



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:06 AM UTC

PDB ID : 8AUW / pdb_00008auw
EMDB ID : EMD-15675
Title : Cryo-EM structure of human BIRC6 in complex with SMAC.
Authors : Ehrmann, J.F.; Grabarczyk, D.B.; Clausen, T.
Deposited on : 2022-08-25
Resolution : 7.20 Å (reported)
Based on initial models : 8ATU, 1G73

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

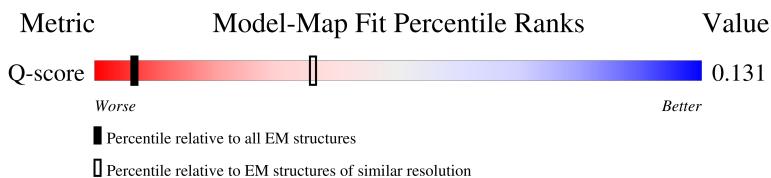
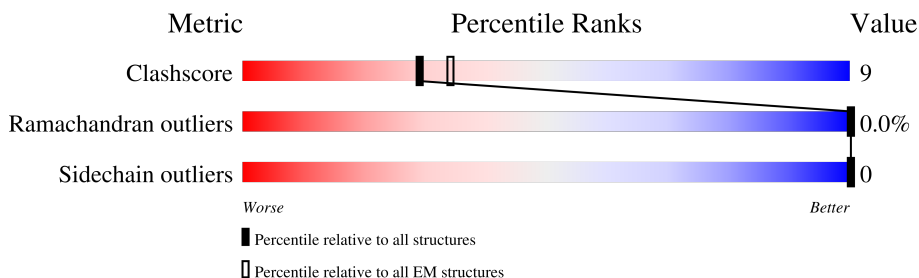
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.20 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	444 (6.70 - 7.70)

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	4867	
1	B	4867	
2	C	184	
2	D	184	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 46869 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 Baculoviral IAP repeat-containing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2900	Total	C	N	O	S	0	0
			22469	14359	3812	4146	152		
1	B	2830	Total	C	N	O	S	0	0
			21887	13991	3697	4048	151		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1332	VAL	LEU	conflict	UNP Q9NR09
A	4858	SER	-	expression tag	UNP Q9NR09
A	4859	ALA	-	expression tag	UNP Q9NR09
A	4860	TRP	-	expression tag	UNP Q9NR09
A	4861	SER	-	expression tag	UNP Q9NR09
A	4862	HIS	-	expression tag	UNP Q9NR09
A	4863	PRO	-	expression tag	UNP Q9NR09
A	4864	GLN	-	expression tag	UNP Q9NR09
A	4865	PHE	-	expression tag	UNP Q9NR09
A	4866	GLU	-	expression tag	UNP Q9NR09
A	4867	LYS	-	expression tag	UNP Q9NR09
B	1332	VAL	LEU	conflict	UNP Q9NR09
B	4858	SER	-	expression tag	UNP Q9NR09
B	4859	ALA	-	expression tag	UNP Q9NR09
B	4860	TRP	-	expression tag	UNP Q9NR09
B	4861	SER	-	expression tag	UNP Q9NR09
B	4862	HIS	-	expression tag	UNP Q9NR09
B	4863	PRO	-	expression tag	UNP Q9NR09
B	4864	GLN	-	expression tag	UNP Q9NR09
B	4865	PHE	-	expression tag	UNP Q9NR09
B	4866	GLU	-	expression tag	UNP Q9NR09
B	4867	LYS	-	expression tag	UNP Q9NR09

- Molecule 2 is a protein called Diablo IAP-binding mitochondrial protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	161	Total	C	N	O	S	0	0
			1269	792	214	258	5		
2	D	157	Total	C	N	O	S	0	0
			1242	773	210	254	5		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	





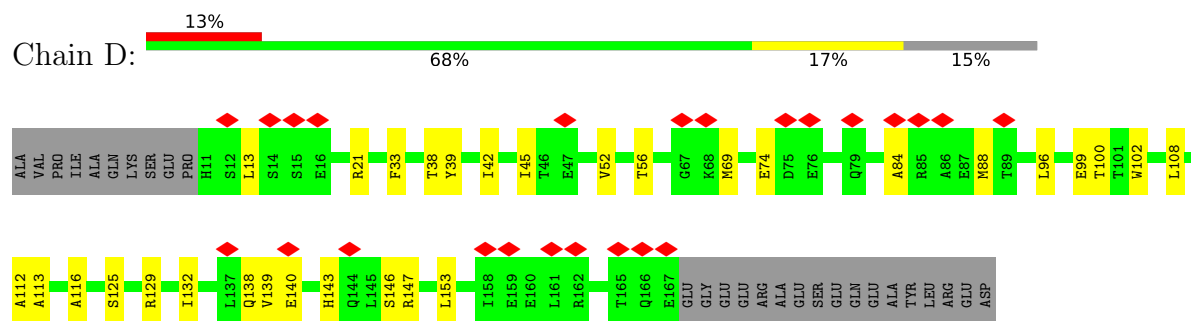








LYS	THR	GLN	L4158	T4228	GLY	L4356	ASN	D4480	ARG	TYR	GLY	THR	TYR	GLY	THR	GLN	ASP	HIS
ILE	ASP	VAL	A4159	D4229	PHE	P4357	GLY	I4481	CYS	ASN	GLU	ASP	THR	ASN	ASP	GLN	GLY	ASP
GLY	SER	SER	A4160	D4230	THR	S4358	GLU	Q4482	ASP	GLY	VAL	SER	THR	GLY	SER	THR	ILE	GLN
THR	TYR	ALA	F4161	Q4231	GLY	V4359	GLU	Q4483	GLY	GLU	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY
SER	LYS	PRO	L4167	V4232	SER	L4360	GLU	T4484	ARG	GLU	ASP	GLU	ASP	GLY	GLY	GLY	GLY	GLY
GLY	ARG	VAL	P4168	L4233	THR	L4361	GLN	A4485	LEU	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	LEU	VAL	L4173	L4234	ALA	E4362	SER	E4486	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	PRO	SER	V4174	R4235	GLY	L4363	GLY	I4487	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ASN	GLU	THR	L4175	R4236	TRP	L4364	CYS	V4488	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
LYS	ASP	THR	L4176	M4237	ASP	S4365	VAL	Y4489	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ILE	HIS	GLU	L4177	A4238	GLU	Q4366	GLU	A4490	THR	PHE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
		LYS	E4177	L4239	GLN	S4367	ALA	T4491	GLY	LYS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
		PRO	R4178	E4240	ALA	C4368	ALA	T4492	GLY	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
		ASP	K4179	I4241	LEU	L4369	LEU	T4493	LYS	THR	THR	THR	THR	THR	THR	THR	THR	THR
		LYS	H4180	L4247	LYS	I4370	LYS	S4494	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		ASP	A4181	L4248	GLN	P4371	GLN	R4495	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
		GLN	Q4182	V4249	THR	M4372	THR	T4496	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		PHE	L4185	S4252	GLY	M4373	THR	R4496	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		TRP	R4186	H4255	ASN	S4374	THR	A4497	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		GLU	L4187	H4256	ASN	S4375	THR	T4498	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		VAL	S4188	H4257	ASN	Y4376	THR	S4499	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		THR	G4190	H4258	ASN	L4377	THR	V4444	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		ILE	VAL	H4259	ASN	R4378	THR	D4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		GLY	THR	S4258	ASN	M4379	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		ASP	ASP	P4259	ASN	ASP	THR	R4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		LEU	ASP	R4260	ASN	VAL	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		CYS	GLY	V4261	ASN	GLY	THR	D4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		MET	GLY	P4262	ASN	ASP	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		ASP	ILE	S4262	ASN	MET	THR	R4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		GLY	SER	H4262	ASN	ALA	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		PRO	ILE	S4262	ASN	ARG	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		ALA	LEU	S4262	ASN	HIS	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		THR	LEU	S4262	ASN	THR	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		GLU	THR	S4262	ASN	VAL	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		THR	THR	S4262	ASN	GLY	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		VAL	THR	S4262	ASN	ASP	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		ALA	THR	S4262	ASN	MET	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		GLU	THR	S4262	ASN	ALA	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		PRO	THR	S4262	ASN	ARG	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		THR	THR	S4262	ASN	LYS	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		ALA	THR	S4262	ASN	THR	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
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		THR	THR	S4262	ASN	GLY	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
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		GLU	THR	S4262	ASN	ALA	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		PRO	THR	S4262	ASN	ARG	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		THR	THR	S4262	ASN	LYS	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		ALA	THR	S4262	ASN	THR	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		GLU	THR	S4262	ASN	VAL	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		THR	THR	S4262	ASN	GLY	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		VAL	THR	S4262	ASN	ASP	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		ALA	THR	S4262	ASN	MET	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		GLU	THR	S4262	ASN	ALA	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		PRO	THR	S4262	ASN	ARG	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		THR	THR	S4262	ASN	LYS	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		ALA	THR	S4262	ASN	THR	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
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		THR	THR	S4262	ASN	GLY	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		VAL	THR	S4262	ASN	ASP	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		ALA	THR	S4262	ASN	MET	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
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		THR	THR	S4262	ASN	LYS	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		ALA	THR	S4262	ASN	THR	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		GLU	THR	S4262	ASN	VAL	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		THR	THR	S4262	ASN	GLY	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		VAL	THR	S4262	ASN	ASP	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		ALA	THR	S4262	ASN	MET	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
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		ALA	THR	S4262	ASN	THR	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		GLU	THR	S4262	ASN	VAL	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		THR	THR	S4262	ASN	GLY	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
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		THR	THR	S4262	ASN	LYS	THR	T4445	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR
		ALA	THR	S4262	ASN	THR	THR	T4445	GLY	THR	THR	THR	THR					



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	56954	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.027	Depositor
Minimum map value	-0.013	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	426.9999, 426.9999, 426.9999	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.423333, 1.423333, 1.423333	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	A	0.24	0/22884	0.57	4/31066 (0.0%)
1	B	0.24	0/22298	0.57	2/30292 (0.0%)
2	C	0.25	0/1284	0.60	0/1737
2	D	0.26	0/1257	0.56	0/1700
All	All	0.24	0/47723	0.57	6/64795 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	MET	CA-CB-CG	6.02	126.15	114.10
1	A	279	ASP	CB-CA-C	5.71	120.31	110.77
1	A	2586	MET	CB-CG-SD	5.61	129.53	112.70
1	B	3488	MET	CA-CB-CG	5.23	124.56	114.10
1	A	279	ASP	CA-CB-CG	5.16	117.75	112.60
1	B	3488	MET	CB-CG-SD	5.02	127.77	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	22469	0	22943	422	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	21887	0	22291	437	0
2	C	1269	0	1270	22	0
2	D	1242	0	1236	22	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	46869	0	47740	875	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (875) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1027:GLU:HA	1:B:1030:ARG:HE	1.46	0.81
1:B:3217:ALA:HA	1:B:3275:ALA:O	1.83	0.79
1:B:1378:LEU:HB3	1:B:1382:ARG:HH21	1.50	0.76
1:A:2817:HIS:HB2	1:A:2859:VAL:HG12	1.68	0.75
1:B:3821:LYS:HD3	1:B:3859:HIS:HB3	1.70	0.74
1:A:157:GLN:HB3	1:A:226:HIS:HB3	1.69	0.73
1:B:1510:LEU:HB3	1:B:1560:LEU:HB2	1.71	0.73
1:A:1806:ILE:HB	1:A:1842:LEU:HB3	1.71	0.73
1:A:1378:LEU:HB3	1:A:1382:ARG:HH21	1.55	0.72
1:B:1806:ILE:HB	1:B:1842:LEU:HB3	1.72	0.71
2:C:26:VAL:HG21	2:D:33:PHE:HB2	1.73	0.71
1:B:1124:LEU:HB3	1:B:1183:CYS:HB3	1.71	0.71
1:B:1776:GLN:HG2	1:B:1875:LEU:HD13	1.71	0.70
2:C:129:ARG:HA	2:C:132:ILE:HD12	1.73	0.70
1:A:829:LYS:HB2	1:A:844:ILE:HD11	1.71	0.70
1:B:3462:ARG:HG3	1:B:3524:LEU:HD21	1.72	0.69
1:A:1557:LEU:HD12	1:A:1560:LEU:HD21	1.73	0.69
1:A:2387:LEU:HD11	1:A:2408:LEU:HD21	1.75	0.69
1:B:1782:ARG:O	1:B:1789:ARG:NH2	2.26	0.69
2:C:31:SER:OG	2:C:131:HIS:ND1	2.25	0.69
1:A:1475:THR:HB	1:A:1479:ARG:HH21	1.58	0.68
1:B:3824:MET:HE1	1:B:4004:LEU:HD12	1.75	0.68
1:B:1557:LEU:HD12	1:B:1560:LEU:HD21	1.75	0.68
1:B:3057:ILE:HG22	1:B:3061:MET:HE1	1.75	0.68
1:B:290:ARG:HH22	1:B:417:LEU:HB2	1.59	0.67
1:A:75:TYR:HB2	1:A:944:ILE:HD12	1.76	0.67
1:A:2389:GLY:HA2	1:A:2655:VAL:HA	1.75	0.67
1:A:3251:LEU:HD22	1:B:2721:LEU:HD21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:ASP:HA	1:A:907:THR:HB	1.77	0.67
1:B:254:SER:HB2	1:B:370:VAL:HG11	1.77	0.67
1:B:1811:ASP:O	1:B:1863:ARG:NH1	2.28	0.67
1:A:3233:ALA:HB2	1:B:3232:LEU:HD21	1.75	0.67
1:A:2165:ILE:HG13	1:A:2166:PRO:HD3	1.75	0.66
1:B:2126:GLN:OE1	1:B:2127:ARG:NH1	2.29	0.66
1:A:2387:LEU:O	1:A:2393:ASN:ND2	2.27	0.66
1:B:75:TYR:HB2	1:B:944:ILE:HD12	1.77	0.66
1:A:250:PRO:HD3	1:A:362:HIS:HB3	1.78	0.66
1:A:1782:ARG:O	1:A:1789:ARG:NH2	2.28	0.66
1:B:1390:ARG:HD2	1:B:2005:LEU:HD11	1.76	0.66
1:A:825:LEU:HB2	1:A:847:GLN:HB3	1.77	0.66
1:B:157:GLN:HB3	1:B:226:HIS:HB3	1.76	0.66
1:B:1821:THR:OG1	1:B:1892:LYS:NZ	2.29	0.65
1:B:1475:THR:HB	1:B:1479:ARG:HH21	1.62	0.65
1:B:568:LEU:HD11	1:B:630:LEU:HB3	1.78	0.64
1:B:1557:LEU:HB3	1:B:1560:LEU:HD11	1.80	0.64
1:A:1813:ALA:HB2	1:A:1863:ARG:HA	1.79	0.64
1:A:2031:LEU:HD21	1:A:2074:ILE:HD11	1.79	0.64
1:A:4377:LEU:HD22	1:A:4440:MET:HE1	1.80	0.64
1:B:3688:ARG:HH22	1:B:3762:ALA:HA	1.62	0.64
1:A:4260:ARG:NH2	1:A:4364:LEU:O	2.30	0.64
1:A:1492:LEU:HD23	1:A:1498:LEU:HD23	1.80	0.63
1:A:93:VAL:O	1:A:102:LEU:N	2.31	0.63
1:A:1436:MET:HE3	1:A:1469:ALA:HB1	1.80	0.63
1:B:98:SER:OG	1:B:212:LYS:NZ	2.30	0.63
1:B:2146:LEU:HG	1:B:2334:LYS:HE2	1.79	0.63
1:A:1556:SER:HB2	1:A:1843:ILE:HG21	1.80	0.63
1:B:1966:GLU:OE1	1:B:1969:ARG:NH2	2.31	0.63
1:A:3202:LEU:O	1:A:3284:ARG:NH1	2.30	0.63
1:B:2381:GLU:OE2	1:B:2645:LYS:NZ	2.31	0.63
1:B:2416:LEU:HD11	1:B:2670:ASN:HD21	1.63	0.63
1:B:2374:ILE:HG22	1:B:2375:VAL:HG13	1.82	0.62
1:A:417:LEU:HD23	1:A:419:LYS:HE3	1.80	0.62
1:A:343:GLU:HG2	1:A:346:SER:H	1.64	0.62
1:A:1927:ARG:HE	1:A:1930:LEU:HD21	1.64	0.62
1:A:2256:MET:HE1	1:A:2271:LEU:HB3	1.82	0.62
1:A:3180:GLU:O	1:A:3184:GLN:NE2	2.32	0.62
1:B:2927:ASN:HB2	1:B:3039:ILE:HG22	1.81	0.62
1:A:4441:LYS:HE3	1:A:4482:GLN:HG2	1.82	0.62
1:B:4260:ARG:NH2	1:B:4364:LEU:O	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:GLU:HG2	1:B:346:SER:H	1.65	0.62
1:B:2817:HIS:HB2	1:B:2859:VAL:HG12	1.81	0.62
1:A:3433:ASP:O	1:A:3437:GLN:NE2	2.33	0.61
1:B:2687:ASN:HB3	1:B:2690:ARG:HG3	1.82	0.61
1:A:3111:MET:HE3	1:A:3330:TRP:HB2	1.82	0.61
1:B:1101:VAL:HA	1:B:1305:ARG:HE	1.65	0.61
1:B:1486:THR:OG1	1:B:1489:GLU:OE1	2.18	0.61
1:B:2787:GLN:NE2	1:B:2791:GLU:OE2	2.34	0.61
1:B:417:LEU:HD23	1:B:419:LYS:HE3	1.81	0.61
1:B:1015:GLN:HG3	1:B:1021:ILE:HD13	1.83	0.61
1:B:2692:PRO:HG2	1:B:2732:MET:HE2	1.81	0.61
1:A:356:PRO:HB2	1:A:363:THR:HG22	1.82	0.61
1:B:1493:GLN:HG2	1:B:1499:TYR:HA	1.82	0.61
1:A:1853:CYS:SG	1:A:1854:ARG:N	2.74	0.60
1:A:3396:LEU:HA	1:A:3399:ILE:HG12	1.83	0.60
1:B:3220:LEU:HD23	1:B:3275:ALA:HB3	1.81	0.60
1:A:568:LEU:HD11	1:A:630:LEU:HB3	1.81	0.60
1:B:2753:VAL:HA	1:B:2758:LEU:HD13	1.82	0.60
1:B:3123:ARG:NH2	1:B:3303:ALA:O	2.34	0.60
1:B:3180:GLU:O	1:B:3184:GLN:NE2	2.33	0.60
1:B:1770:LEU:HD13	1:B:1986:LEU:HD11	1.84	0.60
1:A:55:TRP:HB3	1:A:924:ALA:HB2	1.84	0.60
1:B:1776:GLN:HE21	1:B:1875:LEU:HB2	1.66	0.60
1:B:1819:ILE:HG22	1:B:1856:MET:HG3	1.83	0.60
1:B:2837:VAL:HG12	1:B:2918:LEU:HD13	1.83	0.60
1:A:2121:LEU:HD23	1:A:2124:ILE:HD11	1.84	0.60
1:A:1026:VAL:HG21	1:A:1351:LEU:HD22	1.84	0.60
1:A:2039:HIS:HB2	1:A:2597:ALA:HB2	1.82	0.60
1:A:3118:ILE:HG23	1:B:2344:PHE:HE1	1.66	0.60
1:B:1504:ASP:O	1:B:1981:GLN:NE2	2.34	0.60
1:A:2264:ASN:OD1	2:D:39:TYR:OH	2.19	0.60
1:A:1037:ARG:HH22	1:A:1075:ARG:HB3	1.67	0.60
1:B:1091:PHE:HB2	1:B:1222:ILE:HB	1.82	0.60
1:B:1104:VAL:HG22	1:B:1303:ILE:HD12	1.84	0.59
1:A:3184:GLN:HB2	1:A:3187:PRO:HG3	1.84	0.59
1:B:1398:ARG:NH2	1:B:1846:ASP:OD1	2.36	0.59
1:B:287:ALA:HA	1:B:290:ARG:HE	1.66	0.59
1:B:1436:MET:HE2	1:B:1469:ALA:HB1	1.85	0.59
1:B:1556:SER:HB2	1:B:1843:ILE:HG21	1.84	0.59
1:B:3693:VAL:HG23	1:B:3699:MET:HE3	1.84	0.59
1:B:3279:CYS:SG	1:B:3281:ARG:NH1	2.76	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:TRP:HB3	1:B:924:ALA:HB2	1.84	0.59
1:B:115:VAL:HA	1:B:129:VAL:O	2.02	0.59
1:B:3810:ARG:HA	1:B:3813:LEU:HD12	1.84	0.59
1:B:123:VAL:O	1:B:125:LYS:NZ	2.33	0.59
1:B:1813:ALA:HB2	1:B:1863:ARG:HA	1.85	0.59
1:B:3636:VAL:HG13	1:B:3711:LEU:HD12	1.83	0.59
1:A:3236:PRO:O	1:A:3259:THR:OG1	2.21	0.59
1:A:2038:LEU:HD21	1:A:2085:LEU:HD13	1.84	0.58
1:A:2275:GLN:HG2	1:A:2279:LYS:HE3	1.85	0.58
1:B:2121:LEU:HD23	1:B:2124:ILE:HD11	1.83	0.58
1:A:1015:GLN:HG3	1:A:1021:ILE:HG21	1.85	0.58
1:A:2143:ASP:O	1:A:2334:LYS:NZ	2.34	0.58
1:A:1504:ASP:O	1:A:1981:GLN:NE2	2.37	0.58
1:A:1119:GLN:HG3	1:A:1227:VAL:HG23	1.85	0.58
1:A:1849:PRO:HD2	1:A:2570:ARG:HH22	1.68	0.58
1:A:2772:HIS:ND1	1:B:2873:CYS:O	2.36	0.58
1:A:726:ALA:HA	1:A:731:LEU:HD12	1.85	0.58
1:B:1328:HIS:HA	1:B:1331:LEU:HD12	1.84	0.58
1:A:1505:PRO:O	1:A:1985:ASN:ND2	2.36	0.58
1:A:3077:LEU:HD12	1:A:3082:LEU:HD21	1.85	0.58
1:B:1505:PRO:O	1:B:1985:ASN:ND2	2.36	0.58
1:A:2248:LYS:HB3	1:A:2278:LEU:HD11	1.84	0.57
1:B:3164:ALA:HA	1:B:3298:LEU:HD12	1.86	0.57
1:B:59:ARG:NH2	1:B:927:GLU:O	2.37	0.57
1:A:3547:CYS:HB2	1:A:3616:SER:HA	1.86	0.57
2:C:55:LEU:HD13	2:C:84:ALA:HB3	1.87	0.57
1:A:1788:ARG:HH12	1:A:1790:PHE:HB2	1.70	0.57
1:B:1792:THR:HA	1:B:1856:MET:O	2.04	0.57
1:A:3534:CYS:HA	1:A:3539:LYS:HD2	1.87	0.57
1:B:3817:LEU:HD11	1:B:4185:LEU:HD22	1.86	0.57
1:A:2117:VAL:HA	1:A:2120:LEU:HG	1.87	0.57
1:B:1836:ASP:OD1	1:B:1839:THR:OG1	2.23	0.57
1:B:4173:VAL:HG11	1:B:4220:LEU:HB2	1.87	0.57
1:A:1883:TYR:HE1	1:A:1908:PRO:HG2	1.70	0.57
1:A:1771:GLN:HE22	1:A:1983:GLN:HG2	1.69	0.57
1:A:2716:LEU:HD21	1:B:3254:SER:HA	1.85	0.57
1:B:3191:ARG:HB2	1:B:3193:ARG:HH11	1.70	0.57
1:B:1337:ARG:O	1:B:1337:ARG:NH1	2.36	0.57
1:B:2070:GLY:O	1:B:2075:ARG:NH1	2.38	0.56
1:A:2396:ASP:HB3	1:B:3271:LYS:HE2	1.87	0.56
1:B:1581:ARG:HD2	1:B:1774:PRO:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:CYS:HB2	1:A:514:GLN:HB2	1.87	0.56
1:A:2840:LEU:HD11	1:A:2925:LEU:HD22	1.88	0.56
1:A:3778:GLN:HG2	1:A:4070:PRO:HG3	1.88	0.56
1:A:1817:ILE:HG23	1:A:1831:LEU:HB2	1.86	0.56
1:B:1581:ARG:NH1	1:B:1774:PRO:O	2.37	0.56
1:B:912:VAL:HB	1:B:926:VAL:HB	1.88	0.56
1:B:2985:LEU:HD13	1:B:3052:MET:HB3	1.88	0.56
1:A:2284:LYS:HB2	2:D:21:ARG:HE	1.70	0.56
1:B:929:PRO:HG2	1:B:938:ASP:HB3	1.88	0.56
1:A:1805:LEU:O	1:A:1876:GLY:HA3	2.06	0.56
1:A:3709:ASN:HD21	1:A:3780:LEU:HD21	1.71	0.56
1:A:1452:PHE:O	1:A:1456:ASN:ND2	2.39	0.56
1:A:1770:LEU:HD13	1:A:1986:LEU:HD11	1.86	0.56
1:A:2248:LYS:HE2	2:C:25:LEU:HA	1.88	0.56
1:A:2566:ALA:O	1:A:2584:LYS:NZ	2.38	0.56
1:B:396:CYS:HB3	1:B:512:ILE:HG22	1.88	0.56
1:B:1037:ARG:HH22	1:B:1075:ARG:HB3	1.71	0.56
1:A:1107:LYS:HZ1	1:A:1198:ALA:HB1	1.70	0.55
1:A:2061:GLU:OE2	1:A:2065:HIS:NE2	2.40	0.55
1:A:2259:GLU:HG2	1:A:2271:LEU:HD12	1.86	0.55
1:A:1456:ASN:HA	1:A:1459:LYS:HD3	1.86	0.55
1:A:1771:GLN:OE1	1:A:1983:GLN:NE2	2.39	0.55
1:A:2714:THR:HB	1:A:2719:TRP:HE1	1.71	0.55
1:B:207:THR:HA	1:B:214:ALA:HB2	1.89	0.55
1:A:630:LEU:HD12	1:A:720:LEU:HD22	1.88	0.55
1:A:1124:LEU:HB3	1:A:1183:CYS:HB3	1.88	0.55
1:B:716:LEU:HD21	1:B:719:CYS:HB2	1.87	0.55
1:B:1500:SER:O	1:B:1974:TYR:OH	2.23	0.55
1:A:123:VAL:O	1:A:125:LYS:NZ	2.38	0.55
1:A:3030:ILE:N	1:A:3034:ASP:OD2	2.39	0.55
1:B:2114:GLN:O	1:B:2118:PHE:CB	2.55	0.55
1:B:2635:SER:HA	1:B:2638:MET:HE3	1.88	0.55
1:A:207:THR:HA	1:A:214:ALA:HB2	1.88	0.55
1:A:1812:LEU:O	1:A:1838:SER:OG	2.23	0.55
1:B:1200:MET:HG2	1:B:2577:GLN:HE21	1.71	0.55
1:B:1343:GLN:NE2	1:B:1344:ILE:O	2.39	0.55
1:B:2365:THR:O	1:B:2366:ARG:NH1	2.39	0.55
1:A:380:PRO:HG2	1:A:388:ILE:HG12	1.88	0.55
1:A:2346:CYS:HB3	1:A:2350:LEU:HD11	1.89	0.55
1:A:2755:ASP:OD1	1:A:2755:ASP:N	2.35	0.55
1:B:2035:LEU:HB2	1:B:2081:LEU:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3720:CYS:SG	1:B:3721:HIS:N	2.80	0.55
1:A:2777:HIS:NE2	1:B:3256:PRO:O	2.39	0.55
1:B:1812:LEU:O	1:B:1838:SER:OG	2.24	0.55
2:D:69:MET:HE3	2:D:74:GLU:HG3	1.89	0.55
1:A:3547:CYS:SG	1:A:3846:HIS:NE2	2.71	0.55
1:B:411:ILE:HD11	1:B:567:LEU:HD22	1.89	0.55
1:B:2387:LEU:O	1:B:2393:ASN:ND2	2.40	0.54
1:B:2671:SER:O	1:B:2690:ARG:NH1	2.40	0.54
1:B:3450:ILE:HA	1:B:3453:LEU:HD12	1.89	0.54
1:A:3236:PRO:HG2	1:A:3282:LEU:HD12	1.89	0.54
1:B:1012:LEU:HA	1:B:1015:GLN:HE22	1.73	0.54
1:B:1581:ARG:NH1	1:B:1776:GLN:OE1	2.40	0.54
1:A:239:LEU:HD23	1:A:242:ILE:HD11	1.88	0.54
1:A:2099:VAL:O	1:A:2103:LEU:HB2	2.06	0.54
1:A:3777:ASN:HB3	1:A:3781:MET:HE1	1.89	0.54
1:B:3222:GLU:HG2	1:B:3268:GLN:HA	1.89	0.54
2:C:42:ILE:HG12	2:C:142:VAL:HG21	1.89	0.54
1:A:2235:LEU:HD22	1:A:2293:ARG:HD2	1.90	0.54
1:A:2647:PHE:HE1	1:A:2660:LEU:HD21	1.73	0.54
1:A:2823:ARG:N	1:A:2827:GLN:OE1	2.39	0.54
1:A:163:LEU:HD11	1:A:255:VAL:HG13	1.89	0.54
1:B:1503:PHE:HZ	1:B:1936:GLU:HB2	1.71	0.54
1:A:914:ILE:HB	1:A:924:ALA:HB3	1.90	0.54
1:B:2114:GLN:O	1:B:2118:PHE:HB2	2.07	0.54
1:B:164:GLU:HG2	1:B:258:ARG:HH22	1.73	0.54
1:B:240:LYS:NZ	1:B:284:TYR:OH	2.39	0.54
1:A:287:ALA:HA	1:A:290:ARG:HE	1.73	0.54
1:A:2323:LEU:HD12	1:A:2327:ARG:HH12	1.72	0.54
1:B:1110:LEU:HD21	1:B:1188:LEU:HD21	1.90	0.54
1:B:3703:LEU:HD22	1:B:3708:VAL:HG11	1.89	0.54
1:A:1441:ALA:HB2	1:A:2014:LEU:HD13	1.90	0.53
1:B:914:ILE:HB	1:B:924:ALA:HB3	1.90	0.53
1:B:3694:GLY:HA2	1:B:3699:MET:SD	2.48	0.53
1:A:1406:ARG:HD3	1:A:2576:GLU:HG3	1.90	0.53
1:B:1844:LEU:HD21	1:B:2568:ASP:HB2	1.91	0.53
1:A:1881:HIS:CG	1:A:1993:ARG:HH12	2.27	0.53
1:A:3224:HIS:CE1	1:A:3266:LYS:HG2	2.43	0.53
1:A:296:TRP:CE2	1:A:309:MET:HE1	2.43	0.53
2:C:34:LEU:O	2:C:37:THR:OG1	2.25	0.53
1:A:3701:ASP:OD1	1:A:3774:HIS:NE2	2.35	0.53
1:A:3199:TYR:HB3	1:A:3291:LEU:HD12	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1104:VAL:HB	1:B:1203:LEU:HB2	1.90	0.53
2:C:105:ALA:HA	2:C:108:LEU:HD12	1.89	0.53
1:A:716:LEU:HD21	1:A:719:CYS:HB2	1.91	0.53
1:A:2291:ARG:HH11	2:D:13:LEU:HD11	1.74	0.53
1:B:945:TYR:OH	1:B:950:ASP:OD1	2.26	0.53
1:B:3179:ALA:HB1	1:B:3182:LEU:HD12	1.90	0.53
1:B:3184:GLN:HB2	1:B:3187:PRO:HG3	1.91	0.53
1:B:4155:ALA:HA	1:B:4158:LEU:HD12	1.91	0.53
1:A:3484:TYR:HA	1:A:3487:LEU:HG	1.91	0.53
2:D:129:ARG:HA	2:D:132:ILE:HD12	1.90	0.53
1:A:1209:VAL:HA	1:A:1212:MET:HG3	1.90	0.53
1:A:2252:LEU:HD21	1:A:2275:GLN:HA	1.91	0.53
1:B:1028:LEU:O	1:B:1318:ARG:NH2	2.42	0.53
1:B:1344:ILE:HG12	1:B:1349:GLN:HG3	1.91	0.53
1:A:318:PRO:HA	1:A:325:ARG:HB3	1.91	0.53
1:A:3537:VAL:HA	1:A:3540:LYS:HD2	1.90	0.53
1:B:2041:SER:O	1:B:2044:HIS:ND1	2.41	0.53
1:B:3816:MET:HE3	1:B:4071:LEU:HD12	1.91	0.53
1:A:309:MET:HA	1:A:344:PRO:HB3	1.92	0.52
1:A:1101:VAL:HA	1:A:1305:ARG:HE	1.74	0.52
1:A:4153:ILE:HG23	1:A:4210:PRO:HG3	1.90	0.52
1:B:3075:CYS:O	1:B:3325:LYS:NZ	2.43	0.52
1:B:3967:LEU:HD13	1:B:4004:LEU:HD13	1.92	0.52
1:A:2099:VAL:O	1:A:2103:LEU:CB	2.57	0.52
1:A:2686:TYR:OH	1:A:2727:THR:OG1	2.27	0.52
1:A:116:LYS:NZ	1:A:117:CYS:O	2.42	0.52
1:A:198:ASP:HA	1:A:201:LYS:HE3	1.90	0.52
1:A:2726:LEU:HA	1:A:2729:MET:HG3	1.92	0.52
1:A:2820:SER:HB3	1:A:2826:PHE:HD2	1.74	0.52
1:A:2856:ILE:HG23	1:A:2929:LEU:HD21	1.90	0.52
1:B:1092:GLU:OE2	1:B:1219:SER:OG	2.28	0.52
1:B:2354:VAL:HA	1:B:2357:VAL:HG22	1.91	0.52
1:A:396:CYS:HB3	1:A:512:ILE:HG22	1.91	0.52
1:A:3453:LEU:HD21	1:A:3497:VAL:HG22	1.92	0.52
1:B:2665:LEU:O	1:B:2669:LEU:HB2	2.09	0.52
1:A:1557:LEU:HB3	1:A:1560:LEU:HD11	1.92	0.52
1:A:2780:GLN:HE22	1:A:2834:ASP:H	1.58	0.52
1:B:1480:GLN:HG2	1:B:2015:ILE:HG22	1.92	0.52
1:B:3054:LEU:HD23	1:B:3101:MET:HE2	1.92	0.52
1:A:1028:LEU:O	1:A:1318:ARG:NH2	2.43	0.52
1:A:1818:ASP:HB3	1:A:1857:LYS:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2342:MET:HG3	1:A:2351:LEU:HD11	1.92	0.52
1:A:2693:VAL:HG23	1:A:2694:ILE:HD12	1.90	0.52
1:A:3498:ALA:HB2	1:A:3545:LEU:HD22	1.92	0.52
1:B:2919:MET:HA	1:B:2922:LEU:HG	1.92	0.52
1:A:176:ALA:O	1:A:181:VAL:N	2.42	0.52
1:A:725:PHE:HE2	1:A:846:ILE:HD13	1.75	0.52
1:B:3198:SER:HA	1:B:3291:LEU:O	2.10	0.52
1:B:3236:PRO:O	1:B:3259:THR:OG1	2.27	0.52
1:B:726:ALA:HA	1:B:731:LEU:HD12	1.92	0.52
1:B:855:THR:HB	1:B:908:GLN:HB2	1.91	0.52
1:B:2726:LEU:HA	1:B:2729:MET:HG2	1.92	0.52
1:B:3328:ILE:HD11	1:B:3374:HIS:HB2	1.92	0.52
1:A:2837:VAL:HG12	1:A:2918:LEU:HD13	1.92	0.51
1:A:4235:ARG:HD3	1:A:4356:LEU:HD21	1.92	0.51
1:B:1083:SER:HA	1:B:1086:TRP:HB3	1.92	0.51
1:B:1798:PRO:HD3	1:B:1854:ARG:HE	1.75	0.51
2:C:45:ILE:HG23	2:C:146:SER:HB2	1.92	0.51
1:A:3131:LYS:NZ	1:A:3304:PHE:O	2.34	0.51
1:A:3636:VAL:HG13	1:A:3711:LEU:HD12	1.92	0.51
1:B:3328:ILE:HA	1:B:3331:LEU:HB2	1.92	0.51
1:A:3058:LEU:HA	1:A:3061:MET:HG2	1.93	0.51
1:B:1428:LEU:O	1:B:1432:LEU:HD12	2.10	0.51
1:B:2932:LEU:HD12	1:B:2933:PRO:HD2	1.90	0.51
1:A:372:LEU:HD21	1:A:417:LEU:HA	1.92	0.51
1:A:1091:PHE:HB3	1:A:1222:ILE:HB	1.91	0.51
1:A:3232:LEU:HD21	1:B:3233:ALA:HB2	1.92	0.51
1:B:1290:LEU:HD22	1:B:1294:ASP:HB3	1.91	0.51
1:B:1807:PRO:HG2	1:B:1874:PRO:HB2	1.93	0.51
1:B:3990:LEU:HA	1:B:3993:ARG:HG2	1.92	0.51
1:A:3382:LEU:HD23	1:A:3385:ILE:HD11	1.93	0.51
1:B:1102:GLY:H	1:B:1305:ARG:HA	1.75	0.51
1:B:3224:HIS:HE1	1:B:3266:LYS:HE3	1.76	0.51
1:A:2234:GLN:HB2	2:C:39:TYR:CE2	2.46	0.51
1:B:239:LEU:HD23	1:B:242:ILE:HD11	1.90	0.51
1:B:2578:GLN:HA	1:B:2581:LEU:HG	1.91	0.51
1:A:55:TRP:HE1	1:A:966:ILE:HG23	1.74	0.51
1:A:137:ARG:NH2	1:A:148:THR:O	2.44	0.51
1:A:2994:ILE:HD12	1:A:3040:LEU:HD21	1.93	0.51
1:A:3460:SER:HA	1:A:3486:LEU:HB3	1.92	0.51
1:A:327:MET:HE3	1:A:332:SER:HB3	1.92	0.51
1:A:855:THR:HB	1:A:908:GLN:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1467:SER:HB3	1:A:2050:LEU:HD11	1.93	0.51
1:B:1331:LEU:O	1:B:1334:THR:OG1	2.21	0.51
1:A:1012:LEU:HA	1:A:1015:GLN:HE22	1.76	0.51
1:A:2343:ASP:OD1	1:A:2343:ASP:N	2.43	0.51
1:A:3821:LYS:HA	1:A:3861:PRO:HA	1.93	0.51
1:A:3867:SER:N	1:A:3979:ALA:O	2.41	0.51
1:B:3432:ILE:HG23	1:B:3496:CYS:HB2	1.92	0.51
1:A:3236:PRO:HG3	1:A:3291:LEU:HD22	1.92	0.51
1:B:2585:MET:HA	1:B:2588:THR:HG22	1.93	0.51
1:B:3807:PHE:HA	1:B:3810:ARG:HG2	1.93	0.51
1:B:3534:CYS:HA	1:B:3539:LYS:HD3	1.93	0.50
1:B:4409:VAL:HG12	1:B:4495:LEU:HD22	1.93	0.50
1:A:1494:THR:HG21	1:A:2111:ILE:HG22	1.93	0.50
1:B:380:PRO:HG2	1:B:388:ILE:HG12	1.93	0.50
1:B:1781:GLU:OE1	1:B:1781:GLU:N	2.45	0.50
1:A:254:SER:HB2	1:A:370:VAL:HG11	1.94	0.50
1:B:630:LEU:HD12	1:B:720:LEU:HD22	1.93	0.50
1:A:94:ILE:HA	1:A:101:THR:HA	1.93	0.50
1:A:2724:HIS:O	1:A:2727:THR:OG1	2.28	0.50
1:A:3221:LYS:HG2	1:A:3300:GLY:HA2	1.92	0.50
1:B:3054:LEU:HG	1:B:3058:LEU:HD23	1.93	0.50
1:B:751:THR:HG21	1:B:820:VAL:HG13	1.94	0.50
1:B:2145:LEU:HD21	1:B:2168:ILE:HG13	1.93	0.50
1:B:2724:HIS:O	1:B:2727:THR:OG1	2.26	0.50
1:A:395:SER:HG	1:A:514:GLN:H	1.60	0.50
1:A:3720:CYS:SG	1:A:3721:HIS:N	2.85	0.50
1:A:3867:SER:HB3	1:A:3979:ALA:HB1	1.94	0.50
1:B:1121:GLN:OE1	1:B:1123:THR:OG1	2.28	0.50
1:A:1121:GLN:OE1	1:A:1123:THR:OG1	2.30	0.50
1:A:1444:THR:HG22	1:A:1447:SER:H	1.76	0.50
1:A:3115:THR:HG21	1:A:3361:THR:HB	1.94	0.50
1:B:350:ARG:NE	1:B:1786:GLY:O	2.44	0.49
1:B:3236:PRO:HG3	1:B:3282:LEU:HD23	1.94	0.49
1:B:3550:CYS:HB3	1:B:3557:PHE:HB2	1.93	0.49
1:A:399:PHE:HA	1:A:412:TRP:O	2.13	0.49
1:B:147:ASP:OD2	1:B:218:THR:OG1	2.25	0.49
1:B:1471:ALA:HB2	1:B:2050:LEU:HD11	1.94	0.49
1:B:3700:LYS:NZ	1:B:3769:GLN:O	2.41	0.49
1:B:4357:PRO:HB2	1:B:4359:VAL:HG12	1.94	0.49
1:A:3816:MET:SD	1:A:3816:MET:N	2.85	0.49
1:B:163:LEU:HD11	1:B:255:VAL:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1441:ALA:HB2	1:B:2014:LEU:HD13	1.95	0.49
1:B:1810:GLY:HA2	1:B:1838:SER:HA	1.94	0.49
1:B:2349:ASP:N	1:B:2349:ASP:OD1	2.44	0.49
1:B:3077:LEU:H	1:B:3325:LYS:HZ3	1.61	0.49
1:B:3123:ARG:HH21	1:B:3304:PHE:HA	1.76	0.49
1:B:3984:ALA:HB1	1:B:4067:ILE:H	1.78	0.49
1:A:3079:GLU:HG3	1:A:3080:PRO:HD3	1.94	0.49
1:B:3454:LEU:HA	1:B:3457:VAL:HG12	1.94	0.49
1:A:513:LEU:HD11	1:A:830:MET:HE1	1.95	0.49
1:B:1345:THR:OG1	1:B:1346:GLU:OE1	2.30	0.49
1:B:3224:HIS:CE1	1:B:3266:LYS:HG2	2.47	0.49
1:A:3810:ARG:HA	1:A:3813:LEU:HD12	1.94	0.49
1:A:130:ASP:HB2	1:A:150:LEU:HD13	1.94	0.49
1:A:3256:PRO:O	1:B:2777:HIS:NE2	2.30	0.49
1:A:3436:TYR:HA	1:A:3500:ILE:HD11	1.95	0.49
1:B:1498:LEU:HD13	1:B:1974:TYR:HD1	1.78	0.49
1:A:1914:LEU:HD12	1:A:1994:LEU:HB3	1.94	0.49
1:A:2030:LEU:O	1:A:2033:THR:OG1	2.24	0.49
1:A:3225:ILE:O	1:A:3265:ILE:HB	2.13	0.49
1:B:1812:LEU:HD13	1:B:1862:GLY:HA2	1.95	0.49
1:B:2750:HIS:O	1:B:2754:SER:OG	2.28	0.49
1:B:3206:ALA:O	1:B:3284:ARG:N	2.46	0.49
1:B:3239:VAL:HG22	1:B:3282:LEU:HG	1.94	0.49
2:C:66:LEU:HA	2:C:69:MET:HE1	1.95	0.49
1:B:1498:LEU:HB3	1:B:1974:TYR:HE1	1.77	0.48
1:B:4260:ARG:NH1	1:B:4367:SER:O	2.46	0.48
1:A:630:LEU:HB2	1:A:720:LEU:HB3	1.93	0.48
1:A:2039:HIS:NE2	1:A:2596:GLN:OE1	2.40	0.48
1:A:3206:ALA:O	1:A:3284:ARG:N	2.44	0.48
1:A:4252:SER:HG	1:A:4368:CYS:HG	1.61	0.48
1:B:3867:SER:HB3	1:B:3979:ALA:HB1	1.96	0.48
1:A:1784:HIS:H	1:A:1787:ALA:HB2	1.78	0.48
1:A:4244:LEU:HA	1:A:4247:ILE:HG22	1.95	0.48
1:B:1883:TYR:HE1	1:B:1908:PRO:HG2	1.77	0.48
1:B:3114:SER:OG	1:B:3327:SER:OG	2.26	0.48
1:B:3527:ASN:HA	1:B:3530:MET:SD	2.54	0.48
1:A:3809:ARG:HH22	1:A:4189:LEU:HB2	1.78	0.48
1:B:1763:ILE:HG23	1:B:1920:LEU:HD13	1.95	0.48
1:B:3111:MET:HE3	1:B:3330:TRP:HB2	1.94	0.48
1:B:4252:SER:HG	1:B:4368:CYS:HG	1.56	0.48
1:A:1406:ARG:NH1	1:A:2580:GLU:OE2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3246:ASP:N	1:A:3246:ASP:OD1	2.46	0.48
1:B:2337:LEU:HD13	1:B:2340:LEU:HD21	1.95	0.48
1:A:283:MET:HE1	1:A:329:PHE:HB2	1.94	0.48
1:A:1290:LEU:HD22	1:A:1294:ASP:HB3	1.95	0.48
1:B:85:VAL:HG21	1:B:117:CYS:HB3	1.94	0.48
1:B:1217:TYR:O	1:B:1218:ARG:NH1	2.44	0.48
1:B:4331:ILE:HG21	1:B:4402:ILE:HA	1.95	0.48
1:A:3164:ALA:HA	1:A:3298:LEU:HD12	1.95	0.48
1:A:3429:ASP:HA	1:A:3432:ILE:HD12	1.95	0.48
1:B:2080:LEU:HA	1:B:2083:VAL:HG12	1.95	0.48
1:B:3190:ARG:HH12	2:D:129:ARG:NH2	2.11	0.48
1:A:3302:THR:HG23	1:A:3304:PHE:H	1.78	0.48
1:A:3388:GLN:OE1	1:A:3389:SER:OG	2.30	0.48
1:A:3522:PHE:CZ	1:A:3560:LEU:HB2	2.49	0.48
1:B:383:ASP:OD2	1:B:385:THR:OG1	2.31	0.48
2:D:99:GLU:OE2	2:D:143:HIS:NE2	2.46	0.48
1:A:859:LEU:HB2	1:A:903:LEU:HD11	1.96	0.48
1:A:1098:ALA:HB2	1:A:1218:ARG:HE	1.79	0.48
2:D:96:LEU:O	2:D:100:THR:OG1	2.29	0.48
1:A:1188:LEU:HG	1:A:1192:LEU:HD21	1.95	0.48
1:A:1486:THR:OG1	1:A:1489:GLU:OE1	2.21	0.48
1:A:1888:GLU:HA	1:A:1891:LEU:HG	1.95	0.48
1:A:2062:LEU:HD11	1:A:2082:LEU:HD21	1.96	0.48
1:A:2697:ASN:OD1	1:A:2698:GLN:N	2.47	0.48
1:A:3989:LEU:HB3	1:A:3993:ARG:HH21	1.79	0.48
1:B:2792:PHE:HD2	1:B:2793:LEU:HD22	1.78	0.48
1:B:3536:MET:HG2	1:B:3538:LEU:H	1.79	0.48
1:B:3827:GLN:O	1:B:4005:THR:HA	2.14	0.47
2:D:84:ALA:O	2:D:88:MET:HG2	2.14	0.47
1:A:289:ARG:O	1:A:292:THR:OG1	2.31	0.47
1:A:2080:LEU:HA	1:A:2083:VAL:HG22	1.95	0.47
1:B:1101:VAL:HG22	1:B:1212:MET:HG2	1.96	0.47
1:A:2919:MET:HA	1:A:2922:LEU:HD12	1.96	0.47
1:A:3550:CYS:HB2	1:A:3557:PHE:HB2	1.97	0.47
1:B:1582:ASP:N	1:B:1775:HIS:O	2.47	0.47
1:A:3058:LEU:HA	1:A:3061:MET:HE3	1.96	0.47
1:A:3243:VAL:HG13	1:A:3253:LEU:HD21	1.97	0.47
1:A:1499:TYR:CE2	1:A:2072:PRO:HD3	2.50	0.47
1:A:3077:LEU:HA	1:A:3081:LEU:HD23	1.96	0.47
1:A:625:ARG:NH2	1:A:730:ASN:OD1	2.47	0.47
1:B:2686:TYR:OH	1:B:2727:THR:OG1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3388:GLN:OE1	1:B:3389:SER:OG	2.30	0.47
1:B:3760:GLU:OE2	1:B:3810:ARG:NH1	2.47	0.47
1:A:4080:LEU:HD13	1:A:4083:ILE:HD11	1.96	0.47
1:B:2389:GLY:HA2	1:B:2655:VAL:HG22	1.97	0.47
1:B:2582:MET:HA	1:B:2585:MET:HG3	1.97	0.47
1:B:2590:GLU:O	1:B:2594:ILE:HG12	2.15	0.47
1:B:3866:LEU:HD13	1:B:3967:LEU:HD12	1.97	0.47
1:A:3828:SER:HB3	1:A:3832:LEU:HD21	1.97	0.47
1:A:4324:LEU:HD22	1:A:4398:LEU:HD22	1.95	0.47
1:B:1495:ARG:HD3	1:B:1952:ASN:HD22	1.78	0.47
1:B:1852:VAL:O	1:B:1892:LYS:NZ	2.34	0.47
1:A:58:LEU:HB2	1:A:965:GLN:HB3	1.96	0.47
1:A:164:GLU:HG2	1:A:258:ARG:HH22	1.80	0.47
1:A:1106:PHE:HD2	1:A:1201:LEU:HD13	1.79	0.47
1:A:1573:THR:HG22	1:A:1574:SER:H	1.80	0.47
1:A:1781:GLU:OE1	1:A:1781:GLU:N	2.45	0.47
1:A:1827:ASP:OD1	1:A:1827:ASP:N	2.48	0.47
1:A:2145:LEU:HD12	1:A:2145:LEU:HA	1.77	0.47
1:A:3224:HIS:HE1	1:A:3266:LYS:HE3	1.80	0.47
1:A:3824:MET:N	1:A:3824:MET:SD	2.85	0.47
1:B:1573:THR:HG22	1:B:1574:SER:H	1.80	0.47
1:B:1883:TYR:OH	1:B:1908:PRO:O	2.32	0.47
1:B:2758:LEU:HA	1:B:2761:VAL:HG22	1.97	0.47
1:B:3076:GLN:N	1:B:3076:GLN:OE1	2.45	0.47
1:B:3107:ILE:HG23	1:B:3330:TRP:HB3	1.96	0.47
1:A:2813:LEU:HD21	1:A:2851:VAL:HG11	1.97	0.47
1:A:3263:THR:OG1	1:B:3287:ASP:OD2	2.31	0.47
1:A:4255:SER:O	1:A:4257:HIS:ND1	2.47	0.47
1:B:440:SER:HA	1:B:721:ARG:HH22	1.80	0.47
1:B:1444:THR:HG22	1:B:1447:SER:H	1.79	0.47
1:A:3828:SER:HB2	1:A:4006:VAL:HB	1.95	0.46
1:B:342:ASP:OD2	2:C:1:ALA:N	2.44	0.46
1:B:2141:LEU:O	1:B:2145:LEU:HB2	2.16	0.46
1:A:2668:SER:HB2	1:A:2728:LEU:HD21	1.97	0.46
1:A:4260:ARG:NH1	1:A:4367:SER:O	2.48	0.46
1:B:93:VAL:O	1:B:102:LEU:N	2.46	0.46
2:D:45:ILE:HG23	2:D:146:SER:HB2	1.97	0.46
1:A:1331:LEU:HD12	1:A:1352:VAL:HG13	1.96	0.46
1:A:2408:LEU:HA	1:A:2411:MET:HG3	1.97	0.46
1:A:2650:LEU:HB3	1:A:2655:VAL:HB	1.97	0.46
1:B:2775:ASN:HB3	1:B:2777:HIS:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:55:LEU:HD11	2:C:81:ILE:HG23	1.98	0.46
1:A:2335:LEU:HD23	1:A:2358:LEU:HD13	1.96	0.46
1:B:153:PRO:HG3	1:B:376:PRO:HB2	1.97	0.46
1:B:830:MET:HA	1:B:839:LEU:HD23	1.96	0.46
1:B:1212:MET:HE1	1:B:1218:ARG:HH12	1.79	0.46
1:A:2291:ARG:HA	1:A:2294:ARG:HD2	1.98	0.46
1:A:2787:GLN:O	1:A:2790:GLN:HG3	2.16	0.46
1:A:3845:GLN:HB3	1:A:3849:TYR:HD2	1.79	0.46
1:A:1810:GLY:HA2	1:A:1838:SER:HA	1.96	0.46
1:A:2872:THR:HG22	1:A:3000:LEU:HD22	1.98	0.46
1:A:3443:ASP:OD1	1:A:3446:THR:OG1	2.25	0.46
1:A:2172:VAL:HA	1:A:2175:VAL:HG22	1.97	0.46
1:A:3036:LEU:HA	1:A:3039:ILE:HG22	1.98	0.46
1:B:304:ALA:HA	1:B:309:MET:HE3	1.97	0.46
1:B:2923:LEU:HA	1:B:2926:VAL:HG22	1.98	0.46
1:B:2172:VAL:HA	1:B:2175:VAL:HG22	1.98	0.46
1:B:2399:TRP:O	1:B:2405:GLN:NE2	2.49	0.46
1:A:3355:THR:HG23	1:A:3358:LEU:HB2	1.96	0.46
1:B:1456:ASN:HA	1:B:1459:LYS:HD3	1.97	0.46
1:B:2690:ARG:O	1:B:2731:ASN:ND2	2.49	0.46
1:A:2114:GLN:HA	1:A:2117:VAL:HG22	1.98	0.46
1:A:2274:GLU:O	1:A:2277:LYS:HG3	2.16	0.46
1:A:4409:VAL:HG12	1:A:4495:LEU:HD22	1.97	0.46
1:B:1172:PRO:HA	1:B:1175:GLU:HB2	1.98	0.46
1:B:2714:THR:O	1:B:2719:TRP:NE1	2.49	0.46
1:B:2726:LEU:HB3	1:B:2792:PHE:CE1	2.51	0.46
2:D:38:THR:OG1	2:D:102:TRP:NE1	2.42	0.46
1:A:3771:ILE:HD12	1:A:4070:PRO:HG2	1.98	0.45
1:B:1108:PHE:CZ	1:B:1199:GLY:HA3	2.51	0.45
1:B:2054:PHE:HD2	1:B:2085:LEU:HD22	1.81	0.45
1:B:2324:ALA:H	1:B:2327:ARG:NH2	2.15	0.45
1:B:3199:TYR:HB3	1:B:3291:LEU:HB2	1.98	0.45
1:B:3564:MET:SD	1:B:3564:MET:N	2.89	0.45
1:A:1015:GLN:HG3	1:A:1021:ILE:HD13	1.97	0.45
1:A:2374:ILE:HG22	1:A:2375:VAL:HG13	1.99	0.45
1:A:2930:VAL:HG11	1:A:3039:ILE:HD11	1.98	0.45
1:A:2231:ILE:O	1:A:2235:LEU:HG	2.16	0.45
1:A:2775:ASN:HB3	1:A:2777:HIS:CE1	2.50	0.45
1:A:3221:LYS:HD2	1:A:3301:LEU:HD23	1.98	0.45
1:A:3325:LYS:HD2	1:B:2397:ILE:HD12	1.98	0.45
1:A:3402:ARG:HH21	1:A:3486:LEU:HD21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:934:THR:HG23	1:B:936:GLU:H	1.81	0.45
1:B:3527:ASN:O	1:B:3531:SER:HB3	2.16	0.45
1:B:3547:CYS:HB2	1:B:3616:SER:HA	1.97	0.45
1:A:732:CYS:HB3	1:A:752:CYS:HB2	1.97	0.45
1:A:3379:GLU:HB2	1:A:3434:ILE:HD11	1.99	0.45
1:A:3718:LEU:O	1:A:3722:SER:HB3	2.15	0.45
1:A:4435:THR:O	1:A:4439:LYS:HG3	2.17	0.45
1:B:2827:GLN:NE2	1:B:2828:THR:HG23	2.31	0.45
1:B:3125:MET:O	1:B:3129:ILE:HG13	2.17	0.45
1:A:725:PHE:HA	1:A:728:GLU:HG3	1.97	0.45
1:A:900:LEU:HB3	1:A:917:LEU:HD23	1.99	0.45
1:A:1493:GLN:NE2	1:A:2069:SER:O	2.42	0.45
1:A:3327:SER:HA	1:A:3330:TRP:CE3	2.52	0.45
1:B:829:LYS:HD2	1:B:844:ILE:HD11	1.99	0.45
1:B:1175:GLU:HA	1:B:1178:LYS:HB2	1.99	0.45
1:B:1836:ASP:HB3	1:B:2564:SER:HB3	1.99	0.45
1:A:1467:SER:HB3	1:A:2050:LEU:HD21	1.98	0.45
1:A:2365:THR:O	1:A:2366:ARG:NH1	2.49	0.45
1:A:3250:MET:HE3	1:A:3279:CYS:HB2	1.98	0.45
1:A:4402:ILE:HG13	1:A:4408:MET:HG3	1.99	0.45
1:B:354:ASN:HA	1:B:359:LYS:HE3	1.99	0.45
1:B:1023:THR:HA	1:B:1026:VAL:HG12	1.98	0.45
1:B:3688:ARG:NH2	1:B:3762:ALA:HA	2.28	0.45
2:C:38:THR:HG23	2:C:139:VAL:HG23	1.98	0.45
1:A:120:ILE:HG21	1:A:397:PRO:HB2	1.99	0.45
1:A:2644:ASN:HA	1:A:2647:PHE:CD2	2.52	0.45
1:A:3222:GLU:OE1	1:A:3268:GLN:HA	2.16	0.45
1:B:2734:LEU:HD23	1:B:2734:LEU:HA	1.87	0.45
1:B:3207:TRP:HA	1:B:3282:LEU:O	2.17	0.45
1:A:2284:LYS:HA	2:D:21:ARG:HH21	1.82	0.45
1:B:514:GLN:HA	1:B:837:VAL:HG21	1.98	0.45
1:B:3220:LEU:HD12	1:B:3223:ILE:HD11	1.99	0.45
1:B:3224:HIS:HB2	1:B:3297:LYS:HE2	1.98	0.45
1:A:283:MET:HE3	1:A:283:MET:HB3	1.62	0.45
1:A:749:LEU:O	1:A:823:GLY:CA	2.65	0.45
1:A:2073:LYS:HA	1:A:2073:LYS:HD2	1.81	0.45
1:A:4080:LEU:HD12	1:A:4165:LEU:HD13	1.99	0.45
1:B:250:PRO:HD3	1:B:362:HIS:HB3	1.98	0.45
1:B:1015:GLN:HG3	1:B:1021:ILE:HG21	1.99	0.45
1:B:1459:LYS:HD2	1:B:2037:LEU:HD12	1.99	0.45
1:B:1472:SER:O	1:B:1475:THR:OG1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3707:GLU:HG2	1:B:3708:VAL:HG23	1.99	0.45
1:A:1499:TYR:HD2	1:A:2071:THR:HA	1.81	0.44
1:A:2994:ILE:HG13	1:A:2995:LEU:HD12	1.99	0.44
1:A:3076:GLN:OE1	1:A:3076:GLN:N	2.45	0.44
1:B:272:VAL:HG21	1:B:292:THR:HA	1.97	0.44
1:B:1481:LEU:HD11	1:B:2065:HIS:HB3	1.99	0.44
1:B:1557:LEU:HG	1:B:1805:LEU:HD12	1.99	0.44
1:B:2370:HIS:ND1	1:B:2419:GLU:HG3	2.32	0.44
1:A:1780:ILE:HD13	1:A:1789:ARG:HG3	1.99	0.44
1:A:2012:GLU:HA	1:A:2015:ILE:HB	1.99	0.44
1:A:3160:ILE:HG22	1:A:3299:LEU:HD12	1.99	0.44
1:A:4396:LEU:HD11	1:A:4481:ILE:HG12	1.99	0.44
1:B:1352:VAL:O	1:B:1355:THR:OG1	2.33	0.44
1:B:2033:THR:O	1:B:2036:SER:OG	2.25	0.44
1:B:2834:ASP:OD1	1:B:2834:ASP:N	2.48	0.44
1:B:3225:ILE:HB	1:B:3265:ILE:HB	1.99	0.44
2:C:35:SER:OG	2:C:131:HIS:NE2	2.50	0.44
1:B:280:ARG:HA	1:B:283:MET:HB3	1.99	0.44
1:B:1095:LEU:HD12	1:B:1218:ARG:HA	1.99	0.44
1:A:411:ILE:HD11	1:A:567:LEU:HD22	1.98	0.44
1:B:335:LEU:HB3	2:C:1:ALA:HB1	1.99	0.44
1:B:1572:SER:HB2	1:B:1792:THR:HB	2.00	0.44
1:B:2049:VAL:O	1:B:2053:THR:OG1	2.24	0.44
1:B:2181:TYR:HA	1:B:2184:THR:HG22	1.98	0.44
1:B:3108:CYS:SG	1:B:3355:THR:HG21	2.57	0.44
1:B:3394:LEU:HD21	1:B:3448:ASP:HB3	1.98	0.44
1:A:2687:ASN:HB3	1:A:2690:ARG:HG3	1.99	0.44
1:B:2034:LEU:HA	1:B:2034:LEU:HD23	1.74	0.44
1:B:2073:LYS:O	1:B:2076:LEU:HG	2.18	0.44
1:B:3429:ASP:HA	1:B:3432:ILE:HD12	1.99	0.44
1:B:3711:LEU:HD23	1:B:3715:LEU:HD23	1.99	0.44
1:B:3987:LEU:HD21	1:B:4002:ILE:HD11	2.00	0.44
1:A:1881:HIS:CD2	1:A:1993:ARG:HH12	2.36	0.44
1:A:2096:LEU:HD23	1:A:2096:LEU:HA	1.83	0.44
1:A:2716:LEU:HA	1:A:2719:TRP:HB2	2.00	0.44
1:B:1122:VAL:HG22	1:B:1224:VAL:HG22	1.99	0.44
1:B:1170:LEU:HB3	1:B:1175:GLU:HG2	1.99	0.44
2:C:27:THR:HG21	2:C:116:ALA:HB2	1.99	0.44
1:A:3104:VAL:HA	1:A:3107:ILE:HG12	1.99	0.44
1:B:2084:GLN:NE2	1:B:2600:ASN:O	2.50	0.44
1:A:1808:THR:N	1:A:1841:SER:OG	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1993:ARG:HE	1:A:1994:LEU:HD12	1.83	0.44
1:A:2923:LEU:HA	1:A:2926:VAL:HG22	2.00	0.44
1:A:3209:ASP:OD1	1:A:3209:ASP:N	2.42	0.44
1:B:262:LEU:HA	1:B:376:PRO:HG3	1.99	0.44
1:B:961:LEU:HD23	1:B:961:LEU:HA	1.85	0.44
1:B:1033:THR:HA	1:B:1304:ARG:HG2	1.99	0.44
1:B:1101:VAL:HA	1:B:1305:ARG:NE	2.32	0.44
1:B:1332:VAL:O	1:B:1336:CYS:N	2.43	0.44
1:B:1574:SER:HB3	1:B:1790:PHE:H	1.82	0.44
2:D:140:GLU:OE2	2:D:147:ARG:NH2	2.51	0.44
1:A:2671:SER:HB3	1:A:2693:VAL:HG13	2.00	0.44
1:A:3813:LEU:HD23	1:A:4189:LEU:HD22	2.00	0.44
1:B:834:THR:HG23	1:B:836:ILE:H	1.83	0.44
1:B:3538:LEU:O	1:B:3542:VAL:HG23	2.18	0.44
1:B:3967:LEU:HD22	1:B:4004:LEU:HB3	2.00	0.44
1:A:1104:VAL:HG13	1:A:1203:LEU:HB2	2.00	0.43
1:A:2094:GLN:NE2	1:A:2098:ASN:OD1	2.38	0.43
1:A:3050:VAL:HA	1:A:3053:MET:HE3	1.99	0.43
1:B:4396:LEU:HD11	1:B:4481:ILE:HG12	2.00	0.43
1:A:2387:LEU:HA	1:A:2387:LEU:HD13	1.75	0.43
1:A:2412:LEU:HA	1:A:2415:ILE:HG22	2.00	0.43
1:B:318:PRO:HA	1:B:325:ARG:HB3	1.99	0.43
1:B:1508:PHE:CE1	1:B:2022:GLN:HB2	2.53	0.43
1:B:2749:ALA:HA	1:B:2752:LEU:HG	2.00	0.43
1:B:2875:ASP:OD1	1:B:2875:ASP:N	2.48	0.43
1:B:3058:LEU:HA	1:B:3061:MET:HE2	2.00	0.43
1:B:3240:SER:HB3	1:B:3256:PRO:HG3	1.99	0.43
1:A:1083:SER:HA	1:A:1086:TRP:HB3	2.00	0.43
1:A:3856:ARG:HA	1:A:3856:ARG:HD2	1.82	0.43
1:B:717:VAL:HG11	1:B:836:ILE:HG21	2.00	0.43
1:B:3991:TYR:CE1	1:B:3997:GLN:HA	2.54	0.43
1:A:91:ILE:HD12	1:A:107:LEU:HD21	2.00	0.43
1:A:272:VAL:HG21	1:A:292:THR:HA	2.01	0.43
1:A:3990:LEU:HB3	1:A:3995:LEU:HD22	1.99	0.43
1:B:283:MET:HE2	1:B:315:TYR:HB3	1.99	0.43
1:B:399:PHE:HB3	1:B:411:ILE:HG22	2.00	0.43
1:B:1399:SER:O	1:B:1403:LYS:HG2	2.19	0.43
1:B:1779:ILE:HD11	1:B:1872:LYS:HG2	1.99	0.43
1:B:3241:VAL:HG22	1:B:3280:LEU:HD13	2.00	0.43
1:B:3347:MET:O	1:B:3350:SER:OG	2.29	0.43
1:B:3817:LEU:O	1:B:4182:GLN:NE2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2813:LEU:HD23	1:A:2848:PHE:HE2	1.82	0.43
1:A:2915:ARG:HH22	1:B:2772:HIS:C	2.26	0.43
1:A:3040:LEU:HA	1:A:3040:LEU:HD23	1.73	0.43
1:B:395:SER:HG	1:B:514:GLN:H	1.65	0.43
1:B:414:VAL:HG12	1:B:418:MET:HE1	2.00	0.43
1:B:1029:THR:HG22	1:B:1358:TRP:CE3	2.54	0.43
1:B:3167:GLY:HA2	1:B:3215:PRO:HD3	2.00	0.43
1:B:3866:LEU:HA	1:B:3869:VAL:HG22	2.01	0.43
2:D:38:THR:HG23	2:D:139:VAL:HG23	2.00	0.43
1:A:347:GLU:OE1	1:A:350:ARG:NH1	2.52	0.43
1:A:565:PRO:HD2	1:A:636:LYS:HB2	2.00	0.43
1:A:1480:GLN:O	1:A:1480:GLN:NE2	2.52	0.43
1:A:1581:ARG:HH11	1:A:1776:GLN:HE21	1.67	0.43
1:A:1872:LYS:HD2	1:A:1874:PRO:HD3	2.01	0.43
1:A:3328:ILE:HA	1:A:3331:LEU:HB2	2.00	0.43
1:B:1914:LEU:HD12	1:B:1994:LEU:HB3	2.00	0.43
1:B:2697:ASN:OD1	1:B:2698:GLN:N	2.52	0.43
1:B:2716:LEU:HA	1:B:2719:TRP:HD1	1.84	0.43
1:B:3225:ILE:O	1:B:3265:ILE:HB	2.19	0.43
1:B:749:LEU:O	1:B:823:GLY:CA	2.67	0.43
1:A:838:THR:HG22	1:A:839:LEU:H	1.84	0.43
1:A:934:THR:HG23	1:A:936:GLU:H	1.84	0.43
1:A:4370:ILE:HA	1:A:4373:MET:HG2	2.00	0.43
1:B:289:ARG:O	1:B:292:THR:OG1	2.35	0.43
1:B:859:LEU:HB2	1:B:903:LEU:HD11	1.99	0.43
1:B:1432:LEU:HD22	1:B:1455:LEU:HD13	2.00	0.43
1:B:2366:ARG:HD3	1:B:2366:ARG:HA	1.81	0.43
1:A:3190:ARG:HD3	2:C:117:TYR:CZ	2.53	0.43
1:B:2321:PHE:HB3	1:B:2322:THR:H	1.67	0.43
1:B:2389:GLY:HA2	1:B:2655:VAL:HA	2.01	0.43
1:A:2104:TYR:O	1:A:2167:MET:HE1	2.19	0.43
1:A:2575:LEU:O	1:A:2578:GLN:NE2	2.50	0.43
1:A:2671:SER:OG	1:A:2691:ILE:O	2.27	0.43
1:A:3621:GLU:OE1	1:A:3621:GLU:N	2.47	0.43
1:B:396:CYS:HB2	1:B:514:GLN:HB2	2.00	0.43
1:B:3435:LEU:HA	1:B:3435:LEU:HD23	1.84	0.43
1:B:4432:SER:HB3	1:B:4496:ARG:HH12	1.84	0.43
2:D:42:ILE:HD11	2:D:138:GLN:HB3	2.00	0.43
2:D:52:VAL:HG13	2:D:153:LEU:HD22	2.01	0.43
1:A:1122:VAL:HG22	1:A:1224:VAL:HG22	2.00	0.42
1:A:2758:LEU:HA	1:A:2761:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ILE:HA	1:B:101:THR:HA	2.00	0.42
1:B:2072:PRO:HA	1:B:2075:ARG:HD2	2.00	0.42
1:B:2812:LEU:O	1:B:2816:ILE:HG12	2.19	0.42
1:B:2994:ILE:HD12	1:B:3040:LEU:HD21	1.99	0.42
1:B:3250:MET:HE3	1:B:3279:CYS:HB2	2.01	0.42
1:B:4324:LEU:HD22	1:B:4398:LEU:HD22	2.01	0.42
1:A:1309:THR:HG23	1:A:1311:ILE:H	1.83	0.42
1:A:1931:ALA:HA	1:A:1934:ARG:HH21	1.83	0.42
1:A:3240:SER:OG	1:A:3281:ARG:HB3	2.19	0.42
1:A:3502:TRP:NE1	1:A:3506:GLU:OE2	2.52	0.42
1:B:2915:ARG:HG3	1:B:2919:MET:HE1	2.01	0.42
1:B:3862:VAL:O	1:B:3982:THR:OG1	2.37	0.42
1:A:2073:LYS:O	1:A:2077:HIS:ND1	2.51	0.42
1:A:2354:VAL:HA	1:A:2357:VAL:HG22	2.00	0.42
1:A:2586:MET:HA	1:A:2589:LEU:HG	2.00	0.42
1:A:2715:LEU:O	1:A:2718:THR:OG1	2.29	0.42
1:B:854:ASP:HA	1:B:907:THR:HB	2.02	0.42
1:B:1479:ARG:HA	1:B:2065:HIS:CE1	2.54	0.42
1:B:1492:LEU:HG	1:B:1498:LEU:HB2	2.00	0.42
1:A:1182:LEU:HD13	1:A:1208:LEU:HD12	2.02	0.42
1:A:1332:VAL:HA	1:A:1335:LEU:HD12	2.02	0.42
1:A:1371:LYS:HE3	1:A:1374:ASN:HD22	1.85	0.42
1:A:1935:LEU:HD23	1:A:1939:LEU:HD23	2.00	0.42
1:A:3602:PRO:HB2	1:A:3603:LEU:H	1.70	0.42
1:A:3785:LEU:HA	1:A:3788:LEU:HG	2.00	0.42
1:B:1388:ILE:HA	1:B:1391:VAL:HG22	2.01	0.42
1:B:1470:CYS:SG	1:B:2034:LEU:HD21	2.59	0.42
1:B:2135:LEU:HD13	1:B:2138:LEU:HD21	2.00	0.42
1:B:3400:LEU:HD12	1:B:3401:LEU:HG	2.00	0.42
1:A:951:ARG:HH22	1:A:1132:LEU:HB3	1.84	0.42
1:A:1171:CYS:SG	1:A:1225:LYS:HG3	2.59	0.42
1:A:2121:LEU:HA	1:A:2124:ILE:HG12	2.01	0.42
1:A:4080:LEU:HA	1:A:4083:ILE:HG12	2.01	0.42
1:B:4373:MET:HE3	1:B:4377:LEU:HG	2.00	0.42
1:A:3327:SER:HA	1:A:3330:TRP:HE3	1.85	0.42
1:B:1929:ASN:O	1:B:1933:HIS:HB2	2.20	0.42
1:B:2094:GLN:NE2	1:B:2098:ASN:OD1	2.42	0.42
1:B:2867:VAL:HG11	1:B:2922:LEU:HD11	2.02	0.42
1:B:3856:ARG:HD2	1:B:3856:ARG:HA	1.87	0.42
1:B:4153:ILE:HG23	1:B:4210:PRO:HG3	2.02	0.42
1:B:4393:ARG:HH22	1:B:4484:THR:HG21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1380:LYS:HA	1:A:1380:LYS:HD3	1.82	0.42
1:A:3400:LEU:HD11	1:A:3435:LEU:HD21	2.01	0.42
1:B:184:SER:HA	1:B:189:TYR:CD2	2.55	0.42
1:B:2356:LYS:HA	1:B:2356:LYS:HD3	1.82	0.42
1:B:2934:LEU:N	1:B:2978:ALA:O	2.37	0.42
1:B:3187:PRO:HB2	1:B:3189:HIS:CE1	2.55	0.42
2:C:45:ILE:O	2:C:49:THR:OG1	2.24	0.42
1:A:306:PRO:HA	1:A:309:MET:HE2	2.02	0.42
1:A:2601:THR:OG1	1:A:2602:SER:N	2.53	0.42
1:A:3328:ILE:HA	1:A:3331:LEU:HD12	2.01	0.42
1:B:1041:THR:OG1	1:B:1092:GLU:HB3	2.19	0.42
1:A:2112:PHE:CE2	1:A:2114:GLN:HG2	2.55	0.42
1:A:2121:LEU:HD23	1:A:2121:LEU:HA	1.95	0.42
1:A:2142:LEU:HD21	1:A:2175:VAL:HG11	2.02	0.42
1:A:3454:LEU:HA	1:A:3457:VAL:HG12	2.01	0.42
1:A:3490:SER:HB3	1:A:3493:HIS:ND1	2.35	0.42
1:A:3967:LEU:HB3	1:A:3977:LEU:HD12	2.02	0.42
1:B:1380:LYS:HA	1:B:1380:LYS:HD3	1.82	0.42
1:B:2368:THR:HG21	1:B:2418:GLY:HA3	2.02	0.42
1:B:3341:ILE:HG22	1:B:3343:ASP:H	1.84	0.42
1:B:3991:TYR:HE1	1:B:3997:GLN:HA	1.85	0.42
1:B:70:LEU:HG	1:B:959:GLY:HA2	2.01	0.42
1:B:120:ILE:O	1:B:124:ASP:N	2.53	0.42
1:B:2338:PHE:O	1:B:2342:MET:HE3	2.20	0.42
1:B:2809:SER:HA	1:B:2812:LEU:HG	2.01	0.42
1:A:1359:LEU:HA	1:A:1362:VAL:HG22	2.01	0.41
1:A:2242:LEU:HA	1:A:2242:LEU:HD23	1.77	0.41
1:A:4373:MET:O	1:A:4377:LEU:HG	2.19	0.41
1:B:1092:GLU:OE1	1:B:1127:ASN:ND2	2.53	0.41
1:B:2994:ILE:HG13	1:B:2995:LEU:HD12	2.02	0.41
1:B:3990:LEU:HB3	1:B:3995:LEU:HD22	2.02	0.41
1:A:1345:THR:OG1	1:A:1346:GLU:OE1	2.36	0.41
1:A:4214:PHE:HB3	1:A:4326:VAL:HG21	2.02	0.41
1:B:1569:THR:OG1	1:B:1794:ASP:O	2.22	0.41
1:B:1808:THR:OG1	1:B:1841:SER:OG	2.25	0.41
1:B:3085:ILE:HA	1:B:3088:VAL:HG12	2.01	0.41
1:A:4233:LEU:HA	1:A:4236:ARG:HG2	2.02	0.41
1:B:399:PHE:HA	1:B:412:TRP:O	2.20	0.41
1:B:1218:ARG:HA	1:B:1218:ARG:HD3	1.94	0.41
1:B:2029:TYR:O	1:B:2033:THR:HG23	2.21	0.41
1:B:2351:LEU:HD23	1:B:2351:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3164:ALA:O	1:B:3183:LEU:HD12	2.20	0.41
1:A:1385:LEU:HD21	1:A:1428:LEU:HD13	2.03	0.41
1:A:1778:ILE:HB	1:A:1873:ILE:HB	2.01	0.41
1:A:3129:ILE:HD12	1:A:3129:ILE:HA	1.95	0.41
1:A:3967:LEU:HB2	1:A:3977:LEU:HB2	2.03	0.41
1:B:3124:SER:OG	1:B:3125:MET:N	2.53	0.41
1:B:3555:ASN:N	1:B:3555:ASN:OD1	2.51	0.41
2:C:111:MET:HE1	2:D:108:LEU:HA	2.02	0.41
1:A:98:SER:OG	1:A:212:LYS:NZ	2.53	0.41
1:A:1331:LEU:O	1:A:1334:THR:OG1	2.24	0.41
1:A:2255:GLN:HG3	2:C:21:ARG:NH1	2.35	0.41
1:A:2812:LEU:HD11	1:A:2848:PHE:HZ	1.85	0.41
1:A:3253:LEU:HD13	1:B:2717:ARG:HE	1.85	0.41
1:A:3341:ILE:HG22	1:A:3343:ASP:H	1.84	0.41
1:B:1804:VAL:HG12	1:B:1844:LEU:HB3	2.02	0.41
1:B:1885:LEU:HB2	1:B:1888:GLU:CD	2.46	0.41
1:A:2324:ALA:H	1:A:2327:ARG:NH2	2.17	0.41
1:A:2697:ASN:O	1:A:2701:ILE:HG13	2.20	0.41
1:A:2916:ASP:HA	1:A:2919:MET:HE2	2.02	0.41
1:A:3243:VAL:HG12	1:A:3278:VAL:HG22	2.03	0.41
1:A:3335:HIS:O	1:A:3339:THR:OG1	2.20	0.41
1:A:4072:GLN:HG2	1:A:4175:LEU:HD22	2.01	0.41
1:B:1182:LEU:HD23	1:B:1182:LEU:HA	1.88	0.41
1:B:1784:HIS:H	1:B:1787:ALA:HB2	1.85	0.41
1:B:2121:LEU:HA	1:B:2124:ILE:HG12	2.03	0.41
1:B:2562:SER:OG	1:B:2563:VAL:N	2.51	0.41
1:B:3196:ALA:HB3	1:B:3294:SER:HA	2.03	0.41
2:D:52:VAL:O	2:D:56:THR:OG1	2.34	0.41
1:A:1788:ARG:NH1	1:A:1790:PHE:HB2	2.32	0.41
1:A:3050:VAL:HA	1:A:3053:MET:HG2	2.03	0.41
1:B:2800:LEU:HD23	1:B:2800:LEU:HA	1.69	0.41
1:B:3163:PHE:CZ	1:B:3302:THR:HG23	2.56	0.41
1:B:3197:TRP:CH2	1:B:3199:TYR:HB2	2.55	0.41
1:B:3698:ILE:HD12	1:B:3698:ILE:HA	1.94	0.41
1:B:3756:ARG:HA	1:B:3759:ILE:HG22	2.03	0.41
1:A:391:PHE:HA	1:A:510:LEU:HD12	2.03	0.41
1:A:2344:PHE:CE1	1:B:3120:ASN:HB2	2.55	0.41
1:A:3177:GLN:OE1	1:A:3177:GLN:N	2.53	0.41
1:A:4260:ARG:HG2	1:A:4367:SER:O	2.21	0.41
1:B:565:PRO:HD2	1:B:636:LYS:HB2	2.03	0.41
1:B:1790:PHE:HA	1:B:1858:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2797:GLN:O	1:B:2801:SER:OG	2.21	0.41
1:B:4435:THR:O	1:B:4439:LYS:HG3	2.20	0.41
2:D:116:ALA:HB3	2:D:125:SER:HB2	2.02	0.41
1:A:1104:VAL:HG23	1:A:1303:ILE:HG13	2.02	0.41
1:A:1330:LYS:O	1:A:1333:ASN:HB2	2.21	0.41
1:A:2141:LEU:O	1:A:2145:LEU:HB2	2.20	0.41
1:A:2643:PHE:HB3	1:A:2647:PHE:CZ	2.56	0.41
1:A:2795:ARG:HA	1:A:2798:VAL:HG12	2.03	0.41
1:A:3052:MET:HB3	1:A:3052:MET:HE3	1.80	0.41
1:A:3330:TRP:HA	1:A:3333:LEU:HD12	2.03	0.41
1:B:411:ILE:HD12	1:B:422:LEU:HD12	2.03	0.41
1:B:1182:LEU:HD12	1:B:1220:PHE:HE1	1.85	0.41
1:B:1377:LEU:O	1:B:1381:THR:OG1	2.26	0.41
1:B:1432:LEU:HD23	1:B:1451:TYR:CE1	2.56	0.41
1:B:1534:LEU:HB2	1:B:2119:MET:HE1	2.03	0.41
1:B:2083:VAL:HG21	1:B:2127:ARG:HB2	2.02	0.41
1:B:3177:GLN:N	1:B:3177:GLN:OE1	2.53	0.41
1:B:3526:PHE:HE1	1:B:3612:THR:HG21	1.86	0.41
1:B:3719:LEU:HD13	1:B:3807:PHE:HD2	1.85	0.41
1:B:4237:MET:O	1:B:4241:ILE:HG12	2.21	0.41
1:A:186:THR:HG21	1:A:231:ILE:HA	2.03	0.41
1:A:2041:SER:O	1:A:2044:HIS:ND1	2.53	0.41
1:A:2074:ILE:HD12	1:A:2074:ILE:HA	1.87	0.41
1:A:2813:LEU:HD23	1:A:2848:PHE:CE2	2.56	0.41
1:A:3321:ASP:O	1:A:3325:LYS:NZ	2.47	0.41
1:B:277:SER:HA	1:B:317:GLN:NE2	2.36	0.41
1:B:567:LEU:HB2	1:B:635:ILE:HD11	2.03	0.41
1:B:1046:TRP:CE2	1:B:1079:LEU:HD13	2.55	0.41
1:B:2063:PHE:CZ	1:B:2082:LEU:HD12	2.56	0.41
1:B:2844:LEU:HD23	1:B:2925:LEU:HD13	2.03	0.41
1:B:2846:GLN:HB2	1:B:2848:PHE:CZ	2.56	0.41
1:B:3778:GLN:HB3	1:B:4073:VAL:HG11	2.02	0.41
1:A:85:VAL:HG21	1:A:117:CYS:HB3	2.03	0.40
1:A:129:VAL:HG21	1:A:391:PHE:CG	2.56	0.40
1:A:1347:HIS:O	1:A:1351:LEU:HG	2.21	0.40
1:A:1438:PHE:HB3	1:A:2005:LEU:HD13	2.03	0.40
1:A:2200:GLN:NE2	1:A:2413:GLN:OE1	2.41	0.40
1:A:2794:THR:O	1:A:2797:GLN:HG3	2.21	0.40
1:A:3225:ILE:HB	1:A:3265:ILE:HB	2.03	0.40
1:B:1006:ILE:HD13	1:B:1316:VAL:HG12	2.03	0.40
1:B:1988:HIS:HA	1:B:1991:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:108:LEU:HD21	2:D:112:ALA:HB2	2.02	0.40
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.94	0.40
1:A:1453:VAL:HG13	1:A:2586:MET:SD	2.61	0.40
1:A:1795:PHE:HB3	1:A:1799:ILE:HD12	2.03	0.40
1:A:2838:LYS:HA	1:A:2841:GLU:HG2	2.01	0.40
1:A:3707:GLU:HG2	1:A:3708:VAL:HG23	2.03	0.40
1:B:270:LEU:HD12	1:B:270:LEU:HA	1.93	0.40
1:B:1309:THR:HG23	1:B:1311:ILE:H	1.87	0.40
1:B:1374:ASN:HA	1:B:1377:LEU:HG	2.04	0.40
1:B:3246:ASP:N	1:B:3246:ASP:OD1	2.48	0.40
1:A:163:LEU:HD12	1:A:259:LEU:HD21	2.04	0.40
1:A:627:LEU:HD12	1:A:628:PRO:HD2	2.02	0.40
1:A:1816:SER:HB2	1:A:1833:VAL:HG22	2.03	0.40
1:A:2145:LEU:HD23	1:A:2168:ILE:HD13	2.03	0.40
1:A:3098:PHE:CE1	1:A:3103:GLY:HA3	2.57	0.40
1:B:1074:THR:HG22	1:B:1302:THR:HG23	2.04	0.40
1:B:1105:ASP:OD2	1:B:1304:ARG:NH2	2.39	0.40
1:A:1841:SER:O	1:A:2564:SER:OG	2.35	0.40
1:A:4239:LEU:HD23	1:A:4244:LEU:HD12	2.02	0.40
1:B:1471:ALA:HA	1:B:1474:LEU:HD12	2.04	0.40
1:B:1816:SER:HA	1:B:1832:VAL:O	2.20	0.40
2:D:113:ALA:HB3	2:D:129:ARG:NH1	2.36	0.40
1:A:2840:LEU:HD12	1:A:2840:LEU:HA	1.83	0.40
1:A:3794:GLN:HG2	1:A:4086:ARG:HH12	1.87	0.40
1:A:4225:PRO:HA	1:A:4333:PRO:HG3	2.03	0.40
1:B:2601:THR:OG1	1:B:2602:SER:N	2.54	0.40
1:B:3542:VAL:O	1:B:3546:LEU:HG	2.21	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	2806/4867 (58%)	2734 (97%)	71 (2%)	1 (0%)	100	100
1	B	2738/4867 (56%)	2670 (98%)	68 (2%)	0	100	100
2	C	157/184 (85%)	156 (99%)	1 (1%)	0	100	100
2	D	155/184 (84%)	154 (99%)	1 (1%)	0	100	100
All	All	5856/10102 (58%)	5714 (98%)	141 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2265	LYS

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	2556/4225 (60%)	2556 (100%)	0	100	100
1	B	2491/4225 (59%)	2491 (100%)	0	100	100
2	C	138/157 (88%)	138 (100%)	0	100	100
2	D	135/157 (86%)	135 (100%)	0	100	100
All	All	5320/8764 (61%)	5320 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	202	ASN
1	A	298	HIS
1	A	853	GLN
1	A	1323	GLN
1	A	1347	HIS
1	A	1365	ASN

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Mol	Chain	Res	Type
1	A	1374	ASN
1	A	1771	GLN
1	A	1925	GLN
1	A	1951	ASN
1	A	1983	GLN
1	A	2264	ASN
1	A	2644	ASN
1	A	2651	GLN
1	A	2653	HIS
1	A	2670	ASN
1	A	2931	GLN
1	A	3051	HIS
1	A	3213	HIS
1	A	3224	HIS
1	A	3226	GLN
1	A	3228	HIS
1	A	3335	HIS
1	A	3377	ASN
1	A	3403	ASN
1	A	3451	GLN
1	A	3754	GLN
1	A	3985	GLN
1	A	4332	ASN
1	B	64	HIS
1	B	298	HIS
1	B	853	GLN
1	B	908	GLN
1	B	1111	ASN
1	B	1297	GLN
1	B	1333	ASN
1	B	1376	ASN
1	B	1913	HIS
1	B	1975	GLN
1	B	2596	GLN
1	B	2644	ASN
1	B	2670	ASN
1	B	2790	GLN
1	B	2827	GLN
1	B	2993	GLN
1	B	3224	HIS
1	B	3403	ASN
1	B	3451	GLN

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Mol	Chain	Res	Type
1	B	3527	ASN
1	B	3754	GLN
1	B	3761	ASN
1	B	3769	GLN
1	B	3790	GLN
1	B	3985	GLN
1	B	4072	GLN
2	D	11	HIS
2	D	92	HIS
2	D	118	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are 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.

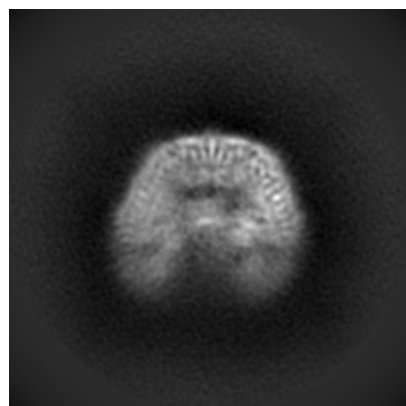
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15675. These allow visual inspection of the internal detail of the map and identification of artifacts.

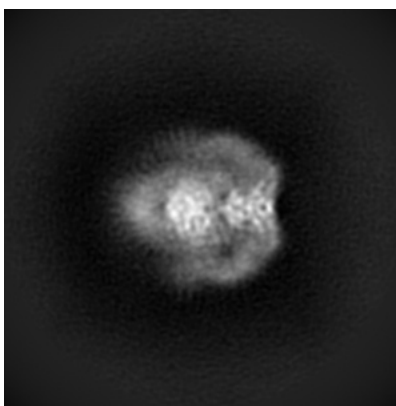
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

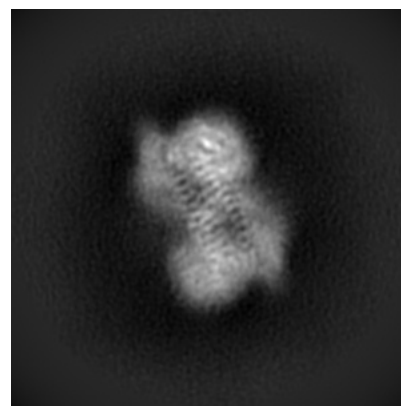
6.1.1 Primary map



X

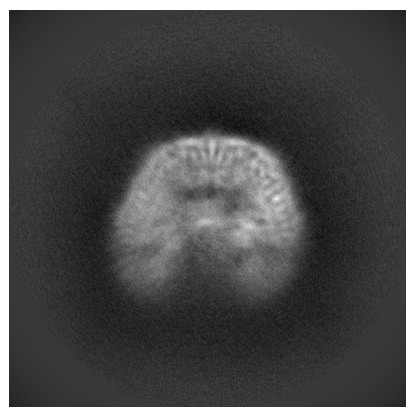


Y

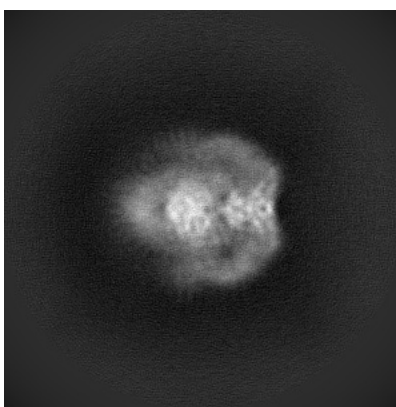


Z

6.1.2 Raw map



X



Y

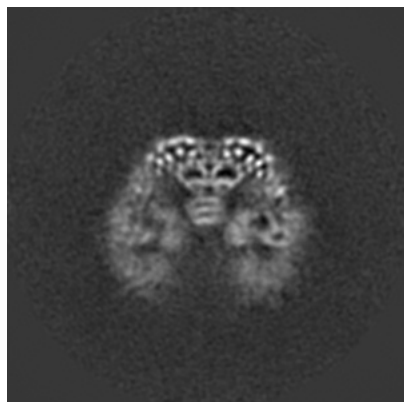


Z

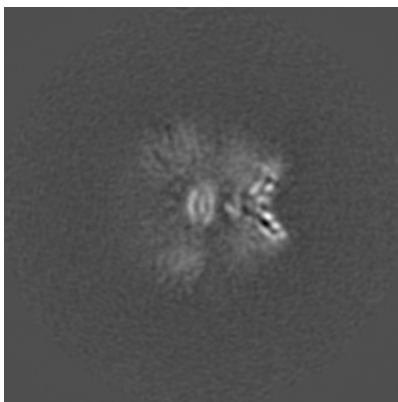
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

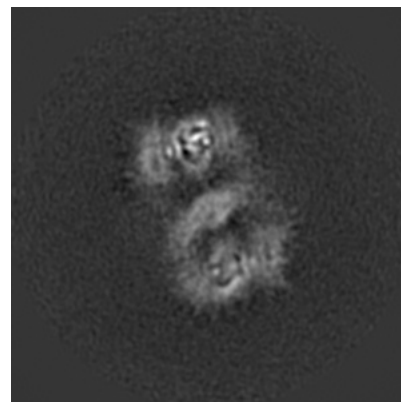
6.2.1 Primary map



X Index: 150

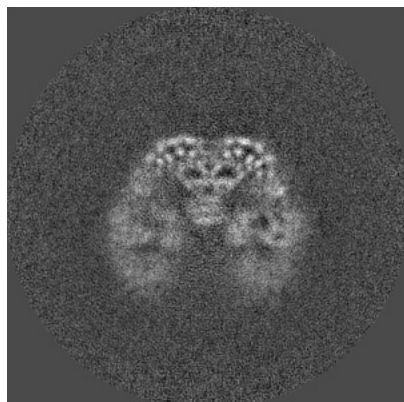


Y Index: 150

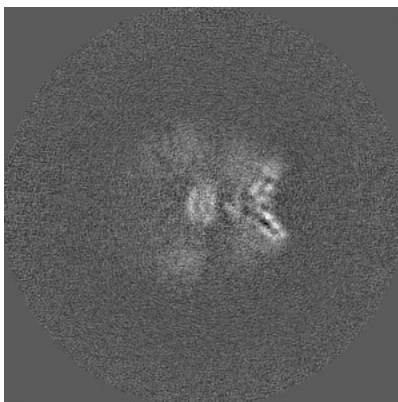


Z Index: 150

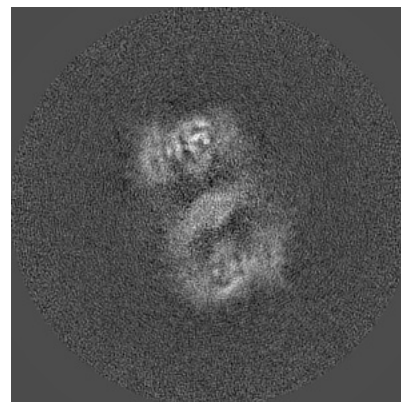
6.2.2 Raw map



X Index: 150



Y Index: 150

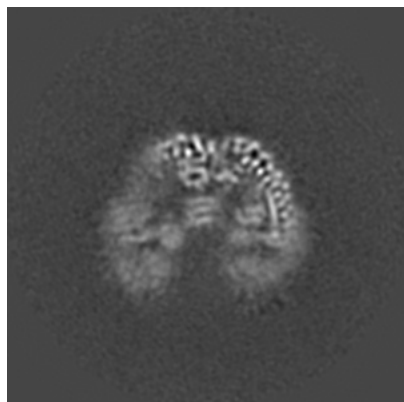


Z Index: 150

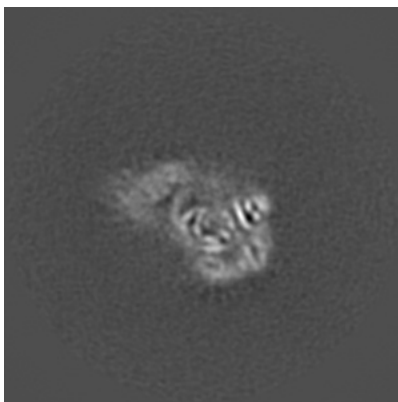
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

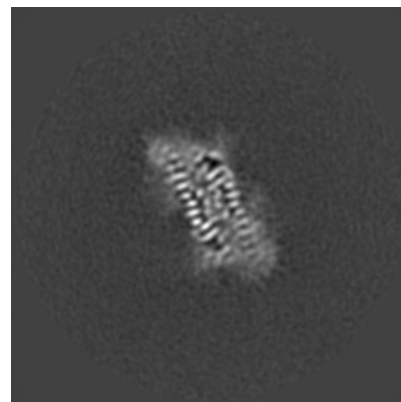
6.3.1 Primary map



X Index: 146

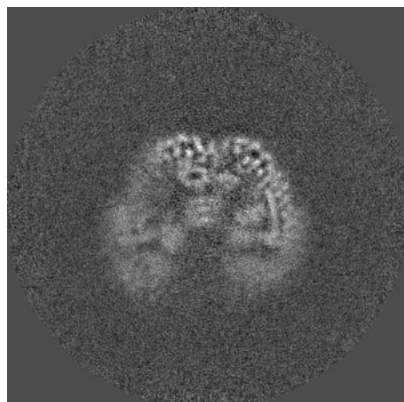


Y Index: 189

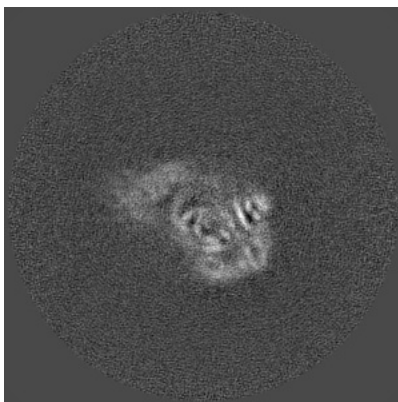


Z Index: 191

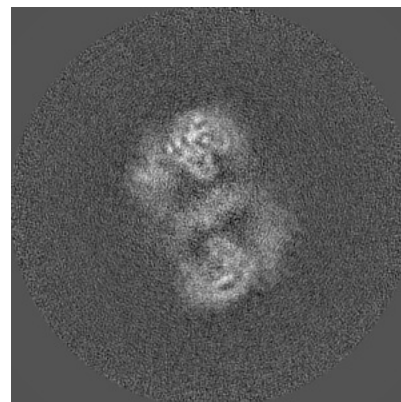
6.3.2 Raw map



X Index: 147



Y Index: 189

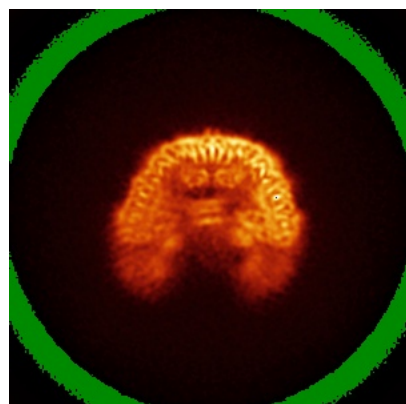


Z Index: 145

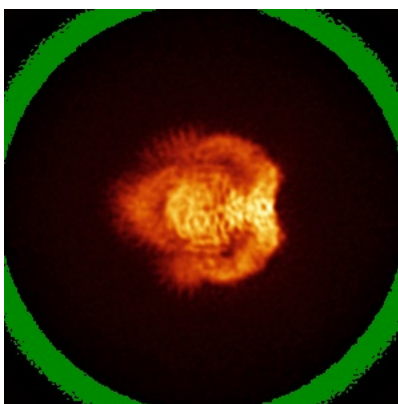
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

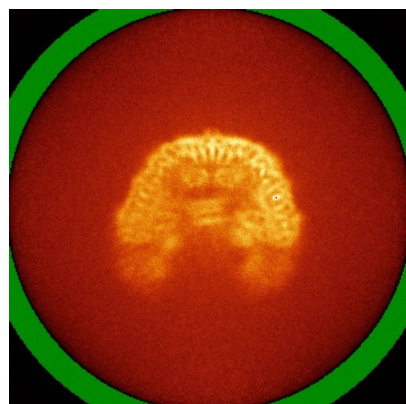


Y

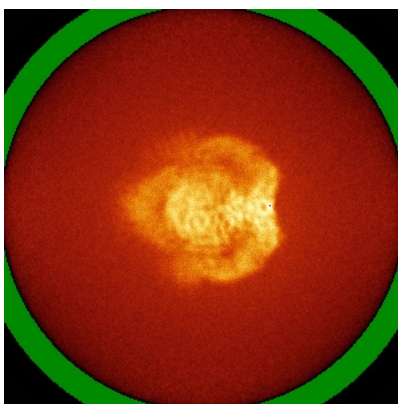


Z

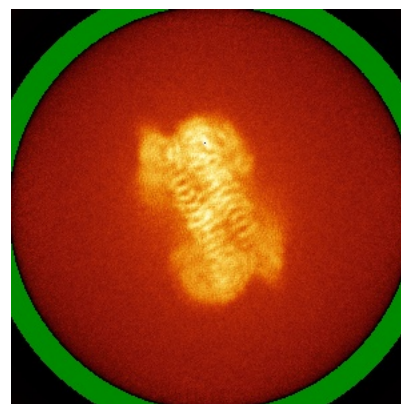
6.4.2 Raw map



X



Y

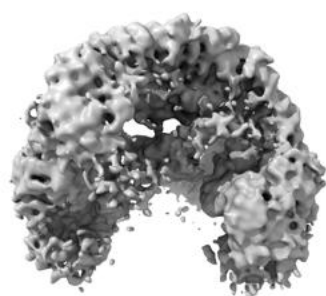


Z

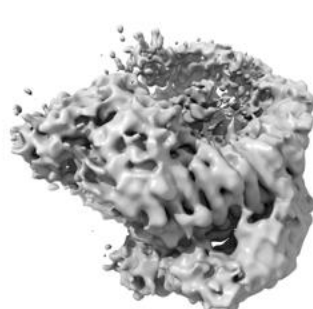
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

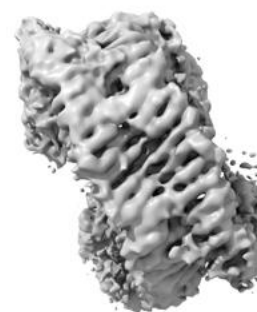
6.5.1 Primary map



X



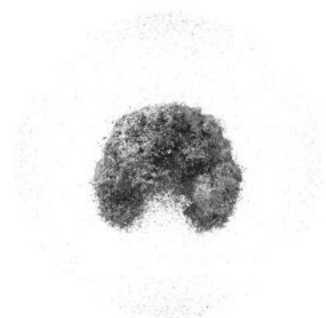
Y



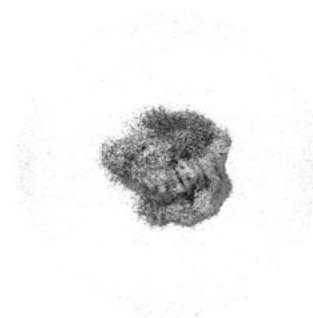
Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

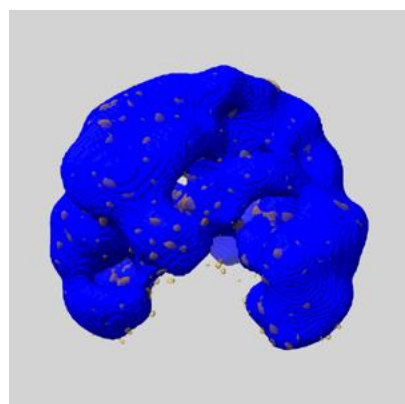
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

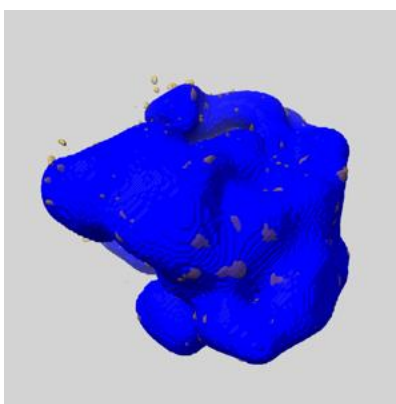
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

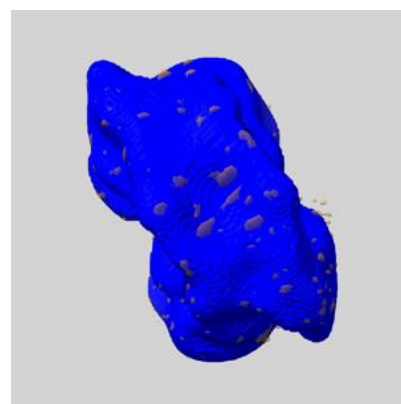
6.6.1 emd_15675_msk_1.map [i](#)



X



Y

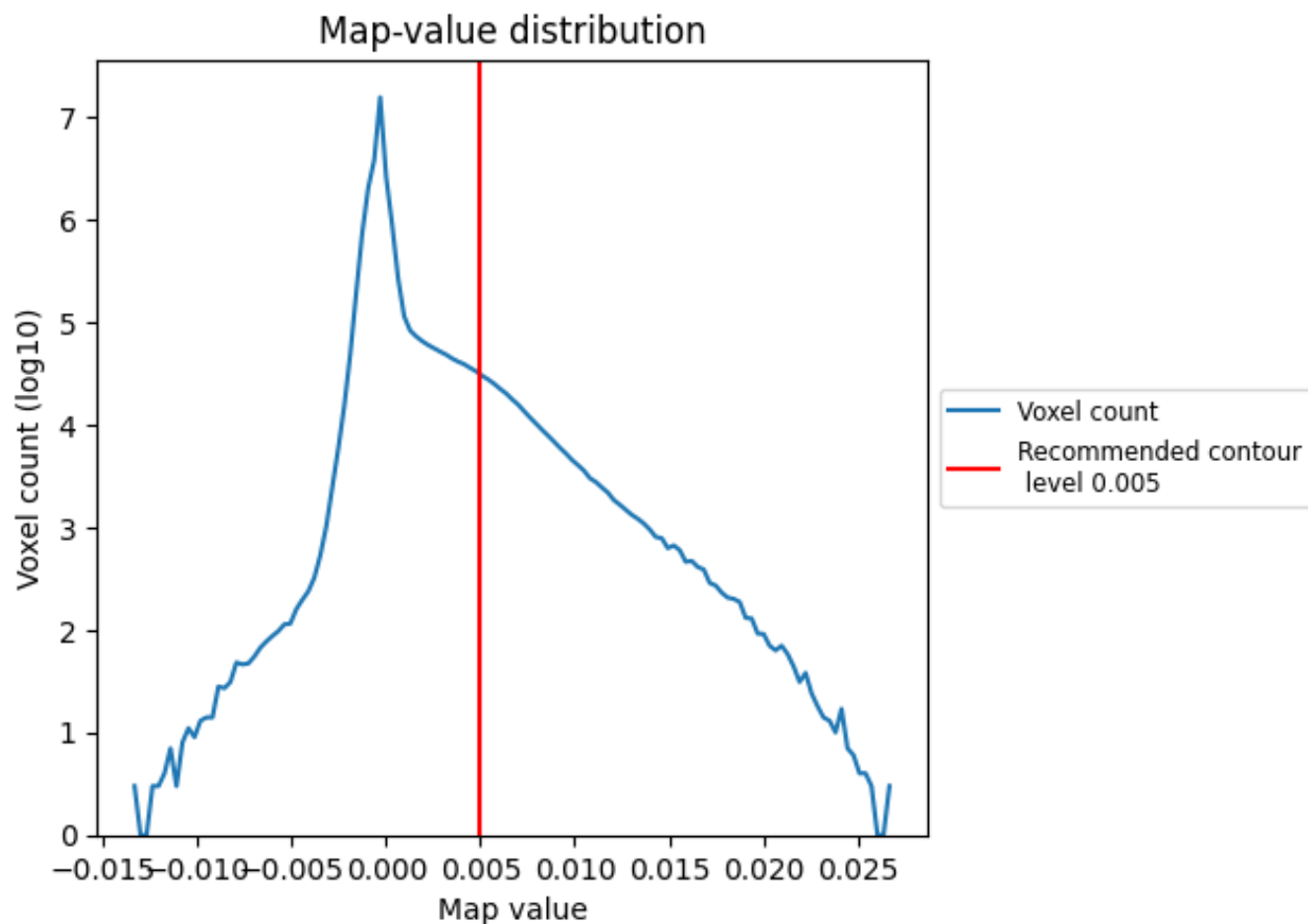


Z

7 Map analysis [i](#)

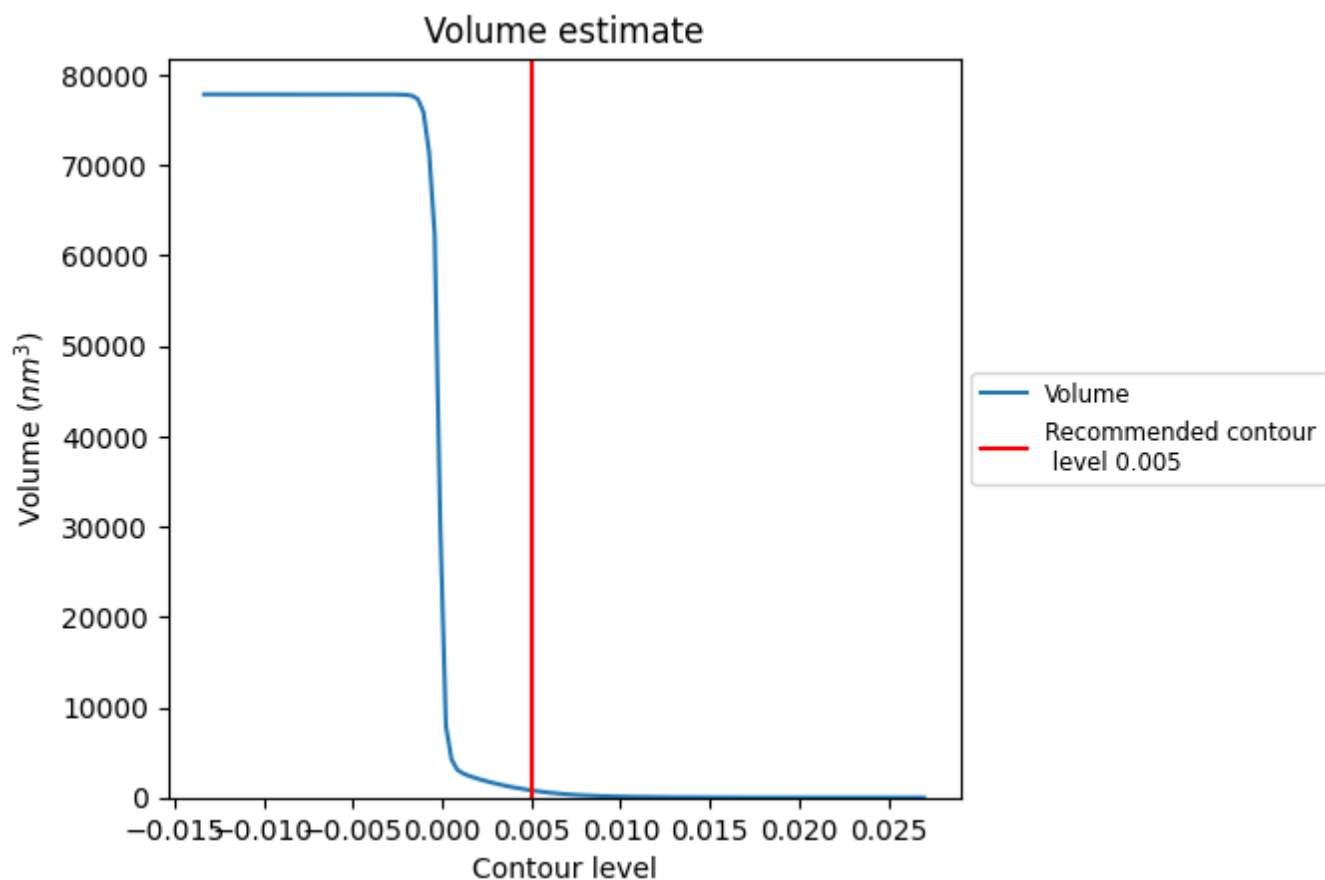
This section contains the results of statistical analysis of the map.

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.

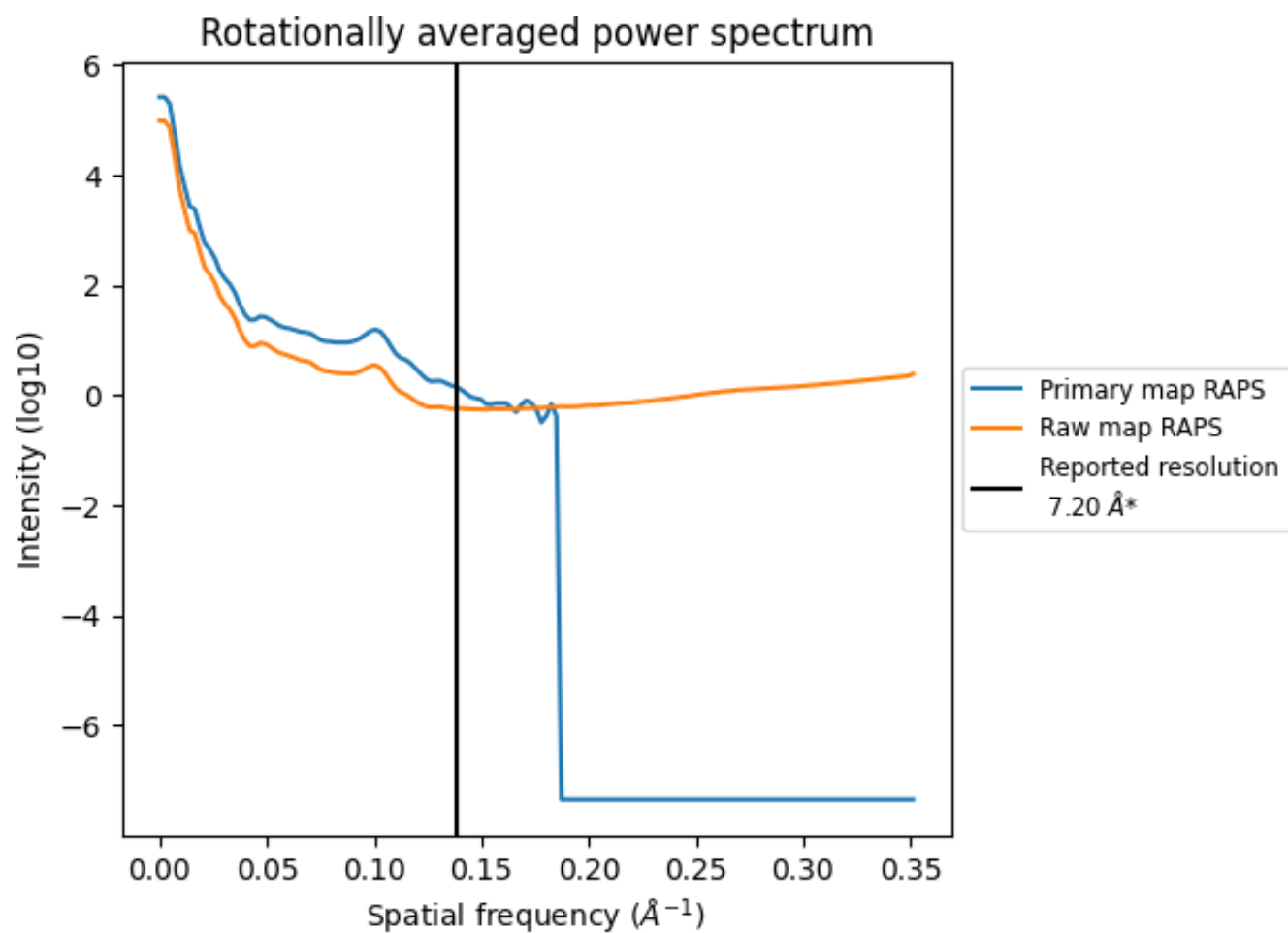
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 800 nm^3 ; this corresponds to an approximate mass of 723 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 ⓘ

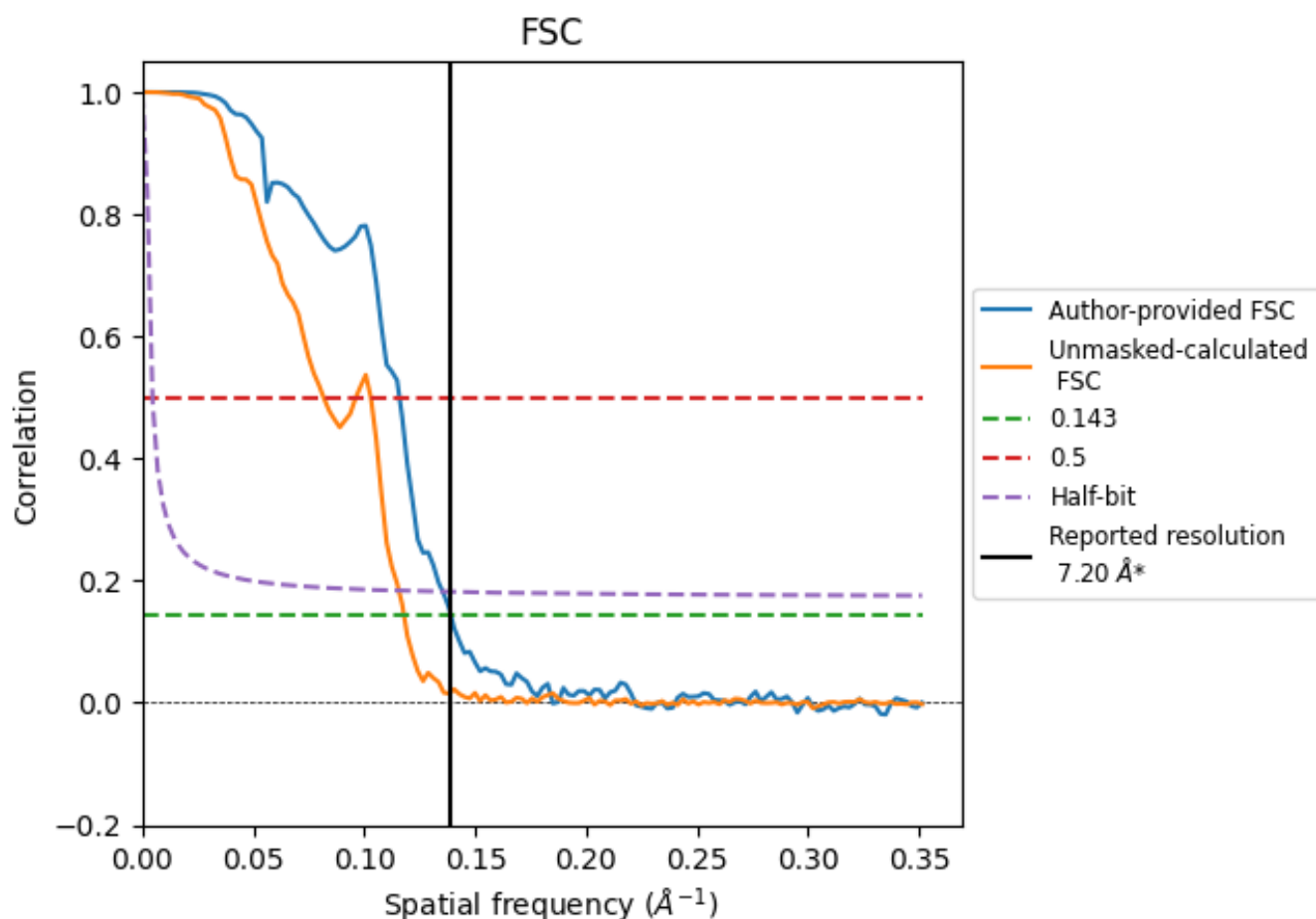


*Reported resolution corresponds to spatial frequency of 0.139 $\text{\AA}^{-1}$

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 0.139 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

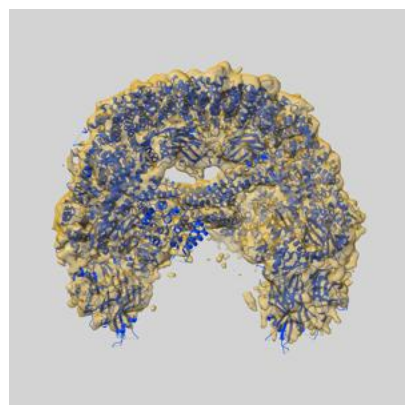
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.20	-	-
Author-provided FSC curve	7.19	8.64	7.39
Unmasked-calculated*	8.48	12.24	8.65

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.48 differs from the reported value 7.2 by more than 10 %

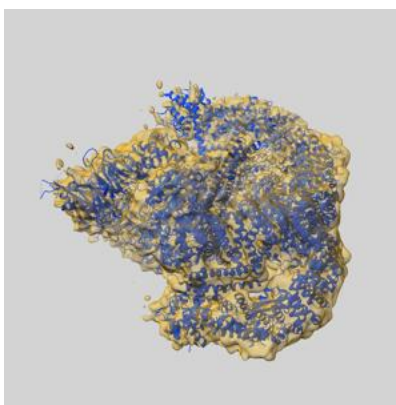
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15675 and PDB model 8AUW. Per-residue inclusion information can be found in section [3](#) on page [5](#).

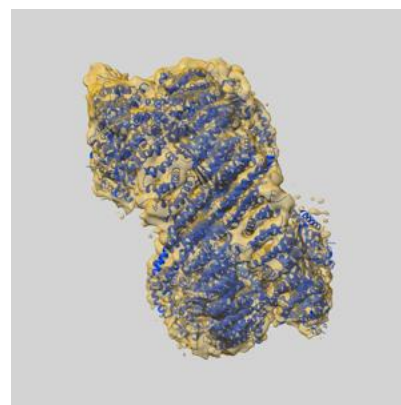
9.1 Map-model overlay [i](#)



X



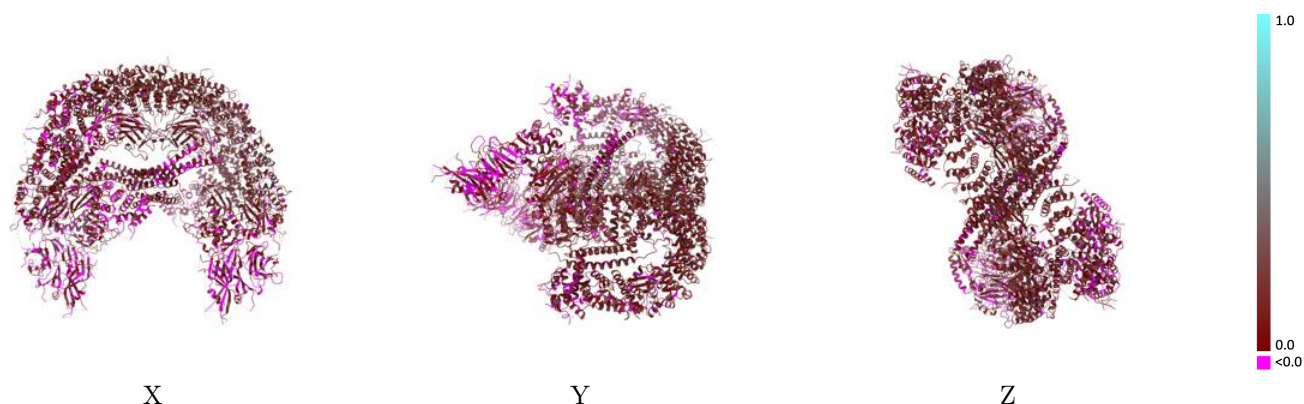
Y



Z

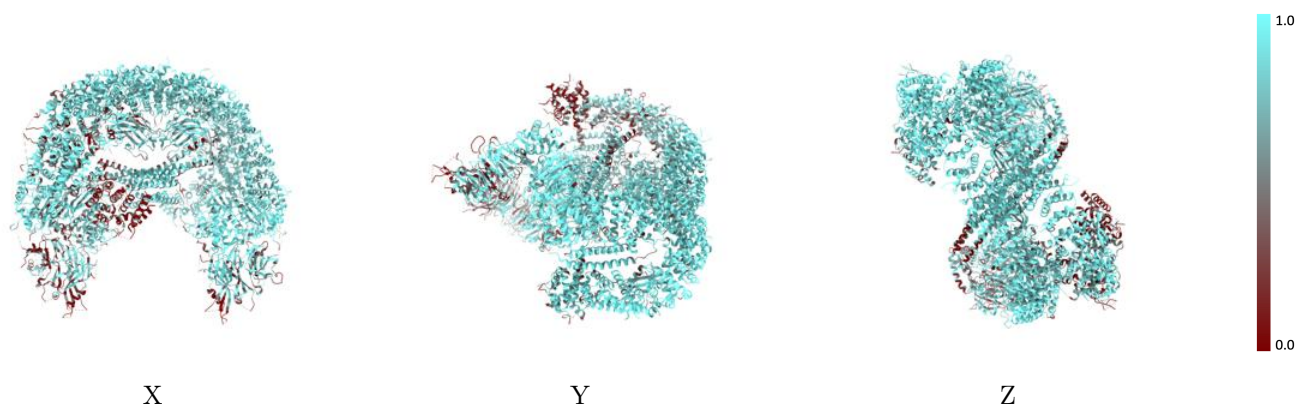
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



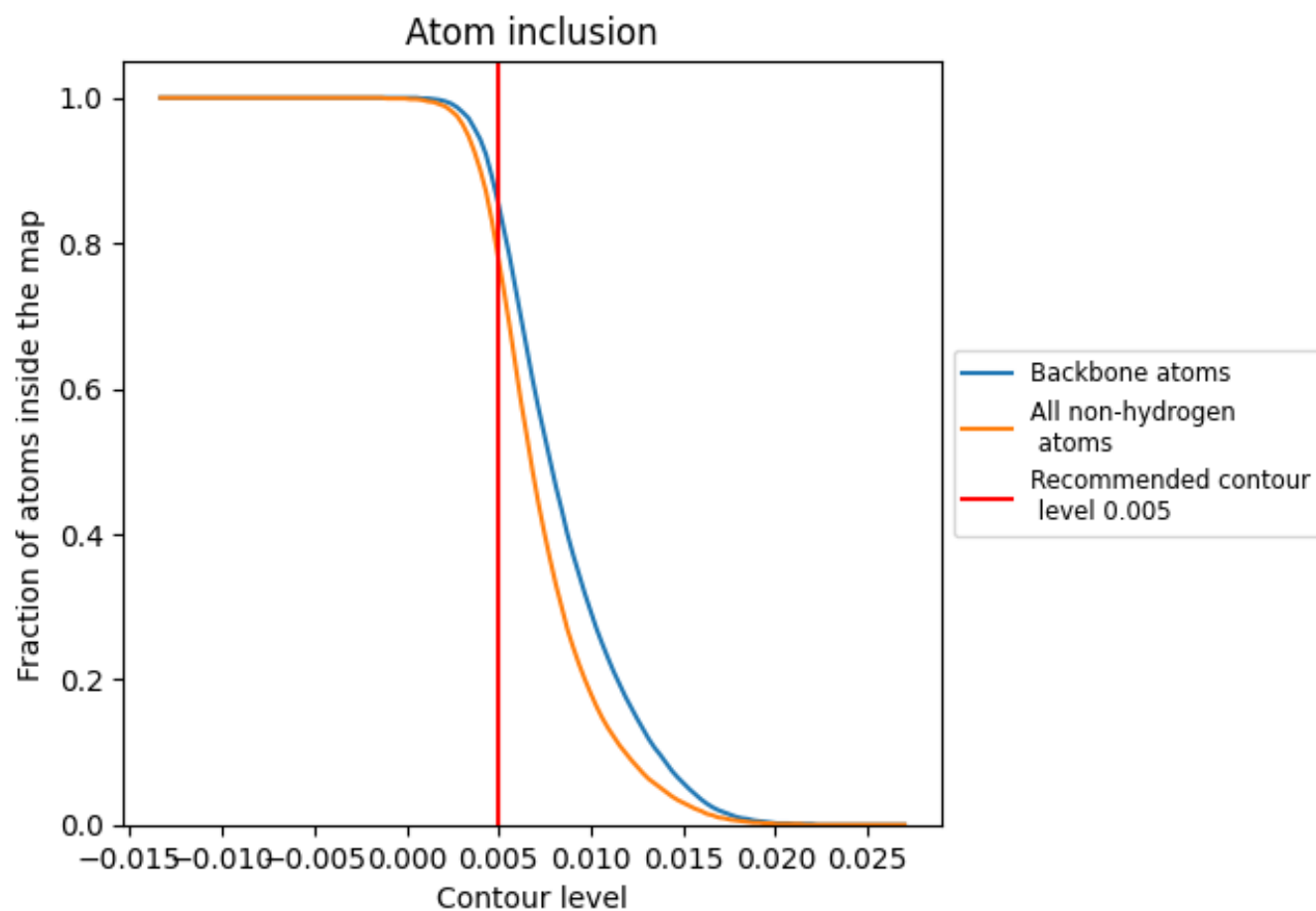
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 78% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7780	0.1310
A	0.7890	0.1330
B	0.7740	0.1320
C	0.6970	0.1120
D	0.7420	0.0950

