H2'	1.65	0.43
3:M:137:ILE:O	3:M:141:LEU:HB2	2.18	0.43
20:B:54:DC:C5'	7:Q:868:ARG:CG	2.88	0.43
20:B:130:DC:H2''	20:B:131:DA:N7	2.34	0.43
8:E:52:ILE:O	8:E:57:ARG:NH2	2.52	0.43
16:R:83:ARG:HB3	21:N:51:DT:P	2.59	0.43
18:Y:80:LEU:HD23	18:Y:80:LEU:HA	1.86	0.43
6:A:196:GLN:HB3	6:A:227:LYS:HB2	2.01	0.42
13:W:37:LEU:HD23	16:V:61:LEU:HD12	2.00	0.42
14:f:75:GLY:HA3	14:f:109:PRO:HG3	2.01	0.42
14:f:166:VAL:CG1	14:f:333:MET:SD	3.07	0.42
16:V:40:ARG:NH2	21:N:82:DG:H21	2.18	0.42
18:U:88:THR:CA	21:N:40:DA:OP1	2.66	0.42
18:U:102:LEU:HA	18:U:103:PRO:HD3	1.89	0.42
19:g:138:ASN:HA	19:g:451:ARG:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:120:DG:H2''	21:N:121:DA:N7	2.34	0.42
7:Q:784:ASP:O	7:Q:785:LEU:CB	2.67	0.42
2:H:149:ASP:OD1	2:H:152:SER:OG	2.36	0.42
8:E:56:GLU:HA	8:E:59:ARG:HG2	2.01	0.42
14:f:73:SER:HA	14:f:162:SER:HB2	2.00	0.42
14:f:178:ALA:HA	14:f:339:LYS:HE3	2.01	0.42
20:B:58:DT:P	7:Q:554:PRO:HG3	2.55	0.42
7:Q:729:MET:O	7:Q:733:ASN:N	2.50	0.42
7:Q:787:PHE:HA	7:Q:793:PHE:HB3	2.01	0.42
2:H:178:LEU:HG	2:D:196:GLY:HA3	2.00	0.42
6:A:446:ARG:HH12	7:J:50:ARG:HH21	1.66	0.42
14:f:36:ILE:HD12	14:f:54:MET:CE	2.43	0.42
14:f:152:SER:O	14:f:172:GLY:N	2.48	0.42
2:D:224:PHE:HZ	7:J:244:GLU:HG2	1.85	0.42
4:I:224:LEU:HD21	4:I:349:ILE:HD12	2.01	0.42
16:R:42:ARG:N	21:N:144:DC:H5'	2.25	0.42
13:S:79:LYS:N	20:B:102:DG:OP1	2.52	0.42
17:T:57:TYR:CG	18:U:113:GLU:HG3	2.53	0.42
19:g:55:SER:HB3	19:g:85:LEU:HD11	2.01	0.42
7:Q:991:GLU:HA	7:Q:994:LEU:HG	2.01	0.42
2:H:466:GLU:HA	2:H:469:LEU:HD12	2.02	0.42
17:T:77:ARG:HG2	18:U:53:GLY:HA3	2.01	0.42
7:Q:477:GLY:HA2	7:Q:480:TRP:HD1	1.84	0.42
5:G:336:ILE:O	5:G:340:LYS:HG3	2.19	0.42
17:O:32:ARG:NH1	20:B:29:DA:H3'	2.34	0.42
18:Y:40:TYR:HH	21:N:122:DG:P	2.41	0.42
18:Y:118:VAL:O	18:Y:122:THR:N	2.50	0.42
20:B:120:DA:H2''	20:B:121:DG:N7	2.35	0.42
7:Q:473:TYR:OH	7:Q:702:VAL:N	2.53	0.42
14:f:124:TYR:HE2	14:f:463:LEU:HD13	1.83	0.42
17:T:77:ARG:HA	18:U:53:GLY:C	2.44	0.42
20:B:56:DC:P	7:Q:840:SER:HB3	2.60	0.42
21:N:110:DA:H1'	21:N:111:DC:H5'	2.01	0.42
2:D:193:THR:HG22	2:D:195:GLN:H	1.85	0.42
14:f:446:LEU:HB3	14:f:451:LEU:HD12	2.01	0.42
16:R:62:ILE:O	16:R:93:GLN:NE2	2.52	0.42
7:Q:937:GLY:HA2	7:Q:941:GLN:HB2	2.01	0.42
14:f:55:ILE:O	14:f:59:ALA:N	2.52	0.42
7:Q:448:TYR:HA	7:Q:452:HIS:HB2	2.01	0.42
7:Q:586:LEU:HD23	7:Q:586:LEU:HA	1.88	0.42
7:Q:656:GLU:O	7:Q:660:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:133:ARG:NH2	12:L:870:PRO:O	2.53	0.42
17:T:33:LEU:HD23	17:T:33:LEU:HA	1.91	0.42
17:O:64:GLU:HG2	18:Y:48:VAL:CG2	2.50	0.42
19:g:42:TYR:O	19:g:53:TYR:HA	2.19	0.42
19:g:132:PHE:HD1	19:g:451:ARG:HH11	1.68	0.42
19:g:323:ILE:HG12	19:g:327:LYS:HE3	2.01	0.42
7:Q:401:ILE:HA	7:Q:404:LEU:HB2	2.02	0.42
7:Q:629:PRO:HG2	7:Q:940:ILE:HG22	2.02	0.42
2:H:365:ARG:HH22	2:D:221:LYS:NZ	2.17	0.41
3:M:189:LEU:HB2	3:M:242:TYR:HE1	1.85	0.41
6:A:445:GLU:HA	6:A:448:LEU:HB3	2.00	0.41
2:D:354:PHE:HA	2:D:357:LEU:HD13	2.02	0.41
2:D:419:GLU:HA	2:D:422:ILE:HG22	2.02	0.41
6:A:423:LEU:HD23	6:A:426:LEU:HD12	2.02	0.41
7:Q:796:LEU:O	7:Q:830:LYS:NZ	2.53	0.41
2:H:424:GLU:HA	8:E:53:ILE:HD11	2.03	0.41
3:M:110:LYS:HG3	10:K:164:ILE:HG23	2.01	0.41
5:G:278:HIS:HA	5:G:298:TRP:O	2.20	0.41
11:X:370:ARG:NH2	11:X:496:ASN:OD1	2.40	0.41
18:U:90:THR:OG1	18:U:93:GLU:OE1	2.33	0.41
2:D:126:ILE:O	2:D:130:ARG:HG2	2.20	0.41
17:O:32:ARG:HG2	20:B:30:DA:OP2	2.16	0.41
18:Y:101:LEU:HD23	18:Y:101:LEU:HA	1.93	0.41
19:g:84:ARG:HA	19:g:135:LEU:HD21	2.01	0.41
19:g:452:GLU:O	19:g:456:MET:HG2	2.20	0.41
20:B:34:DG:H3'	20:B:35:DT:H71	2.01	0.41
21:N:78:DG:H4'	21:N:79:DT:H5'	2.03	0.41
7:Q:876:LEU:HD13	7:Q:901:ALA:HA	2.01	0.41
6:A:10:LEU:HD21	6:A:138:ILE:HG21	2.01	0.41
6:A:107:ILE:HG23	6:A:117:TYR:HE1	1.85	0.41
11:X:378:LEU:HB2	11:X:484:TYR:HB2	2.02	0.41
17:O:32:ARG:CG	20:B:30:DA:OP1	2.68	0.41
19:g:132:PHE:HB3	19:g:451:ARG:HH12	1.84	0.41
7:J:225:ILE:HG12	7:J:231:SER:HB3	2.02	0.41
16:R:126:LEU:HD22	16:V:113:HIS:CG	2.55	0.41
20:B:70:DC:H2''	20:B:71:DG:C8	2.55	0.41
7:Q:535:THR:HA	7:Q:538:PHE:HB2	2.03	0.41
7:Q:598:GLU:HB3	7:Q:600:HIS:CE1	2.55	0.41
7:Q:814:PHE:CA	7:Q:886:ASP:OD2	2.67	0.41
4:I:422:LEU:HA	4:I:429:THR:HG21	2.02	0.41
17:T:80:PRO:CB	18:U:61:ILE:CD1	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:80:LEU:HD23	18:U:80:LEU:HA	1.88	0.41
19:g:335:ILE:HD13	19:g:349:LEU:HD23	2.03	0.41
19:g:359:ILE:CG1	19:g:404:PRO:CG	2.95	0.41
4:I:319:LEU:HA	4:I:322:VAL:HG22	2.03	0.41
6:A:170:THR:HG22	6:A:173:ASP:H	1.86	0.41
14:f:66:GLU:OE1	14:f:68:TYR:OH	2.31	0.41
19:g:350:LEU:HD22	19:g:409:LEU:HG	2.03	0.41
21:N:70:DG:H2''	21:N:71:DA:C8	2.56	0.41
21:N:144:DC:H2'	21:N:145:DA:C8	2.56	0.41
7:Q:936:ASP:O	7:Q:940:ILE:N	2.44	0.41
14:f:69:THR:OG1	14:f:78:TYR:OH	2.33	0.41
18:U:74:ALA:HA	18:U:77:ALA:HB3	2.02	0.41
18:Y:81:ALA:O	18:Y:85:LYS:N	2.54	0.41
18:Y:100:LEU:HD23	18:Y:100:LEU:HA	1.87	0.41
20:B:101:DG:H2''	20:B:102:DG:C8	2.56	0.41
7:Q:397:LYS:HE3	7:Q:685:ARG:HE	1.86	0.41
6:A:35:PHE:H	6:A:75:THR:HG22	1.86	0.40
11:X:504:PRO:HD3	11:X:624:LEU:HB2	2.02	0.40
14:f:157:ILE:HG13	14:f:333:MET:HE1	1.89	0.40
13:S:88:TYR:CD1	18:U:83:TYR:CE2	3.06	0.40
19:g:314:GLY:HA3	19:g:357:HIS:CE1	2.57	0.40
19:g:327:LYS:CE	19:g:403:CYS:HA	2.51	0.40
7:Q:473:TYR:CE2	7:Q:702:VAL:CB	3.04	0.40
5:G:276:ASP:OD1	5:G:301:ASN:ND2	2.47	0.40
5:G:295:ASN:HB2	5:G:376:TRP:HB2	2.01	0.40
14:f:36:ILE:HB	14:f:54:MET:SD	2.61	0.40
14:f:155:PHE:CE2	14:f:333:MET:HE1	2.44	0.40
20:B:66:DC:H2''	20:B:67:DG:C8	2.56	0.40
2:H:180:GLY:HA3	2:D:198:LYS:HE2	2.02	0.40
5:G:283:LEU:O	5:G:293:GLU:HA	2.21	0.40
14:f:87:TRP:HE3	14:f:131:LEU:HD11	1.86	0.40
19:g:152:SER:HA	19:g:434:ILE:HD12	2.03	0.40
7:Q:872:LEU:H	7:Q:900:ARG:NH1	2.19	0.40
4:I:482:ARG:O	4:I:483:LEU:HB3	2.20	0.40
14:f:235:MET:HE1	14:f:288:LYS:HB3	2.03	0.40
16:V:42:ARG:HE	20:B:145:DT:P	2.45	0.40
17:O:42:ARG:HB3	21:N:113:DA:P	2.52	0.40
7:Q:521:PRO:HG2	7:Q:591:TRP:HZ3	1.85	0.40
3:M:353:TYR:CZ	4:I:250:ASN:HB3	2.56	0.40
5:G:225:TYR:HD1	5:G:262:LEU:HD12	1.85	0.40
5:G:337:LEU:HA	5:G:340:LYS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:R:92:LEU:HA	16:R:92:LEU:HD23	1.91	0.40
13:S:62:LEU:HD23	13:S:62:LEU:HA	1.86	0.40
16:V:42:ARG:NE	20:B:144:DC:C3'	2.63	0.40
18:Y:77:ALA:HA	18:Y:80:LEU:HD12	2.03	0.40
19:g:153:MET:CE	19:g:411:LYS:O	2.67	0.40
19:g:323:ILE:HD11	19:g:403:CYS:CA	2.52	0.40
7:Q:684:ARG:HE	7:Q:958:LEU:HD22	1.86	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	F	116/435 (27%)	102 (88%)	14 (12%)	0	100	100
2	D	295/557 (53%)	280 (95%)	15 (5%)	0	100	100
2	H	387/557 (70%)	356 (92%)	31 (8%)	0	100	100
3	M	378/581 (65%)	349 (92%)	29 (8%)	0	100	100
4	I	236/483 (49%)	218 (92%)	18 (8%)	0	100	100
5	G	238/426 (56%)	213 (90%)	25 (10%)	0	100	100
6	A	357/502 (71%)	321 (90%)	36 (10%)	0	100	100
7	J	229/1359 (17%)	201 (88%)	27 (12%)	1 (0%)	30	67
7	P	67/1359 (5%)	66 (98%)	1 (2%)	0	100	100
7	Q	536/1359 (39%)	483 (90%)	52 (10%)	1 (0%)	43	78
8	E	56/78 (72%)	53 (95%)	3 (5%)	0	100	100
9	C	31/883 (4%)	31 (100%)	0	0	100	100
10	K	40/885 (4%)	38 (95%)	2 (5%)	0	100	100
11	X	139/625 (22%)	126 (91%)	13 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	79/889 (9%)	69 (87%)	9 (11%)	1 (1%)	9	42
13	S	80/103 (78%)	77 (96%)	3 (4%)	0	100	100
13	W	86/103 (84%)	81 (94%)	5 (6%)	0	100	100
14	f	391/477 (82%)	382 (98%)	9 (2%)	0	100	100
15	h	46/157 (29%)	43 (94%)	3 (6%)	0	100	100
16	R	94/136 (69%)	90 (96%)	4 (4%)	0	100	100
16	V	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
17	O	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
17	T	102/130 (78%)	101 (99%)	1 (1%)	0	100	100
18	U	91/126 (72%)	88 (97%)	3 (3%)	0	100	100
18	Y	91/126 (72%)	88 (97%)	3 (3%)	0	100	100
19	g	390/467 (84%)	380 (97%)	9 (2%)	1 (0%)	36	72
All	All	4753/13069 (36%)	4430 (93%)	319 (7%)	4 (0%)	49	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	g	154	ILE
7	J	17	PRO
7	Q	994	LEU
12	L	809	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	F	111/388 (29%)	111 (100%)	0	100	100
2	D	285/500 (57%)	285 (100%)	0	100	100
2	H	363/500 (73%)	362 (100%)	1 (0%)	86	86
3	M	349/521 (67%)	347 (99%)	2 (1%)	78	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	I	223/435 (51%)	221 (99%)	2 (1%)	70	79
5	G	226/384 (59%)	226 (100%)	0	100	100
6	A	343/462 (74%)	342 (100%)	1 (0%)	86	86
7	J	187/1228 (15%)	187 (100%)	0	100	100
7	P	63/1228 (5%)	63 (100%)	0	100	100
7	Q	502/1228 (41%)	502 (100%)	0	100	100
8	E	56/75 (75%)	56 (100%)	0	100	100
9	C	32/824 (4%)	32 (100%)	0	100	100
10	K	39/832 (5%)	39 (100%)	0	100	100
11	X	141/578 (24%)	139 (99%)	2 (1%)	59	72
12	L	77/810 (10%)	77 (100%)	0	100	100
13	S	68/79 (86%)	68 (100%)	0	100	100
13	W	72/79 (91%)	72 (100%)	0	100	100
14	f	356/420 (85%)	356 (100%)	0	100	100
15	h	53/140 (38%)	53 (100%)	0	100	100
16	R	84/111 (76%)	84 (100%)	0	100	100
16	V	83/111 (75%)	83 (100%)	0	100	100
17	O	84/102 (82%)	82 (98%)	2 (2%)	43	64
17	T	83/102 (81%)	83 (100%)	0	100	100
18	U	79/105 (75%)	79 (100%)	0	100	100
18	Y	77/105 (73%)	77 (100%)	0	100	100
19	g	362/423 (86%)	361 (100%)	1 (0%)	86	86
All	All	4398/11770 (37%)	4387 (100%)	11 (0%)	84	86

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	262	THR
3	M	104	TYR
3	M	317	LEU
4	I	38	GLU
4	I	267	VAL
6	A	235	THR
11	X	437	LEU

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Mol	Chain	Res	Type
11	X	438	SER
17	O	58	LEU
17	O	65	LEU
19	g	48	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	331	ASN
1	F	396	ASN
2	H	63	GLN
2	H	78	HIS
2	H	123	ASN
2	H	127	ASN
2	H	157	HIS
2	H	167	ASN
2	H	195	GLN
2	H	250	ASN
2	H	314	ASN
2	H	426	GLN
2	D	76	GLN
2	D	239	GLN
2	D	344	HIS
3	M	203	ASN
3	M	251	ASN
3	M	359	HIS
3	M	521	GLN
3	M	539	ASN
3	M	551	GLN
4	I	417	GLN
4	I	432	HIS
4	I	451	ASN
4	I	463	ASN
4	I	473	ASN
4	I	480	GLN
5	G	17	HIS
5	G	177	ASN
5	G	224	ASN
5	G	330	GLN
5	G	352	HIS
5	G	375	ASN
6	A	29	HIS

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Mol	Chain	Res	Type
6	A	112	GLN
6	A	196	GLN
6	A	219	HIS
6	A	412	ASN
6	A	472	ASN
6	A	484	ASN
7	J	90	GLN
7	J	259	GLN
9	C	218	ASN
10	K	160	GLN
11	X	480	ASN
11	X	494	ASN
11	X	514	HIS
11	X	618	ASN
12	L	800	ASN
12	L	810	HIS
14	f	28	GLN
14	f	79	ASN
14	f	137	GLN
14	f	253	GLN
16	R	68	GLN
13	S	75	HIS
17	T	24	GLN
17	T	110	ASN
16	V	68	GLN
18	U	49	HIS
18	U	84	ASN
18	U	109	HIS
18	Y	47	GLN
18	Y	49	HIS
18	Y	109	HIS
19	g	69	GLN
19	g	121	GLN
19	g	179	GLN
19	g	209	GLN
19	g	304	ASN
7	Q	504	GLN
7	Q	600	HIS
7	Q	604	ASN
7	Q	621	ASN
7	Q	650	ASN
7	Q	660	ASN

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Mol	Chain	Res	Type
7	Q	687	HIS
7	Q	722	GLN
7	Q	728	GLN
7	Q	732	HIS
7	Q	764	ASN
7	Q	808	HIS
7	Q	815	GLN
7	Q	896	GLN
7	Q	908	ASN
7	Q	1004	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 ⓘ

There are no chain breaks in this entry.

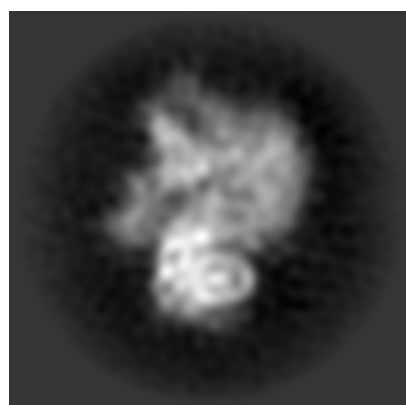
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0779. These allow visual inspection of the internal detail of the map and identification of artifacts.

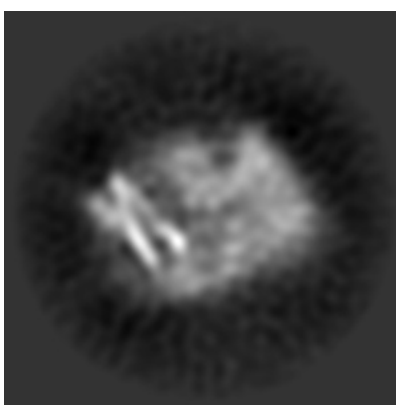
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

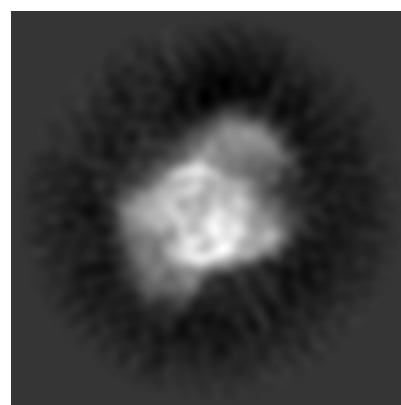
6.1.1 Primary map



X



Y

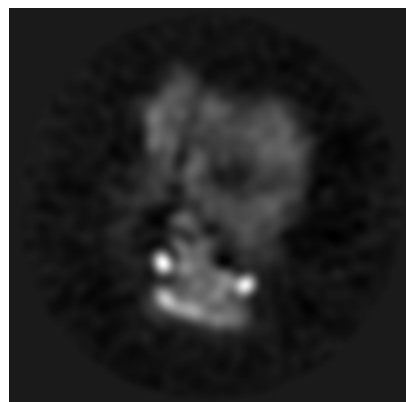


Z

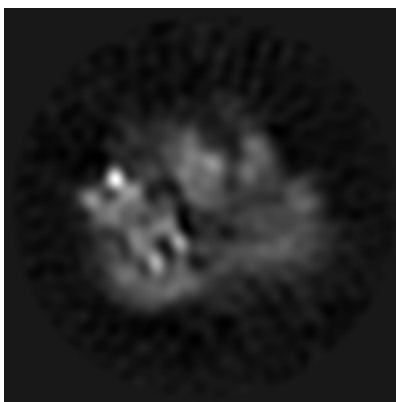
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

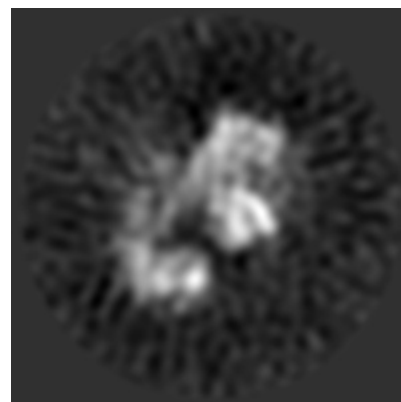
6.2.1 Primary map



X Index: 90



Y Index: 90

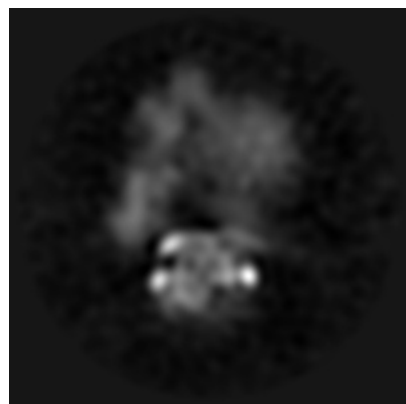


Z Index: 90

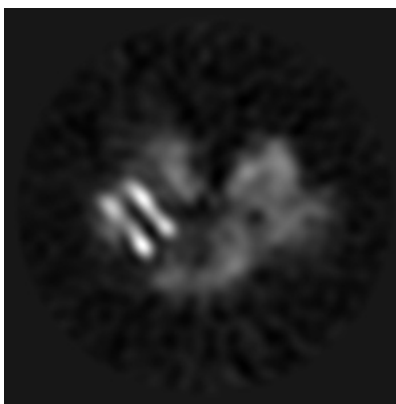
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

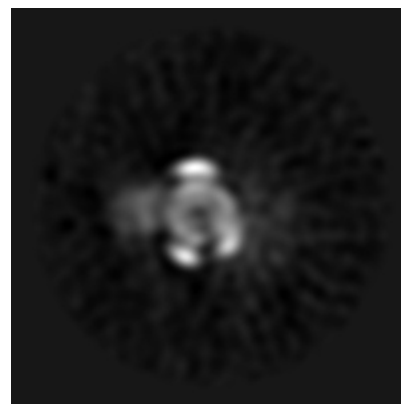
6.3.1 Primary map



X Index: 80



Y Index: 71

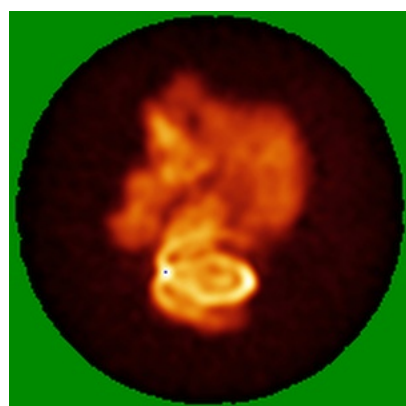


Z Index: 58

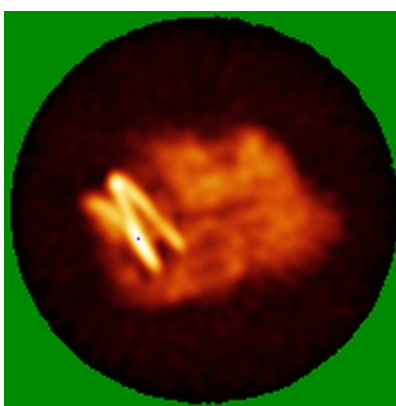
The images above show the largest variance slices of the map in three orthogonal directions.

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

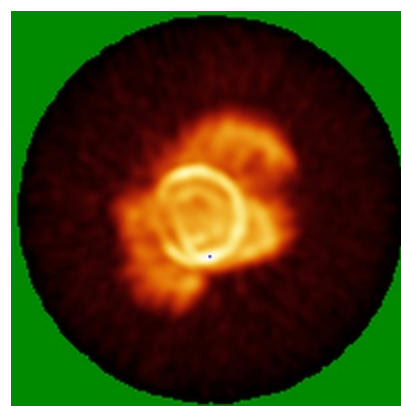
6.4.1 Primary map



X



Y

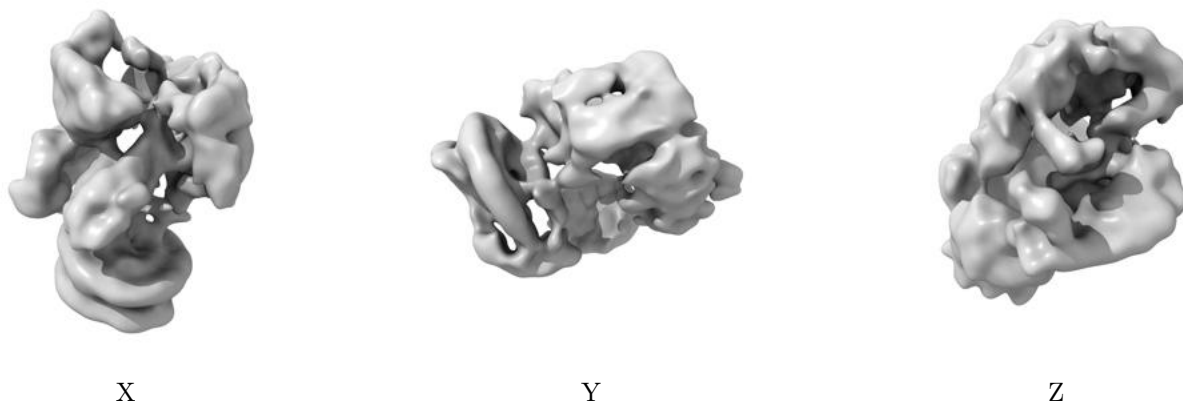


Z

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

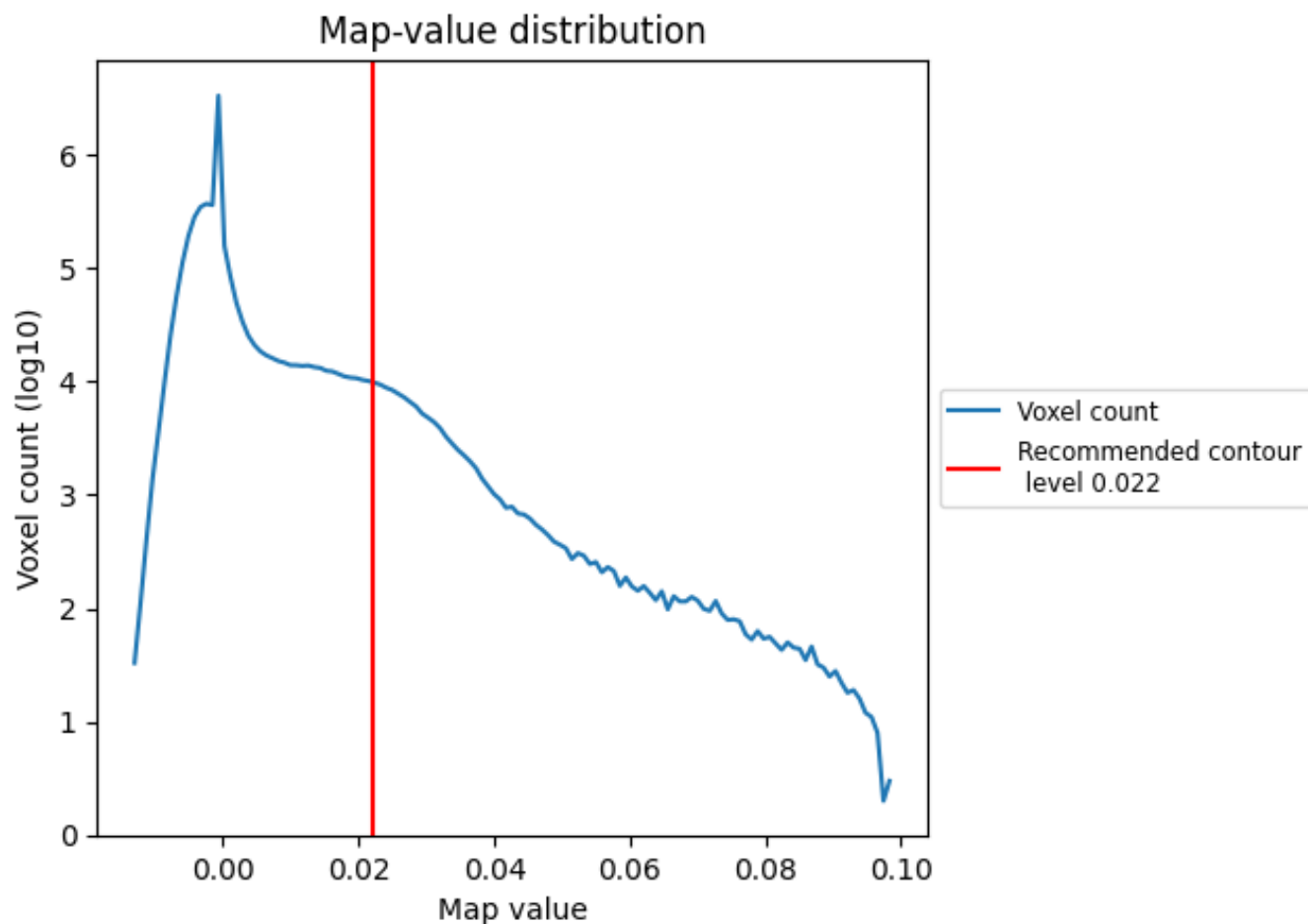
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

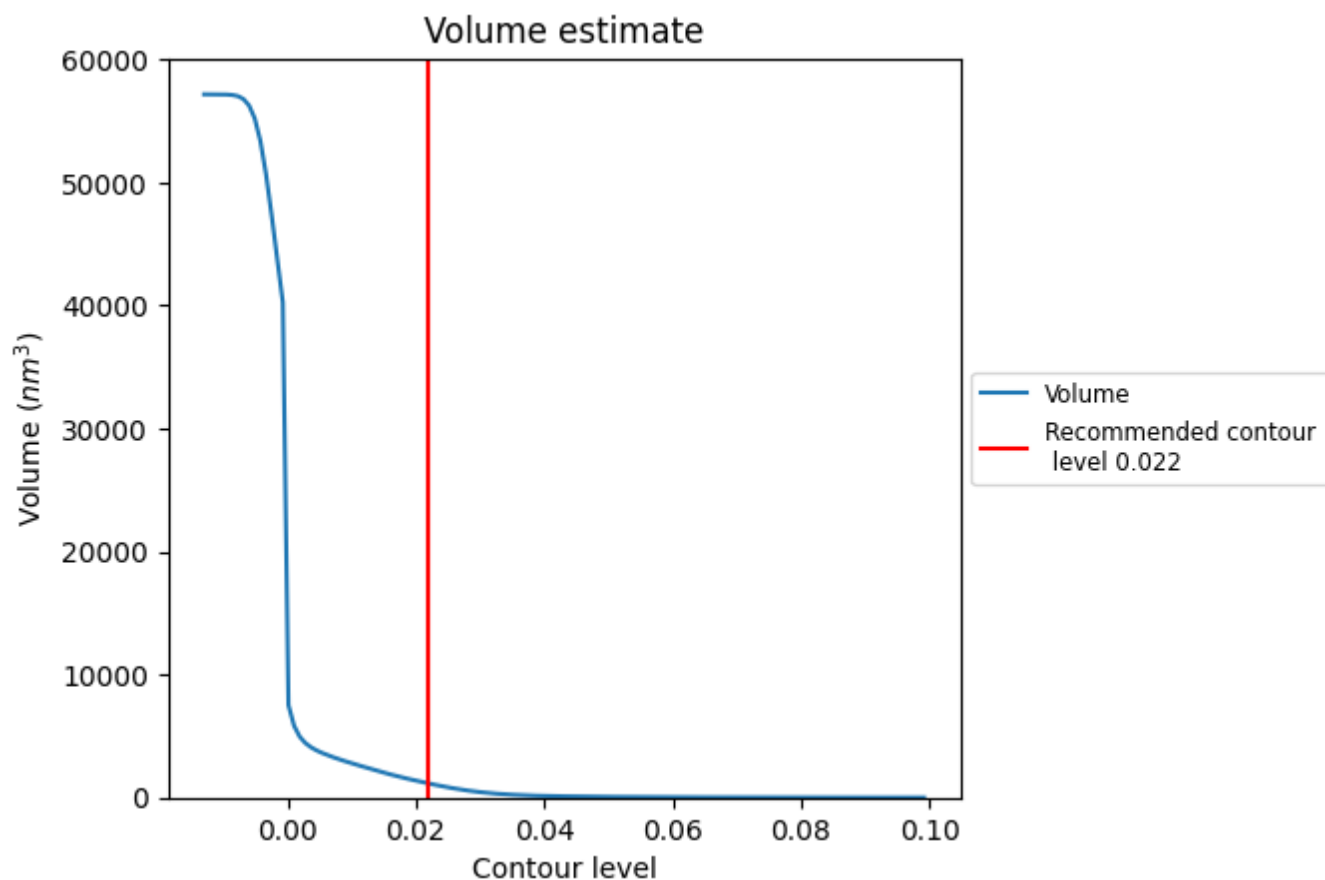
This section contains the results of statistical analysis of the map.

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.

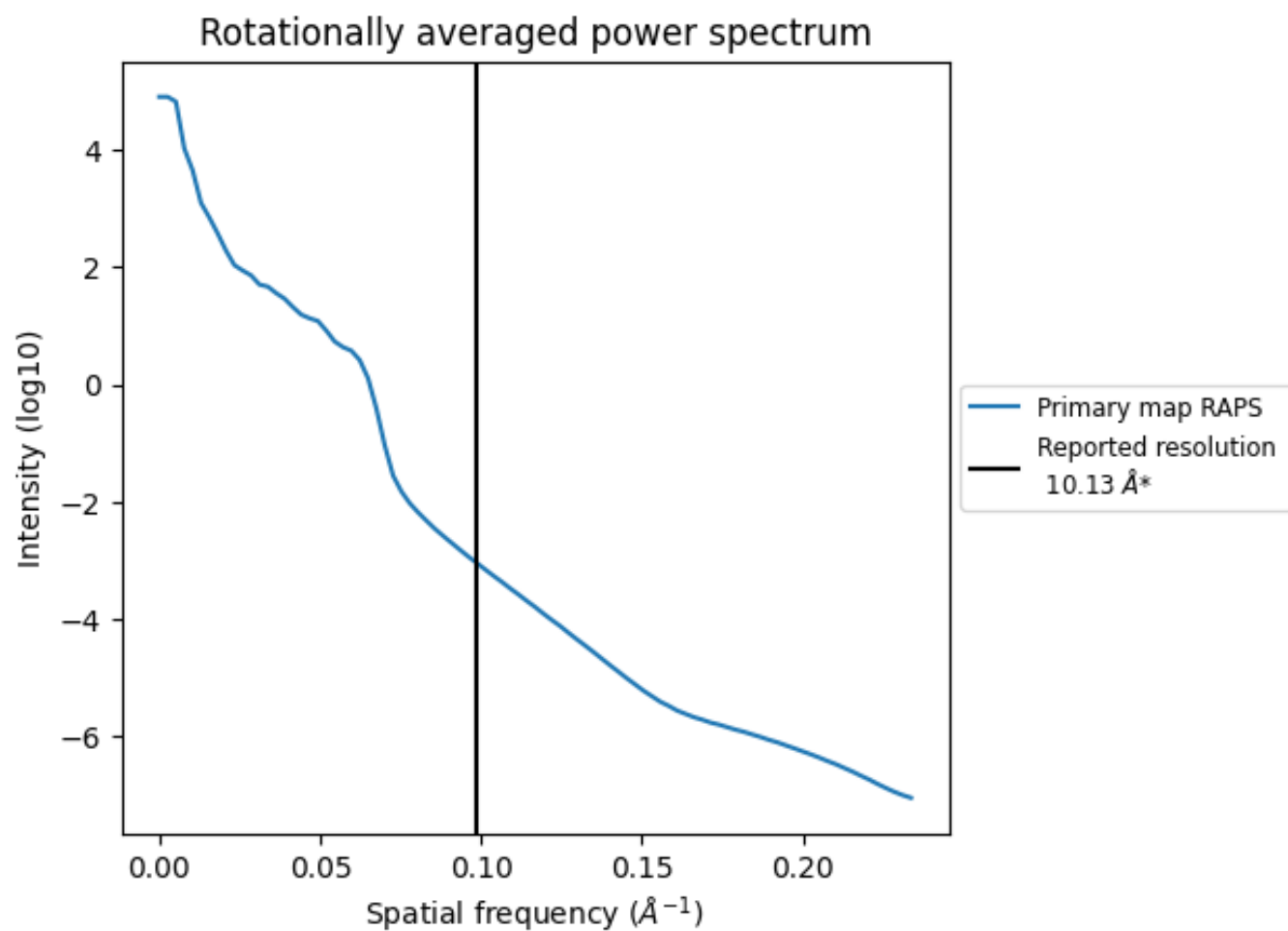
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1145 nm^3 ; this corresponds to an approximate mass of 1035 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 0.099 Å⁻¹

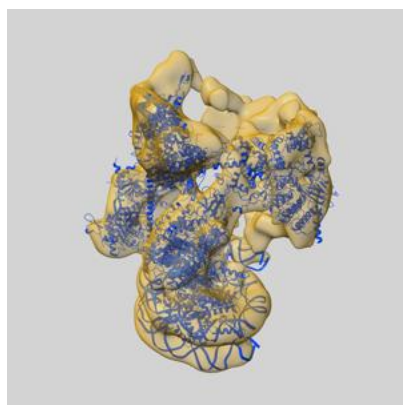
8 Fourier-Shell correlation ⓘ

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

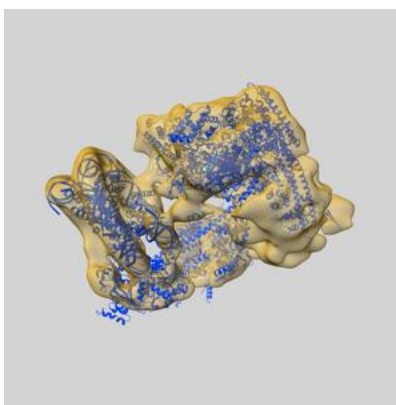
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0779 and PDB model 6KW5. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

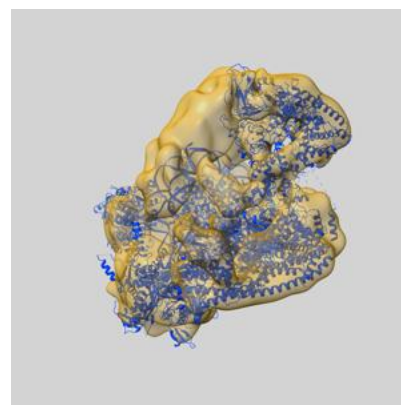
9.1 Map-model overlay [i](#)



X



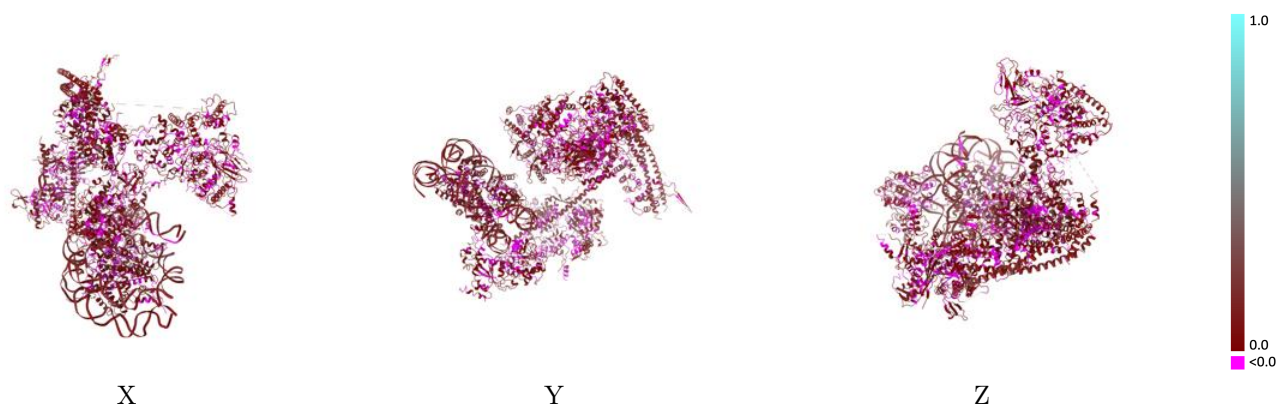
Y



Z

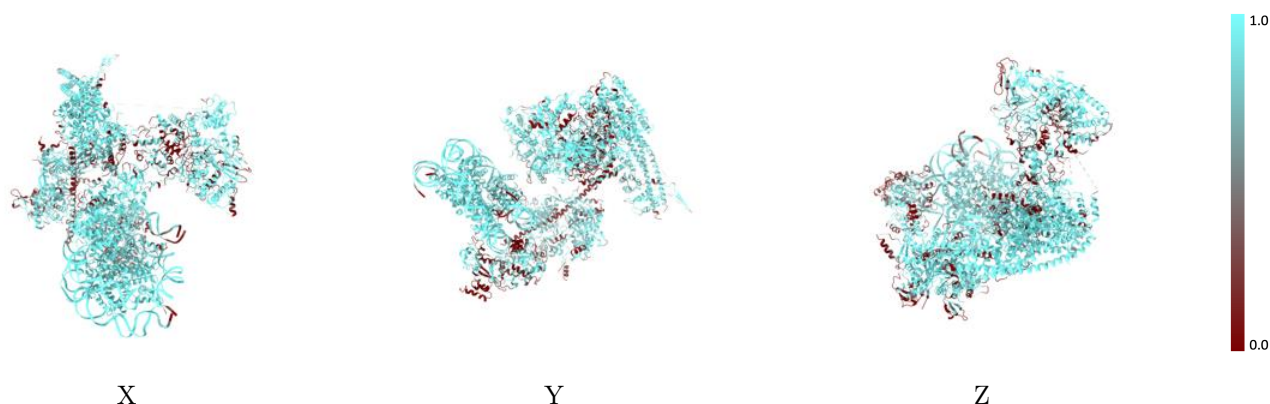
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



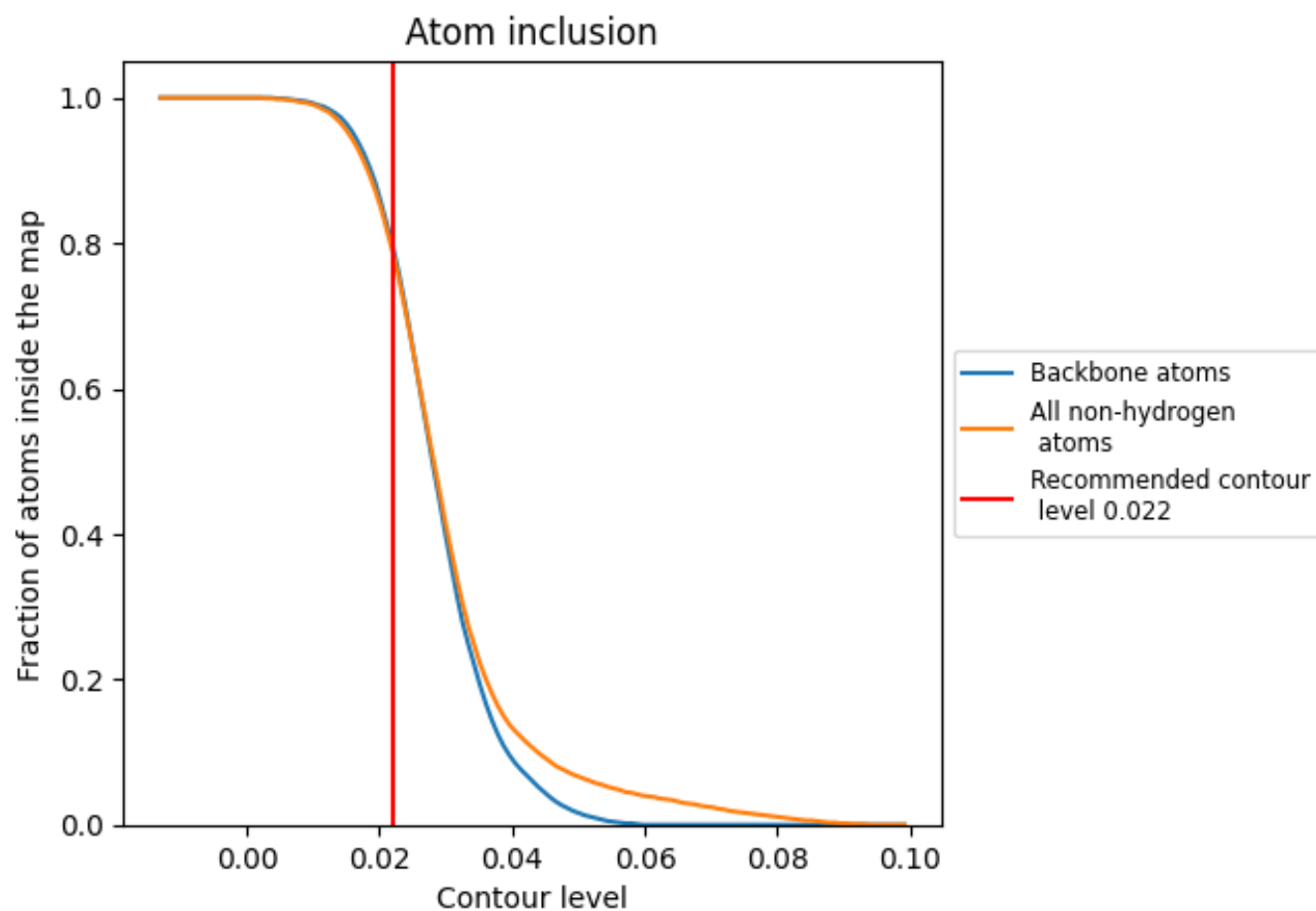
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 79% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7880	 0.0620
A	 0.7660	 0.0490
B	 0.9270	 0.1310
C	 0.5200	 0.0560
D	 0.7980	 0.0510
E	 0.8890	 0.0350
F	 0.8490	 0.0740
G	 0.8630	 0.0750
H	 0.8410	 0.0650
I	 0.8240	 0.0640
J	 0.6160	 0.0340
K	 0.3000	 0.0620
L	 0.8090	 0.0400
M	 0.8050	 0.0490
N	 0.9270	 0.1270
O	 0.9810	 0.0690
P	 0.2500	 0.0520
Q	 0.5630	 0.0360
R	 0.9700	 0.0290
S	 0.9560	 0.0740
T	 0.8450	 0.0490
U	 0.9080	 0.0560
V	 0.9160	 0.0430
W	 0.9280	 0.0710
X	 0.6980	 0.0520
Y	 0.9810	 0.0480
f	 0.7960	 0.0500
g	 0.7020	 0.0390
h	 0.8100	 0.0700

