



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 07:08 AM EST

PDB ID : 6UXV
EMDB ID : EMD-20933
Title : SWI/SNF Body Module
Authors : He, Y.; Han, Y.
Deposited on : 2019-11-08
Resolution : 4.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

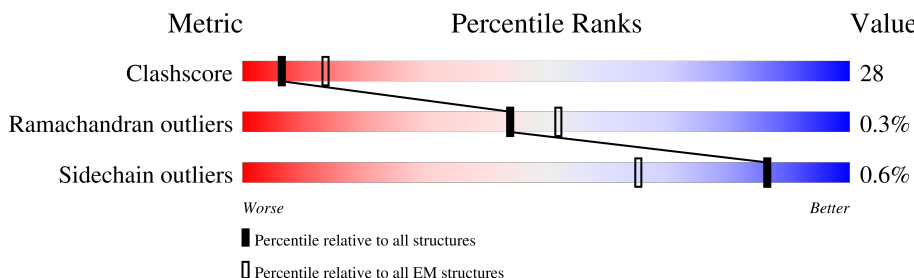
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1703	 5% 16% 21% 63% 92%
2	B	1314	 5% 10% 17% 73% 92%
3	C	905	 9% 11% 81% 92%
4	D	825	 8% 9% 83% 92%
4	E	825	 16% 10% 73% 92%
4	F	825	 14% 9% 76% 92%
4	G	825	 10% 20% 25% 55% 92%
5	H	566	 10% 20% 25% 55% 92%

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Mol	Chain	Length	Quality of chain
6	I	179	<div><div><div></div><div></div><div></div><div></div></div><div>7%34%26%39%</div></div>
7	J	67	<div><div><div></div><div></div></div><div>60%40%</div></div>
8	K	28	<div><div><div></div><div></div></div><div>93%7%</div></div>
9	L	18	<div><div><div></div><div></div></div><div>11%100%</div></div>
9	O	18	<div><div><div></div><div></div></div><div>44%94%6%</div></div>
10	M	83	<div><div><div></div><div></div></div><div>93%7%</div></div>
11	N	30	<div><div><div></div><div></div></div><div>93%7%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 16649 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transcription regulatory protein SNF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	140	Total	C	N	O	S	0	0
			1133	715	196	220	2		

- Molecule 2 is a protein called SWI/SNF chromatin-remodeling complex subunit SWI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	482	Total	C	N	O	S	0	0
			3890	2519	637	723	11		

- Molecule 3 is a protein called SWI/SNF chromatin-remodeling complex subunit SNF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	245	Total	C	N	O	S	0	0
			2005	1256	346	395	8		

- Molecule 4 is a protein called SWI/SNF complex subunit SWI3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	159	Total	C	N	O	S	0	0
			1322	853	225	239	5		
4	E	139	Total	C	N	O	S	0	0
			1152	746	198	205	3		
4	F	221	Total	C	N	O	S	0	0
			1583	987	287	304	5		
4	G	197	Total	C	N	O	S	0	0
			1435	904	258	268	5		

- Molecule 5 is a protein called Transcription regulatory protein SNF12.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	257	Total	C	N	O	S	0	0
			2085	1323	355	400	7		

- Molecule 6 is a protein called Transcription regulatory protein SNF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	109	Total	C	N	O	S	0	0
			818	504	155	156	3		

- Molecule 7 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	J	67	Total	C	N	O	0	0
			336	201	67	68		

- Molecule 8 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	K	28	Total	C	N	O	0	0
			141	84	28	29		

- Molecule 9 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	L	18	Total	C	N	O	0	0
			91	54	18	19		
9	O	18	Total	C	N	O	0	0
			91	54	18	19		

- Molecule 10 is a protein called SWI/SNF global transcription activator complex subunit SWP82.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	M	83	Total	C	N	O	0	0
			416	249	83	84		

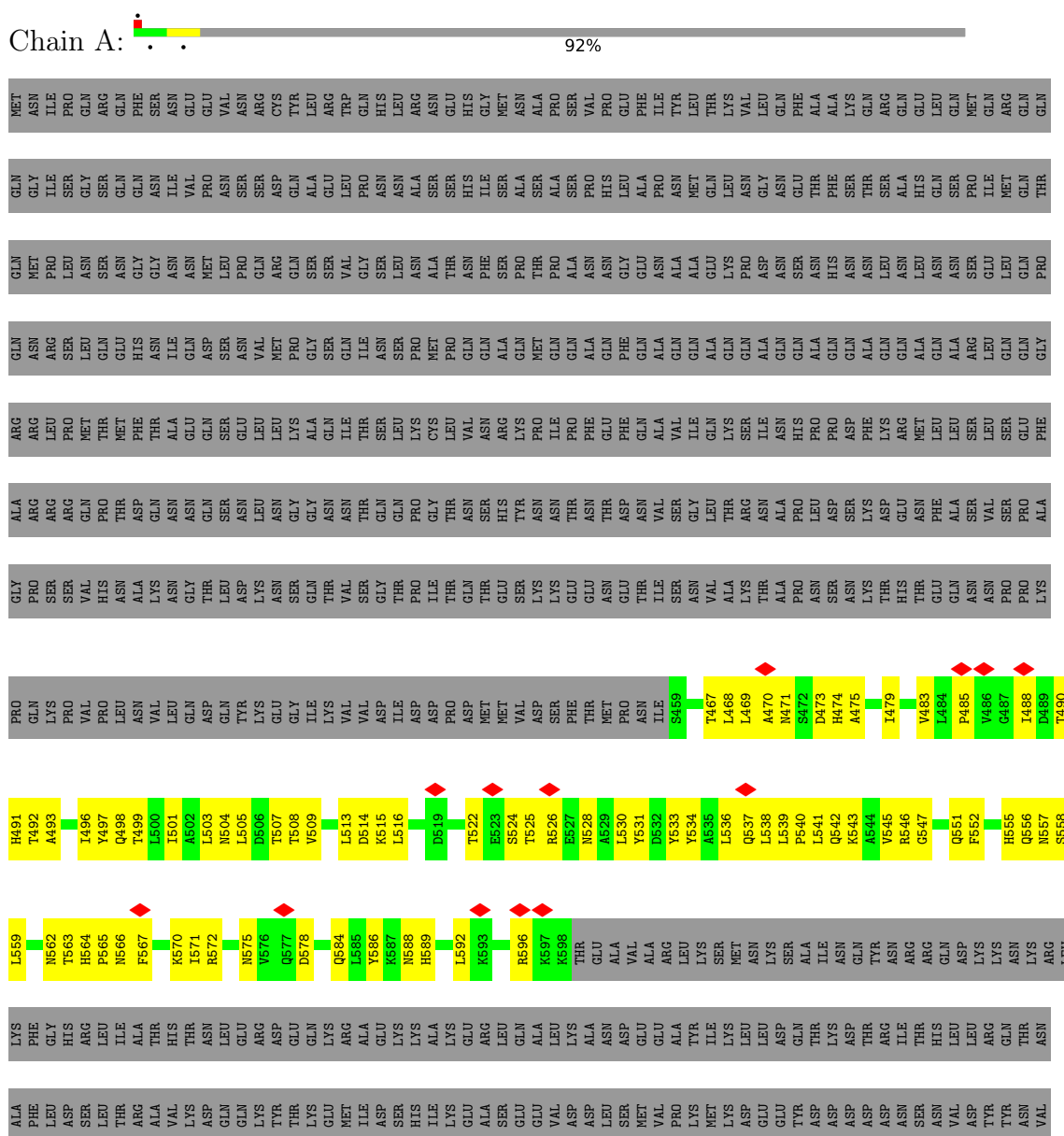
- Molecule 11 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	N	30	Total	C	N	O	0	0
			151	90	30	31		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Transcription regulatory protein SNF2



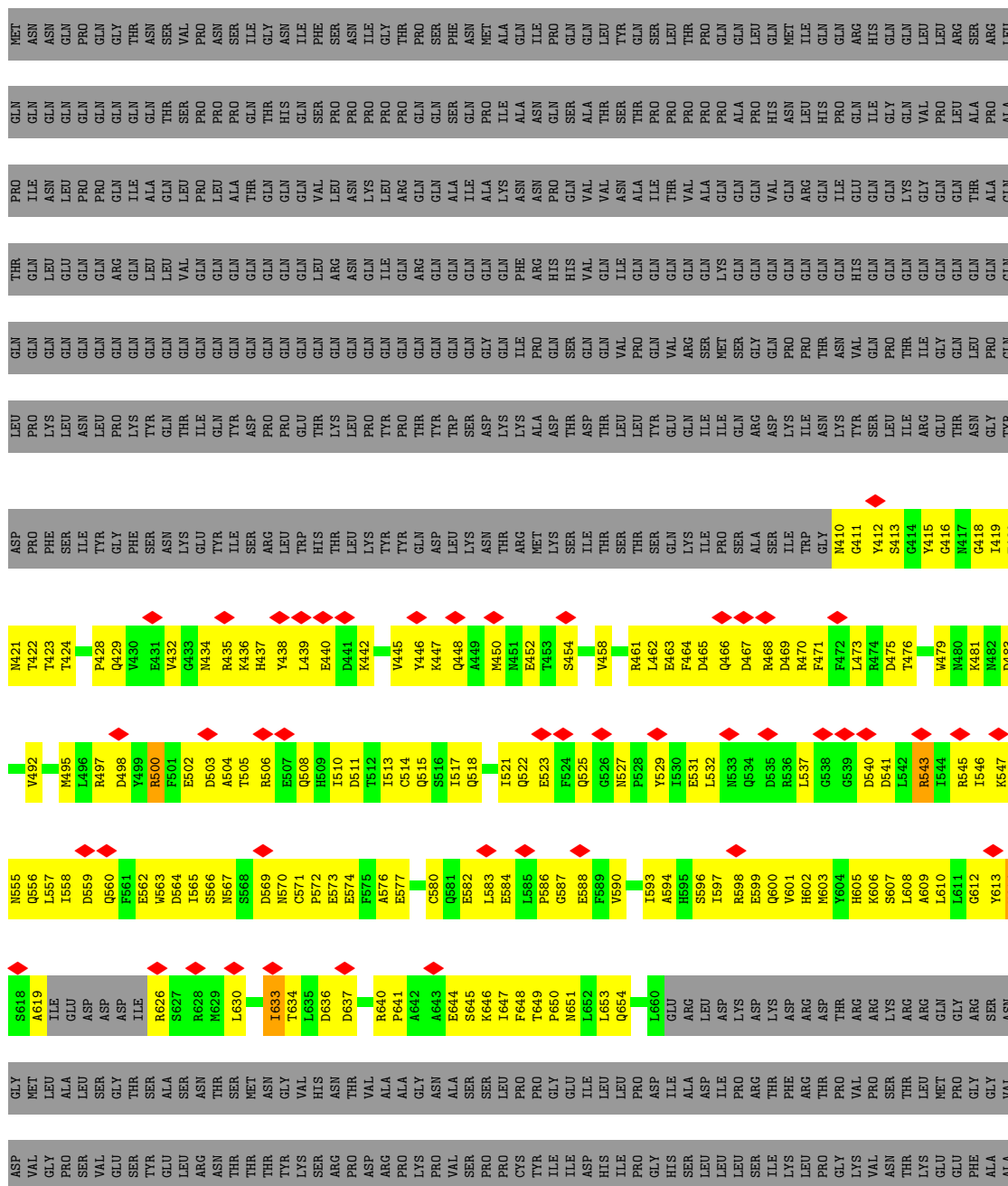
ALA	HIS	ARG	ILE	GLY	ASP	ILE	LYS	PRO	SER	ILE	SER	ILE	LYS	GLY	LEU	THR	ALA	THR	ASP
TYR	LEU	TYR	GLN	THR	LEU	THR	LYS	PRO	GLY	VAL	THR	LEU	VAL	PRO	GLY	THR	ALA	THR	ASP
VAL	VAL	LEU	THR	THR	LEU	THR	LYS	PRO	GLY	VAL	THR	LEU	VAL	PRO	GLY	THR	ALA	THR	ASP
GLN	ASN	ASN	LEU	THR	LEU	THR	LYS	PRO	GLY	VAL	THR	LEU	VAL	PRO	GLY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

● Molecule 2: SWI/SNF chromatin-remodeling complex subunit SWI1



MET	ASP	PHE	THR	ASN	LEU	THR	ASN	THR	ASN	THR	ASN	THR	ASN	THR	ASN	THR	ASN	THR	ASN
ASN	ASN	THR	ASN	GLY	ALA	SER	GLN	PHE	ASN	THR	ASN	THR	ASN	THR	ASN	THR	ASN	THR	ASN
ASN	ALA	PRO	ALA	ASN	VAL	THR	GLY	LYS	ASN	THR	ASN	THR	ASN	THR	ASN	THR	ASN	THR	ASN





ALA	ALA	SER	LYS	SER	VAL	PRO	THR	PRO	SER	LEU	ILE	ALA	PRO	PRO	VAL	ALA	PRO	HIS	ASP	SER	GLU	ALA	THR	LEU	LEU	THR	ASN	SER	ASN	ASN	GLY	SER	SER	ASN	ASN	THR	GLN	ASN	THR
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Chain D: 9% 11% 81%

ASP	ALA	HIS	LYS	ALA	GLU	GLN	GLU	ASP	ILE	ILE	GLU	LYS	THR	GLU	VAL	ASP	SER	SER	GLY	GLU	GLU	ARG	ASN	GLU	GLN	GLU	ARG	GLU	ILE	ILE	MET	ASP	ASN	LYS	SER	HIS	ASP	ASP	GLY	GLU	THR	THR	ILE	ARG	THR	VAL	PRO	GLU	PRO	THR	PHE	GLU	GLU	ILE	ILE	PRO
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A367	A368	A369	A370	A371	A372	A373	A374	A375	A376	A377	A378	A379	A380	A381	A382	A383	A384	A385	A386	A387	A388	A389	A390	A391	A392	A393	A394	A395	A396	A397	A398	A399	A400	A401	A402	A403	A404	A405	A406	A407	A408	A409	A410	A411	A412	A413	A414	A415	A416	A417	A418	A419	A420	A421	A422	A423	A424	A425	A426	A427	A428	A429	A430	A431	A432	A433	A434	A435	A436	A437	A438	A439	A440	A441	A442	A443	A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500
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K441	K442	K443	M444	M445	T446	S447	D448	S449	E450	T452	L453	Y454	K455	Y456	L457	K458	E459	S460	K461	R462	LYS	TYR	ASP	GLU	ILE	THR	HIS	PRO	PRO	SER	THR	THR	ASP	ASP	GLU	ASN	GLY	ASP	LYS	ASN	ASP	ASN	GLY	GLY	LYS	MET	ASN	ASN	GLU	VAL	SER	THR	SER	THR	SER	MET	THR
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[illegible]

	ASN	PHE	LEU	THR	ASN	GLU	LEU	I LE	ARG	G LN	MET	GLI	LYS	LEU	ALA	LYS	ASP	LEU	HIS	ASN	LEU	LYS	PHE	LYS	GLU	LEU	GLY	THR	LYS	ARG	GLN	GLU	ASN	LEU	LEU	T LE	ILE	GLE	VAL	V AL	SER	S ER	LYS	ILE	A SN	C YS
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LEU SER LYS SER LEU CYS LEU ASN LEU ASN SER ASP SER SER ASN ASN ASN ASN VAL ALA ALA GLU LYS GLU GLU LYS GLU ARG SER SER GLN LYS ASP HIS PHE LYS SER SER MET LEU LEU SER LYS PRO PRO GLU GLU THR THR LEU SER SER LYS GLY ASN ASN PRO PHE ASN ASN PRO LYS PRO ASN ASN LYS THR GLU GLY ASN HIS ASN

GLY	GLN	SER	ILE	SER	ASN	GLU	ASN	ASP	VAL	LYS	PRO	ILE	SER	ILE	GLU	ALA	PRO	GLN	PHE	TYR	ARG	TYR	TRP	SER	ALA
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Chain E: 8% 9% 83%

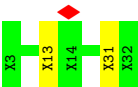
VAL	LYS	GLY	THR	PRO	ASP	LEU	ARG	PRO	GLY	SER	N370	Q301	ASP	VAL	VAL	VAL	SER	PRO	MET
LYS	GLY	THR	GLY	ASP	ASN	GLN	ALA	ILE	THR	GLU	<div><div></div><div>N370</div></div>	Q302	ALA	LYS	ASN	ASN	GLU	ASN	GLY
PRO	MET	GLY	ILE	ASP	THR	ARG	GLN	GLY	SER	SER	<div><div></div><div>G373</div></div>	Q303	HIS	GLU	ASN	THR	ASN	GLY	
ILE	GLY	ASP	GLN	ASP	LEU	PRO	LYS	LYS	THR	LEU	<div><div></div><div>D374</div></div>	E304	LYS	SER	GLY	ASP	ASP	THR	
SER	ASN	ASN	SER	PHE	LEU	LEU	ALA	PHE	LEU	TYR	<div><div></div><div>A375</div></div>	E305	ALA	GLY	GLN	ALA	GLY	GLY	
ILE	GLY	ASP	GLY	LEU	LEU	LYS	GLY	LEU	LYS	LYS	<div><div></div><div>A376</div></div>	V306	GLN	PRO	ASN	GLY	ASN	GLY	
ALA	SER	ALA	SER	TYR	TYR	LYS	LYS	TYR	TYR	TYR	<div><div></div><div>F379</div></div>	<div><div></div><div>P308</div></div>	GLN	ASP	THR	THR	SER	GLY	
PRO	VAL	GLY	ILE	GLY	VAL	LYS	LYS	LYS	VAL	LEU	<div><div></div><div>R380</div></div>	S309	ASP	GLU	PRO	GLU	GLY	SER	
GLN	LEU	ALA	LYS	ASP	LYS	LYS	LYS	ASP	LYS	LYS	<div><div></div><div>L381</div></div>	Y310	ILE	ASN	SER	ASN	THR	GLY	
ASN	ASN	GLY	SER	GLY	ILE	GLY	GLY	GLY	GLY	GLY	<div><div></div><div>H382</div></div>	S311	ILE	THR	ILE	THR	ILE	ASN	
LYS	HIS	TYR	GLN	ASN	LEU	LEU	GLN	ASN	SER	SER	<div><div></div><div>K383</div></div>	K312	GLY	LYS	PRO	GLY	VAL	ASN	
LEU	LEU	GLY	LYS	LYS	GLY	GLY	GLY	GLY	GLY	ARG	<div><div></div><div>T386</div></div>	W313	LYS	MET	THR	THR	ALA	SER	
GLY	LYS	GLY	GLY	LYS	GLY	GLN	GLN	LYS	ARG	LYS	<div><div></div><div>K387</div></div>	<div><div></div><div>N315</div></div>	THR	ASP	ASN	ASN	THR	GLY	
ILE	GLY	GLY	GLY	GLY	ILE	ILE	ILE	ILE	LYS	LYS	<div><div></div><div>G388</div></div>	<div><div></div><div>K318</div></div>	SER	VAL	VAL	VAL	PRO	VAL	
GLY	LEU	GLY	ILE	ASN	ASN	ASP	ASN	ASP	GLY	TYR	<div><div></div><div>G389</div></div>	<div><div></div><div>L319</div></div>	ASP	GLU	GLU	GLY	GLN	GLY	
LEU	LYS	LYS	ASP	ASN	ASN	ASN	TRP	ILE	ILE	ILE	<div><div></div><div>L390</div></div>	<div><div></div><div>E323</div></div>	LYS	GLY	PRO	GLY	GLN	GLY	
PHE	PHE	ASN	GLN	ASN	GLY	GLY	SER	SER	THR	THR	<div><div></div><div>I391</div></div>	<div><div></div><div>V324</div></div>	LYS	ASP	ASN	ASN	MET	GLY	
MET	MET	GLY	PRO	GLY	LEU	LEU	LYS	GLY	HIS	HIS	<div><div></div><div>N392</div></div>	Q325	VAL	GLU	LYS	GLY	GLN	GLY	
GLY	GLY	ILE	ILE	GLY	GLY	GLY	GLY	GLY	LYS	PRO	<div><div></div><div>Y393</div></div>	<div><div></div><div>S326</div></div>	ASP	ASP	PRO	ALA	ASN	ASN	
LEU	GLY	GLY	GLY	PRO	ASP	ASP	ASP	ASP	ASP	PRO	<div><div></div><div>Q394</div></div>	L327	GLY	ASP	ILE	ASP	ASN	ASN	
ARG	HIS	THR	HIS	LEU	LEU	LEU	LEU	LEU	SER	SER	<div><div></div><div>K402</div></div>	P328	GLY	ASN	GLY	GLY	LYS	SER	
LYS	LYS	TYR	LYS	TYR	GLN	GLN	LYS	TYR	THR	THR	<div><div></div><div>N403</div></div>	<div><div></div><div>E329</div></div>	GLU	GLN	ASN	GLY	LEU	ASN	
THR	THR	ALA	GLY	ALA	LYS	LYS	LYS	LYS	THR	THR	<div><div></div><div>I404</div></div>	F330	ARG	PRO	GLY	GLY	ASP	ASP	
LEU	LEU	GLY	GLY	PRO	LYS	LEU	LEU	LEU	ASP	ASP	<div><div></div><div>L408</div></div>	<div><div></div><div>F331</div></div>	ASN	MET	MET	ASP	SER	SER	
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	<div><div></div><div>T409</div></div>	T332	GLY	ILE	ILE	GLY	GLN	ASN	
GLN	GLN	ILE	ILE	PRO	ILE	ILE	ILE	ILE	GLY	GLY	<div><div></div><div>N412</div></div>	<div><div></div><div>R353</div></div>	GLY	PRO	ILE	THR	ASN	ASN	
GLY	GLY	PHE	PHE	PHE	GLN	GLN	GLN	GLN	GLY	GLY	<div><div></div><div>S413</div></div>	R334	ARG	ASP	GLN	GLN	PRO	ALA	
ASN	ASN	ILE	ILE	SER	GLY	GLY	GLY	GLY	ASN	ASN	<div><div></div><div>T414</div></div>	<div><div></div><div>K335</div></div>	GLY						

- Molecule 4: SWI/SNF complex subunit SWI3

Chain F:  16% 10% 73%

[illegible]





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61518	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF amplitude correction was performed following 3D auto refinement in relion.	Depositor
Microscope	JEOL 3200FS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	76.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.035	Depositor
Map size (\AA)	430.08002, 430.08002, 430.08002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.12, 1.12, 1.12	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/1154	0.47	0/1572
2	B	0.38	0/3958	0.52	0/5364
3	C	0.35	0/2040	0.54	0/2756
4	D	0.34	0/1359	0.47	0/1838
4	E	0.40	0/1189	0.51	0/1616
4	F	0.32	0/1596	0.52	5/2154 (0.2%)
4	G	0.33	0/1446	0.51	3/1949 (0.2%)
5	H	0.35	0/2119	0.47	0/2856
6	I	0.32	0/682	0.48	0/913
All	All	0.35	0/15543	0.50	8/21018 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	606	PRO	N-CA-CB	6.95	111.64	103.30
4	G	620	PRO	N-CA-CB	6.10	110.62	103.30
4	F	649	PRO	N-CA-CB	6.07	110.58	103.30
4	F	599	PRO	N-CA-CB	5.89	110.36	103.30
4	F	777	PRO	N-CA-CB	5.72	110.16	103.30
4	G	777	PRO	N-CA-CB	5.68	110.11	103.30
4	G	649	PRO	N-CA-CB	5.59	110.01	103.30
4	F	620	PRO	N-CA-CB	5.34	109.71	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	776	ASP	Peptide
2	B	932	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1133	0	1122	86	0
2	B	3890	0	4008	250	0
3	C	2005	0	1939	164	0
4	D	1322	0	1325	97	0
4	E	1152	0	1137	87	0
4	F	1583	0	1397	72	0
4	G	1435	0	1294	59	0
5	H	2085	0	2104	139	0
6	I	818	0	708	67	0
7	J	336	0	70	19	0
8	K	141	0	33	3	0
9	L	91	0	21	0	0
9	O	91	0	21	2	0
10	M	416	0	92	4	0
11	N	151	0	41	3	0
All	All	16649	0	15312	902	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 28.

All (902) 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)
4:D:412:TYR:CD1	5:H:560:ILE:HG23	1.62	1.34
4:D:412:TYR:CD1	5:H:560:ILE:CG2	2.12	1.32
4:D:412:TYR:CG	5:H:560:ILE:HG21	1.93	1.02
1:A:570:LYS:HE2	6:I:90:LEU:H	1.25	0.98
4:D:412:TYR:HD1	5:H:560:ILE:HG23	1.16	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:412:TYR:CD1	5:H:560:ILE:HG21	1.95	0.94
2:B:933:ASN:HB2	2:B:936:ARG:HE	1.34	0.92
3:C:641:PRO:HG2	4:D:372:SER:OG	1.72	0.89
4:G:519:ILE:HD12	4:G:572:ASP:HB3	1.55	0.88
4:D:412:TYR:CG	5:H:560:ILE:CG2	2.54	0.88
3:C:644:GLU:HA	3:C:647:ILE:CG1	2.04	0.87
3:C:432:VAL:HG12	3:C:436:LYS:H	1.40	0.86
2:B:887:SER:O	2:B:890:LYS:HB3	1.76	0.86
3:C:439:LEU:HD22	4:E:387:LYS:HG2	1.59	0.85
4:G:677:ARG:HH11	4:G:678:GLN:H	1.25	0.84
1:A:557:ASN:HB3	2:B:907:ALA:H	1.44	0.83
1:A:570:LYS:NZ	6:I:88:GLU:O	2.13	0.81
3:C:505:THR:HA	3:C:508:GLN:HB2	1.63	0.81
3:C:644:GLU:HA	3:C:647:ILE:HG13	1.61	0.81
1:A:505:LEU:HB2	4:G:573:LYS:HE2	1.64	0.79
4:D:434:LEU:HD12	4:D:435:PRO:HD2	1.65	0.79
4:D:414:THR:OG1	4:E:309:SER:N	2.15	0.79
3:C:504:ALA:O	3:C:508:GLN:NE2	2.16	0.79
4:D:412:TYR:HB2	5:H:560:ILE:HG22	1.65	0.78
4:E:402:LYS:NZ	4:E:403:ASN:O	2.16	0.77
5:H:394:LYS:NZ	5:H:401:MET:SD	2.58	0.76
3:C:557:LEU:HD11	3:C:651:ASN:HB3	1.68	0.76
2:B:1103:HIS:O	2:B:1104:ASN:ND2	2.20	0.75
4:E:341:GLU:OE1	4:E:341:GLU:N	2.20	0.75
4:F:700:HIS:HA	4:F:703:LYS:HD2	1.69	0.75
6:I:110:ASN:OD1	6:I:113:SER:OG	2.04	0.74
2:B:747:GLU:OE2	3:C:429:GLN:NE2	2.20	0.74
3:C:434:ASN:H	3:C:436:LYS:HG3	1.53	0.74
2:B:715:GLN:HE22	2:B:717:LYS:HB3	1.52	0.74
3:C:481:LYS:NZ	3:C:521:ILE:O	2.18	0.74
2:B:1294:GLN:N	2:B:1294:GLN:OE1	2.18	0.74
1:A:572:ARG:NH2	6:I:93:ILE:O	2.21	0.74
2:B:1051:LYS:HZ2	2:B:1053:ASN:HB2	1.52	0.74
2:B:1084:LEU:O	2:B:1087:ARG:HB3	1.87	0.74
3:C:562:GLU:HG2	3:C:634:THR:HG21	1.70	0.73
4:F:525:GLU:OE2	4:F:564:ARG:NH1	2.21	0.73
4:D:412:TYR:HB2	5:H:560:ILE:CG2	2.18	0.73
4:G:540:GLN:HG3	4:G:541:GLU:HG3	1.70	0.73
5:H:504:PHE:HA	5:H:507:ILE:HD12	1.69	0.73
3:C:633:ILE:HD12	3:C:633:ILE:H	1.54	0.73
4:E:318:LYS:O	4:E:347:ARG:NH2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:605:HIS:O	3:C:609:ALA:N	2.22	0.72
3:C:502:GLU:O	3:C:508:GLN:NE2	2.23	0.72
4:D:414:THR:HG22	4:D:416:HIS:CE1	2.23	0.72
4:F:739:VAL:HA	4:F:742:LYS:HD2	1.72	0.72
2:B:732:THR:HG21	2:B:924:ILE:HG13	1.71	0.71
5:H:379:VAL:O	5:H:400:THR:HA	1.90	0.71
3:C:630:LEU:O	3:C:633:ILE:HD11	1.89	0.71
5:H:79:VAL:O	5:H:83:LYS:NZ	2.23	0.71
3:C:574:GLU:OE1	3:C:574:GLU:N	2.21	0.71
2:B:797:ASP:O	2:B:801:GLU:N	2.18	0.71
2:B:789:VAL:HG12	2:B:790:THR:H	1.57	0.70
5:H:393:LEU:HG	5:H:396:SER:HB3	1.74	0.70
1:A:533:TYR:CZ	1:A:537:GLN:OE1	2.45	0.70
3:C:421:ASN:OD1	4:D:415:ARG:NH2	2.24	0.70
3:C:475:ASP:OD1	4:E:369:ARG:NH1	2.23	0.70
3:C:549:ASP:HA	3:C:557:LEU:O	1.92	0.70
4:E:312:LYS:HG2	5:H:560:ILE:CD1	2.21	0.70
4:F:597:HIS:N	4:F:600:PHE:O	2.25	0.70
2:B:964:CYS:HB3	2:B:967:LYS:HG2	1.74	0.70
3:C:573:GLU:N	3:C:573:GLU:OE2	2.24	0.70
4:G:712:ARG:NH2	5:H:106:SER:OG	2.24	0.69
1:A:552:PHE:O	5:H:554:ARG:NH1	2.25	0.69
3:C:576:ALA:HB1	3:C:590:VAL:HB	1.73	0.69
6:I:157:UNK:O	6:I:161:UNK:N	2.25	0.69
5:H:78:LEU:O	5:H:81:SER:OG	2.08	0.69
3:C:633:ILE:HD12	3:C:633:ILE:N	2.07	0.69
3:C:582:GLU:N	3:C:582:GLU:OE1	2.26	0.69
4:G:720:GLU:HA	4:G:723:LEU:HD12	1.75	0.69
1:A:547:GLY:HA3	4:E:420:ARG:HD2	1.74	0.69
2:B:1196:SER:N	2:B:1197:GLU:OE2	2.27	0.68
3:C:556:GLN:NE2	3:C:654:GLN:OE1	2.25	0.68
4:E:308:PRO:O	4:E:311:SER:OG	2.11	0.68
6:I:74:ASN:HA	6:I:77:ARG:HE	1.59	0.68
3:C:546:ILE:O	3:C:560:GLN:HA	1.94	0.68
7:J:19:UNK:O	7:J:23:UNK:N	2.27	0.68
4:F:667:ARG:NH2	4:G:639:SER:O	2.27	0.68
1:A:498:GLN:HA	1:A:501:ILE:HD12	1.76	0.67
2:B:1137:SER:HA	2:B:1140:ILE:HD12	1.77	0.67
3:C:422:THR:HG22	3:C:423:THR:H	1.59	0.67
2:B:1036:GLN:OE1	2:B:1036:GLN:N	2.27	0.67
2:B:1307:ASN:HA	2:B:1310:LEU:HD12	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:453:ASN:HB2	5:H:457:ARG:HH12	1.59	0.66
3:C:559:ASP:OD1	3:C:560:GLN:N	2.28	0.66
10:M:28:UNK:O	10:M:32:UNK:N	2.28	0.66
1:A:557:ASN:ND2	2:B:907:ALA:O	2.28	0.66
5:H:82:GLU:HA	5:H:85:LEU:HD13	1.78	0.66
2:B:1233:LEU:O	2:B:1236:SER:OG	2.14	0.66
3:C:646:LYS:O	3:C:649:THR:N	2.26	0.66
2:B:891:ILE:O	2:B:895:ILE:N	2.28	0.66
2:B:929:SER:O	2:B:981:ASN:ND2	2.29	0.66
2:B:958:HIS:CE1	2:B:960:GLU:HA	2.30	0.66
1:A:546:ARG:NH2	4:G:566:LEU:O	2.25	0.66
4:E:402:LYS:NZ	7:J:59:UNK:O	2.26	0.66
4:G:538:GLY:O	4:G:542:PHE:HB2	1.95	0.66
6:I:136:LEU:O	6:I:139:GLU:HG2	1.96	0.66
6:I:78:GLN:O	6:I:82:ARG:HG2	1.96	0.65
3:C:465:ASP:OD1	3:C:473:LEU:N	2.30	0.65
2:B:923:MET:O	2:B:927:ASN:ND2	2.30	0.65
5:H:309:SER:OG	5:H:416:LEU:O	2.12	0.65
4:D:417:ASP:OD2	7:J:64:UNK:N	2.29	0.65
4:F:688:ARG:HH11	5:H:86:ASP:HB2	1.62	0.65
4:E:365:THR:HB	4:E:368:ARG:HH21	1.62	0.65
4:G:570:ILE:HG13	4:G:570:ILE:O	1.97	0.65
4:E:309:SER:O	4:E:312:LYS:N	2.23	0.64
3:C:584:GLU:HG3	3:C:586:PRO:HD3	1.79	0.64
4:E:306:VAL:O	4:E:394:GLN:NE2	2.31	0.64
4:F:686:LEU:HD22	6:I:133:LYS:HG2	1.80	0.64
2:B:1300:GLN:OE1	2:B:1304:ASN:ND2	2.31	0.64
3:C:511:ASP:N	3:C:511:ASP:OD1	2.31	0.64
3:C:545:ARG:HH12	3:C:649:THR:HG22	1.62	0.63
1:A:555:HIS:HB2	4:D:422:LEU:HD13	1.79	0.63
2:B:974:ASP:HA	2:B:977:ILE:HD12	1.80	0.63
4:D:412:TYR:CB	5:H:560:ILE:CG2	2.77	0.63
2:B:719:LEU:HD13	5:H:554:ARG:HH21	1.64	0.63
4:D:426:GLU:HB3	4:E:413:SER:H	1.64	0.63
2:B:933:ASN:O	2:B:936:ARG:HG2	1.99	0.63
3:C:454:SER:HB3	4:E:335:ILE:HB	1.80	0.63
3:C:602:HIS:HA	3:C:605:HIS:NE2	2.13	0.63
4:F:676:GLU:OE2	4:F:677:ARG:NH2	2.30	0.63
4:D:354:TYR:OH	4:D:394:GLN:NE2	2.32	0.63
4:E:308:PRO:HB2	4:E:310:TYR:CE2	2.34	0.63
7:J:5:UNK:O	7:J:9:UNK:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:LEU:HA	2:B:726:LEU:HD12	1.78	0.63
2:B:986:LEU:HD11	2:B:1046:LEU:HD13	1.80	0.63
2:B:990:SER:O	2:B:993:ASP:N	2.31	0.63
3:C:515:GLN:OE1	3:C:518:GLN:NE2	2.31	0.63
2:B:1145:THR:HG21	2:B:1239:ILE:HD11	1.80	0.62
2:B:919:SER:O	2:B:922:SER:OG	2.16	0.62
4:E:404:ILE:HD11	4:E:408:LEU:HD22	1.79	0.62
2:B:706:ASN:OD1	2:B:707:LEU:N	2.33	0.62
2:B:886:THR:O	2:B:889:LYS:HB2	1.99	0.62
2:B:915:ASN:HD21	2:B:962:PHE:HA	1.62	0.62
2:B:982:ILE:HB	2:B:1046:LEU:HD11	1.80	0.62
2:B:1092:TYR:O	2:B:1093:ASN:ND2	2.32	0.62
4:D:339:THR:HG23	4:D:342:VAL:H	1.64	0.62
4:G:528:SER:N	4:G:531:ASP:OD2	2.32	0.62
1:A:570:LYS:HG3	6:I:90:LEU:C	2.20	0.62
2:B:1081:ASP:OD1	2:B:1082:LYS:N	2.31	0.62
7:J:4:UNK:O	7:J:8:UNK:N	2.33	0.62
1:A:584:GLN:O	1:A:588:ASN:ND2	2.33	0.62
4:E:301:GLN:HE21	4:E:303:HIS:H	1.47	0.62
4:F:673:THR:O	4:F:677:ARG:HG2	2.00	0.62
3:C:564:ASP:OD1	3:C:566:SER:N	2.31	0.61
1:A:570:LYS:HE2	6:I:90:LEU:N	2.07	0.61
4:E:374:ASP:OD1	4:E:375:ALA:N	2.33	0.61
4:G:525:GLU:O	4:G:564:ARG:NH2	2.25	0.61
3:C:471:PHE:HB3	3:C:473:LEU:HG	1.81	0.61
3:C:583:LEU:HD23	3:C:584:GLU:HG2	1.80	0.61
4:G:557:SER:N	4:G:560:GLN:OE1	2.30	0.61
4:F:670:ILE:HG21	5:H:508:SER:HB3	1.82	0.61
2:B:979:LEU:HA	2:B:982:ILE:HD12	1.82	0.61
3:C:644:GLU:OE1	3:C:644:GLU:N	2.28	0.61
2:B:743:VAL:O	2:B:744:LYS:HD2	2.01	0.61
2:B:744:LYS:HG3	3:C:437:HIS:CE1	2.36	0.61
2:B:1051:LYS:NZ	2:B:1053:ASN:HD22	1.99	0.61
3:C:411:GLY:O	3:C:420:THR:OG1	2.19	0.61
4:E:354:TYR:OH	4:E:394:GLN:N	2.27	0.61
4:G:536:LEU:HA	4:G:539:ILE:HG12	1.82	0.61
2:B:1195:SER:H	2:B:1251:LYS:HE2	1.65	0.61
4:E:415:ARG:HE	4:E:416:HIS:CE1	2.18	0.61
6:I:104:ARG:HH12	8:K:9:UNK:HA	1.65	0.61
4:D:308:PRO:O	4:D:311:SER:OG	2.16	0.60
2:B:1029:GLN:OE1	2:B:1029:GLN:N	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:332:THR:HG23	4:D:334:ARG:H	1.65	0.60
7:J:49:UNK:O	7:J:53:UNK:N	2.34	0.60
2:B:1206:LYS:O	2:B:1210:ILE:HG12	2.01	0.60
3:C:465:ASP:O	3:C:470:ARG:NH2	2.34	0.60
3:C:564:ASP:OD1	3:C:565:ILE:N	2.33	0.60
4:D:422:LEU:HD23	4:D:422:LEU:H	1.67	0.60
4:D:427:SER:OG	4:D:428:TYR:N	2.32	0.60
4:F:673:THR:O	4:F:677:ARG:NH1	2.34	0.60
2:B:1051:LYS:HZ3	2:B:1053:ASN:HD22	1.49	0.60
5:H:457:ARG:HA	5:H:461:ILE:HD11	1.82	0.60
1:A:533:TYR:OH	1:A:537:GLN:OE1	2.16	0.60
2:B:1028:PHE:HZ	2:B:1033:GLY:H	1.48	0.60
4:D:371:VAL:HG13	4:D:373:GLY:H	1.67	0.60
2:B:1294:GLN:O	2:B:1298:GLN:HG2	2.02	0.60
2:B:1143:SER:O	2:B:1146:SER:OG	2.19	0.59
4:D:318:LYS:O	4:D:347:ARG:NH2	2.34	0.59
4:D:318:LYS:HG2	4:D:319:ILE:H	1.67	0.59
4:F:706:LYS:O	4:F:710:LEU:HG	2.01	0.59
4:G:743:CYS:O	4:G:747:ILE:HG13	2.02	0.59
7:J:11:UNK:O	7:J:15:UNK:N	2.36	0.59
1:A:555:HIS:O	1:A:558:SER:OG	2.20	0.59
1:A:567:PHE:HB2	2:B:926:ARG:CZ	2.32	0.59
3:C:410:ASN:HB2	4:D:415:ARG:HD3	1.82	0.59
3:C:543:ARG:HA	3:C:564:ASP:HA	1.85	0.59
4:E:302:ALA:O	4:E:303:HIS:ND1	2.36	0.59
5:H:71:GLU:OE1	5:H:73:TYR:N	2.35	0.59
2:B:926:ARG:O	2:B:929:SER:OG	2.19	0.59
2:B:869:ARG:HA	2:B:953:TRP:CZ3	2.38	0.59
2:B:750:ASP:O	2:B:754:ILE:HG12	2.03	0.59
2:B:896:ASP:C	6:I:110:ASN:HD22	2.06	0.59
3:C:550:ILE:O	3:C:556:GLN:HA	2.03	0.59
4:G:519:ILE:HD12	4:G:572:ASP:CB	2.32	0.59
5:H:109:SER:HA	5:H:112:PHE:CD2	2.37	0.59
6:I:91:SER:OG	6:I:92:ASN:N	2.36	0.59
4:E:311:SER:O	4:E:313:TRP:N	2.32	0.59
4:F:661:ILE:HA	4:F:664:LEU:HD12	1.85	0.59
4:D:426:GLU:OE2	4:E:413:SER:N	2.36	0.58
4:D:447:SER:OG	4:D:451:SER:N	2.36	0.58
4:G:677:ARG:HH11	4:G:678:GLN:N	1.99	0.58
2:B:889:LYS:O	2:B:893:ASP:N	2.29	0.58
2:B:976:VAL:HA	2:B:979:LEU:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:461:ARG:NH1	11:N:31:UNK:O	2.36	0.58
5:H:99:MET:HA	5:H:102:GLN:HE21	1.67	0.58
1:A:483:VAL:HG13	1:A:485:PRO:HD3	1.85	0.58
2:B:896:ASP:CG	6:I:110:ASN:HB3	2.24	0.58
3:C:466:GLN:HE21	3:C:468:ARG:HH21	1.50	0.58
4:F:663:SER:HA	4:F:666:TYR:CD2	2.38	0.58
2:B:1140:ILE:O	2:B:1143:SER:OG	2.17	0.58
2:B:1199:ASN:OD1	2:B:1199:ASN:N	2.31	0.58
4:G:723:LEU:O	4:G:727:LEU:HG	2.03	0.58
2:B:1196:SER:OG	2:B:1251:LYS:NZ	2.37	0.58
3:C:646:LYS:NZ	4:D:370:ASN:O	2.35	0.58
5:H:519:ILE:O	5:H:522:THR:OG1	2.20	0.58
6:I:138:SER:O	6:I:141:THR:OG1	2.18	0.58
3:C:537:LEU:N	4:D:334:ARG:HH22	2.02	0.58
5:H:111:GLU:HA	5:H:114:TYR:CD2	2.39	0.58
2:B:864:LEU:HB2	2:B:865:PRO:HD3	1.86	0.58
2:B:1293:ILE:HA	2:B:1296:ILE:HD12	1.86	0.58
5:H:76:GLN:HG3	5:H:78:LEU:HD23	1.84	0.58
3:C:464:PHE:HB2	3:C:473:LEU:HB2	1.85	0.58
4:E:420:ARG:HD3	4:E:420:ARG:N	2.19	0.58
4:F:692:GLU:HB3	5:H:89:ILE:HG21	1.85	0.58
3:C:517:ILE:O	3:C:521:ILE:HG23	2.03	0.58
2:B:944:LEU:O	2:B:948:ILE:HG12	2.04	0.57
4:D:324:VAL:HG23	4:D:331:PHE:CD1	2.39	0.57
4:E:374:ASP:OD1	4:E:376:ALA:N	2.37	0.57
4:F:667:ARG:HA	4:F:670:ILE:HD12	1.85	0.57
1:A:538:LEU:HD13	1:A:541:LEU:HD13	1.85	0.57
2:B:1264:GLU:HA	2:B:1267:LYS:HD3	1.85	0.57
2:B:1301:LEU:HA	2:B:1304:ASN:HD22	1.69	0.57
4:E:308:PRO:HD3	4:E:393:TYR:CE2	2.39	0.57
2:B:866:GLU:OE1	2:B:866:GLU:N	2.30	0.57
3:C:514:CYS:HA	3:C:517:ILE:HD12	1.87	0.57
4:D:412:TYR:CB	5:H:560:ILE:HG21	2.33	0.57
4:F:732:ASN:O	4:F:736:ILE:HG13	2.04	0.57
5:H:324:THR:HG23	5:H:327:ASP:H	1.69	0.57
4:G:519:ILE:CD1	4:G:572:ASP:HB3	2.31	0.57
6:I:115:ASN:OD1	6:I:119:ASN:ND2	2.29	0.57
2:B:874:GLN:HE22	2:B:959:PRO:HD2	1.70	0.57
2:B:1292:ASP:OD1	2:B:1292:ASP:N	2.37	0.57
3:C:469:ASP:HB2	3:C:471:PHE:HE2	1.68	0.57
3:C:488:ILE:O	3:C:492:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:139:GLU:O	6:I:143:ARG:HD3	2.04	0.57
2:B:1064:LYS:HG3	2:B:1104:ASN:ND2	2.19	0.57
5:H:498:ASN:O	5:H:502:ARG:HG2	2.05	0.57
1:A:589:HIS:ND1	2:B:1050:GLU:HG2	2.20	0.57
2:B:880:HIS:CE1	2:B:958:HIS:HB3	2.39	0.57
4:D:406:PRO:HA	4:E:352:ASN:HD21	1.70	0.57
4:E:364:VAL:HB	4:E:382:HIS:CG	2.39	0.57
4:G:678:GLN:HB2	4:G:679:MET:HE2	1.87	0.57
1:A:556:GLN:OE1	5:H:554:ARG:NH1	2.37	0.56
4:E:354:TYR:CD2	4:E:391:ILE:HA	2.40	0.56
4:F:657:SER:O	4:F:661:ILE:HG12	2.05	0.56
1:A:552:PHE:C	5:H:554:ARG:HH11	2.08	0.56
2:B:896:ASP:O	6:I:110:ASN:ND2	2.32	0.56
1:A:525:THR:HA	1:A:528:ASN:ND2	2.20	0.56
2:B:935:SER:HA	2:B:938:MET:HB2	1.86	0.56
2:B:1058:LYS:HA	2:B:1061:LEU:HD12	1.87	0.56
4:E:402:LYS:HZ3	7:J:59:UNK:C	2.16	0.56
3:C:570:ASN:HD21	4:D:380:ARG:NE	2.04	0.56
5:H:512:VAL:O	5:H:516:ASN:ND2	2.39	0.56
1:A:546:ARG:CZ	5:H:541:ARG:HE	2.18	0.56
2:B:999:ILE:O	2:B:1002:ILE:HG22	2.06	0.56
5:H:307:PHE:HD2	5:H:323:GLY:HA2	1.71	0.56
2:B:785:ASN:HB3	4:E:345:ARG:NH2	2.21	0.56
5:H:490:VAL:HA	5:H:493:ASN:HD22	1.69	0.56
4:D:437:MET:O	4:D:441:LYS:N	2.37	0.56
3:C:649:THR:OG1	4:D:369:ARG:HA	2.06	0.56
4:G:530:GLU:HA	4:G:533:GLN:HB2	1.88	0.56
5:H:335:TYR:O	5:H:339:ASN:ND2	2.39	0.56
6:I:138:SER:O	6:I:142:ILE:HG12	2.06	0.56
1:A:559:LEU:HD21	2:B:722:ILE:HG23	1.86	0.56
2:B:880:HIS:HE1	2:B:958:HIS:O	1.89	0.56
4:D:363:SER:OG	4:D:364:VAL:N	2.39	0.56
4:F:710:LEU:HD23	4:F:713:LYS:HZ3	1.70	0.56
1:A:505:LEU:O	1:A:508:THR:OG1	2.17	0.55
2:B:1243:GLN:NE2	2:B:1247:CYS:SG	2.79	0.55
4:E:420:ARG:O	4:E:420:ARG:NH1	2.37	0.55
5:H:117:LEU:O	5:H:118:ASN:ND2	2.39	0.55
3:C:584:GLU:HB2	4:D:401:PRO:HG3	1.88	0.55
2:B:912:VAL:HG12	2:B:963:THR:HG21	1.88	0.55
4:D:412:TYR:HD1	5:H:560:ILE:CG2	1.83	0.55
3:C:567:ASN:ND2	3:C:570:ASN:OD1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:424:PRO:HG2	4:E:425:PHE:CE2	2.42	0.55
4:G:519:ILE:CD1	4:G:572:ASP:CB	2.85	0.55
5:H:532:ASP:OD1	5:H:532:ASP:N	2.37	0.55
6:I:170:UNK:O	6:I:174:UNK:N	2.39	0.55
3:C:415:TYR:CE2	3:C:418:GLY:HA2	2.42	0.55
3:C:609:ALA:HA	3:C:614:ASN:HD21	1.72	0.55
4:G:735:LYS:O	4:G:739:VAL:HG23	2.06	0.55
5:H:399:ASP:HB2	5:H:401:MET:HG2	1.89	0.55
4:D:438:ALA:O	4:D:442:LYS:N	2.40	0.55
1:A:499:THR:HG21	4:E:427:SER:HB3	1.89	0.55
2:B:745:TYR:CD2	2:B:936:ARG:HD3	2.42	0.54
2:B:1055:ASN:OD1	2:B:1055:ASN:N	2.38	0.54
2:B:742:LEU:HB2	2:B:745:TYR:CZ	2.42	0.54
2:B:941:ASN:O	2:B:944:LEU:N	2.39	0.54
2:B:1278:THR:OG1	2:B:1281:GLU:HG2	2.07	0.54
3:C:599:GLU:HG2	3:C:603:MET:HE3	1.90	0.54
2:B:1034:LYS:O	2:B:1037:THR:OG1	2.16	0.54
2:B:1237:ILE:O	2:B:1240:SER:OG	2.18	0.54
2:B:745:TYR:N	2:B:745:TYR:CD1	2.74	0.54
2:B:879:ILE:O	2:B:881:ARG:NE	2.35	0.54
4:F:703:LYS:HA	4:F:707:PHE:CE2	2.42	0.54
4:E:306:VAL:H	4:E:394:GLN:NE2	2.05	0.54
5:H:311:SER:OG	5:H:314:LEU:HG	2.08	0.54
2:B:963:THR:OG1	2:B:964:CYS:N	2.41	0.54
2:B:1197:GLU:H	2:B:1199:ASN:CG	2.11	0.54
4:D:426:GLU:HB3	4:E:412:TYR:HA	1.90	0.54
4:F:710:LEU:HB3	5:H:107:LYS:HD3	1.88	0.54
2:B:947:PHE:HD2	2:B:948:ILE:HD13	1.72	0.54
5:H:328:ALA:O	5:H:331:SER:OG	2.19	0.54
6:I:71:GLN:O	6:I:74:ASN:HB2	2.08	0.54
2:B:761:SER:O	2:B:764:SER:OG	2.18	0.53
4:F:666:TYR:O	4:F:670:ILE:HG13	2.07	0.53
5:H:465:GLU:O	5:H:469:ASN:ND2	2.42	0.53
2:B:915:ASN:ND2	2:B:963:THR:HG23	2.23	0.53
2:B:953:TRP:CD1	2:B:957:ILE:HD12	2.44	0.53
2:B:1037:THR:OG1	2:B:1038:PHE:N	2.41	0.53
2:B:1136:PHE:CE2	2:B:1140:ILE:HD11	2.44	0.53
4:F:708:MET:HG3	4:F:712:ARG:HH21	1.71	0.53
1:A:542:GLN:OE1	1:A:546:ARG:NH2	2.36	0.53
4:G:546:TRP:HA	4:G:549:VAL:HG22	1.90	0.53
4:F:719:GLN:HA	4:F:722:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:952:LEU:HD12	2:B:996:LEU:HD12	1.90	0.53
4:F:643:GLU:O	4:F:647:GLN:N	2.33	0.53
5:H:485:LYS:O	5:H:488:THR:OG1	2.26	0.53
10:M:21:UNK:HA	10:M:22:UNK:C	2.37	0.53
1:A:505:LEU:O	1:A:509:VAL:HG23	2.08	0.53
6:I:133:LYS:HD2	6:I:133:LYS:N	2.24	0.53
3:C:475:ASP:OD1	3:C:476:THR:N	2.40	0.53
4:D:344:MET:HG2	4:D:347:ARG:HH12	1.73	0.53
4:F:702:LYS:HD3	4:F:706:LYS:HE3	1.90	0.53
4:F:733:SER:O	4:F:737:VAL:HG23	2.09	0.53
4:G:689:LEU:HB3	6:I:143:ARG:HE	1.73	0.53
3:C:469:ASP:HB2	3:C:471:PHE:CE2	2.44	0.53
4:D:449:SER:HA	4:D:452:THR:HB	1.90	0.53
2:B:710:LEU:HD22	2:B:747:GLU:HG3	1.90	0.52
2:B:1205:LEU:O	2:B:1208:SER:OG	2.25	0.52
2:B:1279:ASP:HA	2:B:1282:ILE:HD12	1.91	0.52
3:C:439:LEU:O	3:C:442:LYS:HG2	2.10	0.52
3:C:644:GLU:CA	3:C:647:ILE:HG12	2.38	0.52
5:H:310:TYR:HB3	5:H:314:LEU:HB2	1.91	0.52
3:C:464:PHE:HB2	3:C:473:LEU:HD12	1.90	0.52
3:C:518:GLN:HA	3:C:521:ILE:HG12	1.91	0.52
3:C:577:GLU:O	3:C:580:CYS:HB3	2.09	0.52
1:A:504:ASN:O	1:A:507:THR:OG1	2.22	0.52
3:C:641:PRO:HG2	3:C:646:LYS:HD3	1.91	0.52
4:D:449:SER:O	4:D:453:LEU:N	2.28	0.52
1:A:497:TYR:CE2	1:A:501:ILE:HD11	2.45	0.52
4:D:365:THR:HA	4:D:368:ARG:HG3	1.91	0.52
4:E:417:ASP:HB3	4:E:419:PRO:HD2	1.90	0.52
4:F:681:PHE:HE1	5:H:497:SER:HB2	1.73	0.52
7:J:27:UNK:O	7:J:31:UNK:N	2.41	0.52
5:H:497:SER:HA	5:H:500:ARG:HD3	1.92	0.52
3:C:495:MET:HE2	4:E:365:THR:HG22	1.90	0.52
5:H:464:ALA:O	5:H:468:GLU:HG3	2.10	0.52
6:I:73:LEU:O	6:I:77:ARG:HG3	2.10	0.52
2:B:715:GLN:NE2	2:B:717:LYS:HB3	2.22	0.52
2:B:1029:GLN:HE21	2:B:1032:TRP:HE1	1.57	0.52
5:H:98:ARG:O	5:H:102:GLN:HG3	2.10	0.52
7:J:42:UNK:O	7:J:46:UNK:N	2.43	0.52
3:C:497:ARG:HH12	3:C:503:ASP:HA	1.75	0.52
1:A:575:ASN:N	1:A:578:ASP:OD2	2.43	0.52
2:B:715:GLN:OE1	2:B:717:LYS:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:438:TYR:HB2	4:E:383:LYS:HD2	1.92	0.52
4:D:364:VAL:O	4:D:367:ALA:N	2.43	0.52
4:D:448:ASP:OD1	4:D:448:ASP:N	2.40	0.51
2:B:727:ASN:O	2:B:731:VAL:HG23	2.10	0.51
2:B:745:TYR:CD1	2:B:746:PRO:HD3	2.45	0.51
4:F:735:LYS:O	4:F:739:VAL:HG23	2.11	0.51
4:G:564:ARG:HA	4:G:567:GLN:HE21	1.75	0.51
2:B:932:ASP:HA	2:B:934:ASN:OD1	2.11	0.51
2:B:1054:LEU:HA	2:B:1057:PHE:CD2	2.45	0.51
4:F:549:VAL:HA	4:F:552:ASN:HD22	1.74	0.51
6:I:102:SER:O	6:I:105:SER:OG	2.20	0.51
4:D:365:THR:OG1	4:D:368:ARG:NH2	2.43	0.51
1:A:572:ARG:NH1	6:I:95:HIS:HB2	2.24	0.51
2:B:1134:ASP:O	2:B:1138:PRO:HD3	2.11	0.51
3:C:483:ASP:OD1	3:C:484:LYS:N	2.43	0.51
4:F:525:GLU:HB2	4:F:564:ARG:CZ	2.41	0.51
2:B:741:SER:O	2:B:936:ARG:NH2	2.36	0.51
2:B:1080:LYS:HA	2:B:1083:LYS:HG2	1.93	0.51
2:B:1202:SER:OG	2:B:1204:LEU:HB2	2.11	0.51
3:C:510:ILE:HA	3:C:513:ILE:HD12	1.92	0.51
3:C:529:TYR:HA	3:C:532:LEU:HB2	1.92	0.51
3:C:630:LEU:O	3:C:633:ILE:CD1	2.59	0.51
3:C:646:LYS:O	3:C:650:PRO:HD3	2.11	0.51
4:D:344:MET:HG2	4:D:347:ARG:NH1	2.26	0.51
4:D:426:GLU:CB	4:E:413:SER:H	2.23	0.51
2:B:1047:PHE:CE1	2:B:1058:LYS:HD2	2.46	0.51
4:E:339:THR:HG22	4:E:342:VAL:HG12	1.93	0.51
6:I:78:GLN:HG3	9:O:3:UNK:C	2.40	0.51
3:C:450:MET:HG2	3:C:485:LEU:HD11	1.92	0.51
3:C:597:ILE:O	3:C:601:VAL:HG12	2.11	0.51
4:D:350:MET:O	4:D:353:SER:OG	2.27	0.51
4:D:361:TYR:HB2	4:D:395:VAL:HG11	1.91	0.51
4:G:738:ASN:O	4:G:741:SER:OG	2.23	0.51
5:H:311:SER:HB3	5:H:414:HIS:HB3	1.93	0.51
5:H:336:ILE:HD11	5:H:385:LEU:HD21	1.93	0.51
6:I:74:ASN:O	6:I:78:GLN:HG2	2.11	0.51
1:A:551:GLN:HG3	4:E:419:PRO:HG3	1.91	0.51
1:A:570:LYS:NZ	1:A:571:ILE:HG12	2.26	0.51
4:E:332:THR:HG23	4:E:334:ARG:H	1.75	0.51
1:A:467:THR:OG1	1:A:468:LEU:N	2.44	0.50
1:A:563:THR:HG22	1:A:564:HIS:H	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1064:LYS:HG3	2:B:1104:ASN:HD22	1.76	0.50
2:B:1258:CYS:SG	2:B:1259:LEU:N	2.84	0.50
1:A:470:ALA:O	6:I:128:CYS:HB2	2.11	0.50
4:G:691:MET:HA	4:G:694:LEU:HD12	1.92	0.50
4:D:317:GLU:OE1	4:D:317:GLU:N	2.44	0.50
4:F:565:PHE:HE1	4:F:634:ALA:H	1.59	0.50
4:F:674:ASN:OD1	5:H:504:PHE:HB3	2.11	0.50
4:G:730:ASN:O	4:G:733:SER:OG	2.27	0.50
3:C:547:LYS:O	3:C:548:LEU:HD23	2.10	0.50
5:H:381:LEU:HD11	5:H:401:MET:SD	2.52	0.50
5:H:506:LYS:HA	5:H:509:GLU:HG2	1.93	0.50
5:H:375:GLN:HG2	5:H:402:LYS:HE3	1.91	0.50
3:C:603:MET:HA	3:C:606:LYS:HB3	1.94	0.50
1:A:564:HIS:CD2	2:B:966:ARG:HH12	2.30	0.50
2:B:952:LEU:HB3	2:B:996:LEU:HD12	1.94	0.50
3:C:458:VAL:N	3:C:479:TRP:O	2.44	0.50
3:C:636:ASP:OD1	3:C:637:ASP:N	2.44	0.50
1:A:471:ASN:CG	6:I:129:ASP:HB3	2.32	0.50
1:A:488:ILE:HD11	4:G:622:THR:HA	1.94	0.50
2:B:742:LEU:HB2	2:B:745:TYR:CE1	2.47	0.50
2:B:1105:LEU:HD23	2:B:1106:LEU:HD23	1.94	0.50
4:D:415:ARG:NH1	4:D:416:HIS:O	2.45	0.50
5:H:75:PHE:HA	5:H:78:LEU:HD21	1.93	0.50
1:A:565:PRO:HG2	1:A:567:PHE:HE1	1.77	0.50
2:B:1028:PHE:CE2	2:B:1030:LEU:HA	2.47	0.50
3:C:410:ASN:HB2	4:D:415:ARG:CD	2.42	0.50
3:C:445:VAL:O	3:C:448:GLN:NE2	2.45	0.50
4:E:389:GLY:O	4:E:393:TYR:HB2	2.12	0.50
4:G:705:GLU:O	4:G:709:GLU:HG2	2.11	0.50
6:I:110:ASN:O	6:I:114:SER:OG	2.20	0.50
4:F:675:GLU:O	4:F:679:MET:HG2	2.12	0.49
4:F:738:ASN:O	4:F:741:SER:OG	2.25	0.49
2:B:1059:SER:O	2:B:1062:LEU:HB2	2.13	0.49
3:C:588:GLU:HA	4:E:369:ARG:O	2.11	0.49
7:J:44:UNK:O	7:J:48:UNK:N	2.45	0.49
2:B:869:ARG:HG2	2:B:953:TRP:CD2	2.48	0.49
3:C:412:TYR:HB2	3:C:419:ILE:HA	1.94	0.49
3:C:527:ASN:HB3	3:C:531:GLU:CD	2.33	0.49
1:A:541:LEU:O	1:A:545:VAL:HG22	2.12	0.49
2:B:1189:LEU:HB2	2:B:1191:PHE:CE2	2.48	0.49
3:C:518:GLN:O	3:C:522:GLN:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:613:TYR:CE1	3:C:619:ALA:HA	2.46	0.49
4:F:659:ILE:HD13	4:G:633:SER:H	1.77	0.49
4:F:707:PHE:O	4:F:711:GLU:HG2	2.12	0.49
6:I:139:GLU:HG3	6:I:143:ARG:NH1	2.27	0.49
1:A:566:ASN:HD22	6:I:94:ILE:HG12	1.77	0.49
2:B:1056:TYR:O	2:B:1060:ILE:HG13	2.13	0.49
4:D:361:TYR:CG	4:D:362:PHE:N	2.80	0.49
4:F:724:ILE:O	4:F:727:LEU:HG	2.12	0.49
2:B:745:TYR:HD2	2:B:936:ARG:HD3	1.76	0.49
2:B:956:LEU:HD12	2:B:996:LEU:HD13	1.95	0.49
2:B:1035:TYR:O	2:B:1038:PHE:N	2.45	0.49
5:H:326:HIS:O	5:H:329:ILE:HG12	2.13	0.49
2:B:1292:ASP:O	2:B:1296:ILE:HG13	2.13	0.49
5:H:410:ILE:HD13	5:H:414:HIS:HB2	1.95	0.49
1:A:570:LYS:O	6:I:92:ASN:ND2	2.46	0.49
2:B:1275:LEU:HG	2:B:1276:PHE:CG	2.48	0.49
4:G:712:ARG:O	4:G:716:GLU:HG2	2.12	0.49
5:H:100:VAL:O	5:H:104:GLU:HG3	2.11	0.49
2:B:786:GLN:HG2	2:B:787:TYR:H	1.77	0.49
2:B:1232:VAL:C	2:B:1235:PRO:HD2	2.33	0.49
3:C:645:SER:O	3:C:648:PHE:HD2	1.96	0.49
4:D:327:LEU:HB3	4:D:329:GLU:OE2	2.12	0.49
4:F:702:LYS:HD3	4:F:706:LYS:HZ1	1.77	0.49
2:B:745:TYR:HE2	2:B:936:ARG:HB2	1.78	0.48
5:H:512:VAL:HG13	5:H:513:LYS:H	1.78	0.48
3:C:518:GLN:O	3:C:521:ILE:HG12	2.13	0.48
4:F:530:GLU:OE2	4:F:530:GLU:N	2.28	0.48
5:H:85:LEU:O	5:H:89:ILE:HG12	2.12	0.48
2:B:942:PHE:HA	2:B:945:LYS:HE3	1.95	0.48
2:B:1088:LEU:HA	2:B:1091:LEU:HB2	1.95	0.48
4:D:340:PRO:O	4:D:344:MET:HG3	2.14	0.48
6:I:74:ASN:HA	6:I:77:ARG:NE	2.26	0.48
7:J:18:UNK:O	7:J:22:UNK:N	2.46	0.48
2:B:1278:THR:HG21	5:H:113:LEU:HD21	1.96	0.48
4:F:563:LEU:O	4:F:567:GLN:N	2.47	0.48
5:H:529:LEU:HD21	6:I:107:LEU:HB3	1.96	0.48
4:F:651:GLU:O	4:F:655:GLU:HG2	2.14	0.48
4:G:703:LYS:O	4:G:706:LYS:HG3	2.13	0.48
5:H:329:ILE:HA	5:H:332:ILE:HG12	1.96	0.48
2:B:915:ASN:ND2	2:B:963:THR:H	2.11	0.48
2:B:1006:GLN:NE2	2:B:1029:GLN:HE22	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:125:THR:OG1	6:I:126:VAL:N	2.47	0.48
3:C:461:ARG:C	3:C:462:LEU:HD22	2.34	0.48
3:C:594:ALA:O	3:C:597:ILE:HB	2.13	0.48
4:D:358:PRO:HB2	4:D:394:GLN:NE2	2.28	0.48
4:E:306:VAL:H	4:E:394:GLN:HE22	1.60	0.48
2:B:761:SER:OG	2:B:762:ASN:N	2.47	0.48
2:B:1144:LEU:O	2:B:1147:ILE:HG22	2.14	0.48
4:E:402:LYS:HA	7:J:59:UNK:CB	2.43	0.48
1:A:542:GLN:HG3	1:A:543:LYS:N	2.28	0.48
1:A:586:TYR:CZ	2:B:1048:SER:HA	2.49	0.48
2:B:902:ILE:O	2:B:904:THR:N	2.46	0.48
2:B:993:ASP:O	2:B:997:ILE:HG12	2.14	0.48
4:E:335:ILE:HD12	4:E:336:PRO:HD2	1.96	0.48
4:F:710:LEU:HA	4:F:713:LYS:HZ3	1.78	0.48
5:H:90:HIS:HA	5:H:93:ASN:OD1	2.14	0.48
5:H:92:ARG:O	5:H:96:MET:HG2	2.13	0.48
6:I:139:GLU:HG3	6:I:143:ARG:HH12	1.79	0.48
4:E:364:VAL:HB	4:E:382:HIS:ND1	2.29	0.47
4:G:721:ASN:O	4:G:725:GLN:HG2	2.13	0.47
5:H:123:LYS:HD2	5:H:454:ASN:ND2	2.29	0.47
6:I:88:GLU:OE2	6:I:89:GLN:NE2	2.37	0.47
1:A:492:THR:OG1	1:A:493:ALA:N	2.47	0.47
4:F:662:SER:OG	4:F:663:SER:N	2.46	0.47
5:H:76:GLN:HE21	5:H:78:LEU:HA	1.79	0.47
2:B:898:PRO:HB2	2:B:899:PHE:CE2	2.49	0.47
2:B:973:LYS:O	2:B:977:ILE:HG13	2.13	0.47
2:B:1062:LEU:HD23	2:B:1106:LEU:HD12	1.97	0.47
4:G:685:GLU:HA	4:G:688:ARG:HH12	1.79	0.47
5:H:76:GLN:HG3	5:H:78:LEU:H	1.79	0.47
5:H:453:ASN:O	5:H:457:ARG:NH1	2.47	0.47
6:I:81:GLU:HB2	6:I:82:ARG:NH1	2.28	0.47
2:B:718:ASN:HB2	2:B:770:TYR:CD2	2.49	0.47
2:B:1306:LYS:O	2:B:1310:LEU:HG	2.14	0.47
3:C:593:ILE:O	3:C:596:SER:OG	2.22	0.47
2:B:1124:SER:OG	2:B:1126:SER:O	2.31	0.47
3:C:605:HIS:HA	3:C:608:LEU:HB3	1.96	0.47
4:F:725:GLN:HE22	4:F:728:ASN:HD22	1.62	0.47
5:H:99:MET:O	5:H:102:GLN:NE2	2.48	0.47
1:A:570:LYS:O	1:A:572:ARG:N	2.47	0.47
2:B:762:ASN:HB2	2:B:767:VAL:HG13	1.96	0.47
2:B:1106:LEU:HA	2:B:1109:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:446:TYR:CE1	3:C:485:LEU:HB3	2.50	0.47
4:E:348:ASN:HA	4:E:351:VAL:HG12	1.97	0.47
4:F:549:VAL:HA	4:F:552:ASN:ND2	2.29	0.47
4:F:727:LEU:HD21	5:H:122:VAL:HG21	1.96	0.47
4:G:532:LEU:O	4:G:536:LEU:HG	2.14	0.47
1:A:562:ASN:OD1	1:A:563:THR:N	2.48	0.47
2:B:703:GLY:O	3:C:424:THR:HG23	2.14	0.47
2:B:863:LEU:H	2:B:863:LEU:HD23	1.80	0.47
4:D:426:GLU:HB3	4:E:413:SER:N	2.28	0.47
4:F:683:THR:HA	6:I:133:LYS:HE3	1.97	0.47
4:G:714:THR:O	4:G:718:GLN:HG3	2.15	0.47
5:H:75:PHE:CZ	5:H:77:GLN:HA	2.50	0.47
3:C:466:GLN:O	3:C:470:ARG:NH2	2.45	0.47
3:C:447:LYS:HD2	4:E:328:PRO:HG3	1.97	0.47
4:D:318:LYS:NZ	4:D:319:ILE:O	2.47	0.47
3:C:416:GLY:N	4:E:393:TYR:CZ	2.82	0.47
3:C:602:HIS:HA	3:C:605:HIS:CE1	2.49	0.47
3:C:646:LYS:HG2	4:D:372:SER:HB3	1.97	0.47
4:D:429:LYS:HE3	4:E:420:ARG:HH22	1.79	0.47
4:D:433:GLN:N	4:D:433:GLN:OE1	2.48	0.47
4:D:458:LYS:HA	4:D:461:LYS:HE2	1.97	0.47
4:F:563:LEU:O	4:F:568:LEU:N	2.44	0.47
4:F:689:LEU:O	4:F:693:LYS:HG2	2.15	0.47
6:I:104:ARG:NH1	8:K:9:UNK:HA	2.30	0.47
4:E:362:PHE:N	4:E:392:ASN:OD1	2.41	0.46
5:H:314:LEU:HA	5:H:317:ILE:HD12	1.97	0.46
2:B:866:GLU:H	2:B:866:GLU:CD	2.16	0.46
4:G:563:LEU:HG	4:G:567:GLN:NE2	2.30	0.46
2:B:724:THR:O	2:B:728:THR:HG22	2.16	0.46
2:B:1028:PHE:HE1	2:B:1032:TRP:HD1	1.63	0.46
1:A:473:ASP:CG	1:A:475:ALA:H	2.16	0.46
1:A:570:LYS:HG3	6:I:90:LEU:O	2.16	0.46
3:C:562:GLU:CG	3:C:634:THR:HG21	2.43	0.46
4:F:655:GLU:HA	4:F:658:GLU:OE1	2.15	0.46
5:H:78:LEU:HD13	5:H:84:ARG:NH1	2.31	0.46
2:B:1051:LYS:O	2:B:1053:ASN:N	2.45	0.46
2:B:1195:SER:H	2:B:1251:LYS:CE	2.28	0.46
4:D:307:ILE:HD11	4:D:312:LYS:HA	1.96	0.46
4:D:374:ASP:O	4:D:378:LEU:HG	2.15	0.46
4:G:742:LYS:O	4:G:746:LEU:HG	2.14	0.46
1:A:556:GLN:HB3	2:B:718:ASN:HD21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:440:GLU:OE1	3:C:440:GLU:N	2.29	0.46
3:C:475:ASP:OD2	4:E:368:ARG:NH1	2.48	0.46
5:H:308:MET:SD	5:H:415:LEU:HG	2.55	0.46
5:H:489:SER:O	5:H:493:ASN:ND2	2.49	0.46
1:A:490:THR:OG1	1:A:491:HIS:N	2.48	0.46
3:C:446:TYR:HE1	3:C:485:LEU:HB3	1.79	0.46
4:F:528:SER:H	4:F:531:ASP:HB2	1.80	0.46
2:B:920:THR:O	2:B:924:ILE:HG22	2.15	0.46
3:C:523:GLU:O	3:C:606:LYS:HE3	2.15	0.46
4:E:361:TYR:CG	4:E:362:PHE:N	2.83	0.46
4:F:683:THR:O	4:F:687:ILE:HG12	2.15	0.46
4:F:685:GLU:O	4:F:689:LEU:HG	2.15	0.46
1:A:471:ASN:HB3	6:I:129:ASP:HB3	1.97	0.46
2:B:718:ASN:O	2:B:722:ILE:HG12	2.16	0.46
4:D:321:SER:HA	4:D:324:VAL:HG12	1.97	0.46
3:C:563:TRP:HZ3	4:D:376:ALA:HB2	1.81	0.46
3:C:613:TYR:C	3:C:615:PHE:H	2.19	0.46
4:G:525:GLU:C	4:G:527:TRP:H	2.18	0.46
5:H:71:GLU:O	5:H:72:LEU:HD23	2.16	0.46
2:B:708:HIS:CE1	2:B:710:LEU:HD11	2.51	0.45
2:B:1255:PHE:HA	2:B:1258:CYS:SG	2.56	0.45
3:C:640:ARG:NH2	10:M:72:UNK:O	2.49	0.45
6:I:143:ARG:HD2	6:I:146:MET:HE1	1.97	0.45
1:A:540:PRO:HB2	4:D:430:PRO:O	2.16	0.45
2:B:784:SER:O	2:B:784:SER:OG	2.33	0.45
2:B:1198:GLU:O	5:H:98:ARG:NH1	2.43	0.45
3:C:613:TYR:OH	3:C:626:ARG:HG2	2.16	0.45
5:H:525:ALA:HA	5:H:528:VAL:HG12	1.97	0.45
1:A:536:LEU:HD13	1:A:536:LEU:HA	1.78	0.45
2:B:907:ALA:CB	2:B:913:LEU:HB2	2.46	0.45
3:C:529:TYR:CD1	3:C:532:LEU:HB2	2.51	0.45
2:B:735:ASP:OD1	2:B:735:ASP:N	2.49	0.45
3:C:527:ASN:OD1	3:C:531:GLU:N	2.50	0.45
4:E:312:LYS:HG2	5:H:560:ILE:HD11	1.97	0.45
2:B:795:MET:O	2:B:798:LYS:HB2	2.17	0.45
2:B:1197:GLU:N	2:B:1199:ASN:OD1	2.39	0.45
2:B:1265:ILE:HG13	2:B:1266:LEU:H	1.82	0.45
3:C:463:GLU:HA	3:C:473:LEU:O	2.16	0.45
4:F:708:MET:HG3	4:F:712:ARG:NH2	2.30	0.45
5:H:77:GLN:OE1	5:H:79:VAL:HB	2.17	0.45
2:B:1266:LEU:O	2:B:1270:ALA:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:653:LEU:HB2	11:N:13:UNK:HA	1.97	0.45
4:D:381:LEU:O	4:D:385:LEU:HG	2.17	0.45
4:F:528:SER:N	4:F:531:ASP:OD2	2.50	0.45
5:H:389:LEU:HB2	5:H:409:LEU:HD21	1.98	0.45
2:B:745:TYR:HD1	2:B:745:TYR:H	1.64	0.45
4:E:324:VAL:HG12	4:E:331:PHE:CZ	2.52	0.45
4:E:429:LYS:NZ	4:E:433:GLN:HE21	2.14	0.45
4:G:687:ILE:HA	4:G:690:GLN:OE1	2.16	0.45
5:H:86:ASP:OD1	5:H:87:HIS:N	2.50	0.45
5:H:537:GLU:HG3	5:H:538:ASP:H	1.82	0.45
2:B:917:GLN:O	2:B:921:ILE:HG12	2.16	0.45
2:B:1265:ILE:O	2:B:1269:ILE:N	2.30	0.45
3:C:498:ASP:O	3:C:500:ARG:NH1	2.48	0.45
5:H:121:ASN:OD1	5:H:122:VAL:HG23	2.17	0.45
5:H:338:LEU:HD12	5:H:339:ASN:N	2.32	0.45
2:B:1119:LEU:H	2:B:1122:VAL:HG22	1.82	0.45
4:E:327:LEU:HD23	4:E:327:LEU:HA	1.81	0.45
6:I:133:LYS:HD2	6:I:133:LYS:H	1.81	0.45
2:B:934:ASN:O	2:B:938:MET:N	2.49	0.45
4:E:350:MET:O	4:E:353:SER:OG	2.25	0.45
5:H:378:ILE:HB	5:H:400:THR:HG22	1.98	0.45
6:I:88:GLU:HB3	6:I:89:GLN:HE22	1.82	0.45
2:B:899:PHE:HE1	5:H:517:GLU:HB2	1.81	0.44
1:A:473:ASP:OD1	1:A:474:HIS:N	2.50	0.44
2:B:1034:LYS:HD3	2:B:1034:LYS:HA	1.74	0.44
3:C:587:GLY:O	3:C:590:VAL:HG22	2.16	0.44
4:F:545:ASP:OD1	4:F:545:ASP:N	2.51	0.44
4:F:685:GLU:OE2	5:H:83:LYS:HD3	2.17	0.44
1:A:496:ILE:HG13	1:A:497:TYR:N	2.32	0.44
2:B:718:ASN:HD22	2:B:719:LEU:HD23	1.83	0.44
2:B:785:ASN:HD22	4:E:341:GLU:HB3	1.82	0.44
2:B:1027:GLU:HG3	2:B:1118:PRO:HD2	1.99	0.44
4:E:323:GLU:O	4:E:327:LEU:N	2.50	0.44
4:F:655:GLU:HA	4:F:658:GLU:CD	2.38	0.44
5:H:99:MET:CE	5:H:103:TRP:HE1	2.30	0.44
5:H:325:SER:HB3	5:H:415:LEU:HD22	2.00	0.44
2:B:878:LYS:HG2	2:B:881:ARG:HD3	1.99	0.44
3:C:452:GLU:HA	4:E:334:ARG:NH1	2.32	0.44
4:F:709:GLU:C	4:F:713:LYS:HZ2	2.20	0.44
5:H:418:LEU:HD23	5:H:418:LEU:HA	1.82	0.44
2:B:710:LEU:HD12	2:B:711:SER:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:903:ASN:ND2	2:B:906:GLY:O	2.51	0.44
3:C:571:CYS:HB2	3:C:574:GLU:OE2	2.18	0.44
3:C:651:ASN:HD21	4:D:368:ARG:HH22	1.66	0.44
4:F:527:TRP:HE3	4:F:531:ASP:HB3	1.81	0.44
6:I:115:ASN:O	6:I:119:ASN:ND2	2.51	0.44
2:B:919:SER:O	2:B:923:MET:HG3	2.18	0.44
4:D:343:TYR:HA	4:D:346:TYR:CD2	2.53	0.44
4:G:737:VAL:O	4:G:740:LEU:HG	2.17	0.44
2:B:862:ASP:OD1	2:B:862:ASP:N	2.49	0.44
2:B:1025:PHE:HD1	2:B:1025:PHE:HA	1.67	0.44
2:B:1030:LEU:N	2:B:1120:GLN:OE1	2.51	0.44
4:D:369:ARG:NH2	4:D:370:ASN:HD21	2.16	0.44
4:D:402:LYS:O	4:D:404:ILE:HG23	2.17	0.44
5:H:403:LEU:O	5:H:407:LEU:HG	2.18	0.44
1:A:575:ASN:O	2:B:1135:GLN:NE2	2.51	0.44
5:H:81:SER:HA	5:H:83:LYS:HE2	1.99	0.44
5:H:452:PHE:O	5:H:455:THR:OG1	2.36	0.44
7:J:30:UNK:O	7:J:34:UNK:N	2.51	0.44
2:B:910:PRO:O	2:B:913:LEU:HB3	2.17	0.44
4:G:521:GLU:N	4:G:521:GLU:OE1	2.51	0.44
6:I:138:SER:OG	6:I:139:GLU:N	2.51	0.44
1:A:546:ARG:NH1	5:H:541:ARG:HE	2.15	0.43
1:A:558:SER:O	1:A:559:LEU:HD23	2.17	0.43
1:A:589:HIS:CE1	2:B:1050:GLU:HG2	2.53	0.43
2:B:779:TYR:O	4:E:319:ILE:HG12	2.18	0.43
4:D:402:LYS:HE2	4:D:402:LYS:HB2	1.71	0.43
6:I:75:LYS:HA	9:O:3:UNK:N	2.32	0.43
1:A:566:ASN:OD1	1:A:566:ASN:N	2.51	0.43
2:B:1202:SER:H	2:B:1274:ASN:CB	2.31	0.43
3:C:525:GLN:N	3:C:525:GLN:OE1	2.51	0.43
3:C:548:LEU:HD21	3:C:600:GLN:HG3	1.99	0.43
4:D:308:PRO:HD3	4:D:393:TYR:CD2	2.53	0.43
6:I:79:ASP:O	6:I:83:VAL:HG12	2.18	0.43
2:B:879:ILE:HG22	2:B:880:HIS:N	2.34	0.43
2:B:890:LYS:O	2:B:894:GLU:N	2.32	0.43
3:C:412:TYR:HB2	3:C:420:THR:H	1.83	0.43
3:C:567:ASN:OD1	3:C:569:ASP:N	2.46	0.43
3:C:572:PRO:HD2	3:C:598:ARG:HH22	1.83	0.43
4:E:338:LYS:HA	4:E:338:LYS:HD3	1.78	0.43
4:E:386:THR:OG1	4:E:391:ILE:HD11	2.18	0.43
5:H:344:ASN:OD1	5:H:344:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:483:GLN:O	5:H:487:ILE:HG12	2.18	0.43
1:A:559:LEU:HD12	2:B:916:ASP:OD1	2.18	0.43
2:B:984:HIS:O	2:B:986:LEU:HD12	2.19	0.43
2:B:1148:LEU:HD23	2:B:1148:LEU:HA	1.77	0.43
2:B:1211:ILE:HG21	2:B:1237:ILE:HB	2.00	0.43
4:G:535:LEU:O	4:G:539:ILE:HG23	2.17	0.43
4:G:682:LEU:HA	4:G:685:GLU:CD	2.38	0.43
4:G:726:ARG:HG2	4:G:730:ASN:HD21	1.82	0.43
5:H:513:LYS:HA	5:H:516:ASN:HD22	1.83	0.43
6:I:142:ILE:HA	6:I:145:LEU:HG	1.99	0.43
2:B:777:TYR:CD1	2:B:777:TYR:N	2.86	0.43
2:B:1253:ILE:HG13	2:B:1254:CYS:N	2.33	0.43
3:C:547:LYS:HB2	3:C:560:GLN:NE2	2.33	0.43
3:C:603:MET:O	3:C:607:SER:N	2.26	0.43
3:C:640:ARG:HA	3:C:641:PRO:HD3	1.45	0.43
4:G:743:CYS:HA	4:G:746:LEU:HD12	1.98	0.43
3:C:466:GLN:O	3:C:468:ARG:N	2.47	0.43
4:D:347:ARG:HG3	4:D:348:ASN:N	2.32	0.43
4:D:352:ASN:O	4:D:356:LEU:HG	2.18	0.43
4:E:416:HIS:CE1	7:J:36:UNK:HA	2.53	0.43
5:H:312:PRO:HA	5:H:315:THR:HG22	2.01	0.43
5:H:413:THR:HB	5:H:414:HIS:CE1	2.53	0.43
1:A:503:LEU:O	1:A:507:THR:HG23	2.19	0.43
1:A:522:THR:O	1:A:526:ARG:HG3	2.19	0.43
3:C:411:GLY:O	4:D:415:ARG:NH2	2.45	0.43
3:C:511:ASP:O	3:C:515:GLN:HG2	2.19	0.43
3:C:549:ASP:HB2	3:C:558:ILE:HD13	2.01	0.43
3:C:607:SER:HA	3:C:610:LEU:HG	2.00	0.43
3:C:641:PRO:HB2	3:C:646:LYS:CE	2.49	0.43
5:H:512:VAL:HG13	5:H:513:LYS:N	2.34	0.43
1:A:539:LEU:HD13	4:G:570:ILE:HG21	1.99	0.43
2:B:1023:LEU:HD22	2:B:1111:SER:HB3	1.99	0.43
3:C:447:LYS:HD2	3:C:447:LYS:HA	1.83	0.43
3:C:554:GLN:NE2	3:C:555:ASN:HB2	2.33	0.43
4:D:308:PRO:HG3	4:D:393:TYR:CE1	2.54	0.43
4:D:339:THR:HG22	4:D:342:VAL:HG22	2.00	0.43
4:E:329:GLU:OE2	4:E:380:ARG:NE	2.48	0.43
4:E:415:ARG:NH2	7:J:39:UNK:C	2.82	0.43
4:G:681:PHE:HA	4:G:684:ASN:ND2	2.34	0.43
5:H:388:LEU:HG	5:H:414:HIS:CE1	2.54	0.43
1:A:514:ASP:OD1	1:A:515:LYS:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:415:TYR:OH	3:C:419:ILE:N	2.52	0.43
3:C:435:ARG:NH1	3:C:438:TYR:OH	2.51	0.43
4:E:379:PHE:CZ	4:E:383:LYS:HD3	2.53	0.43
1:A:513:LEU:O	1:A:516:LEU:HG	2.18	0.43
3:C:446:TYR:CD1	3:C:485:LEU:HD22	2.53	0.43
2:B:899:PHE:CE2	5:H:506:LYS:HD2	2.54	0.42
3:C:467:ASP:HA	3:C:470:ARG:NH2	2.34	0.42
4:G:529:LYS:O	4:G:533:GLN:HG3	2.19	0.42
2:B:748:LEU:O	2:B:751:SER:OG	2.33	0.42
2:B:1117:ILE:HB	2:B:1118:PRO:HD3	2.00	0.42
2:B:1295:ILE:H	2:B:1295:ILE:HD12	1.84	0.42
4:E:402:LYS:HA	4:E:402:LYS:HD2	1.88	0.42
5:H:468:GLU:HA	5:H:471:ARG:NH1	2.33	0.42
1:A:559:LEU:HD21	2:B:722:ILE:HD12	2.02	0.42
2:B:711:SER:OG	2:B:712:MET:N	2.51	0.42
2:B:945:LYS:HE3	2:B:945:LYS:HB2	1.82	0.42
2:B:952:LEU:HA	2:B:955:VAL:HG12	2.00	0.42
3:C:541:ASP:OD1	3:C:541:ASP:N	2.52	0.42
4:E:362:PHE:CE1	4:E:366:THR:HB	2.55	0.42
2:B:992:ILE:O	2:B:996:LEU:HD23	2.18	0.42
4:D:420:ARG:O	4:D:420:ARG:HG3	2.19	0.42
1:A:530:LEU:HG	1:A:534:TYR:CE2	2.54	0.42
1:A:546:ARG:NH1	1:A:546:ARG:HB2	2.35	0.42
1:A:592:LEU:O	1:A:596:ARG:HG3	2.18	0.42
3:C:555:ASN:OD1	3:C:654:GLN:N	2.48	0.42
3:C:613:TYR:CZ	3:C:619:ALA:HA	2.55	0.42
4:D:347:ARG:O	4:D:351:VAL:HG12	2.19	0.42
4:E:339:THR:HG23	4:E:342:VAL:H	1.84	0.42
4:F:718:GLN:HE22	4:G:719:GLN:HB2	1.85	0.42
5:H:115:PRO:HG2	5:H:116:HIS:CD2	2.54	0.42
5:H:541:ARG:HG2	5:H:545:PHE:HE2	1.84	0.42
1:A:586:TYR:OH	2:B:1048:SER:HA	2.20	0.42
2:B:1214:ILE:HD13	2:B:1214:ILE:HA	1.90	0.42
3:C:505:THR:OG1	3:C:506:ARG:NH1	2.52	0.42
4:D:311:SER:O	4:D:313:TRP:N	2.49	0.42
5:H:84:ARG:O	5:H:87:HIS:HB2	2.19	0.42
5:H:106:SER:O	5:H:110:GLN:HG2	2.19	0.42
6:I:81:GLU:HB2	6:I:82:ARG:HH12	1.83	0.42
2:B:763:LEU:HD11	2:B:961:ASN:HB2	2.00	0.42
2:B:939:SER:O	2:B:945:LYS:NZ	2.46	0.42
4:D:420:ARG:NH2	10:M:6:UNK:H	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:111:GLU:O	5:H:114:TYR:N	2.47	0.42
2:B:789:VAL:HG12	2:B:790:THR:N	2.28	0.42
2:B:1202:SER:H	2:B:1274:ASN:ND2	2.17	0.42
4:F:726:ARG:CZ	6:I:161:UNK:HA	2.49	0.42
6:I:136:LEU:O	6:I:140:LYS:HG2	2.19	0.42
7:J:34:UNK:O	7:J:35:UNK:C	2.67	0.42
2:B:787:TYR:CE1	4:E:345:ARG:HB3	2.55	0.42
3:C:469:ASP:N	3:C:469:ASP:OD1	2.50	0.42
3:C:584:GLU:HG3	3:C:586:PRO:CD	2.50	0.42
4:F:551:LYS:HA	4:F:551:LYS:HD3	1.62	0.42
5:H:397:SER:HB2	5:H:399:ASP:OD1	2.19	0.42
5:H:450:LEU:HG	5:H:451:LYS:H	1.85	0.42
1:A:479:ILE:HG12	8:K:23:UNK:O	2.20	0.42
2:B:1271:SER:O	2:B:1272:ILE:HD13	2.20	0.42
4:D:414:THR:HG22	4:D:416:HIS:HE1	1.81	0.42
4:G:682:LEU:O	4:G:686:LEU:HG	2.20	0.42
5:H:108:LEU:HD23	5:H:108:LEU:HA	1.90	0.42
5:H:313:GLN:H	5:H:313:GLN:CD	2.22	0.42
5:H:335:TYR:O	5:H:338:LEU:HG	2.19	0.42
6:I:74:ASN:HA	6:I:77:ARG:HH21	1.85	0.42
1:A:531:TYR:HA	1:A:534:TYR:CD2	2.55	0.41
2:B:897:ASP:N	2:B:897:ASP:OD1	2.53	0.41
2:B:990:SER:OG	2:B:991:SER:N	2.52	0.41
2:B:1267:LYS:HB3	4:G:717:ARG:CZ	2.50	0.41
3:C:541:ASP:HA	3:C:543:ARG:HH11	1.85	0.41
4:F:557:SER:H	4:F:560:GLN:CD	2.24	0.41
4:F:702:LYS:HD3	4:F:706:LYS:NZ	2.35	0.41
6:I:102:SER:O	6:I:105:SER:N	2.51	0.41
6:I:144:TYR:HA	6:I:147:GLN:NE2	2.34	0.41
1:A:469:LEU:HA	6:I:128:CYS:SG	2.60	0.41
2:B:1035:TYR:N	2:B:1036:GLN:OE1	2.52	0.41
2:B:1053:ASN:HB3	2:B:1057:PHE:CZ	2.54	0.41
4:E:424:PRO:HG2	4:E:425:PHE:CD2	2.56	0.41
5:H:99:MET:HG3	5:H:103:TRP:CD1	2.55	0.41
6:I:110:ASN:HA	6:I:113:SER:OG	2.20	0.41
2:B:760:LEU:HD11	2:B:951:LEU:HA	2.01	0.41
2:B:876:PRO:O	2:B:877:LEU:HD22	2.20	0.41
3:C:636:ASP:HA	4:D:337:SER:OG	2.20	0.41
4:D:355:ARG:O	4:D:358:PRO:HD3	2.20	0.41
4:F:532:LEU:HA	4:F:535:LEU:HB3	2.02	0.41
4:G:677:ARG:HA	4:G:677:ARG:HD2	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:3:UNK:O	7:J:7:UNK:N	2.54	0.41
3:C:588:GLU:HG3	4:E:370:ASN:HD22	1.85	0.41
3:C:613:TYR:C	3:C:615:PHE:N	2.74	0.41
3:C:653:LEU:HD12	11:N:13:UNK:HA	2.03	0.41
4:F:702:LYS:HD3	4:F:706:LYS:CE	2.50	0.41
6:I:71:GLN:O	6:I:75:LYS:HG3	2.20	0.41
2:B:882:THR:HA	2:B:883:PRO:HD3	1.88	0.41
2:B:896:ASP:OD2	6:I:110:ASN:HB3	2.21	0.41
2:B:1292:ASP:HB2	2:B:1295:ILE:HB	2.02	0.41
4:F:670:ILE:CG2	5:H:508:SER:HB3	2.47	0.41
4:G:526:ASN:O	4:G:527:TRP:HD1	2.02	0.41
5:H:80:ASP:O	5:H:82:GLU:N	2.45	0.41
5:H:311:SER:CB	5:H:414:HIS:HB3	2.51	0.41
7:J:35:UNK:O	7:J:36:UNK:C	2.69	0.41
2:B:798:LYS:O	2:B:802:LYS:N	2.50	0.41
3:C:498:ASP:OD2	4:E:363:SER:HB2	2.21	0.41
4:F:726:ARG:HD3	4:F:726:ARG:HA	1.94	0.41
5:H:406:LEU:O	5:H:410:ILE:N	2.45	0.41
1:A:556:GLN:HG3	2:B:719:LEU:HD22	2.03	0.41
5:H:121:ASN:OD1	5:H:122:VAL:N	2.53	0.41
1:A:564:HIS:HB3	2:B:966:ARG:HH22	1.85	0.41
2:B:878:LYS:HG2	2:B:881:ARG:CZ	2.51	0.41
3:C:466:GLN:H	3:C:466:GLN:CD	2.24	0.41
4:D:320:HIS:HD2	4:D:321:SER:N	2.19	0.41
4:G:571:GLU:OE1	4:G:571:GLU:HA	2.20	0.41
1:A:546:ARG:NH1	5:H:541:ARG:HH11	2.19	0.41
2:B:701:GLU:O	2:B:702:LEU:HD23	2.20	0.41
2:B:785:ASN:HB3	4:E:345:ARG:HH21	1.86	0.41
2:B:890:LYS:HB3	2:B:890:LYS:HE3	1.88	0.41
2:B:905:ARG:HA	2:B:905:ARG:NE	2.36	0.41
2:B:1027:GLU:HG2	2:B:1115:SER:HA	2.03	0.41
2:B:1057:PHE:O	2:B:1061:LEU:HG	2.20	0.41
2:B:1265:ILE:HG13	2:B:1266:LEU:HD22	2.03	0.41
3:C:447:LYS:CD	4:E:328:PRO:HG3	2.51	0.41
3:C:540:ASP:N	3:C:566:SER:OG	2.44	0.41
3:C:606:LYS:O	3:C:609:ALA:HB3	2.21	0.41
4:D:344:MET:HE2	4:D:344:MET:HB2	1.80	0.41
4:F:681:PHE:CZ	5:H:498:ASN:HA	2.56	0.41
4:G:542:PHE:CD2	4:G:548:LYS:HD3	2.56	0.41
5:H:86:ASP:HA	5:H:89:ILE:HG12	2.02	0.41
5:H:109:SER:HA	5:H:112:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:309:SER:O	5:H:415:LEU:HD12	2.21	0.41
5:H:491:LEU:HD23	5:H:491:LEU:HA	1.70	0.41
6:I:142:ILE:HG22	6:I:146:MET:SD	2.61	0.41
1:A:572:ARG:HH22	6:I:95:HIS:N	2.19	0.41
2:B:738:LEU:HD13	2:B:738:LEU:HA	1.95	0.41
2:B:741:SER:OG	2:B:742:LEU:N	2.53	0.41
2:B:883:PRO:O	2:B:886:THR:HG23	2.21	0.41
3:C:438:TYR:HB3	4:E:383:LYS:HZ1	1.86	0.41
3:C:630:LEU:O	3:C:633:ILE:CG1	2.69	0.41
4:D:453:LEU:HD12	4:D:456:TYR:HB2	2.01	0.41
4:E:315:ASN:HB2	4:E:318:LYS:HG2	2.03	0.41
2:B:879:ILE:HG22	2:B:880:HIS:CD2	2.55	0.40
3:C:413:SER:H	3:C:420:THR:HG23	1.85	0.40
4:G:704:LEU:O	4:G:708:MET:HG2	2.21	0.40
1:A:493:ALA:HA	1:A:496:ILE:HG12	2.02	0.40
1:A:522:THR:C	1:A:524:SER:H	2.24	0.40
2:B:1128:ASP:HA	2:B:1131:LEU:HD13	2.03	0.40
4:E:304:GLU:OE1	4:E:304:GLU:N	2.54	0.40
5:H:472:GLU:O	5:H:475:GLN:HB3	2.21	0.40
2:B:707:LEU:HD23	3:C:428:PRO:HA	2.04	0.40
2:B:1086:ARG:HA	2:B:1089:LEU:HG	2.03	0.40
4:D:329:GLU:OE1	4:D:329:GLU:N	2.42	0.40
4:D:407:PRO:C	4:D:408:LEU:HD22	2.41	0.40
4:E:376:ALA:HB1	4:E:380:ARG:HH12	1.86	0.40
5:H:487:ILE:HD13	5:H:487:ILE:HA	1.91	0.40
6:I:123:LEU:HD23	6:I:123:LEU:HA	1.82	0.40
2:B:933:ASN:O	2:B:937:ILE:HG13	2.21	0.40
2:B:1029:GLN:O	2:B:1029:GLN:HG2	2.21	0.40
5:H:472:GLU:O	5:H:476:ILE:HG23	2.21	0.40
6:I:107:LEU:HD13	6:I:107:LEU:HA	1.93	0.40
2:B:755:LEU:O	2:B:759:LEU:HG	2.22	0.40
2:B:874:GLN:HE22	2:B:959:PRO:CD	2.35	0.40
3:C:537:LEU:H	4:D:334:ARG:HH22	1.68	0.40
4:D:406:PRO:CA	4:E:352:ASN:HD21	2.34	0.40
4:F:654:LYS:HE2	4:F:654:LYS:H	1.87	0.40
5:H:377:SER:OG	5:H:403:LEU:HG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	138/1703 (8%)	118 (86%)	20 (14%)	0	100	100
2	B	468/1314 (36%)	364 (78%)	104 (22%)	0	100	100
3	C	241/905 (27%)	176 (73%)	63 (26%)	2 (1%)	19	60
4	D	157/825 (19%)	131 (83%)	26 (17%)	0	100	100
4	E	137/825 (17%)	113 (82%)	24 (18%)	0	100	100
4	F	215/825 (26%)	186 (86%)	27 (13%)	2 (1%)	17	56
4	G	189/825 (23%)	164 (87%)	24 (13%)	1 (0%)	29	68
5	H	249/566 (44%)	217 (87%)	32 (13%)	0	100	100
6	I	78/179 (44%)	67 (86%)	11 (14%)	0	100	100
All	All	1872/7967 (24%)	1536 (82%)	331 (18%)	5 (0%)	44	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	606	PRO
3	C	614	ASN
4	G	572	ASP
4	F	648	LYS
3	C	612	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	129/1520 (8%)	129 (100%)	0	100	100
2	B	460/1218 (38%)	458 (100%)	2 (0%)	91	94
3	C	222/823 (27%)	219 (99%)	3 (1%)	67	81
4	D	150/751 (20%)	150 (100%)	0	100	100
4	E	129/751 (17%)	128 (99%)	1 (1%)	81	89
4	F	138/751 (18%)	138 (100%)	0	100	100
4	G	127/751 (17%)	125 (98%)	2 (2%)	62	79
5	H	239/517 (46%)	238 (100%)	1 (0%)	91	94
6	I	79/133 (59%)	78 (99%)	1 (1%)	69	82
All	All	1673/7215 (23%)	1663 (99%)	10 (1%)	86	92

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	772	ARG
2	B	941	ASN
3	C	500	ARG
3	C	543	ARG
3	C	633	ILE
4	E	420	ARG
4	G	571	GLU
4	G	706	LYS
5	H	562	SER
6	I	143	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	460	HIS
1	A	510	ASN
1	A	528	ASN
1	A	564	HIS
1	A	588	ASN
2	B	718	ASN
2	B	791	GLN
2	B	874	GLN
2	B	880	HIS
2	B	915	ASN
2	B	984	HIS

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Mol	Chain	Res	Type
2	B	1006	GLN
2	B	1026	ASN
2	B	1053	ASN
2	B	1093	ASN
2	B	1104	ASN
2	B	1215	ASN
2	B	1243	GLN
2	B	1274	ASN
2	B	1298	GLN
2	B	1300	GLN
2	B	1304	ASN
3	C	437	HIS
3	C	448	GLN
3	C	466	GLN
3	C	508	GLN
3	C	556	GLN
3	C	595	HIS
3	C	614	ASN
4	D	348	ASN
4	D	394	GLN
4	D	416	HIS
4	E	352	ASN
4	E	357	ASN
4	E	394	GLN
4	E	411	GLN
4	E	433	GLN
4	F	552	ASN
4	F	567	GLN
4	F	718	GLN
4	F	728	ASN
4	F	738	ASN
4	G	526	ASN
4	G	533	GLN
4	G	555	ASN
4	G	567	GLN
4	G	699	ASN
4	G	725	GLN
4	G	730	ASN
4	G	745	ASN
5	H	76	GLN
5	H	102	GLN
5	H	118	ASN

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Mol	Chain	Res	Type
5	H	313	GLN
5	H	326	HIS
5	H	469	ASN
5	H	493	ASN
5	H	516	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	I	1
10	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	150:HIS	C	152:UNK	N	20.17

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	22:UNK	C	24:UNK	N	7.86

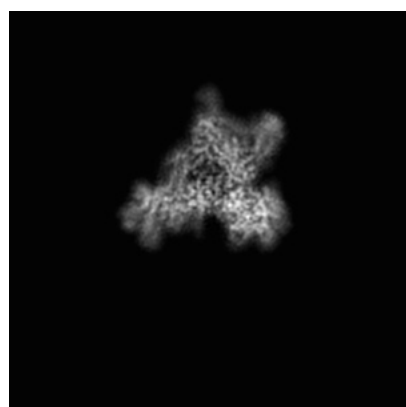
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20933. These allow visual inspection of the internal detail of the map and identification of artifacts.

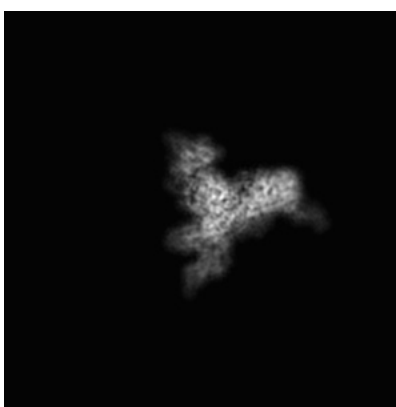
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

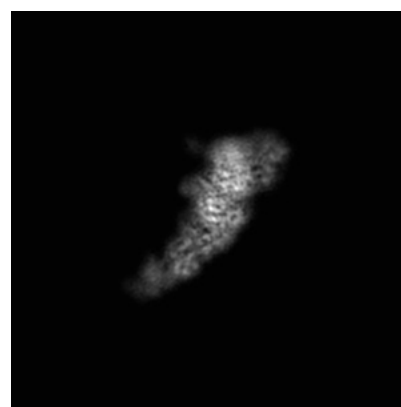
6.1.1 Primary map



X



Y

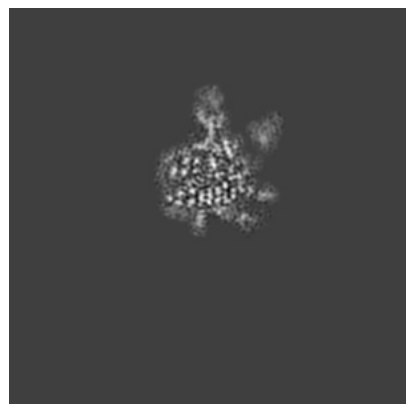


Z

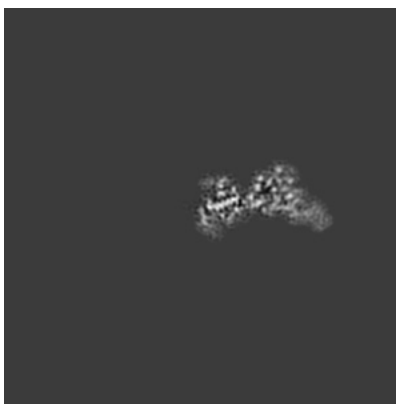
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

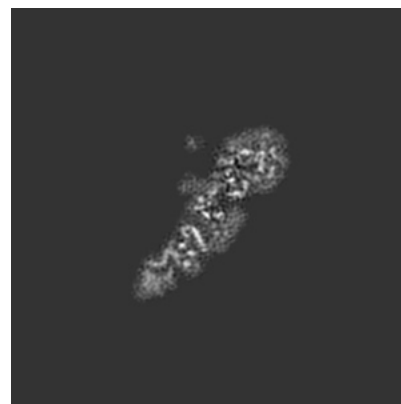
6.2.1 Primary map



X Index: 192



Y Index: 192

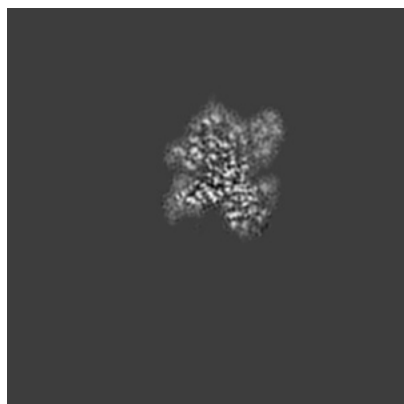


Z Index: 192

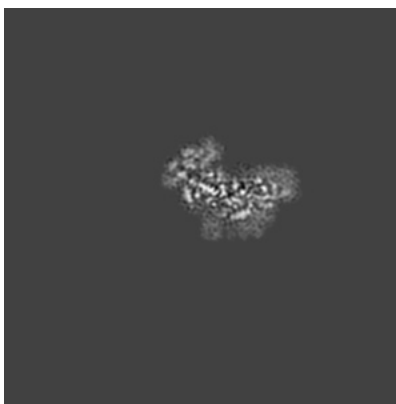
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 204



Y Index: 218

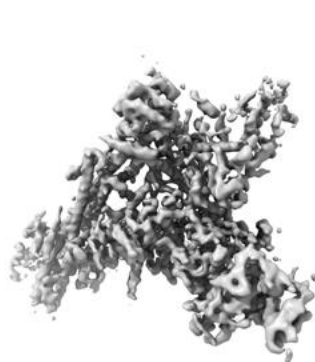


Z Index: 197

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

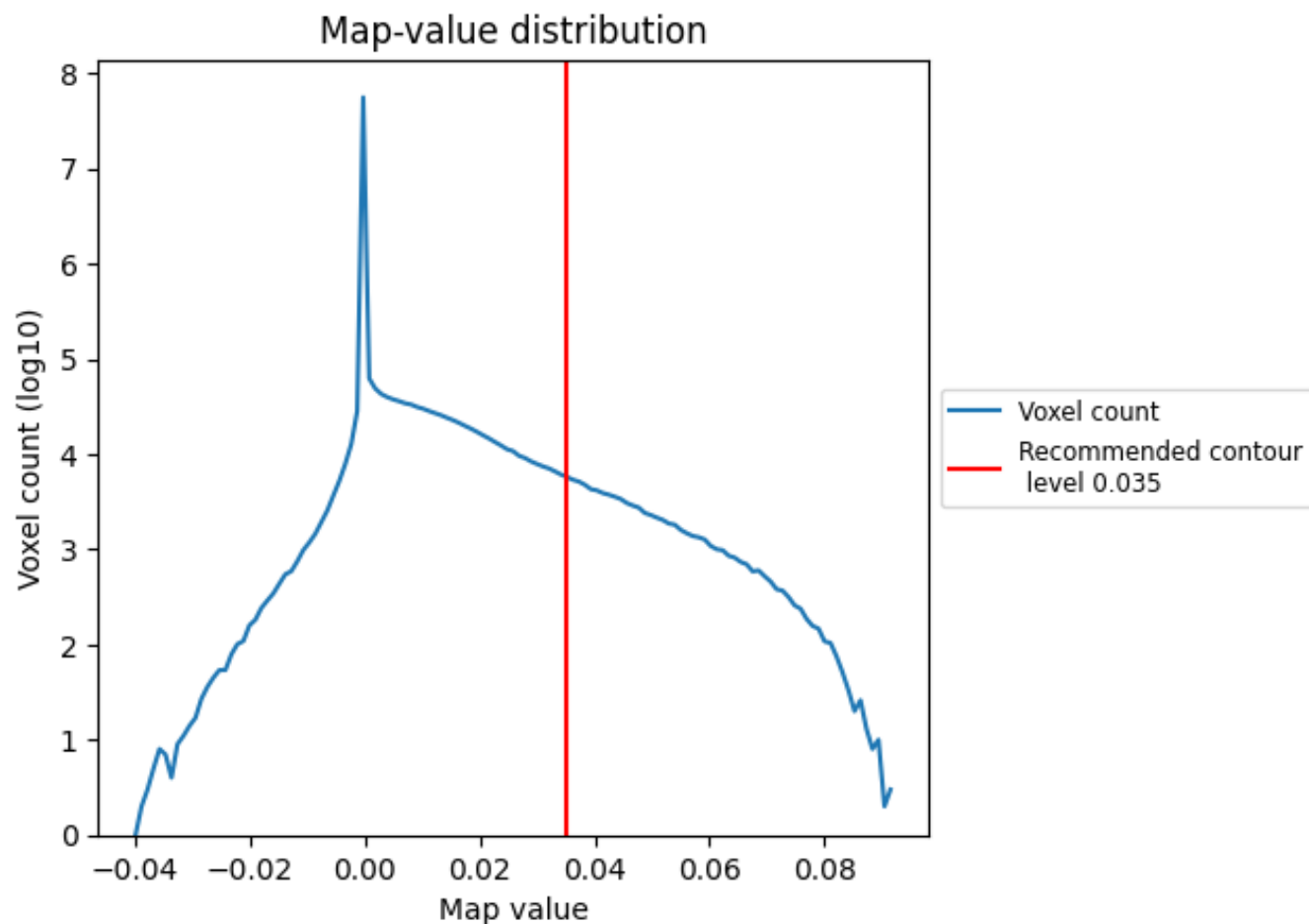
6.5 Mask visualisation

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

7 Map analysis [i](#)

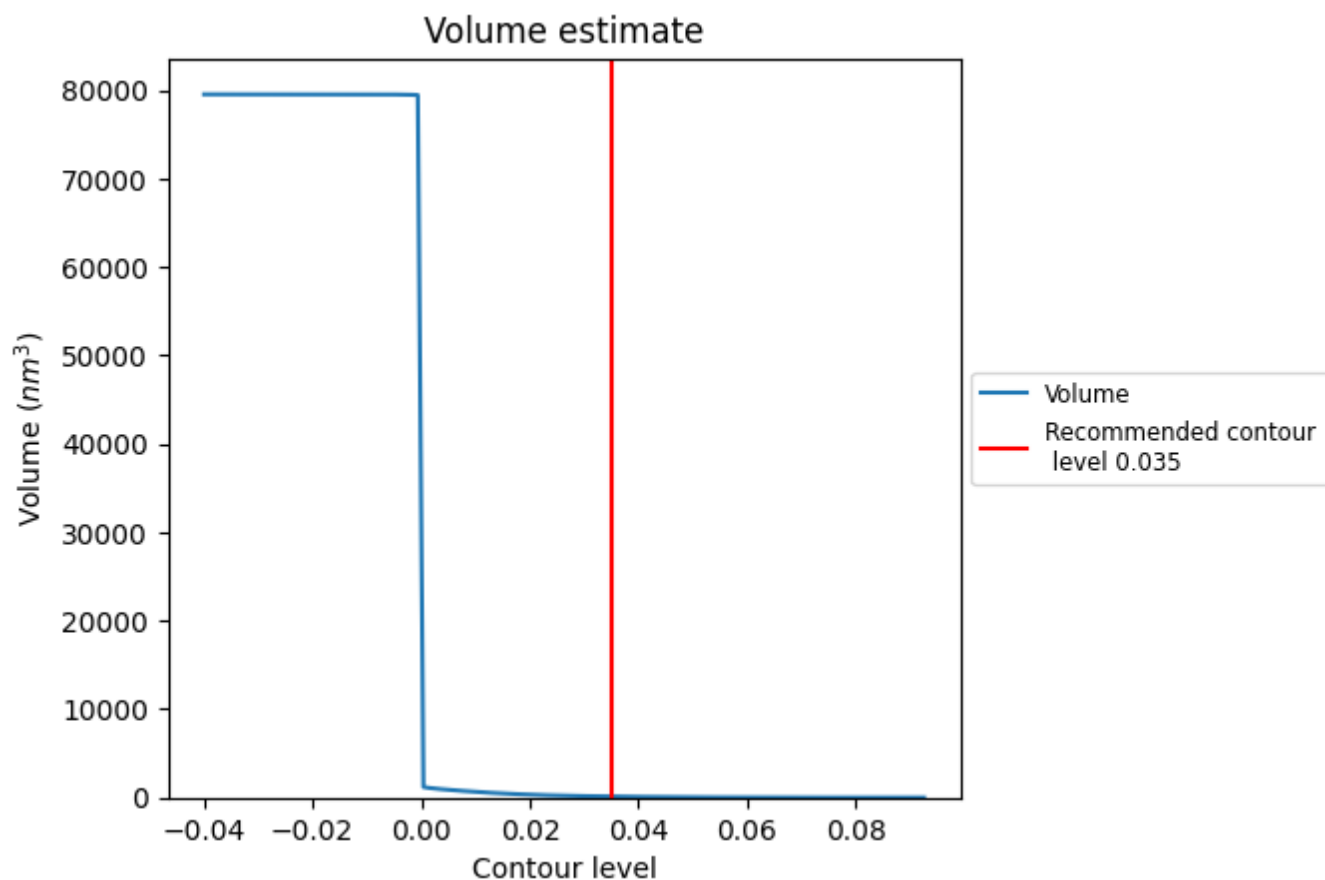
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

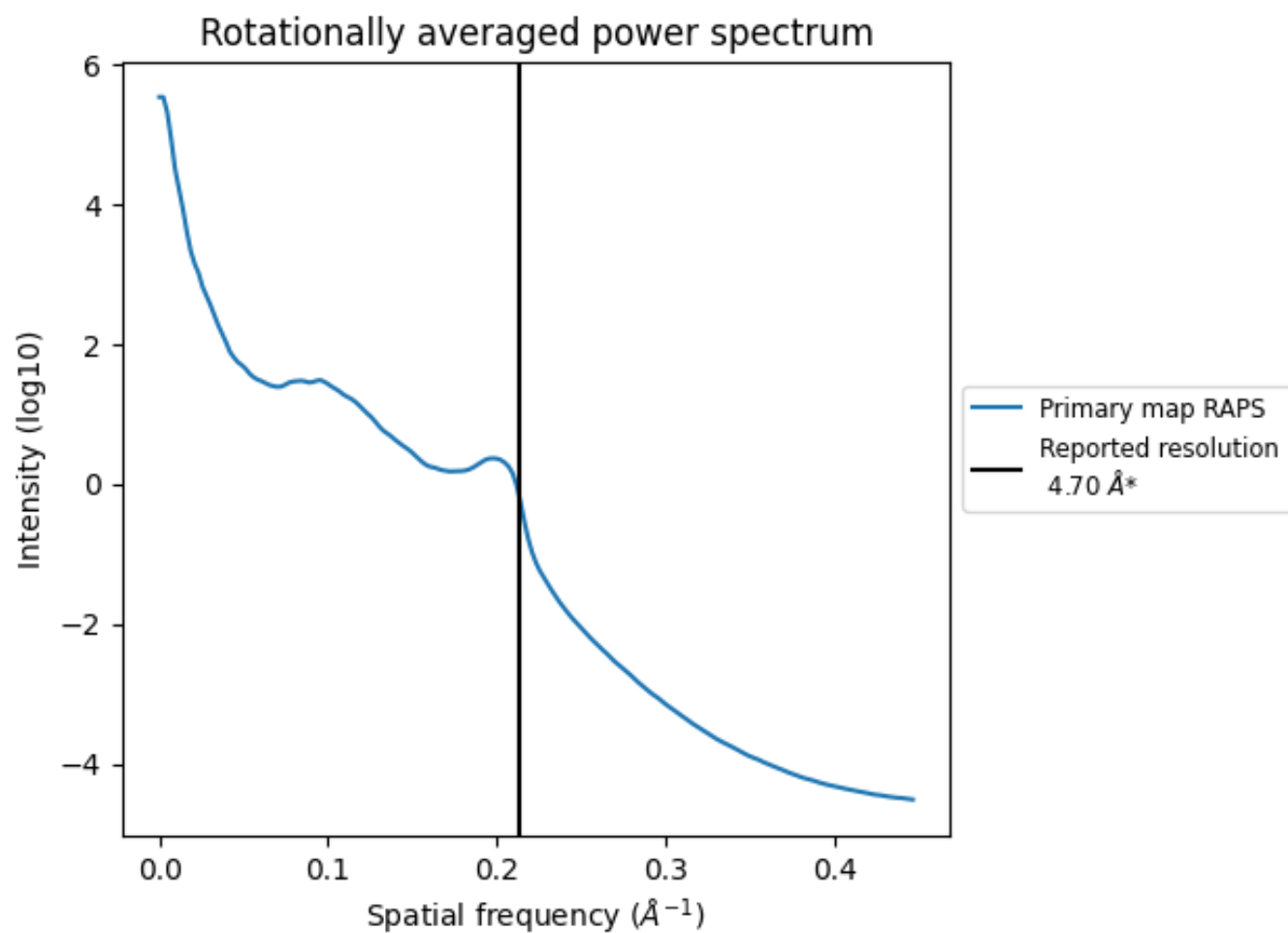
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 118 nm³; this corresponds to an approximate mass of 107 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 ⓘ

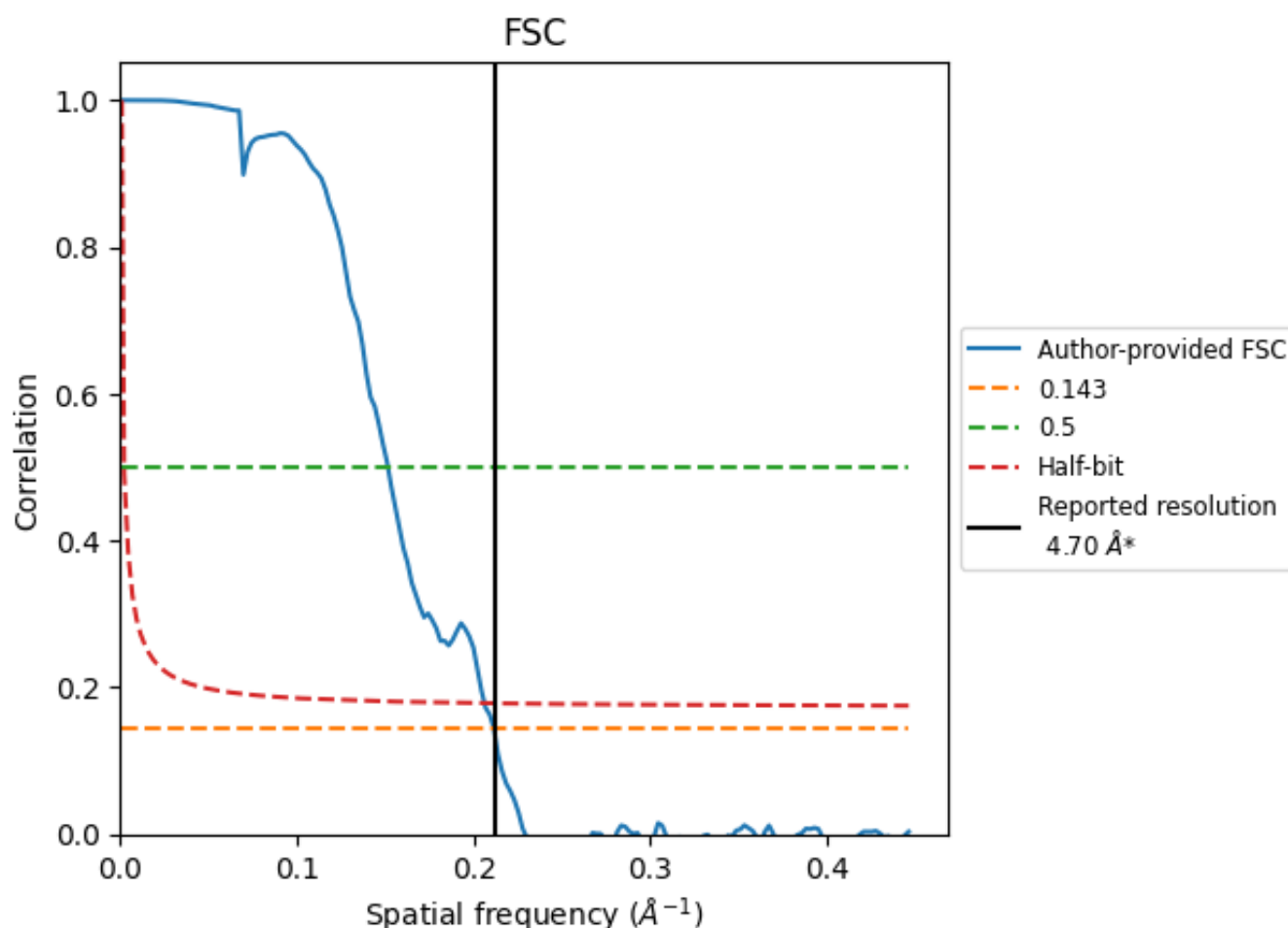


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

8.2 Resolution estimates [i](#)

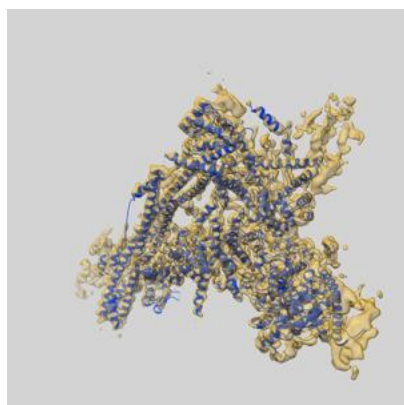
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.73	6.60	4.85
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

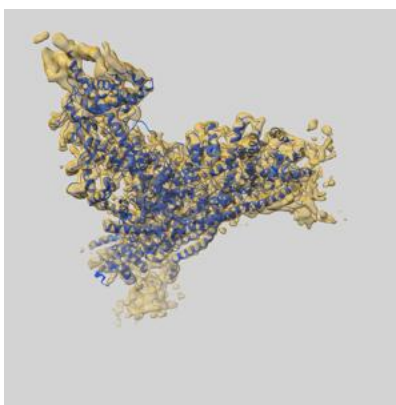
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20933 and PDB model 6UXV. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

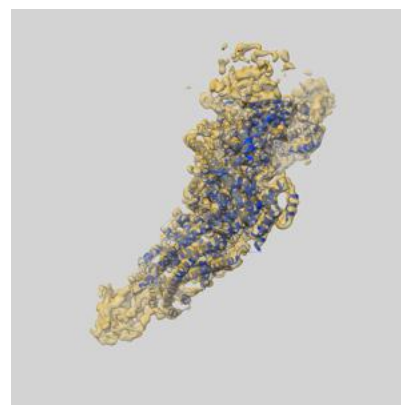
9.1 Map-model overlay [i](#)



X



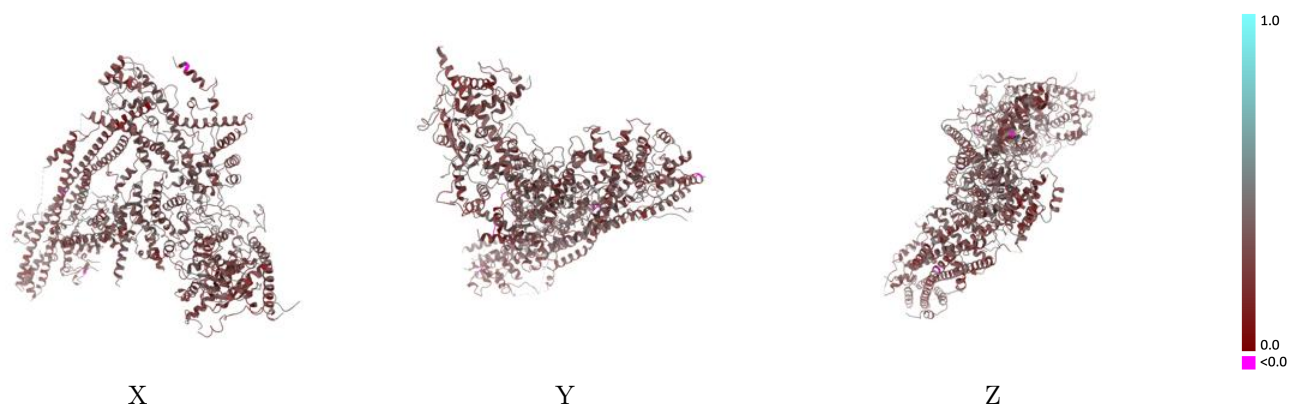
Y



Z

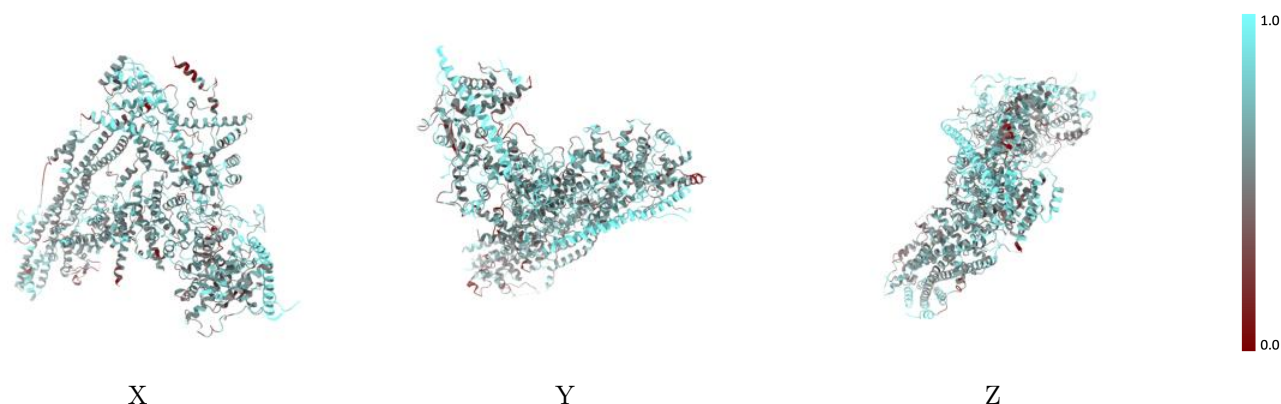
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



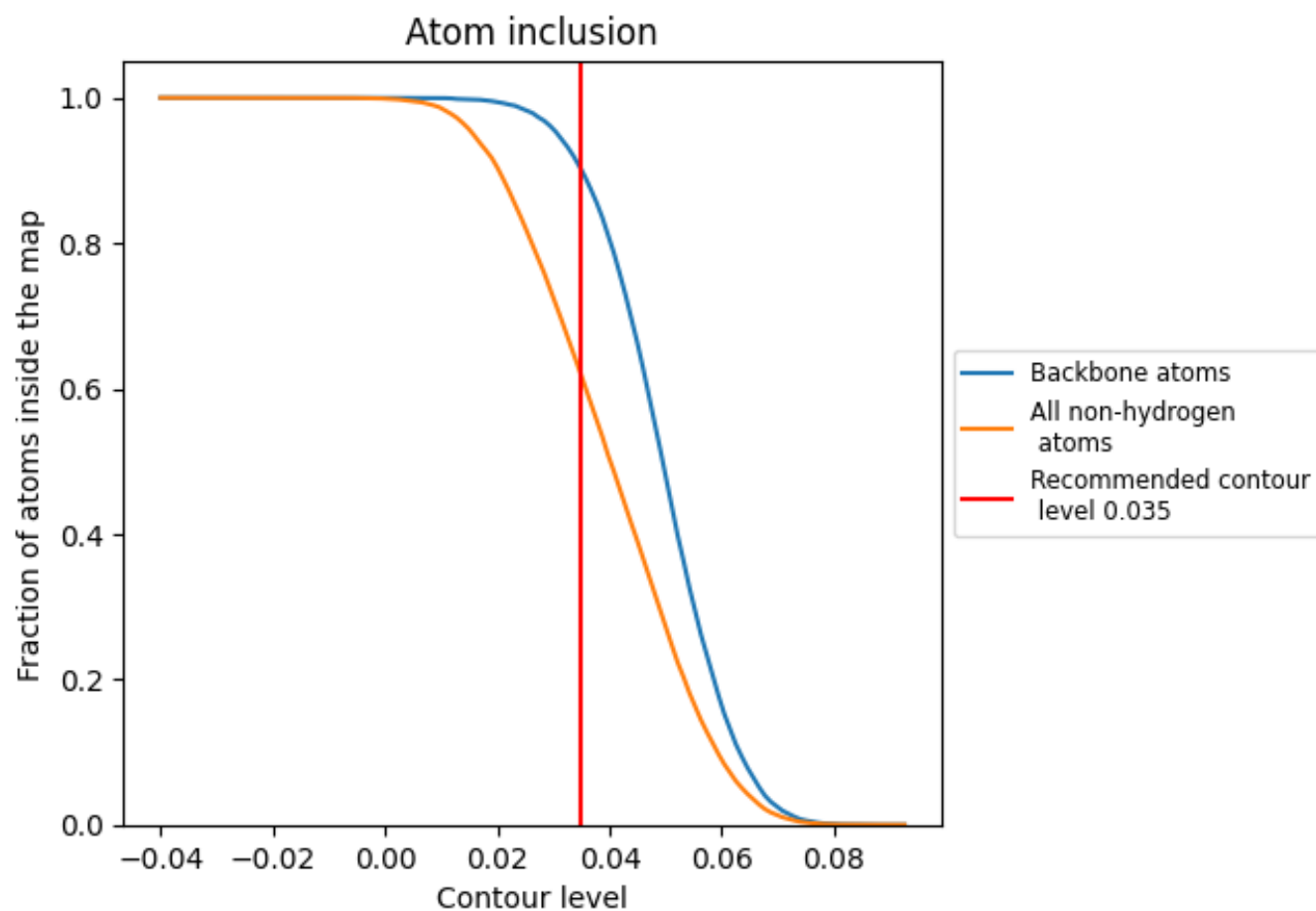
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 62% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6173	 0.3220
A	 0.6270	 0.3330
B	 0.5991	 0.3360
C	 0.5545	 0.3140
D	 0.5775	 0.3070
E	 0.6415	 0.3420
F	 0.6224	 0.2950
G	 0.6533	 0.3150
H	 0.5501	 0.2930
I	 0.6317	 0.3310
J	 0.9167	 0.3710
K	 0.8652	 0.4030
L	 0.7582	 0.2930
M	 0.8654	 0.3650
N	 0.8742	 0.4630
O	 0.4396	 0.1680

