



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 09:10 pm BST

PDB ID : 8AUW  
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 : 1G73, 8ATU

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

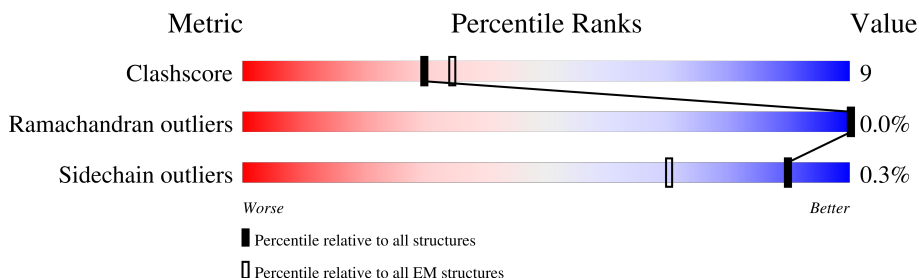
# 1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	<div> <div>8%</div> <div>46%</div> <div>13%</div> <div>40%</div> </div>
1	B	4867	<div> <div>9%</div> <div>44%</div> <div>14%</div> <div>42%</div> </div>
2	C	184	<div> <div>19%</div> <div>72%</div> <div>15%</div> <div>12%</div> </div>
2	D	184	<div> <div>13%</div> <div>70%</div> <div>15%</div> <div>15%</div> </div>

## 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		

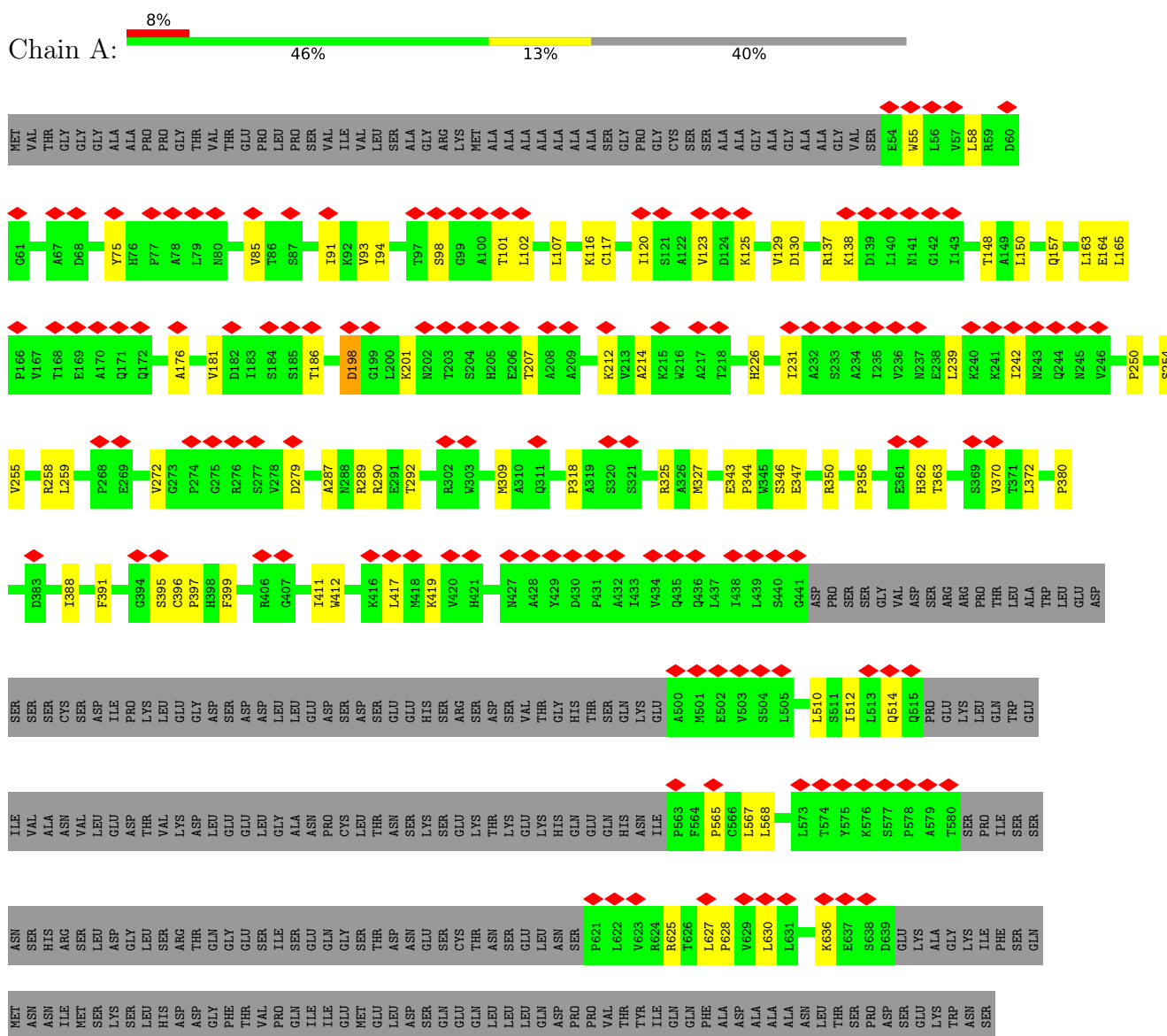
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

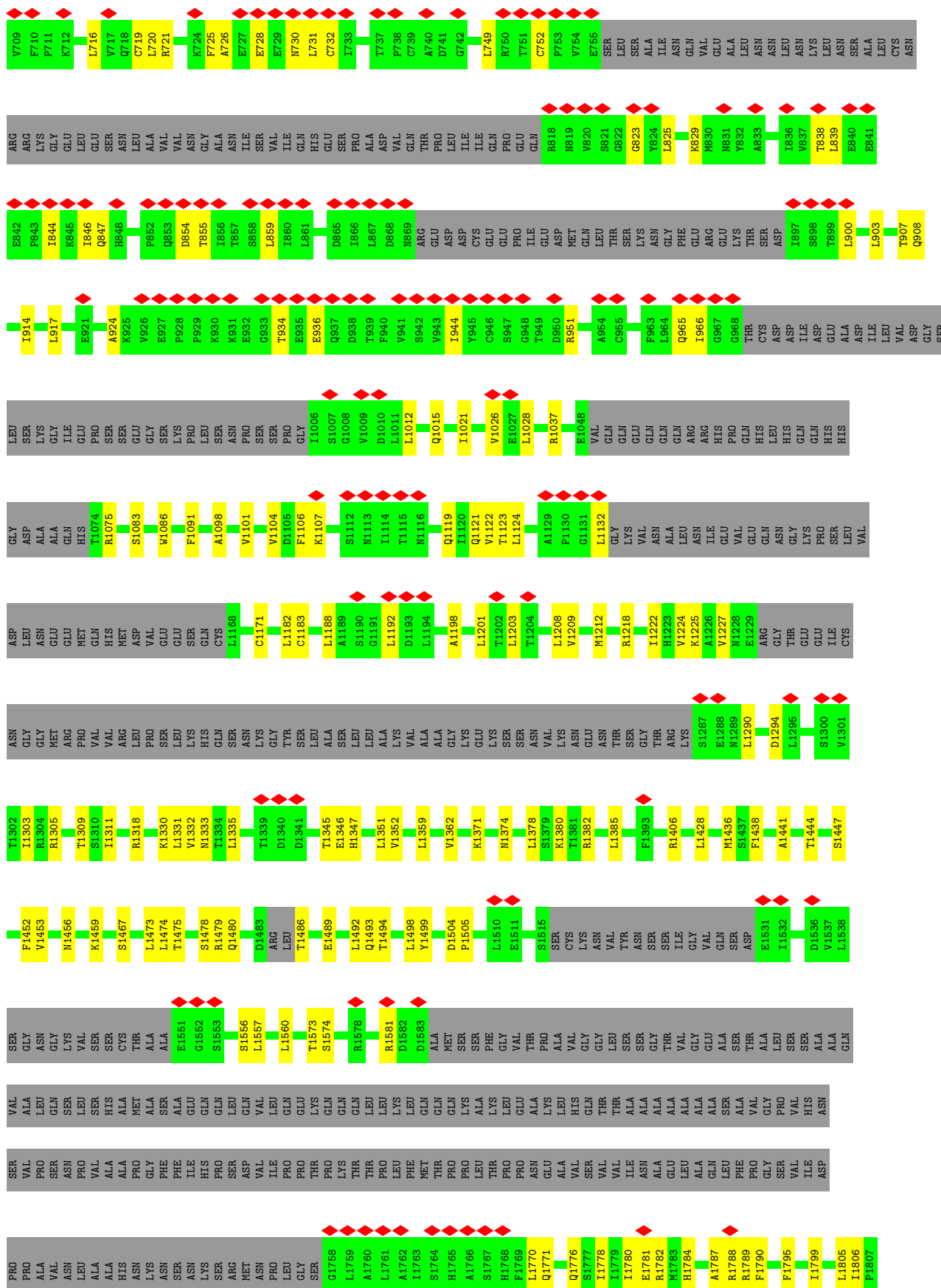
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	

### 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: Baculoviral IAP repeat-containing protein 6











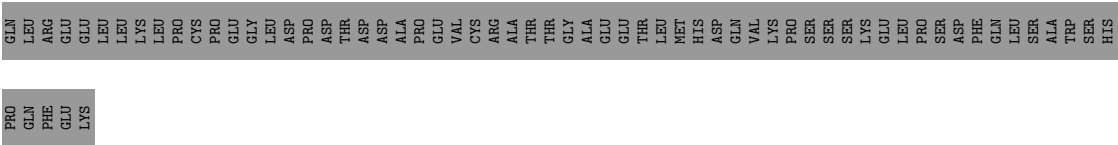


THR	GLY	HIS	THR	SER	GLN	LYS	GLU	A500	M501	E502	V503	D506	I512	L513	Q514	Q515	PRO	GLU	LYS	LEU	GLN	TRP	GLU	ILE	VAL	ALA	ASN	VAL	VAL	LEU	LEU	ASP	THR	VAL	LYS	ARG	ASP	LEU	GLU	GLU	LEU	GLY	ALA	ASN	PRO	CYS	LEU	THR	THR	LYS	LYS	PRO	GLU	LYS	HIS
GLN	GLU	GLN	HIS	ASN	ILE	P563	F564	P565	C566	L567	L568	L573	T574	Y575	K576	S577	P578	A579	T580	SER	PRO	ILE	ILE	SER	ASN	MET	ASN	ILE	MET	SER	LYS	HIS	ARG	SER	LEU	ASP	GLY	LEU	THR	GLN	GLY	GLU	ILE	SER	GLU	GLN	GLY	THR	THR	ASN	PRO	GLU	LEU	ASN	
SER	P621	L622	V623	R624	L630	I635	K636	E637	S638	D639	GLU	LYS	ALA	CYS	GLY	LYS	ILE	PHE	SER	GLN	MET	ASN	ILE	MET	SER	LYS	VAL	SER	LEU	HIS	ASP	ASN	GLY	PHE	THR	VAL	GLN	ILE	ILE	SER	GLU	LEU	ASP	SER	GLN	GLN	LEU	LEU	GLN	GLN	PRO	VAL	THR		
TYR	ILE	GLN	GLN	PHE	ALA	ASP	ALA	ALA	ALA	ALA	THR	SER	PRO	ASP	LYS	GLU	GLY	TRP	ASN	V709	K712	L716	V717	Q718	C719	L720	R721	A726	E729	N730	L731	D734	S735	I736	T737	P738	C739	A740	D741	G742	I743	L749	R750	T751	V754	E755	SER	LEU	SER	ALA					
ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ASN	ASN	LYS	LEU	ASN	SER	ALA	CYS	ASN	ARG	ARG	GLY	GLU	LEU	GLU	SER	ASN	ALA	VAL	VAL	ASN	GLY	ALA	ASN	ILE	SER	VAL	ILE	HIS	GLU	SER	PRO	ALA	ASP	VAL	GLN	THR	PRO	LEU	ILE	ILE	GLN	PRO	GLU	GLU	R819	N819	
V820	G823	Y824	L825	K829	M830	N831	Y832	A833	T834	R835	I836	V837	T838	L839	E840	E841	T844	Q847	K850	Q853	D854	T855	I856	T857	S858	L859	I860	L861	L862	P863	P864	D865	I866	L867	D868	N869	ARG	GLU	ASP	ASP	CYS	GLU	PRO	PRO	ILE	GLU	GLU	GLN	R819	N819					
ASN	GLY	PHE	GLU	ARG	GLU	LYS	THR	SER	ASP	T897	S898	T899	L903	T906	T907	Q908	V912	K913	I914	F920	E921	I922	L923	A924	K925	V926	E927	P928	P929	K930	K931	E932	G933	T934	E935	E936	Q937	D938	S942	Y943	I944	Y945	C946	D950	G959	E960	L961	Q965	G968	THR	LYS				
CYS	ASP	ASP	ILE	GLU	ASP	ALA	ILE	LEU	VAL	ASP	GLY	SER	LEU	LYS	GLY	ILE	PRO	SER	GLY	SER	LYS	PRO	LEU	SER	ASN	PRO	SER	PRO	GLY	I1006	S1007	L1012	Q1015	I1021	L1022	T1023	V1026	E1027	L1028	T1029	R1030	T1033	R1037	T1041	V1046										
V1047	E1048	VAL	GLN	GLN	GLN	GLN	GLN	ARG	ARG	HIS	PRO	GLN	HIS	HIS	GLN	HIS	GLY	ASP	ALA	ALA	GLN	HIS	T1074	R1075	L1079	S1083	W1086	F1091	E1092	L1095	V1101	G1102	H1103	V1104	D1105	F1108	V1109	L1110	Q1121	V1122	T1123	L1124	W1127	L1132	GLY										
LYS	VAL	ASN	ALA	LEU	ASN	ILE	GLU	VAL	GLN	GLN	ASN	GLY	GLY	VAL	ASP	LEU	PRO	ASN	SER	GLU	MET	GLN	HIS	MET	ASP	VAL	GLU	HIS	GLN	GLY	L1168	R1169	L1170	G1171	P1172	E1175	K1178	L1182	C1183	L1188	A1189	S1190	G1199	M1200	L1203	M1212	Y1217	R1218							
S1219	F1220	T1221	T1222	H1223	V1224	E1229	ARG	THR	GLU	GLU	ASN	GLY	ILE	CYS	ASN	GLY	MET	ARG	PRO	VAL	VAL	ARG	LEU	PRO	SER	LEU	LYS	HIS	GLN	ASN	GLN	L1168	R1169	L1170	G1171	P1172	E1175	K1178	L1182	C1183	L1188	A1189	S1190	G1199	M1200	L1203	M1212	Y1217	R1218						
SER	GLY	THR	ARG	LYS	S1287	L1290	D1294	T1302	I1303	R1304	R1305	T1309	S1310	S1311	V1316	Q1317	R1318	H1328	L1331	V1332	N1333	Q1343	T1344	E1346	Q1349	W1358	N1374	L1377	L1378	S1379	K1380	T1381	R1382	T1388	V1389	R1390	V1391																		
R1398	S1399	K1403	L1428	L1432	A1441	T1444	S1447	Y1451	L1455	M1456	K1459	C1470	A1471	L1474	T1475	R1479	Q1480	L1481	Q1482	D1483	ARG	T1486	E1489	L1492	Q1493	T1494	R1495	L1498	Y1499	S1500	F1503	D1504	P1505	F1508	D1509	L1510	S1515	SER	CYS	LYS															

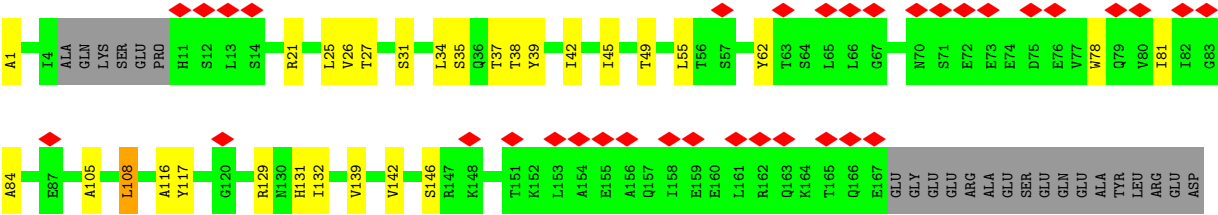




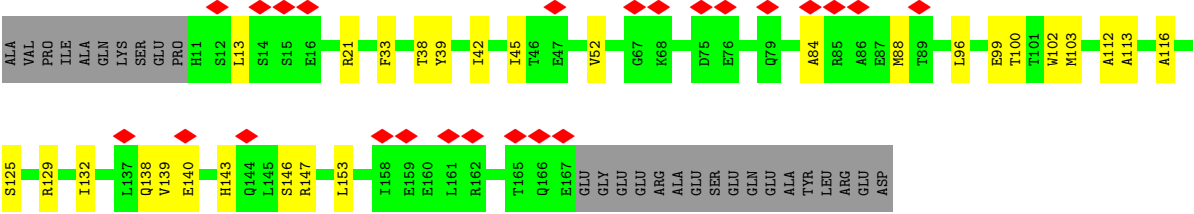




● Molecule 2: Diablo IAP-binding mitochondrial protein



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## 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

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.30	0/22884	0.67	20/31066 (0.1%)
1	B	0.31	0/22298	0.67	27/30292 (0.1%)
2	C	0.30	0/1284	0.65	1/1737 (0.1%)
2	D	0.31	0/1257	0.59	1/1700 (0.1%)
All	All	0.30	0/47723	0.67	49/64795 (0.1%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	ASP	CB-CG-OD1	10.06	127.35	118.30
1	A	2922	LEU	CA-CB-CG	7.95	133.57	115.30
1	B	3487	LEU	CA-CB-CG	7.91	133.50	115.30
1	A	327	MET	CA-CB-CG	7.56	126.15	113.30
1	B	1432	LEU	CA-CB-CG	7.07	131.56	115.30
1	A	2387	LEU	CB-CG-CD1	-6.78	99.47	111.00
1	B	3488	MET	CA-CB-CG	6.63	124.56	113.30
1	B	2146	LEU	CA-CB-CG	6.58	130.44	115.30
1	B	1982	LEU	CA-CB-CG	6.50	130.25	115.30
2	C	108	LEU	CA-CB-CG	6.28	129.74	115.30
2	D	103	MET	CA-CB-CG	6.23	123.90	113.30
1	A	4323	LEU	CB-CG-CD1	6.22	121.57	111.00
1	A	2732	MET	CG-SD-CE	6.19	110.10	100.20
1	A	2633	LEU	CA-CB-CG	6.04	129.19	115.30
1	B	2922	LEU	CA-CB-CG	6.02	129.15	115.30
1	B	2167	MET	CA-CB-CG	5.93	123.38	113.30
1	B	2149	LEU	CA-CB-CG	5.93	128.93	115.30
1	B	1428	LEU	CA-CB-CG	5.89	128.85	115.30
1	A	2076	LEU	CA-CB-CG	5.77	128.58	115.30
1	A	3682	LEU	CA-CB-CG	5.76	128.55	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2342	MET	CG-SD-CE	5.74	109.38	100.20
1	A	2586	MET	CB-CG-SD	5.71	129.53	112.40
1	B	2005	LEU	CA-CB-CG	5.70	128.42	115.30
1	B	2800	LEU	CA-CB-CG	-5.70	102.18	115.30
1	B	2812	LEU	CA-CB-CG	5.62	128.23	115.30
1	B	198	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	198	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	3287	ASP	CB-CG-OD1	5.54	123.28	118.30
1	B	2066	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	2174	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	2408	LEU	CA-CB-CG	5.38	127.67	115.30
1	B	2815	LEU	CA-CB-CG	5.37	127.65	115.30
1	B	2397	ILE	CG1-CB-CG2	-5.36	99.60	111.40
1	B	3530	MET	CA-CB-CG	5.34	122.37	113.30
1	A	3981	MET	CA-CB-CG	5.33	122.37	113.30
1	B	2633	LEU	CA-CB-CG	5.29	127.48	115.30
1	A	1939	LEU	CA-CB-CG	5.23	127.33	115.30
1	B	2732	MET	CA-CB-CG	5.23	122.19	113.30
1	B	2352	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	2031	LEU	CA-CB-CG	5.19	127.23	115.30
1	A	2350	LEU	CA-CB-CG	5.17	127.20	115.30
1	B	3711	LEU	CA-CB-CG	5.13	127.10	115.30
1	B	3488	MET	CB-CG-SD	5.12	127.77	112.40
1	A	3400	LEU	CA-CB-CG	5.09	127.00	115.30
1	B	3034	ASP	CB-CG-OD1	5.06	122.85	118.30
1	B	2589	LEU	CA-CB-CG	5.03	126.86	115.30
1	B	2839	LEU	CA-CB-CG	5.02	126.85	115.30
1	A	2639	LEU	CA-CB-CG	5.02	126.85	115.30
1	B	2878	MET	CA-CB-CG	5.02	121.83	113.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	22469	0	22943	408	0
1	B	21887	0	22291	415	0
2	C	1269	0	1270	21	0
2	D	1242	0	1236	19	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	46869	0	47740	838	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 (838) 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:1557:LEU:HD12	1:B:1560:LEU:HD21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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:B:1101:VAL:HA	1:B:1305:ARG:HE	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1556:SER:HB2	1:B:1843:ILE:HG21	1.84	0.59
1:B:3279:CYS:SG	1:B:3281:ARG:NH1	2.76	0.59
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3236:PRO:O	1:A:3259:THR:OG1	2.21	0.57
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
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:A:395:SER:HG	1:A:514:GLN:H	1.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:1436:MET:HE1	1:A:1473:LEU:HG	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:2750:HIS:O	1:A:2754:SER:OG	2.22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:116:LYS:NZ	1:A:117:CYS:O	2.42	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:3816:MET:HE3	1:B:4071:LEU:HD12	1.93	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:855:THR:HB	1:A:908:GLN:HB2	1.92	0.51
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:1107:LYS:HZ1	1:A:1198:ALA:HB1	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2692:PRO:HG2	1:B:2732:MET:HE2	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
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: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
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: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
1:A:1188:LEU:HG	1:A:1192:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:289:ARG:O	1:A:292:THR:OG1	2.31	0.47
1:A:3243:VAL:HG13	1:A:3253:LEU:HD21	1.97	0.47
1:B:147:ASP:OD2	1:B:218:THR:OG1	2.25	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
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
2:C:62:TYR:HH	2:C:78:TRP:HE1	1.62	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:B:2834:ASP:OD1	1:B:2834:ASP:N	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:B:108:SER:OG	1:B:147:ASP:O	2.33	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:1377:LEU:O	1:B:1381:THR:OG1	2.26	0.46
1:B:2775:ASN:HB3	1:B:2777:HIS:CE1	2.51	0.46
1:B:2875:ASP:OD1	1:B:2875:ASP:N	2.48	0.46
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: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: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:3335:HIS:O	1:A:3339:THR:OG1	2.20	0.46
1:A:3355:THR:HG23	1:A:3358:LEU:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4437:LEU:HA	1:A:4440:MET:HE3	1.98	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2365:THR:O	1:A:2366:ARG:NH1	2.49	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
1:B:4373:MET:HE3	1:B:4377:LEU:HG	1.99	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:B:3335:HIS:O	1:B:3339:THR:OG1	2.31	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: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: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:2033:THR:O	1:B:2036:SER:OG	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:2562:SER:OG	1:B:2563:VAL:N	2.51	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
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:1474:LEU:O	1:A:1478:SER:OG	2.28	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:A:4377:LEU:HD22	1:A:4440:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:2724:HIS:O	1:B:2727:THR:OG1	2.26	0.43
1:B:3241:VAL:HG22	1:B:3280:LEU:HD13	2.00	0.43
1:B:3817:LEU:O	1:B:4182:GLN:NE2	2.48	0.43
1:A:2813:LEU:HD23	1:A:2848:PHE:HE2	1.82	0.43
1:A:3040:LEU:HA	1:A:3040:LEU:HD23	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:138:LYS:HZ2	1:A:372:LEU:HB3	1.84	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: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
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: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:3862:VAL:O	1:B:3982:THR:OG1	2.37	0.42
2:D:96:LEU:O	2:D:100:THR:OG1	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:1808:THR:OG1	1:B:1841:SER:OG	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
1:A:98:SER:OG	1:A:212:LYS:NZ	2.53	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: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:3243:VAL:HG12	1:A:3278:VAL:HG22	2.03	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:3196:ALA:HB3	1:B:3294:SER:HA	2.03	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:A:4003:ASP:N	1:A:4003:ASP:OD1	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:3330:TRP:HA	1:A:3333:LEU:HD12	2.03	0.41
1:B:395:SER:HG	1:B:514:GLN:H	1.69	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:1432:LEU:HD23	1:B:1451:TYR:CE1	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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%)	2546 (100%)	10 (0%)	89	91
1	B	2491/4225 (59%)	2487 (100%)	4 (0%)	92	94
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%)	5306 (100%)	14 (0%)	90	92

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	721	ARG
1	A	1829	ARG
1	A	1872	LYS
1	A	1989	ASN
1	A	2264	ASN
1	A	2277	LYS
1	A	3190	ARG

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Mol	Chain	Res	Type
1	A	3191	ARG
1	A	3993	ARG
1	A	4000	ARG
1	B	1829	ARG
1	B	2116	ARG
1	B	3193	ARG
1	B	4000	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1925	GLN
1	A	3224	HIS
1	A	3228	HIS
1	B	1343	GLN
1	B	3224	HIS
1	B	3228	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

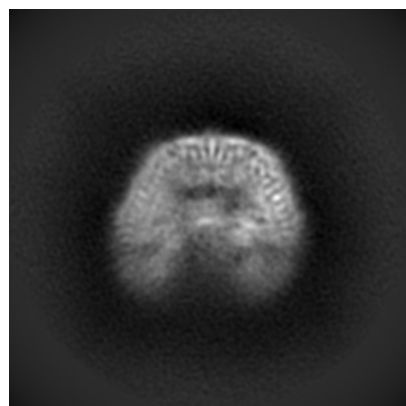
## 6 Map visualisation [i](#)

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.

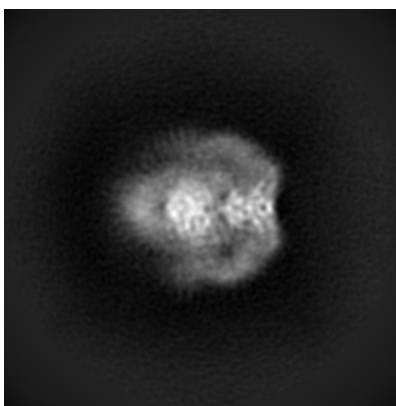
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

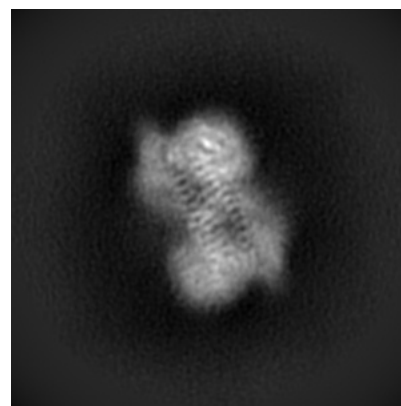
#### 6.1.1 Primary map



X

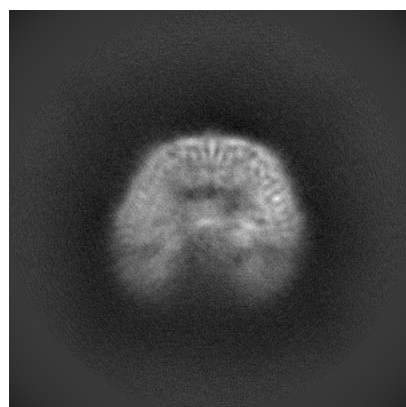


Y

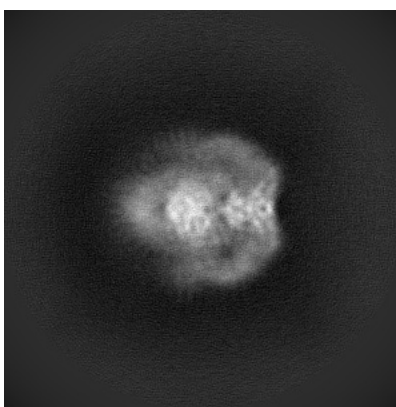


Z

#### 6.1.2 Raw map



X



Y

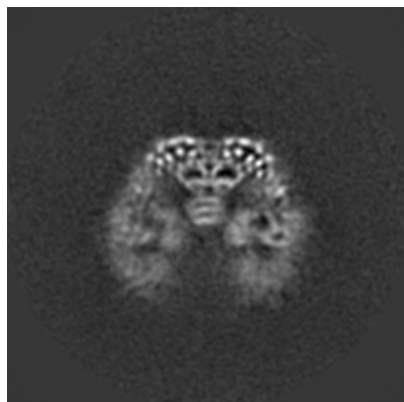


Z

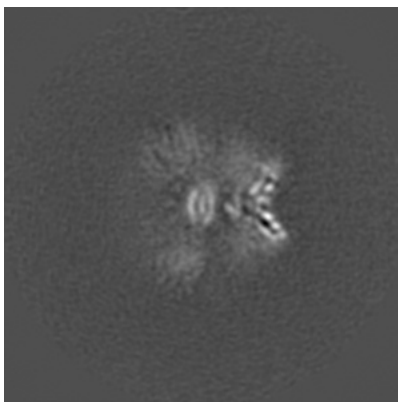
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

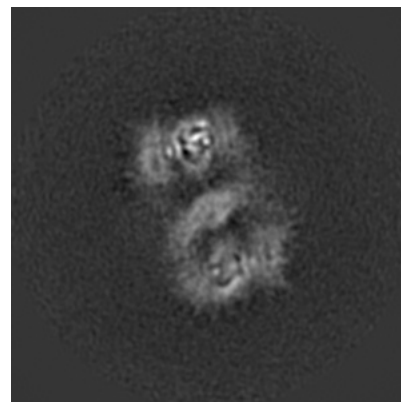
### 6.2.1 Primary map



X Index: 150

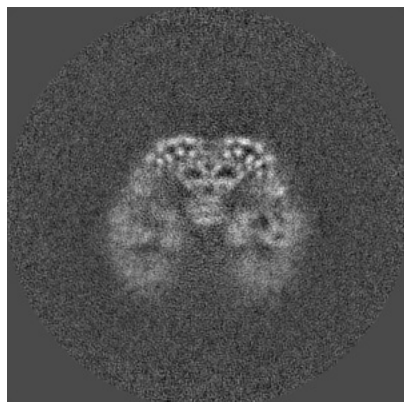


Y Index: 150

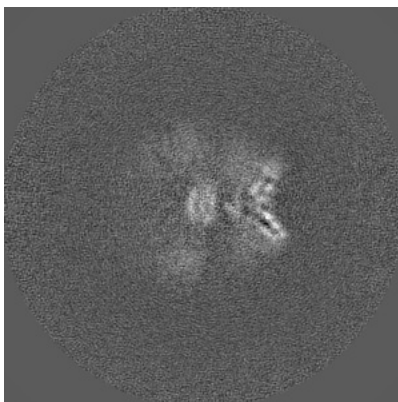


Z Index: 150

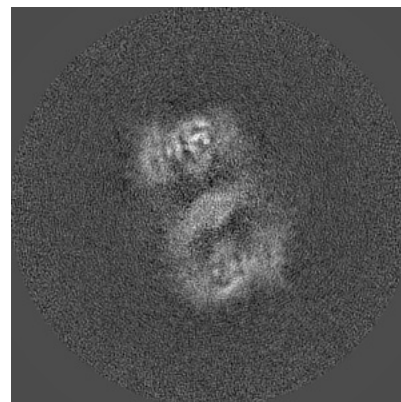
### 6.2.2 Raw map



X Index: 150



Y Index: 150

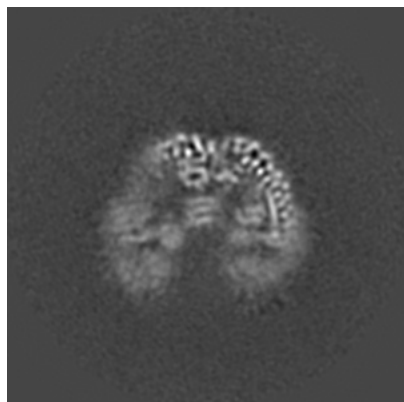


Z Index: 150

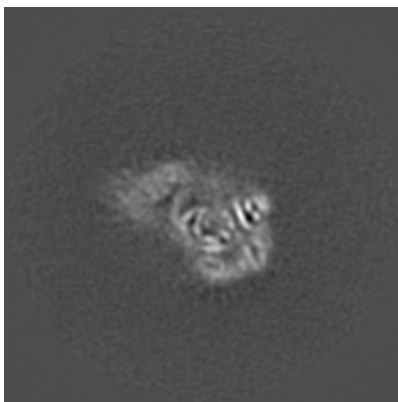
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

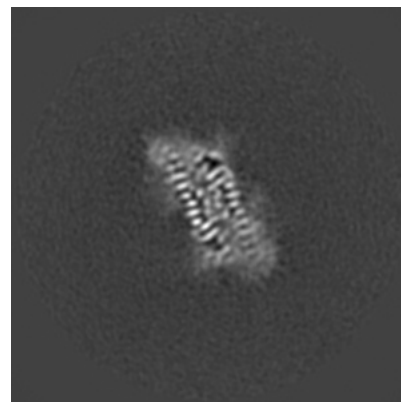
### 6.3.1 Primary map



X Index: 146

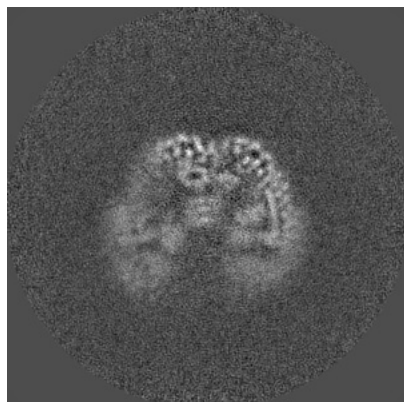


Y Index: 189

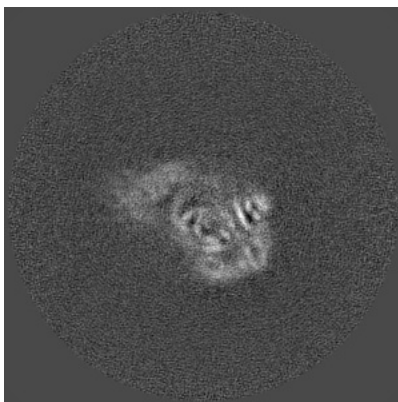


Z Index: 191

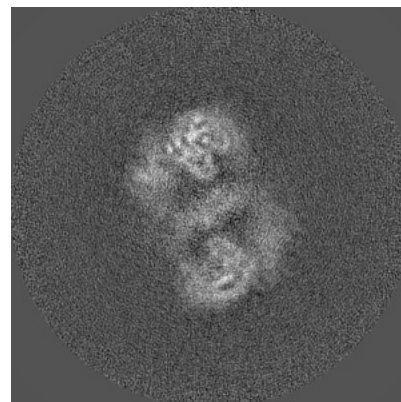
### 6.3.2 Raw map



X Index: 147



Y Index: 189

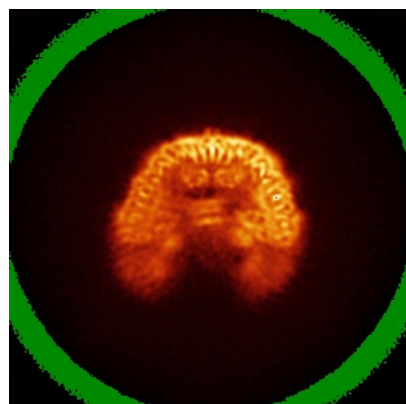


Z Index: 145

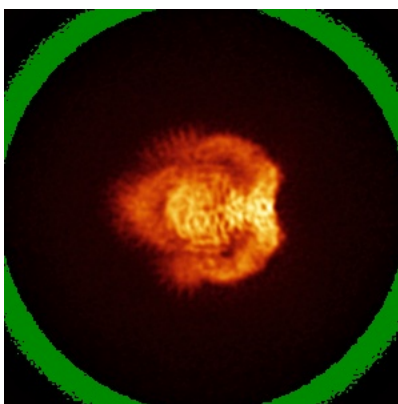
The images above show the largest variance slices of the map in three orthogonal directions.

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

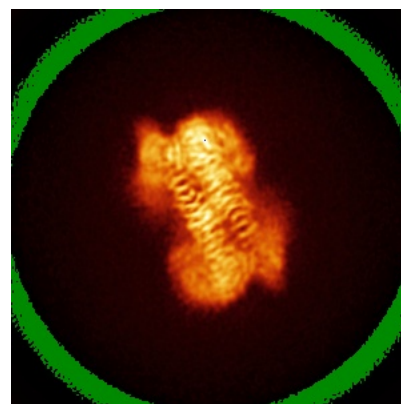
### 6.4.1 Primary map



X

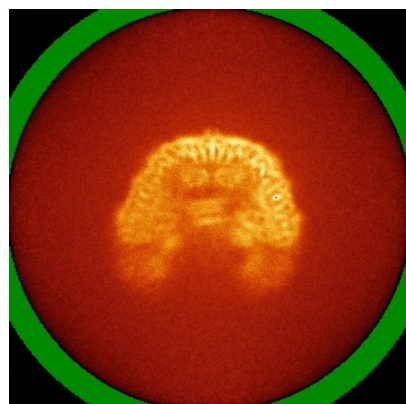


Y

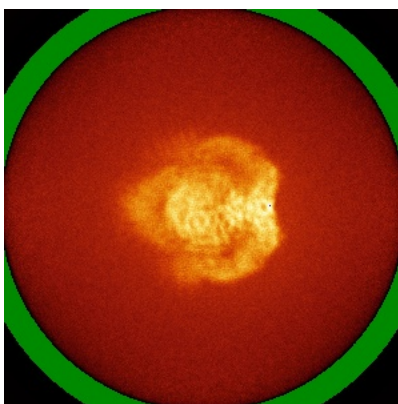


Z

### 6.4.2 Raw map



X



Y



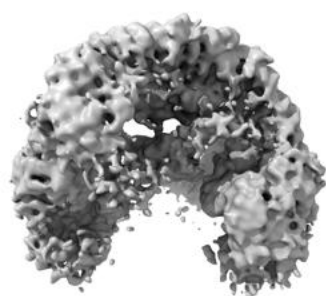
Z

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.

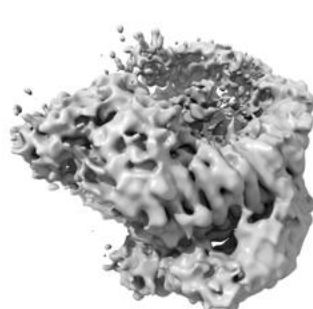


## 6.5 Orthogonal surface views [i](#)

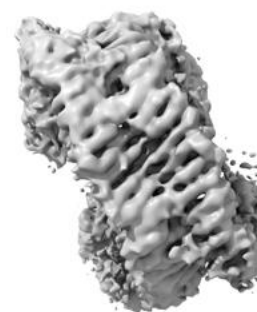
### 6.5.1 Primary map



X



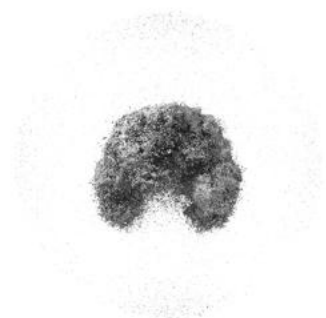
Y



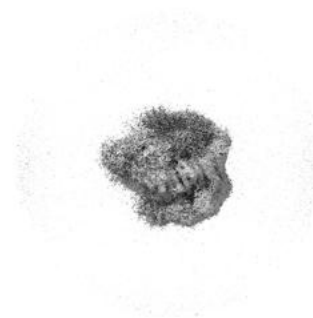
Z

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.

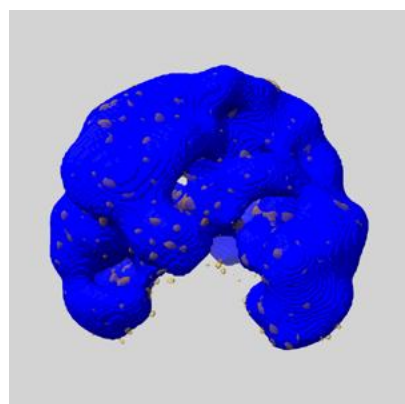
## 6.6 Mask visualisation [i](#)

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

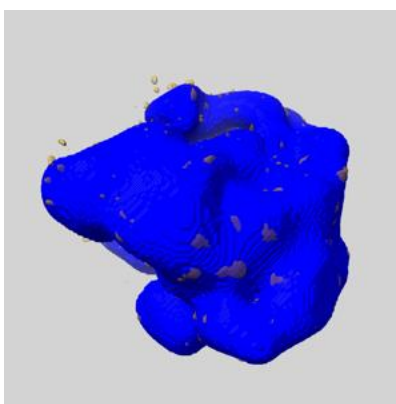
A mask typically either:

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

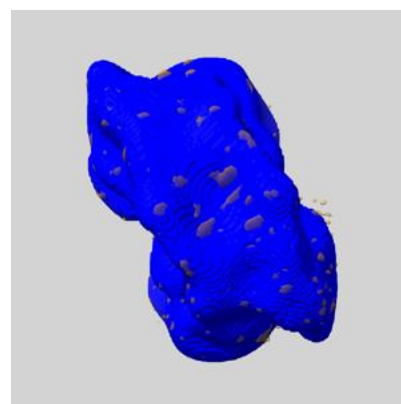
### 6.6.1 emd\_15675\_msk\_1.map [i](#)



X



Y

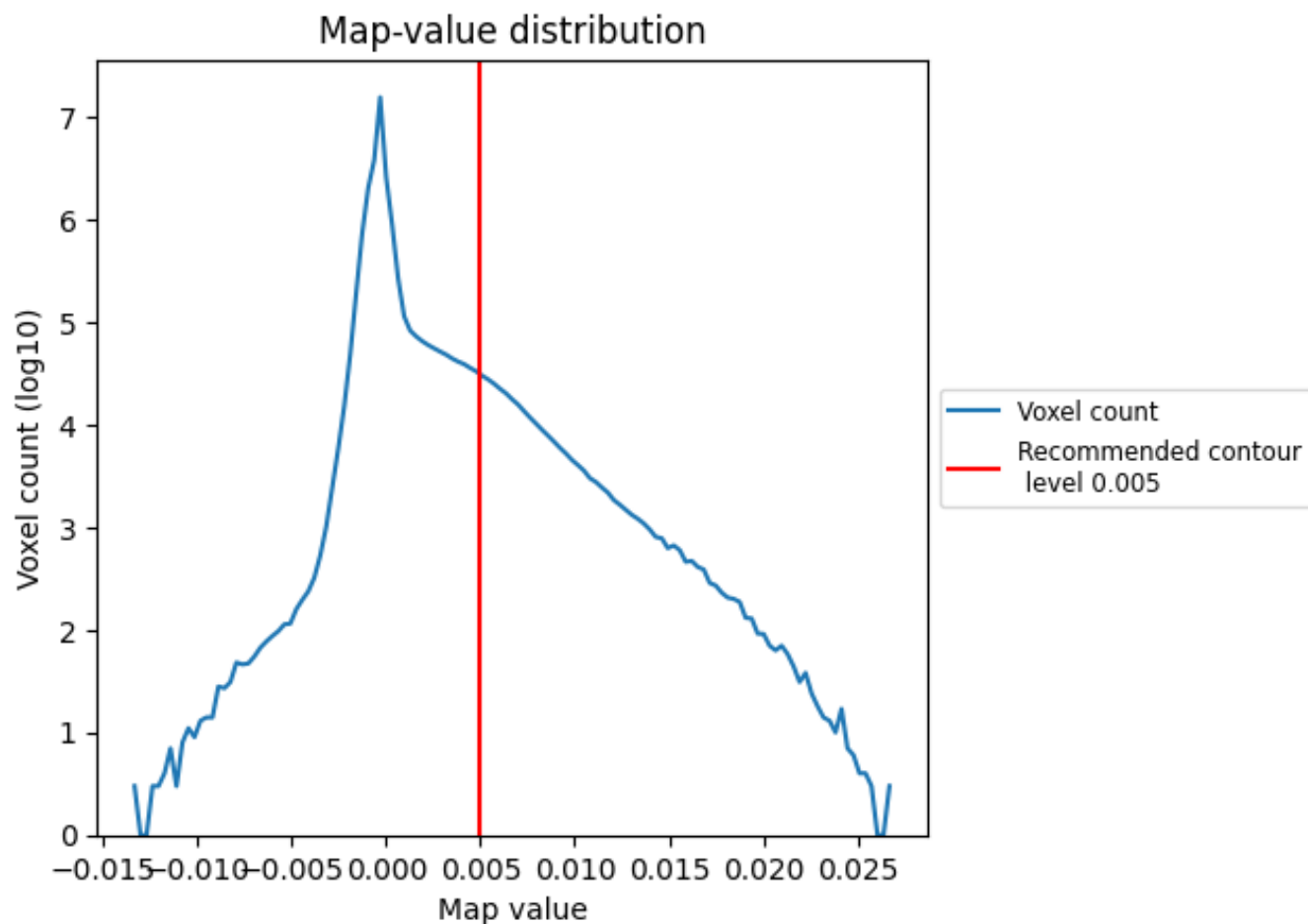


Z

## 7 Map analysis [i](#)

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

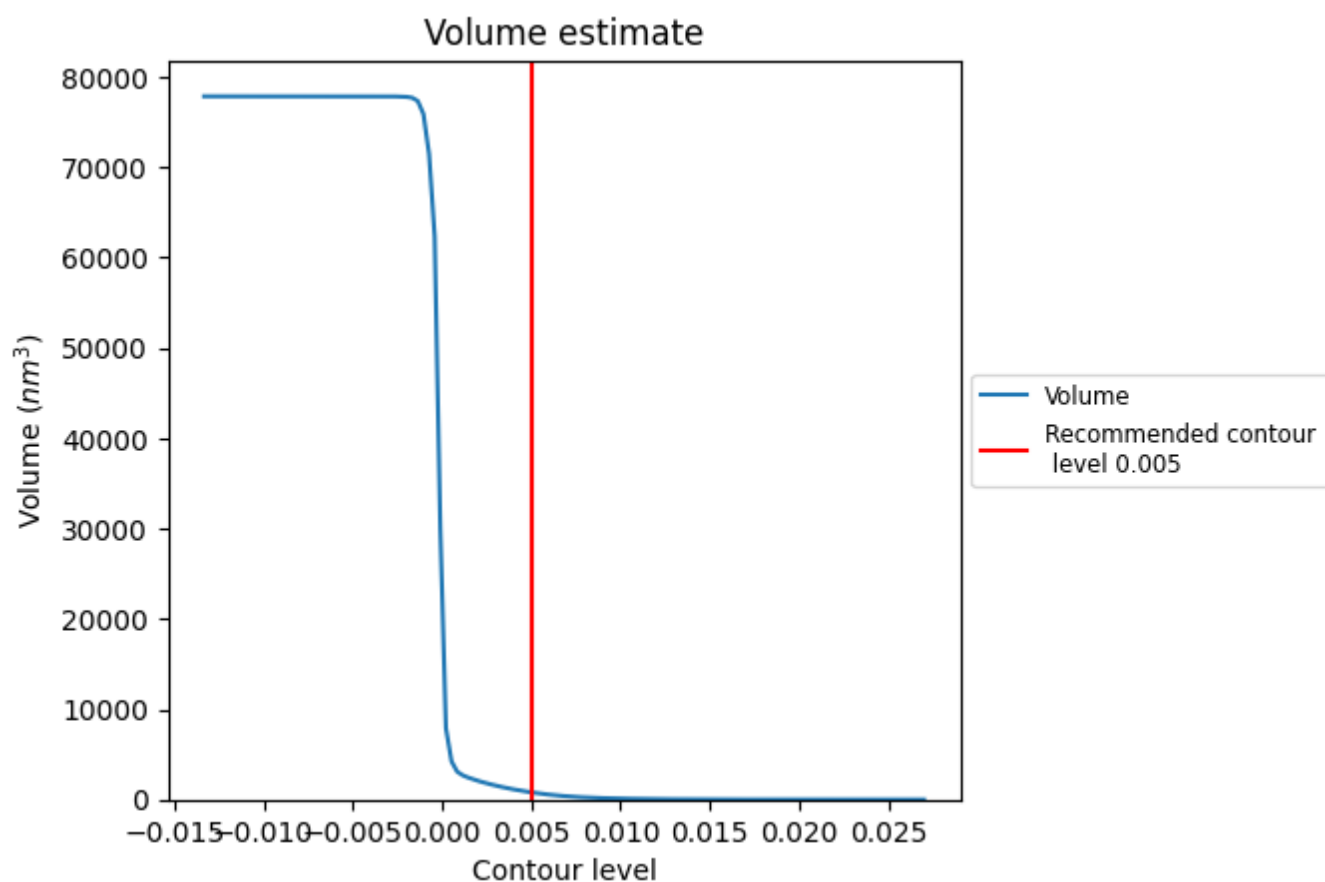
### 7.1 Map-value distribution [i](#)



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.



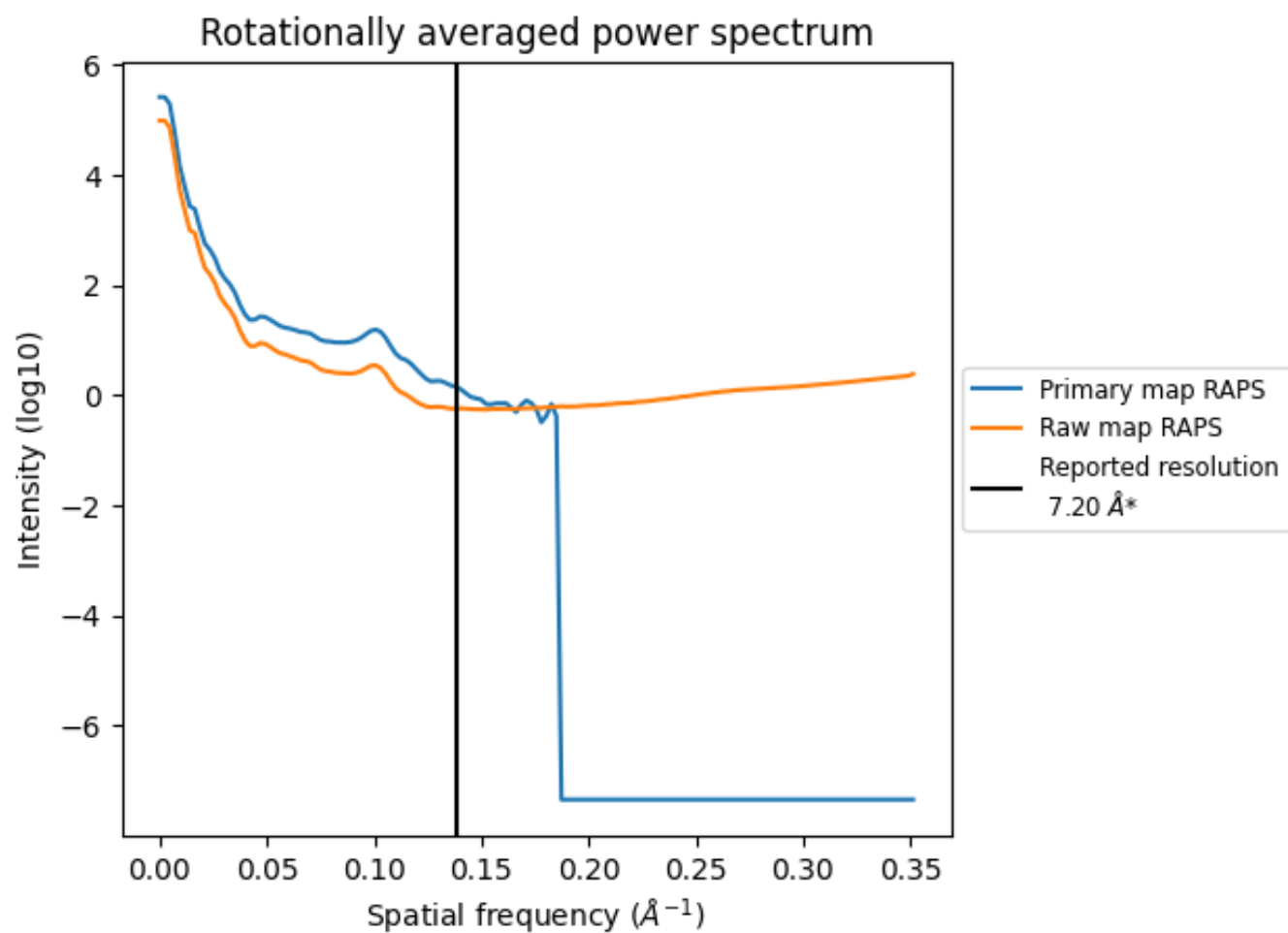
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $800 \text{ nm}^3$ ; 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 ⓘ

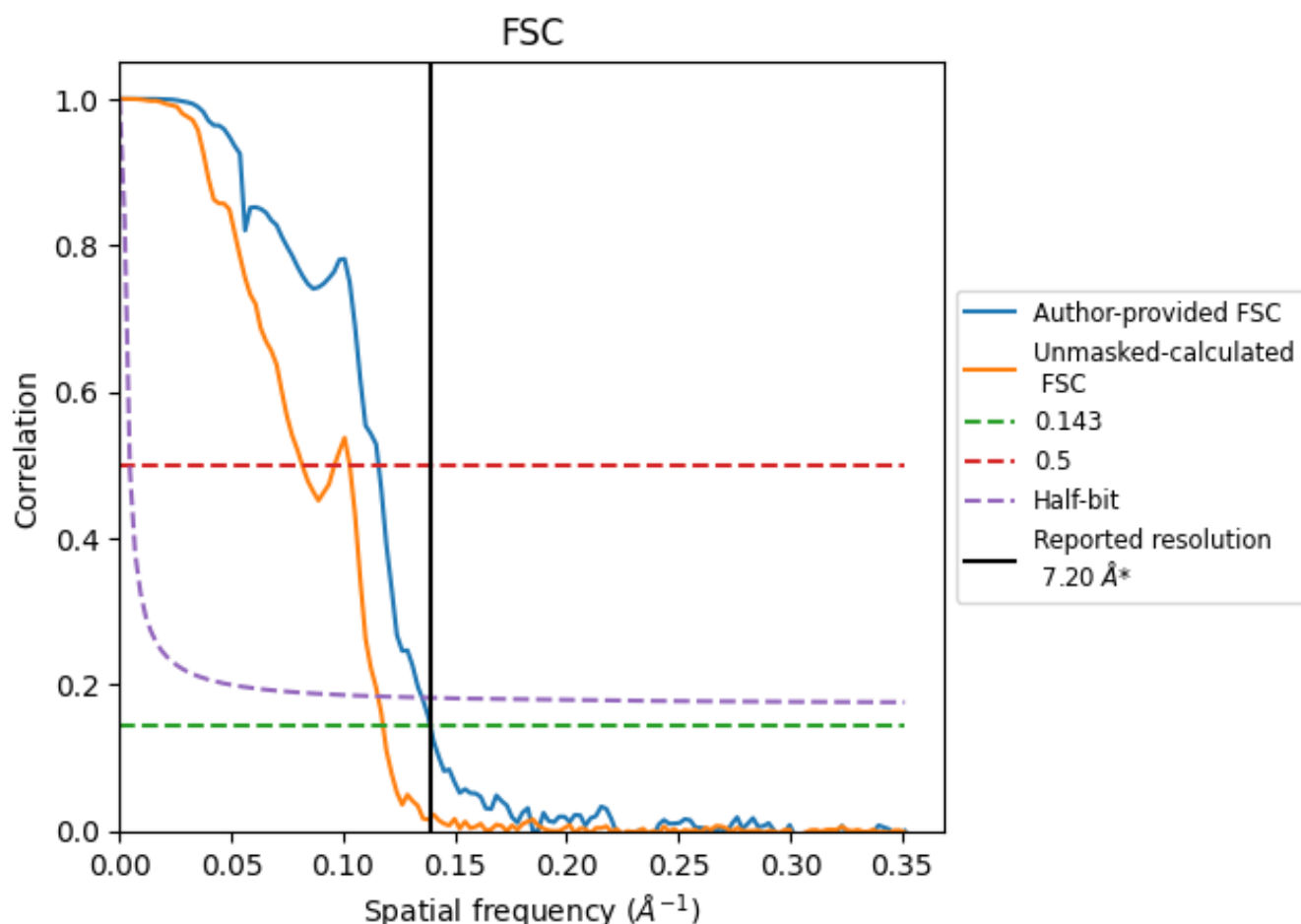


\*Reported resolution corresponds to spatial frequency of 0.139  $\text{\AA}^{-1}$

## 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](#)

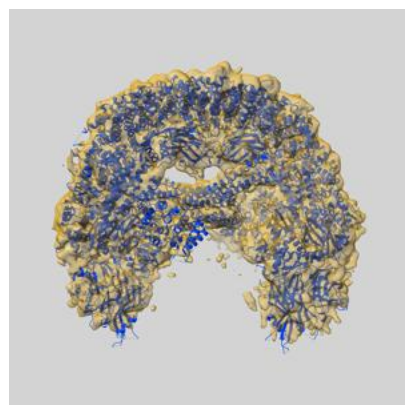
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.20	-	-
Author-provided FSC curve	7.19	8.64	7.39
Unmasked-calculated*	8.48	12.24	8.65

\*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 %

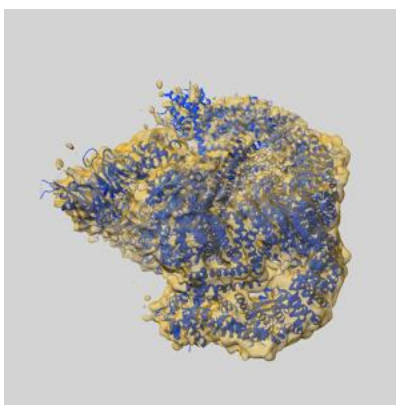
## 9 Map-model fit [i](#)

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](#).

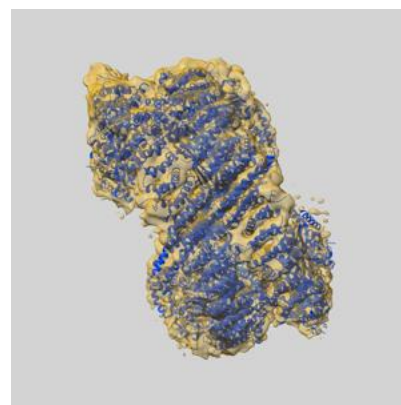
### 9.1 Map-model overlay [i](#)



X



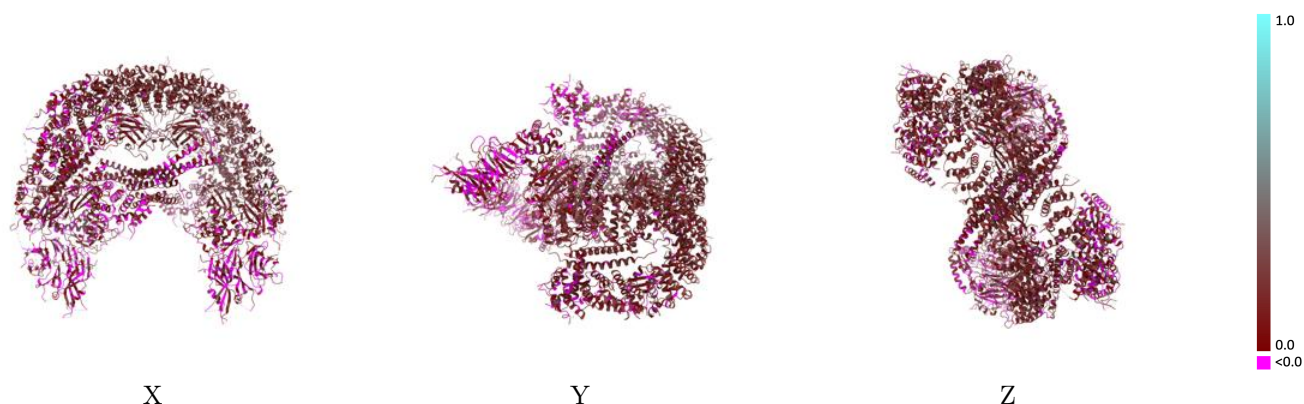
Y



Z

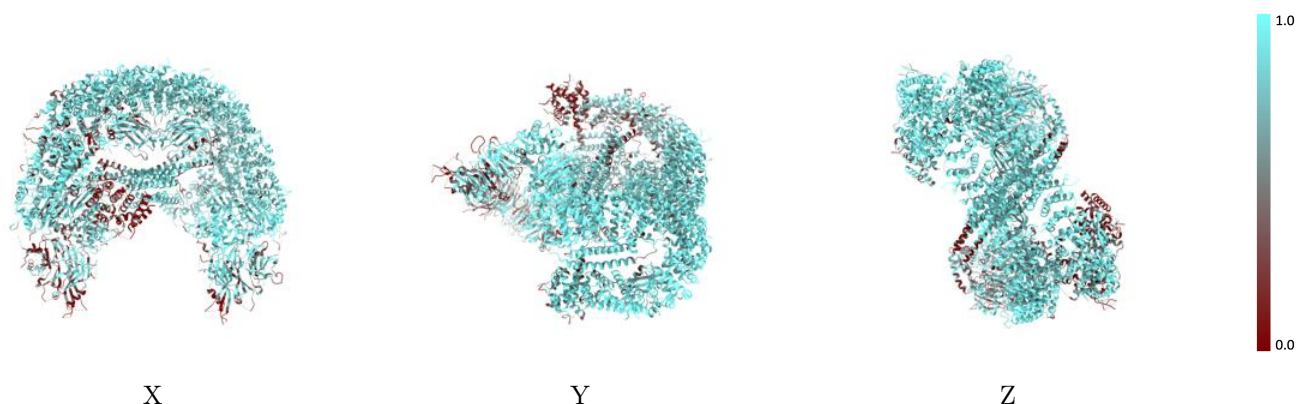
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



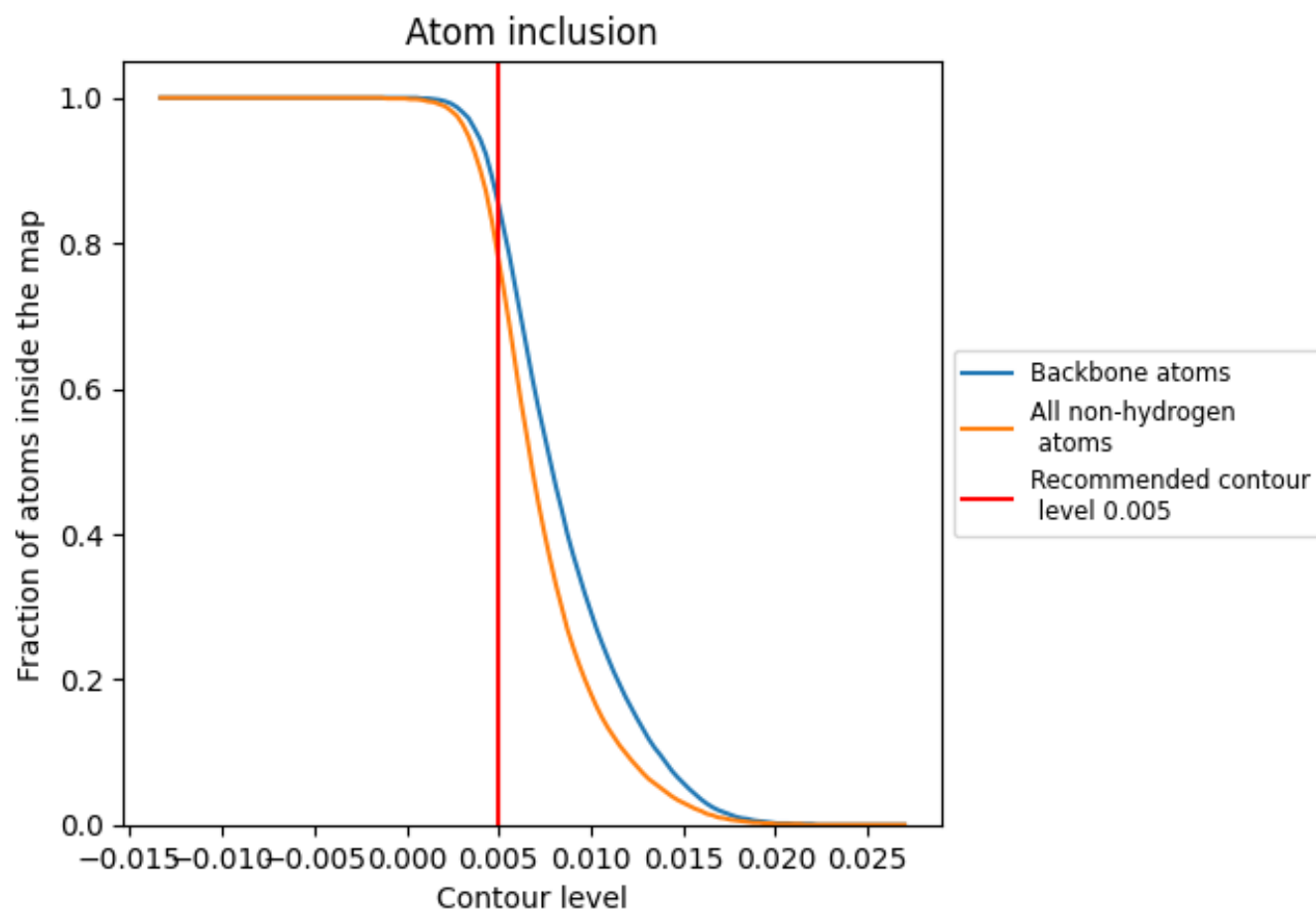
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div></div> 0.7780	<div></div> 0.1310
A	<div></div> 0.7890	<div></div> 0.1330
B	<div></div> 0.7740	<div></div> 0.1320
C	<div></div> 0.6970	<div></div> 0.1120
D	<div></div> 0.7420	<div></div> 0.0950

