



## Full wwPDB EM Validation Report ⓘ

Jul 15, 2024 – 11:41 am BST

PDB ID : 8ATU  
EMDB ID : EMD-15663  
Title : Cryo-EM structure of human BIRC6  
Authors : Ehrmann, J.F.; Grabarczyk, D.B.; Clausen, T.  
Deposited on : 2022-08-24  
Resolution : 3.30 Å(reported)

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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.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

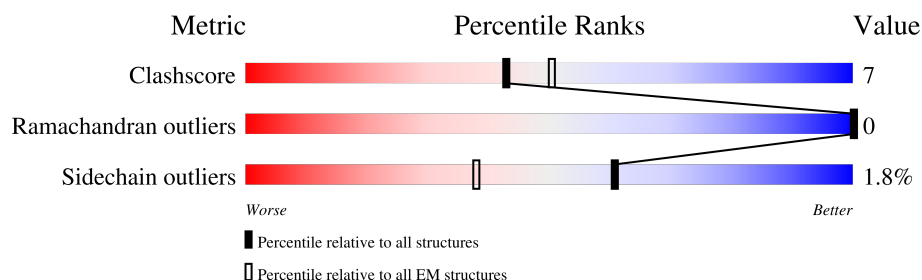
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>34%</div> <div>47%</div> <div>11%</div> <div>42%</div> </div>
1	B	4867	<div> <div>34%</div> <div>47%</div> <div>11%</div> <div>42%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 43882 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	2837	Total	C	N	O	S	0	0
			21940	14019	3711	4059	151		
1	B	2837	Total	C	N	O	S	0	0
			21940	14019	3711	4059	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 ZINC ION (three-letter code: ZN) (formula: Zn).

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











G4231	V4232	L4233	R4235	R4236	M4237	L4238	L4239	E4240	I4241	G4242	A4243	L4244	H4245	L4246	I4247	L4248	V4249	C4250	L4251	S4252	A4253	L4254	S4255	H4256	H4257	S4258	P4259	R4260	V4261	P4262	ASN	SER	SER	VAL	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
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K241	K242	N243	N244	N245	N246	A247	A248	L249	P250	V251	A252	S253	S254	V255	M256	D257	R258	L259	S260	Y261	L262	L263	P264	S265	A266	R267	P268	E269	L270	G271	V272	G273	P274	G275	R276	S277	V278	D279	R280	S281	L282	M283	Y284	S285	E286	A287	N288	R289	R290	E291	T292	F293	T294	S295	P296	H297	V298	V299	G300
Y301	R302	W303	A304	Q305	P306	D307	P308	M309	A310	Q311	A312	G313	F314	Y315	H316	Q317	P318	A319	S320	S321	G322	D323	D324	R325	A326	M327	C328	F329	T330	C331	S332	V333	C334	L335	V336	C337	W338	E339	P340	T341	L342	E343	P344	W345	S346	E347	H348	E349	R350	H351	S352	P353	N354	C355	P356	F357	V358	K359	G360
E361	H362	T363	Q364	N365	V366	P367	L368	S369	V370	T371	L372	A373	T374	S375	P376	A377	Q378	F379	P380	C381	L382	D383	G384	T385	A386	R387	I388	S389	C390	F391	G392	S393	G394	S395	C396	P397	H398	F399	L400	A401	L402	A403	T404	K405	R406	G407	K408	I409	C410	I411	W412	D413	V414	S415	K416	L417	M418	K419	V420
H421	L422	K423	F424	E425	I426	M427	A428	Y429	D430	P431	A432	I433	V434	Q435	Q436	L437	I438	L439	S440	G441	ASP	PRO	SER	SER	GLY	VAL	SER	ARG	PRO	THR	LEU	ALA	TRP	LEU	GLU	SER	SER	CYS	SER	ASN	VAL	ILE	PRO	PRO	LYS	LEU	ASP	THR	LEU	GLY	ASP	SER	ASP	GLY	ALA				
ASP	SER	GLU	THR	HIS	SER	ARG	SER	SER	VAL	THR	GLY	HIS	THR	GLN	LYS	ASP	M500	M501	E502	V503	S504	L505	D506	I507	T508	A509	L510	S511	I512	ARG	PRO	THR	LEU	ALA	GLU	LYS	VAL	ILE	VAL	ASN	VAL	ILE	LEU	LEU	ASP	LEU	GLU	THR	GLY	ALA									
ASN	PRO	CYS	LEU	THR	ASN	SER	LYS	SER	GLU	THR	LYS	GLN	GLN	GLN	HIS	ASN	P563	F564	P565	C566	L567	L568	A569	G570	G571	L572	L573	T574	V575	K576	S577	P578	A579	T580	PRO	PRO	ILE	SER	ASN	VAL	THR	SER	GLN	THR	GLY	ASP													
SER	ILE	GLU	GLY	GLY	THR	ASP	ASP	ASN	GLU	CYS	THR	ASN	GLU	LEU	ASN	SER	P621	L622	V623	R624	R625	T626	L627	P628	V629	L630	L631	L632	V633	S634	L635	K636	E637	S638	D639	GLU	LYS	ALA	GLY	ILE	PHE	SER	GLN	VAL	GLY	ASN	THR	ASP											
GLY	PHE	THR	VAL	PRO	GLN	ILE	ILE	LEU	MET	LEU	GLU	THR	GLU	LEU	GLN	ASN	P621	L622	V623	R624	R625	T626	L627	P628	V629	L630	L631	L632	V633	S634	L635	K636	E637	S638	D639	GLU	LYS	ALA	GLY	ILE	PHE	SER	GLN	VAL	GLY	ASN	THR	ASP											
R721	L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	T737	P738	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ALA	ILE	ASN	VAL	GLN	THR	LEU	ASN	ARG													
LYS	GLY	GLU	LEU	SER	ASN	LEU	ALA	VAL	ASN	GLY	ALA	ILE	SER	VAL	ILE	GLN	HIS	GLU	ALA	ASP	VAL	THR	PRO	LEU	ILE	ILE	PRO	GLN	GLN	R818	N819	V820	S821	G822	G823	Y824	L825	W826	L827	Y828	K829	M830	N831	Y832	A833	T834	R835	L836	V837	T838	L839	E840							
E841	F842	P843	T844	K845	L846	Q847	H848	L849	K850	D851	P852	K853	D854	T855	I856	T857	S858	L859	T860	L861	P863	P864	D865	D866	L867	P868	P869	ARG	GLU	ASP	ASP	CYS	GLU	GLU	PRO	ILE	GLY	ASP	MET	GLN	LEU	THR	SER	LYS	ARG	GLU	LYS	THR	SER	ASP	L897	S898	T899	L900					
G901	H902	L903	V904	I905	T906	T907	G908	G909	G910	Y911	V912	K913	I914	L915	D916	L917	S918	N919	F920	E921	L922	L923	A924	K925	E927	P928	P929	K930	K931	E932	G933	P934	E935	E936	Q937	D938	T939	F940	Y941	S942	Y943	I944	Y945	C946	S947	O948	T949	D950	R951	L952	C953	A954	C955	T956	K957	G958	G959	E960	
L961	H962	F963	L964	Q965	I966	G967	G968	THR	CYS	ASP	ASP	ASP	ALA	ASP	ILE	LEU	VAL	ASP	GLY	SER	SER	LYS	GLY	GLU	PRO	SER	SER	SER	LYS	PRO	LEU	ASN	ASN	PRO	SER	PRO	GLY	I1006	S1007	G1008	V1009	D1010	L1011	L1012	V1013	D1014	Q1015	P1016	F1017	T1018	L1019	E1020							









VAL	CYS	ARG	ALA	THR	GLY	ALA	GLU	GLU	THR	LEU	MET	HIS	ASP	GLN	VAL	LYS	PRO	SER	SER	SER	LYS	GLU	LEU	PRO	SER	ASP	PHE	GLN	LEU	SER	ALA	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	136799	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)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	425.87997, 425.87997, 425.87997	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.17, 1.17, 1.17	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	0.25	0/22350	0.54	13/30362 (0.0%)
1	B	0.25	0/22350	0.54	13/30362 (0.0%)
All	All	0.25	0/44700	0.54	26/60724 (0.0%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1807	PRO	CA-N-CD	-12.39	94.15	111.50
1	B	1807	PRO	CA-N-CD	-12.38	94.16	111.50
1	B	1426	PRO	CA-N-CD	-9.27	98.52	111.50
1	A	1426	PRO	CA-N-CD	-9.24	98.56	111.50
1	A	2187	ASP	CB-CG-OD2	8.00	125.50	118.30
1	B	2187	ASP	CB-CG-OD2	7.97	125.47	118.30
1	B	3232	LEU	CA-CB-CG	6.75	130.83	115.30
1	A	3232	LEU	CA-CB-CG	6.75	130.83	115.30
1	B	2146	LEU	CA-CB-CG	6.38	129.97	115.30
1	A	2146	LEU	CA-CB-CG	6.37	129.94	115.30
1	A	2571	LEU	CA-CB-CG	6.16	129.47	115.30
1	B	2571	LEU	CA-CB-CG	6.15	129.45	115.30
1	A	1019	LEU	CA-CB-CG	5.86	128.78	115.30
1	B	1019	LEU	CA-CB-CG	5.84	128.72	115.30
1	A	1429	LEU	CA-CB-CG	5.75	128.52	115.30
1	B	1429	LEU	CA-CB-CG	5.74	128.50	115.30
1	B	2351	LEU	CA-CB-CG	5.74	128.50	115.30
1	A	2351	LEU	CA-CB-CG	5.73	128.48	115.30
1	A	3034	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	3034	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	1807	PRO	N-CD-CG	-5.17	95.44	103.20
1	B	1807	PRO	N-CD-CG	-5.16	95.47	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3564	MET	CA-CB-CG	5.10	121.98	113.30
1	A	3564	MET	CA-CB-CG	5.08	121.93	113.30
1	A	2030	LEU	CA-CB-CG	5.01	126.81	115.30
1	B	2030	LEU	CA-CB-CG	5.00	126.81	115.30

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	21940	0	22350	326	0
1	B	21940	0	22350	320	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	43882	0	44700	629	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 7.

All (629) 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:A:3984:ALA:HB1	1:A:4067:ILE:H	1.52	0.74
1:B:3984:ALA:HB1	1:B:4067:ILE:H	1.51	0.72
1:A:2145:LEU:HD21	1:A:2167:MET:HG3	1.75	0.68
1:B:2145:LEU:HD21	1:B:2167:MET:HG3	1.75	0.67
1:B:3224:HIS:HB2	1:B:3297:LYS:HB2	1.77	0.66
1:A:3224:HIS:HB2	1:A:3297:LYS:HB2	1.77	0.66
1:B:3547:CYS:HG	1:B:3846:HIS:HE2	1.44	0.65
1:A:3429:ASP:HA	1:A:3432:ILE:HD12	1.79	0.65
1:B:3429:ASP:HA	1:B:3432:ILE:HD12	1.79	0.65
1:B:1193:ASP:OD1	1:B:2565:GLN:NE2	2.30	0.65
1:A:3242:GLU:HG2	1:A:3252:PRO:HA	1.79	0.65
1:B:3242:GLU:HG2	1:B:3252:PRO:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:GLU:HG2	1:B:346:SER:H	1.63	0.64
1:A:1193:ASP:OD1	1:A:2565:GLN:NE2	2.30	0.63
1:A:343:GLU:HG2	1:A:346:SER:H	1.63	0.63
1:A:1819:ILE:HD12	1:A:1853:CYS:HB2	1.80	0.63
1:A:3462:ARG:HG3	1:A:3524:LEU:HD21	1.81	0.63
1:A:3547:CYS:HG	1:A:3846:HIS:HE2	1.46	0.62
1:A:1456:ASN:HD21	1:A:2033:THR:HG22	1.64	0.62
1:B:75:TYR:HB2	1:B:944:ILE:HD12	1.82	0.62
1:A:55:TRP:HE1	1:A:966:ILE:HG23	1.64	0.62
1:B:3462:ARG:HG3	1:B:3524:LEU:HD21	1.81	0.62
1:B:1819:ILE:HD12	1:B:1853:CYS:HB2	1.80	0.62
1:B:55:TRP:HE1	1:B:966:ILE:HG23	1.64	0.61
1:A:75:TYR:HB2	1:A:944:ILE:HD12	1.82	0.61
1:A:2658:GLU:HB2	1:A:2718:THR:HG22	1.82	0.61
1:B:1456:ASN:HD21	1:B:2033:THR:HG22	1.65	0.61
1:B:1853:CYS:SG	1:B:1854:ARG:N	2.74	0.61
1:B:2658:GLU:HB2	1:B:2718:THR:HG22	1.82	0.61
1:A:1980:LEU:HA	1:A:1983:GLN:HE21	1.66	0.61
1:A:3639:LEU:HD11	1:A:3711:LEU:HG	1.82	0.61
1:B:3639:LEU:HD11	1:B:3711:LEU:HG	1.82	0.61
1:A:1853:CYS:SG	1:A:1854:ARG:N	2.74	0.60
1:B:1980:LEU:HA	1:B:1983:GLN:HE21	1.66	0.60
1:A:2397:ILE:HD12	1:B:3325:LYS:HB2	1.84	0.60
1:B:3720:CYS:SG	1:B:3721:HIS:N	2.75	0.60
1:A:3720:CYS:SG	1:A:3721:HIS:N	2.75	0.59
1:B:1844:LEU:HD21	1:B:1847:LEU:HD21	1.85	0.59
1:A:1099:CYS:SG	1:A:1100:MET:N	2.75	0.59
1:A:1329:GLU:HB3	1:A:1380:LYS:HG3	1.85	0.59
1:B:1329:GLU:HB3	1:B:1380:LYS:HG3	1.85	0.59
1:A:2668:SER:HA	1:A:2693:VAL:HG22	1.85	0.59
1:A:3325:LYS:HB2	1:B:2397:ILE:HD12	1.85	0.58
1:B:1813:ALA:HB2	1:B:1863:ARG:HA	1.85	0.58
1:A:1844:LEU:HD21	1:A:1847:LEU:HD21	1.85	0.58
1:A:3396:LEU:HD11	1:A:3438:LEU:HD11	1.85	0.58
1:A:3534:CYS:HA	1:A:3539:LYS:HD2	1.85	0.58
1:A:417:LEU:HD23	1:A:419:LYS:HE3	1.85	0.58
1:A:2768:GLY:HA3	1:A:2831:GLY:HA2	1.86	0.58
1:B:3534:CYS:HA	1:B:3539:LYS:HD2	1.85	0.58
1:A:1813:ALA:HB2	1:A:1863:ARG:HA	1.85	0.58
1:B:1452:PHE:O	1:B:1456:ASN:ND2	2.36	0.58
1:B:3396:LEU:HD11	1:B:3438:LEU:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2768:GLY:HA3	1:B:2831:GLY:HA2	1.86	0.57
1:A:1829:ARG:NH2	1:A:1852:VAL:O	2.38	0.57
1:A:1771:GLN:NE2	1:A:1983:GLN:OE1	2.35	0.57
1:B:1099:CYS:SG	1:B:1100:MET:N	2.75	0.57
1:B:2668:SER:HA	1:B:2693:VAL:HG22	1.85	0.57
1:B:1328:HIS:HA	1:B:1331:LEU:HD12	1.87	0.57
1:A:1799:ILE:HD11	1:A:1882:THR:HA	1.87	0.57
1:B:2349:ASP:N	1:B:2349:ASP:OD1	2.38	0.57
1:B:1829:ARG:NH2	1:B:1852:VAL:O	2.38	0.56
1:A:1328:HIS:HA	1:A:1331:LEU:HD12	1.86	0.56
1:B:417:LEU:HD23	1:B:419:LYS:HE3	1.85	0.56
1:A:3242:GLU:HB2	1:A:3279:CYS:HB3	1.88	0.56
1:A:3396:LEU:HA	1:A:3399:ILE:HG12	1.87	0.56
1:A:630:LEU:HD12	1:A:720:LEU:HD22	1.88	0.56
1:B:3396:LEU:HA	1:B:3399:ILE:HG12	1.87	0.56
1:A:3627:LEU:HD12	1:A:3698:ILE:HD12	1.88	0.56
1:B:1015:GLN:HG3	1:B:1021:ILE:HD13	1.87	0.56
1:A:2349:ASP:OD1	1:A:2349:ASP:N	2.38	0.56
1:A:1452:PHE:O	1:A:1456:ASN:ND2	2.36	0.56
1:B:630:LEU:HD12	1:B:720:LEU:HD22	1.88	0.56
1:B:3242:GLU:HB2	1:B:3279:CYS:HB3	1.88	0.56
1:B:1883:TYR:O	1:B:1993:ARG:NH2	2.39	0.56
1:B:1494:THR:HG21	1:B:2111:ILE:HG22	1.88	0.56
1:B:1557:LEU:HD22	1:B:1805:LEU:HD13	1.87	0.56
1:B:3774:HIS:HB3	1:B:3777:ASN:HB2	1.88	0.56
1:A:1015:GLN:HG3	1:A:1021:ILE:HD13	1.87	0.55
1:A:1494:THR:HG21	1:A:2111:ILE:HG22	1.88	0.55
1:A:1883:TYR:O	1:A:1993:ARG:NH2	2.39	0.55
1:B:1799:ILE:HD11	1:B:1882:THR:HA	1.87	0.55
1:B:3716:LEU:HD13	1:B:3788:LEU:HD11	1.88	0.55
1:A:1429:LEU:HD23	1:A:1433:LEU:HD23	1.88	0.55
1:A:1885:LEU:HB2	1:A:1888:GLU:HG3	1.89	0.55
1:B:1885:LEU:HB2	1:B:1888:GLU:HG3	1.89	0.55
1:B:3627:LEU:HD12	1:B:3698:ILE:HD12	1.88	0.55
1:A:1557:LEU:HD22	1:A:1805:LEU:HD13	1.87	0.55
1:A:3716:LEU:HD13	1:A:3788:LEU:HD11	1.88	0.55
1:A:3774:HIS:HB3	1:A:3777:ASN:HB2	1.88	0.55
1:B:1771:GLN:NE2	1:B:1983:GLN:OE1	2.35	0.55
1:A:576:LYS:HE3	1:A:624:ARG:HE	1.72	0.55
1:B:1429:LEU:HD23	1:B:1433:LEU:HD23	1.88	0.55
1:A:2374:ILE:HG22	1:A:2375:VAL:HG13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2384:LEU:HB3	1:A:2646:LEU:HD11	1.89	0.54
1:A:1346:GLU:HA	1:A:1349:GLN:HE21	1.73	0.54
1:B:576:LYS:HE3	1:B:624:ARG:HE	1.72	0.54
1:B:2374:ILE:HG22	1:B:2375:VAL:HG13	1.88	0.54
1:B:2384:LEU:HB3	1:B:2646:LEU:HD11	1.89	0.54
1:A:2336:VAL:HG22	1:A:2358:LEU:HD11	1.90	0.54
1:A:2582:MET:HA	1:A:2585:MET:HG3	1.90	0.54
1:A:1124:LEU:HB3	1:A:1183:CYS:HB2	1.89	0.54
1:B:2582:MET:HA	1:B:2585:MET:HG3	1.90	0.54
1:A:3700:LYS:NZ	1:A:3769:GLN:O	2.41	0.54
1:B:514:GLN:HA	1:B:837:VAL:HG21	1.90	0.54
1:B:1806:ILE:HB	1:B:1842:LEU:HB3	1.90	0.54
1:A:3209:ASP:OD1	1:A:3209:ASP:N	2.36	0.54
1:A:154:VAL:HG23	1:A:263:LEU:HD13	1.91	0.53
1:A:2084:GLN:NE2	1:A:2600:ASN:O	2.41	0.53
1:A:2566:ALA:O	1:A:2584:LYS:NZ	2.41	0.53
1:B:1124:LEU:HB3	1:B:1183:CYS:HB2	1.89	0.53
1:B:1346:GLU:HA	1:B:1349:GLN:HE21	1.73	0.53
1:B:2775:ASN:O	1:B:2777:HIS:ND1	2.42	0.53
1:A:239:LEU:HD23	1:A:242:ILE:HD11	1.91	0.53
1:B:239:LEU:HD23	1:B:242:ILE:HD11	1.91	0.53
1:B:2084:GLN:NE2	1:B:2600:ASN:O	2.41	0.53
1:B:2934:LEU:HA	1:B:2942:ALA:HA	1.90	0.53
1:B:3700:LYS:NZ	1:B:3769:GLN:O	2.41	0.53
1:B:3616:SER:O	1:B:3616:SER:OG	2.26	0.53
1:A:3828:SER:HB2	1:A:4006:VAL:HB	1.91	0.53
1:B:3450:ILE:HA	1:B:3453:LEU:HD12	1.90	0.53
1:A:514:GLN:HA	1:A:837:VAL:HG21	1.90	0.53
1:A:2826:PHE:O	1:A:2915:ARG:NH2	2.42	0.53
1:B:2336:VAL:HG22	1:B:2358:LEU:HD11	1.90	0.53
1:A:1806:ILE:HB	1:A:1842:LEU:HB3	1.90	0.52
1:A:2775:ASN:O	1:A:2777:HIS:ND1	2.42	0.52
1:A:2713:ASN:HB2	1:B:2869:HIS:CE1	2.45	0.52
1:A:2934:LEU:HA	1:A:2942:ALA:HA	1.90	0.52
1:B:2777:HIS:CD2	1:B:2778:SER:H	2.28	0.52
1:B:2826:PHE:O	1:B:2915:ARG:NH2	2.42	0.52
1:B:154:VAL:HG23	1:B:263:LEU:HD13	1.91	0.52
1:A:80:ASN:HD21	1:A:948:GLY:HA3	1.75	0.52
1:B:3828:SER:HB2	1:B:4006:VAL:HB	1.91	0.52
1:A:2813:LEU:HD12	1:A:2851:VAL:HG11	1.92	0.52
1:A:2777:HIS:CD2	1:A:2778:SER:H	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ASN:HD21	1:B:948:GLY:HA3	1.75	0.51
1:B:1556:SER:HB2	1:B:1843:ILE:HG21	1.92	0.51
1:A:2688:ALA:O	1:A:2731:ASN:ND2	2.43	0.51
1:B:2927:ASN:HB2	1:B:3039:ILE:HG22	1.92	0.51
1:A:2869:HIS:CE1	1:B:2713:ASN:HB2	2.46	0.51
1:B:2121:LEU:HD23	1:B:2124:ILE:HD11	1.92	0.51
1:B:2813:LEU:HD12	1:B:2851:VAL:HG11	1.92	0.51
1:A:1556:SER:HB2	1:A:1843:ILE:HG21	1.92	0.51
1:B:1917:MET:HB3	1:B:1991:VAL:HG12	1.93	0.51
1:B:2688:ALA:O	1:B:2731:ASN:ND2	2.43	0.51
1:B:3494:LEU:HB2	1:B:3541:ALA:HB1	1.92	0.51
1:A:1126:LYS:HB2	1:A:1182:LEU:HD12	1.92	0.51
1:A:1182:LEU:HD13	1:A:1208:LEU:HD23	1.92	0.51
1:A:3169:ILE:HB	1:A:3183:LEU:HD11	1.93	0.51
1:B:3512:ASP:OD1	1:B:3512:ASP:N	2.40	0.51
1:A:2416:LEU:HD21	1:A:2639:LEU:HD11	1.93	0.51
1:A:2927:ASN:HB2	1:A:3039:ILE:HG22	1.92	0.51
1:B:1126:LYS:HB2	1:B:1182:LEU:HD12	1.92	0.51
1:B:3002:ASN:ND2	1:B:3321:ASP:OD2	2.42	0.51
1:A:1364:SER:HA	1:A:1414:ASN:HD22	1.76	0.51
1:A:3401:LEU:HD11	1:A:3453:LEU:HD23	1.93	0.51
1:A:3494:LEU:HB2	1:A:3541:ALA:HB1	1.92	0.51
1:A:3819:ASP:OD1	1:A:3819:ASP:N	2.43	0.51
1:B:2390:THR:HB	1:B:2656:GLN:HG2	1.93	0.51
1:A:2121:LEU:HD23	1:A:2124:ILE:HD11	1.92	0.51
1:A:4068:GLN:O	1:A:4072:GLN:NE2	2.40	0.51
1:B:1356:LEU:HD23	1:B:1359:LEU:HD21	1.92	0.51
1:A:914:ILE:HB	1:A:924:ALA:HB3	1.93	0.51
1:A:3450:ILE:HA	1:A:3453:LEU:HD12	1.91	0.51
1:B:3401:LEU:HD11	1:B:3453:LEU:HD23	1.93	0.51
1:A:2175:VAL:HG23	1:A:2357:VAL:HG21	1.93	0.50
1:B:1364:SER:HA	1:B:1414:ASN:HD22	1.76	0.50
1:B:2416:LEU:HD21	1:B:2639:LEU:HD11	1.93	0.50
1:A:1356:LEU:HD23	1:A:1359:LEU:HD21	1.92	0.50
1:A:2390:THR:HB	1:A:2656:GLN:HG2	1.93	0.50
1:B:289:ARG:O	1:B:292:THR:OG1	2.29	0.50
1:A:2880:ARG:HA	1:A:2880:ARG:HH11	1.76	0.50
1:B:2566:ALA:O	1:B:2584:LYS:NZ	2.40	0.50
1:B:153:PRO:HG3	1:B:376:PRO:HB2	1.93	0.50
1:A:3262:LEU:HD11	1:B:3286:ARG:HH21	1.76	0.50
1:B:3169:ILE:HB	1:B:3183:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:914:ILE:HB	1:B:924:ALA:HB3	1.93	0.50
1:A:163:LEU:HD11	1:A:255:VAL:HG13	1.94	0.50
1:A:2872:THR:HG22	1:A:3000:LEU:HD12	1.94	0.50
1:B:163:LEU:HD11	1:B:255:VAL:HG13	1.94	0.50
1:B:1331:LEU:HD22	1:B:1352:VAL:HG23	1.94	0.50
1:B:2006:SER:HG	1:B:2009:SER:HG	1.52	0.50
1:A:164:GLU:HG3	1:A:258:ARG:HH12	1.77	0.50
1:A:1917:MET:HB3	1:A:1991:VAL:HG12	1.92	0.50
1:A:3616:SER:O	1:A:3616:SER:OG	2.26	0.50
1:B:2389:GLY:HA2	1:B:2655:VAL:HA	1.94	0.50
1:A:289:ARG:O	1:A:292:THR:OG1	2.29	0.49
1:A:3124:SER:OG	1:A:3125:MET:N	2.45	0.49
1:A:3429:ASP:OD2	1:A:3853:HIS:ND1	2.42	0.49
1:B:1182:LEU:HD13	1:B:1208:LEU:HD23	1.93	0.49
1:A:2389:GLY:HA2	1:A:2655:VAL:HA	1.94	0.49
1:B:1914:LEU:HD12	1:B:1994:LEU:HB3	1.92	0.49
1:A:1122:VAL:HG22	1:A:1224:VAL:HG22	1.94	0.49
1:B:3124:SER:OG	1:B:3125:MET:N	2.45	0.49
1:B:3209:ASP:OD1	1:B:3209:ASP:N	2.36	0.49
1:A:153:PRO:HG3	1:A:376:PRO:HB2	1.93	0.49
1:A:3286:ARG:HH21	1:B:3262:LEU:HD11	1.78	0.49
1:B:2180:ASP:OD1	1:B:2356:LYS:NZ	2.38	0.49
1:B:2872:THR:HG22	1:B:3000:LEU:HD12	1.94	0.49
1:A:1914:LEU:HD12	1:A:1994:LEU:HB3	1.92	0.49
1:B:1510:LEU:HB3	1:B:1560:LEU:HB2	1.95	0.49
1:B:2690:ARG:O	1:B:2731:ASN:ND2	2.45	0.49
1:B:164:GLU:HG3	1:B:258:ARG:HH12	1.77	0.49
1:B:1335:LEU:HB3	1:B:1388:ILE:HG22	1.94	0.49
1:B:3778:GLN:HG2	1:B:4070:PRO:HG3	1.95	0.49
1:B:4173:VAL:HG11	1:B:4220:LEU:HB2	1.94	0.49
1:A:3002:ASN:ND2	1:A:3321:ASP:OD2	2.42	0.49
1:B:749:LEU:HD12	1:B:824:TYR:HB2	1.95	0.49
1:B:2713:ASN:OD1	1:B:2772:HIS:ND1	2.37	0.49
1:B:2852:SER:HA	1:B:2940:TYR:HA	1.95	0.49
1:B:3429:ASP:OD2	1:B:3853:HIS:ND1	2.42	0.49
1:A:2690:ARG:O	1:A:2731:ASN:ND2	2.45	0.49
1:B:240:LYS:NZ	1:B:284:TYR:OH	2.45	0.49
1:B:1101:VAL:HA	1:B:1305:ARG:HH21	1.78	0.49
1:B:2354:VAL:O	1:B:2358:LEU:HB2	2.13	0.49
1:B:3819:ASP:N	1:B:3819:ASP:OD1	2.43	0.49
1:B:137:ARG:NH2	1:B:148:THR:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2880:ARG:HH11	1:B:2880:ARG:HA	1.76	0.49
1:B:2175:VAL:HG23	1:B:2357:VAL:HG21	1.93	0.48
1:A:1510:LEU:HB3	1:A:1560:LEU:HB2	1.95	0.48
1:A:3778:GLN:HG2	1:A:4070:PRO:HG3	1.95	0.48
1:B:1075:ARG:HH21	1:B:1077:TRP:HZ2	1.61	0.48
1:A:240:LYS:NZ	1:A:284:TYR:OH	2.45	0.48
1:A:1075:ARG:HH21	1:A:1077:TRP:HZ2	1.61	0.48
1:A:1335:LEU:HB3	1:A:1388:ILE:HG22	1.94	0.48
1:A:1505:PRO:O	1:A:1985:ASN:ND2	2.46	0.48
1:A:2755:ASP:OD1	1:A:2755:ASP:N	2.46	0.48
1:A:1331:LEU:HD22	1:A:1352:VAL:HG23	1.94	0.48
1:A:4173:VAL:HG11	1:A:4220:LEU:HB2	1.94	0.48
1:B:1505:PRO:O	1:B:1985:ASN:ND2	2.46	0.48
1:A:3039:ILE:O	1:A:3043:LEU:HB2	2.13	0.48
1:B:2755:ASP:N	1:B:2755:ASP:OD1	2.46	0.48
1:B:1122:VAL:HG22	1:B:1224:VAL:HG22	1.94	0.48
1:A:1101:VAL:HA	1:A:1305:ARG:HH21	1.78	0.48
1:A:2354:VAL:O	1:A:2358:LEU:HB2	2.13	0.48
1:A:2371:LEU:HA	1:A:2374:ILE:HB	1.95	0.48
1:A:2852:SER:HA	1:A:2940:TYR:HA	1.95	0.48
1:A:4060:SER:N	1:A:4063:GLU:OE1	2.47	0.48
1:B:2371:LEU:HA	1:B:2374:ILE:HB	1.95	0.48
1:A:3755:GLN:O	1:A:3759:ILE:HG12	2.14	0.48
1:A:2601:THR:OG1	1:A:2602:SER:N	2.47	0.48
1:B:2820:SER:HB3	1:B:2826:PHE:HD2	1.79	0.48
1:B:3755:GLN:O	1:B:3759:ILE:HG12	2.14	0.48
1:A:137:ARG:NH2	1:A:148:THR:O	2.46	0.48
1:A:3338:LEU:HD12	1:A:3381:VAL:HG23	1.96	0.48
1:B:3196:ALA:HB3	1:B:3294:SER:HA	1.96	0.48
1:B:3443:ASP:OD1	1:B:3446:THR:OG1	2.27	0.48
1:A:1027:GLU:HA	1:A:1030:ARG:HE	1.79	0.47
1:A:1359:LEU:HA	1:A:1362:VAL:HG22	1.96	0.47
1:A:1398:ARG:NH1	1:A:1846:ASP:OD1	2.47	0.47
1:A:2180:ASP:OD1	1:A:2356:LYS:NZ	2.38	0.47
1:B:3039:ILE:O	1:B:3043:LEU:HB2	2.13	0.47
1:B:3338:LEU:HD12	1:B:3381:VAL:HG23	1.96	0.47
1:B:1791:VAL:HG23	1:B:1858:ILE:HB	1.97	0.47
1:B:157:GLN:HB3	1:B:226:HIS:HB3	1.96	0.47
1:B:1359:LEU:HA	1:B:1362:VAL:HG22	1.96	0.47
1:B:1412:ILE:HD13	1:B:1424:PHE:HB3	1.96	0.47
1:B:4260:ARG:NH1	1:B:4367:SER:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4441:LYS:HE3	1:B:4482:GLN:HG2	1.96	0.47
1:A:749:LEU:HD12	1:A:824:TYR:HB2	1.95	0.47
1:A:2820:SER:HB3	1:A:2826:PHE:HD2	1.79	0.47
1:A:4441:LYS:HE3	1:A:4482:GLN:HG2	1.96	0.47
1:B:2362:ALA:HA	1:B:2369:ILE:HD12	1.97	0.47
1:A:147:ASP:OD2	1:A:218:THR:OG1	2.32	0.47
1:A:916:ASP:HB2	1:A:923:LEU:HD11	1.97	0.47
1:A:1353:LEU:HD21	1:A:1404:CYS:HB2	1.96	0.47
1:A:2697:ASN:OD1	1:A:2698:GLN:N	2.48	0.47
1:A:3481:THR:HA	1:B:2162:VAL:HG13	1.96	0.47
1:B:95:ASP:OD2	1:B:212:LYS:NZ	2.45	0.47
1:B:215:LYS:HD2	1:B:215:LYS:HA	1.73	0.47
1:B:2687:ASN:HB3	1:B:2690:ARG:HG3	1.97	0.47
1:A:323:ASP:OD1	1:A:323:ASP:N	2.42	0.47
1:A:3623:ILE:HG23	1:A:3698:ILE:HD11	1.95	0.47
1:B:147:ASP:OD2	1:B:218:THR:OG1	2.32	0.47
1:B:945:TYR:OH	1:B:950:ASP:OD1	2.28	0.47
1:B:1398:ARG:NH1	1:B:1846:ASP:OD1	2.47	0.47
1:B:2601:THR:OG1	1:B:2602:SER:N	2.47	0.47
1:A:513:LEU:HD11	1:A:568:LEU:HD22	1.96	0.47
1:A:1811:ASP:HA	1:A:1863:ARG:HD3	1.96	0.47
1:A:2162:VAL:HG13	1:B:3481:THR:HA	1.96	0.47
1:A:2697:ASN:OD1	1:A:2699:ALA:N	2.45	0.47
1:A:2726:LEU:HD22	1:A:2752:LEU:HD21	1.97	0.47
1:A:3196:ALA:HB3	1:A:3294:SER:HA	1.96	0.47
1:A:3709:ASN:HD21	1:A:3780:LEU:HD21	1.79	0.47
1:A:3967:LEU:HD12	1:A:4004:LEU:HB3	1.97	0.47
1:B:513:LEU:HD11	1:B:568:LEU:HD22	1.96	0.47
1:B:912:VAL:HB	1:B:926:VAL:HB	1.96	0.47
1:B:1378:LEU:HD13	1:B:1382:ARG:HH21	1.79	0.47
1:B:2697:ASN:OD1	1:B:2698:GLN:N	2.48	0.47
1:A:4260:ARG:NH1	1:A:4367:SER:O	2.47	0.47
1:B:3709:ASN:HD21	1:B:3780:LEU:HD21	1.79	0.47
1:A:1791:VAL:HG23	1:A:1858:ILE:HB	1.96	0.47
1:B:1027:GLU:HA	1:B:1030:ARG:HE	1.79	0.47
1:A:2834:ASP:OD1	1:A:2834:ASP:N	2.47	0.47
1:A:4396:LEU:HB3	1:A:4484:THR:HG21	1.97	0.47
1:B:1353:LEU:HD21	1:B:1404:CYS:HB2	1.96	0.47
1:B:2726:LEU:HD22	1:B:2752:LEU:HD21	1.97	0.47
1:B:3433:ASP:OD2	1:B:3853:HIS:NE2	2.48	0.47
1:B:4060:SER:N	1:B:4063:GLU:OE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:GLN:HB3	1:A:226:HIS:HB3	1.96	0.46
1:A:912:VAL:HB	1:A:926:VAL:HB	1.97	0.46
1:A:1077:TRP:HB2	1:A:1299:VAL:HG12	1.97	0.46
1:A:1213:ALA:HA	1:A:1315:ARG:HD3	1.97	0.46
1:A:2109:LEU:H	1:A:2109:LEU:HD23	1.81	0.46
1:A:3433:ASP:OD2	1:A:3853:HIS:NE2	2.48	0.46
1:B:174:LEU:HD22	1:B:200:LEU:HD12	1.98	0.46
1:B:916:ASP:HB2	1:B:923:LEU:HD11	1.97	0.46
1:B:1504:ASP:O	1:B:1981:GLN:NE2	2.44	0.46
1:B:1811:ASP:HA	1:B:1863:ARG:HD3	1.96	0.46
1:B:3279:CYS:SG	1:B:3281:ARG:NH1	2.89	0.46
1:A:4244:LEU:HA	1:A:4247:ILE:HG22	1.97	0.46
1:B:1091:PHE:HB2	1:B:1222:ILE:HG13	1.97	0.46
1:A:3279:CYS:SG	1:A:3281:ARG:NH1	2.89	0.46
1:B:1302:THR:HG21	1:B:1304:ARG:HH21	1.80	0.46
1:B:3623:ILE:HG23	1:B:3698:ILE:HD11	1.95	0.46
1:B:3967:LEU:HD12	1:B:4004:LEU:HB3	1.97	0.46
1:A:1091:PHE:HB2	1:A:1222:ILE:HG13	1.97	0.46
1:A:1378:LEU:HD13	1:A:1382:ARG:HH21	1.79	0.46
1:A:3856:ARG:HD2	1:A:3856:ARG:HA	1.75	0.46
1:B:1089:HIS:HB2	1:B:1224:VAL:HB	1.98	0.46
1:A:174:LEU:HD22	1:A:200:LEU:HD12	1.98	0.46
1:A:1412:ILE:HD13	1:A:1424:PHE:HB3	1.96	0.46
1:A:2926:VAL:HA	1:A:2929:LEU:HB2	1.97	0.46
1:B:323:ASP:OD1	1:B:323:ASP:N	2.43	0.46
1:B:900:LEU:HB2	1:B:917:LEU:HB3	1.98	0.46
1:B:2834:ASP:OD1	1:B:2834:ASP:N	2.47	0.46
1:A:1439:LEU:HD22	1:A:2026:ILE:HD11	1.98	0.46
1:A:2687:ASN:HB3	1:A:2690:ARG:HG3	1.97	0.46
1:B:1782:ARG:O	1:B:1789:ARG:NH2	2.48	0.46
1:B:2863:VAL:HG11	1:B:2926:VAL:HG11	1.98	0.46
1:B:4244:LEU:HA	1:B:4247:ILE:HG22	1.97	0.46
1:A:1089:HIS:HB2	1:A:1224:VAL:HB	1.98	0.46
1:A:2362:ALA:HA	1:A:2369:ILE:HD12	1.97	0.46
1:A:4153:ILE:HG23	1:A:4210:PRO:HG3	1.98	0.46
1:A:3846:HIS:CD2	1:A:3847:PRO:HD2	2.51	0.46
1:B:1439:LEU:HD22	1:B:2026:ILE:HD11	1.98	0.46
1:B:4396:LEU:HB3	1:B:4484:THR:HG21	1.97	0.46
1:A:1490:ALA:O	1:A:1494:THR:HG23	2.15	0.46
1:A:2671:SER:O	1:A:2690:ARG:NH1	2.49	0.46
1:A:2863:VAL:HG11	1:A:2926:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2204:ILE:HD13	1:B:2356:LYS:HD2	1.98	0.46
1:B:3846:HIS:CD2	1:B:3847:PRO:HD2	2.51	0.46
1:B:1490:ALA:O	1:B:1494:THR:HG23	2.15	0.45
1:B:2109:LEU:HD23	1:B:2109:LEU:H	1.80	0.45
1:B:3502:TRP:HH2	1:B:3619:SER:HB3	1.81	0.45
1:A:900:LEU:HB2	1:A:917:LEU:HB3	1.98	0.45
1:B:4068:GLN:O	1:B:4072:GLN:NE2	2.40	0.45
1:A:3684:ALA:HB2	1:A:3759:ILE:HD13	1.99	0.45
1:B:1388:ILE:HA	1:B:1391:VAL:HG22	1.99	0.45
1:B:1456:ASN:HA	1:B:1459:LYS:HD3	1.99	0.45
1:B:3817:LEU:HD11	1:B:4185:LEU:HD23	1.98	0.45
1:A:245:ASN:ND2	1:A:361:GLU:OE1	2.50	0.45
1:A:3225:ILE:HB	1:A:3265:ILE:HB	1.98	0.45
1:B:3331:LEU:HD21	1:B:3378:ILE:HG23	1.98	0.45
1:A:1302:THR:HG21	1:A:1304:ARG:HH21	1.80	0.45
1:B:245:ASN:ND2	1:B:361:GLU:OE1	2.50	0.45
1:B:1077:TRP:HB2	1:B:1299:VAL:HG12	1.97	0.45
1:B:1213:ALA:HA	1:B:1315:ARG:HD3	1.97	0.45
1:A:324:ASP:N	1:A:324:ASP:OD1	2.50	0.45
1:A:1489:GLU:HA	1:A:1492:LEU:HD12	1.98	0.45
1:B:1780:ILE:HD11	1:B:1873:ILE:HD11	1.99	0.45
1:A:391:PHE:HA	1:A:510:LEU:HD12	1.99	0.45
1:A:1388:ILE:HA	1:A:1391:VAL:HG22	1.99	0.45
1:B:2926:VAL:HA	1:B:2929:LEU:HB2	1.97	0.45
1:A:95:ASP:OD2	1:A:212:LYS:NZ	2.45	0.45
1:B:94:ILE:HG12	1:B:101:THR:HG23	1.99	0.45
1:B:4153:ILE:HG23	1:B:4210:PRO:HG3	1.98	0.45
1:A:116:LYS:HE2	1:A:116:LYS:HB2	1.86	0.45
1:A:2655:VAL:HG11	1:A:2660:LEU:HD12	1.99	0.45
1:B:3684:ALA:HB2	1:B:3759:ILE:HD13	1.99	0.45
1:A:162:GLN:OE1	1:A:222:HIS:ND1	2.48	0.45
1:A:1504:ASP:O	1:A:1981:GLN:NE2	2.44	0.45
1:A:2028:ARG:HB2	1:A:2074:ILE:HG22	1.99	0.45
1:A:2204:ILE:HD13	1:A:2356:LYS:HD2	1.98	0.45
1:A:2368:THR:HG21	1:A:2418:GLY:HA3	1.99	0.45
1:A:2713:ASN:HD21	1:A:2772:HIS:HB3	1.82	0.45
1:B:2655:VAL:HG11	1:B:2660:LEU:HD12	1.99	0.45
1:B:3220:LEU:HD21	1:B:3223:ILE:HD11	1.99	0.45
1:A:1015:GLN:HG3	1:A:1021:ILE:HG21	1.99	0.44
1:A:3817:LEU:HD11	1:A:4185:LEU:HD23	1.98	0.44
1:B:2713:ASN:HD21	1:B:2772:HIS:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3258:VAL:HG23	1:B:2777:HIS:CD2	2.53	0.44
1:A:3502:TRP:HH2	1:A:3619:SER:HB3	1.81	0.44
1:A:1473:LEU:HB3	1:A:2030:LEU:HD11	1.99	0.44
1:A:1809:CYS:H	1:A:1837:ILE:HG22	1.82	0.44
1:A:3602:PRO:HB2	1:A:3603:LEU:H	1.59	0.44
1:B:1473:LEU:HB3	1:B:2030:LEU:HD11	1.99	0.44
1:A:144:LEU:HD12	1:A:216:TRP:HH2	1.82	0.44
1:A:1557:LEU:HD11	1:A:1803:ASP:HB3	2.00	0.44
1:A:2039:HIS:HB2	1:A:2597:ALA:HB2	1.99	0.44
1:A:2771:PRO:HG2	1:B:2869:HIS:HE1	1.82	0.44
1:A:1456:ASN:HA	1:A:1459:LYS:HD3	1.98	0.44
1:A:2173:MET:HB3	1:A:2173:MET:HE2	1.94	0.44
1:A:2985:LEU:HD13	1:A:3052:MET:HG3	2.00	0.44
1:A:3220:LEU:HD21	1:A:3223:ILE:HD11	1.99	0.44
1:B:1429:LEU:HD11	1:B:1462:ASP:H	1.83	0.44
1:B:1943:ASP:N	1:B:1943:ASP:OD1	2.51	0.44
1:B:2671:SER:O	1:B:2690:ARG:NH1	2.49	0.44
1:B:2985:LEU:HD13	1:B:3052:MET:HG3	2.00	0.44
1:B:3526:PHE:O	1:B:3530:MET:HG2	2.18	0.44
1:A:2324:ALA:HB3	1:A:2327:ARG:HE	1.82	0.44
1:B:1489:GLU:HA	1:B:1492:LEU:HD12	1.98	0.44
1:B:1809:CYS:H	1:B:1837:ILE:HG22	1.82	0.44
1:B:3225:ILE:HB	1:B:3265:ILE:HB	1.98	0.44
1:A:1377:LEU:O	1:A:1381:THR:OG1	2.34	0.44
1:A:1429:LEU:HD11	1:A:1462:ASP:H	1.83	0.44
1:A:1780:ILE:HD11	1:A:1873:ILE:HD11	1.99	0.44
1:A:2027:ILE:HD13	1:A:2066:LEU:HD21	1.99	0.44
1:A:2366:ARG:HA	1:A:2366:ARG:HD3	1.85	0.44
1:B:2039:HIS:HB2	1:B:2597:ALA:HB2	1.99	0.44
1:A:3331:LEU:HD21	1:A:3378:ILE:HG23	1.98	0.44
1:B:2028:ARG:HB2	1:B:2074:ILE:HG22	1.99	0.44
1:A:94:ILE:HG12	1:A:101:THR:HG23	1.99	0.44
1:A:1943:ASP:OD1	1:A:1943:ASP:N	2.51	0.44
1:A:3813:LEU:HA	1:A:3817:LEU:HD22	2.00	0.44
1:A:3547:CYS:HB2	1:A:3616:SER:HA	2.00	0.43
1:A:1782:ARG:O	1:A:1789:ARG:NH2	2.48	0.43
1:A:2713:ASN:OD1	1:A:2772:HIS:ND1	2.37	0.43
1:B:1767:SER:HB3	1:B:1920:LEU:HD11	2.00	0.43
1:A:2820:SER:HA	1:A:2826:PHE:HB2	2.01	0.43
1:A:4080:LEU:HD12	1:A:4165:LEU:HD13	2.00	0.43
1:B:827:LEU:HB3	1:B:845:LYS:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1026:VAL:HG21	1:B:1351:LEU:HD22	2.01	0.43
1:B:1563:VAL:HG12	1:B:1879:TYR:HD1	1.83	0.43
1:B:2027:ILE:HD13	1:B:2066:LEU:HD21	1.99	0.43
1:B:2324:ALA:HB3	1:B:2327:ARG:HE	1.82	0.43
1:B:3179:ALA:HB1	1:B:3182:LEU:HD12	2.01	0.43
1:B:3679:THR:OG1	1:B:3680:ALA:N	2.51	0.43
1:A:2717:ARG:NH2	1:B:2876:LYS:HB3	2.33	0.43
1:A:3512:ASP:OD1	1:A:3512:ASP:N	2.40	0.43
1:A:3526:PHE:O	1:A:3530:MET:HG2	2.18	0.43
1:B:2368:THR:HG21	1:B:2418:GLY:HA3	1.99	0.43
1:B:2864:THR:HA	1:B:2867:VAL:HG12	2.00	0.43
1:B:3521:LEU:HD23	1:B:3525:LEU:HD13	2.01	0.43
1:B:3813:LEU:HD22	1:B:4189:LEU:HD22	2.01	0.43
1:B:4184:LEU:HD11	1:B:4212:LEU:HB3	2.01	0.43
1:A:1380:LYS:HA	1:A:1380:LYS:HD3	1.87	0.43
1:A:2869:HIS:HE1	1:B:2771:PRO:HG2	1.83	0.43
1:A:3521:LEU:HD23	1:A:3525:LEU:HD13	2.01	0.43
1:B:144:LEU:HD12	1:B:216:TRP:HH2	1.82	0.43
1:B:391:PHE:HA	1:B:510:LEU:HD12	1.99	0.43
1:B:1015:GLN:HG3	1:B:1021:ILE:HG21	1.99	0.43
1:B:3856:ARG:HD2	1:B:3856:ARG:HA	1.75	0.43
1:A:2876:LYS:HB3	1:B:2717:ARG:NH2	2.34	0.43
1:A:3756:ARG:HE	1:A:3756:ARG:HB3	1.64	0.43
1:B:324:ASP:OD1	1:B:324:ASP:N	2.50	0.43
1:B:2820:SER:HA	1:B:2826:PHE:HB2	2.01	0.43
1:A:1026:VAL:HG21	1:A:1351:LEU:HD22	2.01	0.43
1:A:568:LEU:HD11	1:A:630:LEU:HB3	2.01	0.43
1:A:827:LEU:HB3	1:A:845:LYS:HB3	2.00	0.43
1:A:1777:SER:HA	1:A:1874:PRO:HA	2.01	0.43
1:A:3813:LEU:HD22	1:A:4189:LEU:HD22	2.01	0.43
1:B:1498:LEU:HD13	1:B:1974:TYR:CG	2.54	0.43
1:B:3813:LEU:HA	1:B:3817:LEU:HD22	2.00	0.43
1:A:2777:HIS:CD2	1:B:3258:VAL:HG23	2.54	0.43
1:B:162:GLN:OE1	1:B:222:HIS:ND1	2.48	0.43
1:B:2697:ASN:OD1	1:B:2699:ALA:N	2.45	0.43
1:A:1563:VAL:HG12	1:A:1879:TYR:HD1	1.83	0.43
1:A:2034:LEU:HD23	1:A:2034:LEU:HA	1.88	0.43
1:A:3179:ALA:HB1	1:A:3182:LEU:HD12	2.01	0.43
1:A:3443:ASP:OD1	1:A:3446:THR:OG1	2.27	0.43
1:A:3679:THR:OG1	1:A:3680:ALA:N	2.51	0.43
1:B:1030:ARG:HH12	1:B:1891:LEU:HD22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1557:LEU:HD11	1:B:1803:ASP:HB3	2.00	0.43
1:B:2665:LEU:HD12	1:B:2728:LEU:HD22	2.00	0.43
1:A:1992:GLN:O	1:A:1996:VAL:HG22	2.19	0.42
1:A:2864:THR:HA	1:A:2867:VAL:HG12	2.00	0.42
1:B:3400:LEU:HD23	1:B:3400:LEU:HA	1.88	0.42
1:B:4080:LEU:HD12	1:B:4165:LEU:HD13	2.00	0.42
1:A:1030:ARG:HH12	1:A:1891:LEU:HD22	1.83	0.42
1:B:192:PHE:HD2	1:B:231:ILE:HG21	1.84	0.42
1:B:2351:LEU:HD11	1:B:2399:TRP:CZ3	2.54	0.42
1:B:3982:THR:HG22	1:B:3985:GLN:HG3	2.00	0.42
1:A:632:LEU:HD23	1:A:632:LEU:HA	1.89	0.42
1:A:1034:LEU:HD23	1:A:1038:PHE:HD2	1.85	0.42
1:B:2669:LEU:O	1:B:2690:ARG:NH1	2.51	0.42
1:A:1396:ALA:HB1	1:A:1400:ILE:HB	2.02	0.42
1:B:1193:ASP:HA	1:B:2581:LEU:HD21	2.02	0.42
1:B:1992:GLN:O	1:B:1996:VAL:HG22	2.20	0.42
1:B:3253:LEU:HB3	1:B:3254:SER:H	1.70	0.42
1:B:4260:ARG:NH2	1:B:4364:LEU:O	2.53	0.42
1:A:1445:GLY:HA3	1:A:1509:ASP:HB3	2.02	0.42
1:A:1498:LEU:HD13	1:A:1974:TYR:CG	2.54	0.42
1:A:1831:LEU:HD23	1:A:1831:LEU:HA	1.86	0.42
1:A:2099:VAL:HG22	1:A:2103:LEU:HD12	2.01	0.42
1:A:2665:LEU:HD12	1:A:2728:LEU:HD22	2.00	0.42
1:A:2669:LEU:O	1:A:2690:ARG:NH1	2.51	0.42
1:A:3683:VAL:HA	1:A:3686:ILE:HG22	2.02	0.42
1:B:568:LEU:HD11	1:B:630:LEU:HB3	2.01	0.42
1:B:2099:VAL:HG22	1:B:2103:LEU:HD12	2.01	0.42
1:B:3547:CYS:HB2	1:B:3616:SER:HA	2.00	0.42
1:B:4260:ARG:HH21	1:B:4365:SER:HA	1.84	0.42
1:A:191:LEU:HD12	1:A:191:LEU:HA	1.90	0.42
1:A:630:LEU:HB2	1:A:720:LEU:HB3	2.00	0.42
1:A:853:GLN:HE21	1:A:909:GLY:HA3	1.85	0.42
1:A:945:TYR:OH	1:A:950:ASP:OD1	2.28	0.42
1:A:1473:LEU:HD12	1:A:1473:LEU:HA	1.88	0.42
1:A:1474:LEU:HD12	1:A:2062:LEU:HD11	2.02	0.42
1:A:2029:TYR:O	1:A:2033:THR:HG23	2.20	0.42
1:A:2705:LEU:HD23	1:A:2705:LEU:HA	1.94	0.42
1:A:3124:SER:HB2	1:B:2347:HIS:CG	2.55	0.42
1:A:3432:ILE:HG23	1:A:3496:CYS:HB2	2.01	0.42
1:A:3982:THR:HG22	1:A:3985:GLN:HG3	2.00	0.42
1:A:4260:ARG:HH21	1:A:4365:SER:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:VAL:HG11	1:A:398:HIS:HA	2.02	0.42
1:A:193:ILE:HD13	1:A:193:ILE:HA	1.92	0.42
1:B:1337:ARG:NH2	1:B:1349:GLN:OE1	2.53	0.42
1:B:2173:MET:HB3	1:B:2173:MET:HE2	1.94	0.42
1:B:2650:LEU:HD13	1:B:2707:VAL:HG11	2.01	0.42
1:A:834:THR:OG1	1:A:835:ARG:N	2.53	0.42
1:A:1935:LEU:O	1:A:1939:LEU:HB2	2.20	0.42
1:A:1978:ILE:HD13	1:A:1978:ILE:HA	1.92	0.42
1:B:630:LEU:HB2	1:B:720:LEU:HB3	2.00	0.42
1:B:3127:SER:O	1:B:3131:LYS:HB2	2.20	0.42
1:A:1767:SER:HB3	1:A:1920:LEU:HD11	2.00	0.42
1:A:1800:LEU:HB2	1:A:1881:HIS:HB2	2.02	0.42
1:A:2795:ARG:HA	1:A:2795:ARG:HD2	1.84	0.42
1:A:4184:LEU:HD11	1:A:4212:LEU:HB3	2.01	0.42
1:A:4260:ARG:NH2	1:A:4364:LEU:O	2.53	0.42
1:B:1396:ALA:HB1	1:B:1400:ILE:HB	2.02	0.42
1:B:2029:TYR:O	1:B:2033:THR:HG23	2.20	0.42
1:B:3525:LEU:HD21	1:B:3545:LEU:HD23	2.02	0.42
1:A:192:PHE:HD2	1:A:231:ILE:HG21	1.84	0.42
1:A:1193:ASP:HA	1:A:2581:LEU:HD21	2.02	0.42
1:A:1353:LEU:HD23	1:A:1403:LYS:HB3	2.01	0.42
1:A:2142:LEU:O	1:A:2146:LEU:HD23	2.20	0.42
1:A:2351:LEU:HD11	1:A:2399:TRP:CZ3	2.54	0.42
1:A:3127:SER:O	1:A:3131:LYS:HB2	2.20	0.42
1:B:853:GLN:HE21	1:B:909:GLY:HA3	1.85	0.42
1:B:2142:LEU:O	1:B:2146:LEU:HD23	2.20	0.42
1:B:2582:MET:O	1:B:2586:MET:HG3	2.20	0.42
1:B:2705:LEU:HD23	1:B:2705:LEU:HA	1.94	0.42
1:B:3865:THR:HA	1:B:3982:THR:HA	2.02	0.42
1:A:3525:LEU:HD21	1:A:3545:LEU:HD23	2.02	0.41
1:B:834:THR:OG1	1:B:835:ARG:N	2.53	0.41
1:B:3085:ILE:HA	1:B:3088:VAL:HG12	2.02	0.41
1:B:3432:ILE:HG23	1:B:3496:CYS:HB2	2.02	0.41
1:A:1337:ARG:NH2	1:A:1349:GLN:OE1	2.53	0.41
1:A:2840:LEU:HD11	1:A:2922:LEU:HD23	2.02	0.41
1:A:3169:ILE:HG13	1:A:3212:ILE:HG12	2.01	0.41
1:A:3689:PHE:O	1:A:3693:VAL:HG22	2.20	0.41
1:B:1038:PHE:HA	1:B:1096:PRO:HD3	2.02	0.41
1:B:1353:LEU:HD23	1:B:1403:LYS:HB3	2.01	0.41
1:B:1777:SER:HA	1:B:1874:PRO:HA	2.01	0.41
1:B:1939:LEU:HD23	1:B:1939:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1182:LEU:HD23	1:A:1182:LEU:HA	1.91	0.41
1:A:1477:VAL:HG13	1:A:2023:LEU:HD22	2.03	0.41
1:B:173:LEU:HD23	1:B:248:ALA:HB1	2.02	0.41
1:B:3169:ILE:HG13	1:B:3212:ILE:HG12	2.01	0.41
1:A:91:ILE:HD12	1:A:107:LEU:HD21	2.02	0.41
1:A:365:ASN:OD1	1:A:365:ASN:N	2.54	0.41
1:A:1783:MET:SD	1:A:1783:MET:N	2.94	0.41
1:A:1812:LEU:HD13	1:A:1862:GLY:HA2	2.02	0.41
1:B:2840:LEU:HD11	1:B:2922:LEU:HD23	2.02	0.41
1:B:3030:ILE:N	1:B:3034:ASP:OD1	2.54	0.41
1:A:3085:ILE:HA	1:A:3088:VAL:HG12	2.02	0.41
1:A:3695:ASN:OD1	1:A:3769:GLN:NE2	2.43	0.41
1:A:4241:ILE:HD12	1:A:4241:ILE:HA	1.94	0.41
1:B:1935:LEU:O	1:B:1939:LEU:HB2	2.20	0.41
1:B:2099:VAL:O	1:B:2103:LEU:HB2	2.21	0.41
1:A:1290:LEU:HD22	1:A:1294:ASP:HB3	2.01	0.41
1:A:2347:HIS:CG	1:B:3124:SER:HB2	2.56	0.41
1:A:2764:LYS:HA	1:A:2764:LYS:HD3	1.81	0.41
1:B:246:VAL:HG23	1:B:248:ALA:H	1.86	0.41
1:B:858:SER:OG	1:B:906:THR:OG1	2.35	0.41
1:B:1445:GLY:HA3	1:B:1509:ASP:HB3	2.02	0.41
1:B:1477:VAL:HG13	1:B:2023:LEU:HD22	2.03	0.41
1:B:1783:MET:SD	1:B:1783:MET:N	2.94	0.41
1:A:1190:SER:O	1:A:1190:SER:OG	2.38	0.41
1:A:2099:VAL:O	1:A:2103:LEU:HB2	2.21	0.41
1:A:2582:MET:O	1:A:2586:MET:HG3	2.20	0.41
1:A:3823:THR:HB	1:A:4001:SER:HA	2.01	0.41
1:A:3865:THR:HA	1:A:3982:THR:HA	2.01	0.41
1:B:91:ILE:HD12	1:B:107:LEU:HD21	2.02	0.41
1:B:1569:THR:OG1	1:B:1794:ASP:O	2.34	0.41
1:B:2812:LEU:HD12	1:B:2812:LEU:HA	1.92	0.41
1:B:3484:TYR:HA	1:B:3487:LEU:HG	2.02	0.41
1:B:3823:THR:HB	1:B:4001:SER:HA	2.01	0.41
1:A:1038:PHE:HA	1:A:1096:PRO:HD3	2.02	0.41
1:A:1398:ARG:HD2	1:A:1562:GLU:HB2	2.03	0.41
1:A:2354:VAL:HA	1:A:2357:VAL:HG12	2.03	0.41
1:A:3035:GLY:O	1:A:3039:ILE:HG23	2.21	0.41
1:A:3074:THR:OG1	1:A:3075:CYS:N	2.53	0.41
1:B:1309:THR:HG23	1:B:1311:ILE:H	1.85	0.41
1:B:1812:LEU:HD13	1:B:1862:GLY:HA2	2.02	0.41
1:B:3689:PHE:O	1:B:3693:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LYS:HD2	1:A:215:LYS:HA	1.73	0.41
1:A:1569:THR:OG1	1:A:1794:ASP:O	2.34	0.41
1:A:1863:ARG:HG2	1:A:1866:SER:HB3	2.03	0.41
1:A:2650:LEU:HD13	1:A:2707:VAL:HG11	2.01	0.41
1:A:2873:CYS:O	1:B:2713:ASN:ND2	2.54	0.41
1:A:3454:LEU:HA	1:A:3457:VAL:HG12	2.03	0.41
1:B:1474:LEU:HD12	1:B:2062:LEU:HD11	2.02	0.41
1:B:2354:VAL:HA	1:B:2357:VAL:HG12	2.03	0.41
1:B:3175:THR:OG1	1:B:3177:GLN:O	2.33	0.41
1:B:3635:LEU:HD11	1:B:3690:LEU:HD21	2.02	0.41
1:B:3683:VAL:HA	1:B:3686:ILE:HG22	2.02	0.41
1:A:173:LEU:HD23	1:A:248:ALA:HB1	2.02	0.41
1:A:1309:THR:HG23	1:A:1311:ILE:H	1.85	0.41
1:A:3030:ILE:N	1:A:3034:ASP:OD1	2.54	0.41
1:B:1398:ARG:HD2	1:B:1562:GLU:HB2	2.03	0.41
1:B:2716:LEU:HA	1:B:2719:TRP:HB2	2.03	0.41
1:B:3870:LEU:HD21	1:B:3967:LEU:HD21	2.02	0.41
1:A:934:THR:HG23	1:A:936:GLU:H	1.86	0.40
1:A:2096:LEU:HD23	1:A:2096:LEU:HA	1.91	0.40
1:A:3635:LEU:HD11	1:A:3690:LEU:HD21	2.02	0.40
1:B:207:THR:HA	1:B:214:ALA:HB2	2.03	0.40
1:B:510:LEU:HD22	1:B:567:LEU:HD11	2.03	0.40
1:B:2050:LEU:HA	1:B:2053:THR:HG22	2.03	0.40
1:A:207:THR:HA	1:A:214:ALA:HB2	2.03	0.40
1:A:2050:LEU:HA	1:A:2053:THR:HG22	2.03	0.40
1:A:2716:LEU:HA	1:A:2719:TRP:HB2	2.03	0.40
1:B:123:VAL:HG11	1:B:398:HIS:HA	2.02	0.40
1:B:1034:LEU:HD23	1:B:1038:PHE:HD2	1.85	0.40
1:B:1290:LEU:HD22	1:B:1294:ASP:HB3	2.01	0.40
1:B:1989:ASN:HD22	1:B:1989:ASN:HA	1.66	0.40
1:B:2172:VAL:HA	1:B:2175:VAL:HG22	2.03	0.40
1:B:3990:LEU:HD12	1:B:3995:LEU:HB2	2.04	0.40
1:A:1799:ILE:HD12	1:A:1799:ILE:HA	1.97	0.40
1:B:1207:LYS:HD3	1:B:1207:LYS:HA	1.87	0.40
1:B:3167:GLY:HA2	1:B:3215:PRO:HD3	2.04	0.40
1:B:3454:LEU:HA	1:B:3457:VAL:HG12	2.03	0.40
1:B:3627:LEU:HD23	1:B:3627:LEU:HA	1.88	0.40
1:B:3035:GLY:O	1:B:3039:ILE:HG23	2.21	0.40
1:B:3198:SER:HA	1:B:3291:LEU:O	2.22	0.40
1:B:3224:HIS:HD2	1:B:3299:LEU:HG	1.87	0.40
1:A:1009:VAL:HG12	1:A:1313:LYS:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:LYS:HZ2	1:B:372:LEU:HB3	1.87	0.40
1:B:3074:THR:OG1	1:B:3075:CYS:N	2.53	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2745/4867 (56%)	2649 (96%)	96 (4%)	0	100	100
1	B	2745/4867 (56%)	2650 (96%)	95 (4%)	0	100	100
All	All	5490/9734 (56%)	5299 (96%)	191 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	2497/4225 (59%)	2452 (98%)	45 (2%)	59	78
1	B	2497/4225 (59%)	2451 (98%)	46 (2%)	59	78
All	All	4994/8450 (59%)	4903 (98%)	91 (2%)	61	78

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	A	65	CYS
1	A	192	PHE
1	A	201	LYS
1	A	1017	PHE
1	A	1030	ARG
1	A	1046	TRP
1	A	1106	PHE
1	A	1126	LYS
1	A	1343	GLN
1	A	1467	SER
1	A	1770	LEU
1	A	1818	ASP
1	A	1829	ARG
1	A	1881	HIS
1	A	1887	TRP
1	A	1914	LEU
1	A	2003	LYS
1	A	2030	LEU
1	A	2097	SER
1	A	2344	PHE
1	A	2407	SER
1	A	2582	MET
1	A	2633	LEU
1	A	2711	TYR
1	A	2811	PHE
1	A	2852	SER
1	A	2935	SER
1	A	3052	MET
1	A	3193	ARG
1	A	3201	PHE
1	A	3334	LEU
1	A	3371	CYS
1	A	3374	HIS
1	A	3436	TYR
1	A	3462	ARG
1	A	3488	MET
1	A	3490	SER
1	A	3550	CYS
1	A	3616	SER
1	A	3720	CYS
1	A	3810	ARG
1	A	3830	CYS

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Mol	Chain	Res	Type
1	A	4000	ARG
1	A	4440	MET
1	B	60	ASP
1	B	65	CYS
1	B	192	PHE
1	B	201	LYS
1	B	1017	PHE
1	B	1030	ARG
1	B	1046	TRP
1	B	1106	PHE
1	B	1126	LYS
1	B	1343	GLN
1	B	1467	SER
1	B	1770	LEU
1	B	1818	ASP
1	B	1829	ARG
1	B	1881	HIS
1	B	1887	TRP
1	B	1914	LEU
1	B	2003	LYS
1	B	2030	LEU
1	B	2097	SER
1	B	2344	PHE
1	B	2407	SER
1	B	2582	MET
1	B	2633	LEU
1	B	2711	TYR
1	B	2811	PHE
1	B	2852	SER
1	B	2935	SER
1	B	3052	MET
1	B	3193	ARG
1	B	3201	PHE
1	B	3268	GLN
1	B	3334	LEU
1	B	3371	CYS
1	B	3374	HIS
1	B	3436	TYR
1	B	3462	ARG
1	B	3488	MET
1	B	3490	SER
1	B	3550	CYS

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Mol	Chain	Res	Type
1	B	3616	SER
1	B	3720	CYS
1	B	3810	ARG
1	B	3830	CYS
1	B	4000	ARG
1	B	4440	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3228	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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.

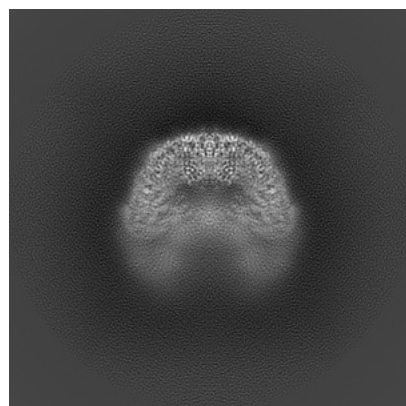
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15663. These allow visual inspection of the internal detail of the map and identification of artifacts.

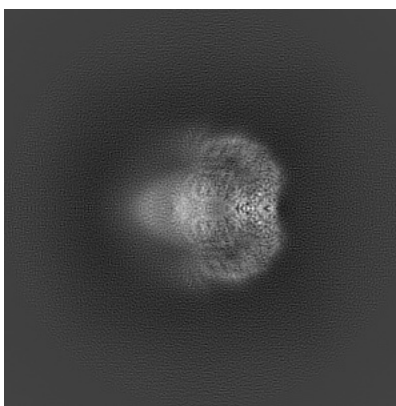
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

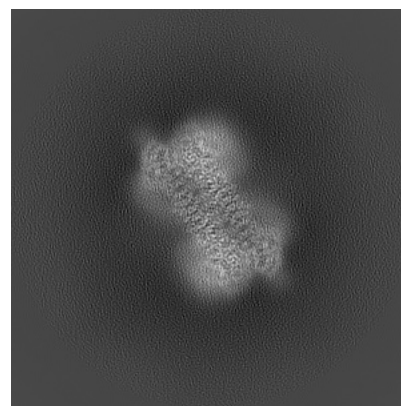
#### 6.1.1 Primary map



X

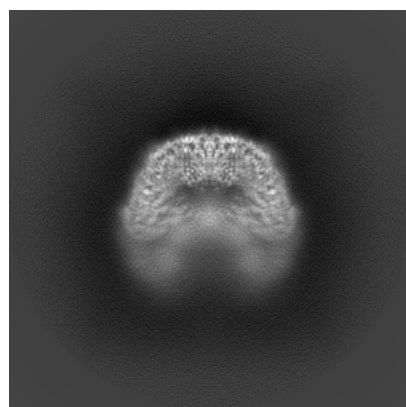


Y

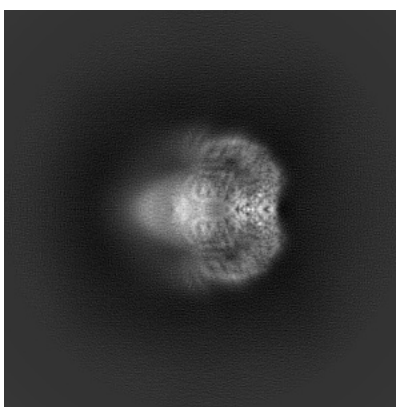


Z

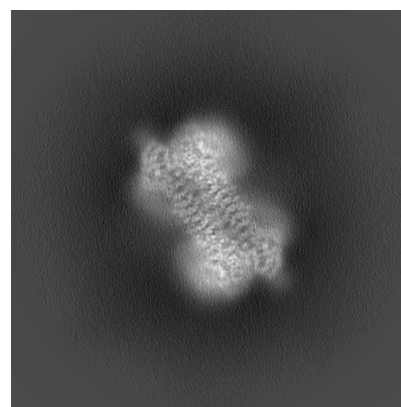
#### 6.1.2 Raw map



X



Y



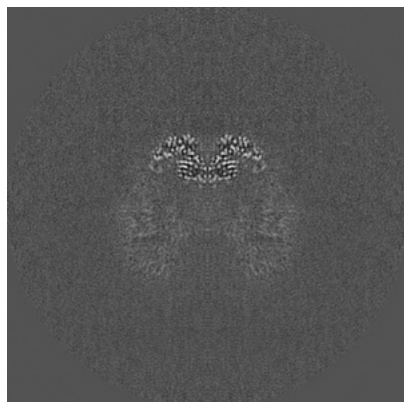
Z

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

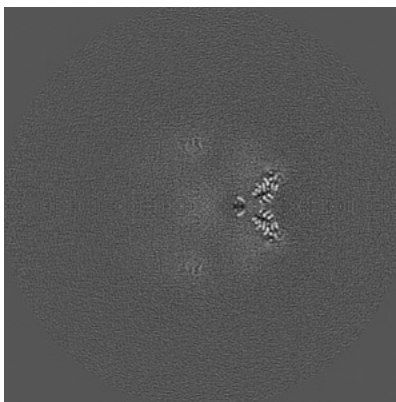


## 6.2 Central slices [i](#)

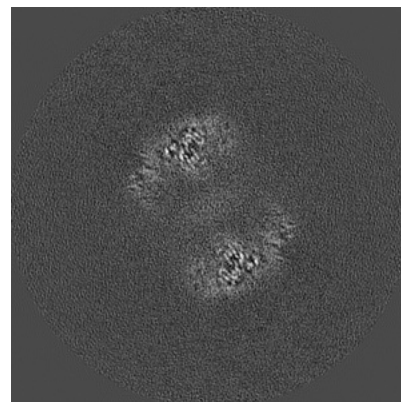
### 6.2.1 Primary map



X Index: 182

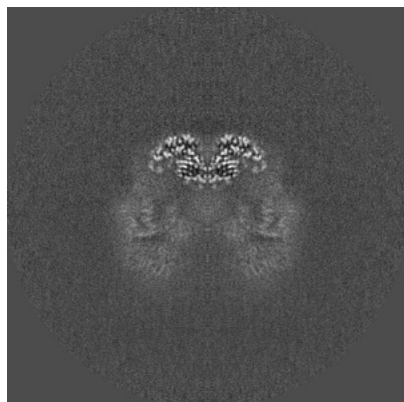


Y Index: 182

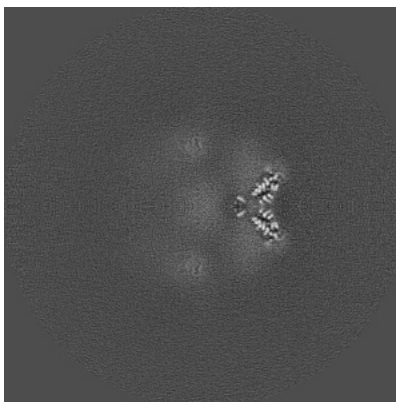


Z Index: 182

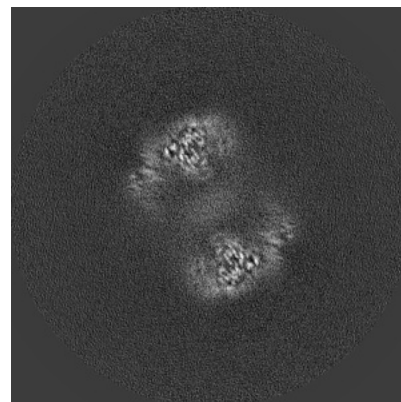
### 6.2.2 Raw map



X Index: 182



Y Index: 182

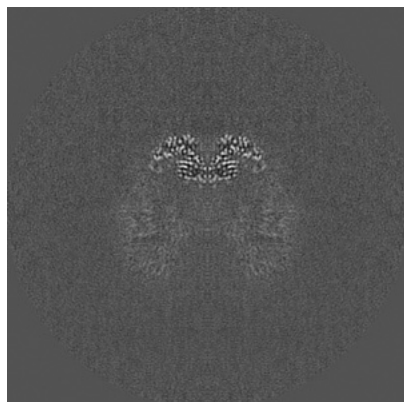


Z Index: 182

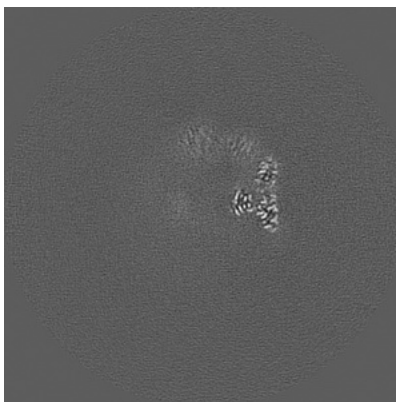
The images above show central slices of the map in three orthogonal directions.

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

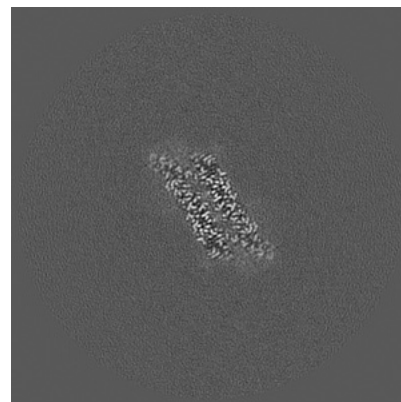
### 6.3.1 Primary map



X Index: 182

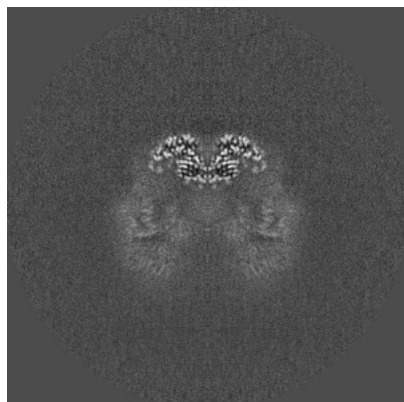


Y Index: 161

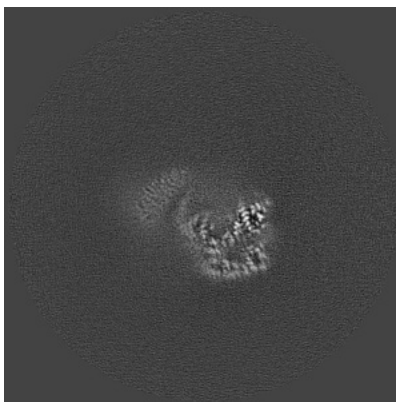


Z Index: 236

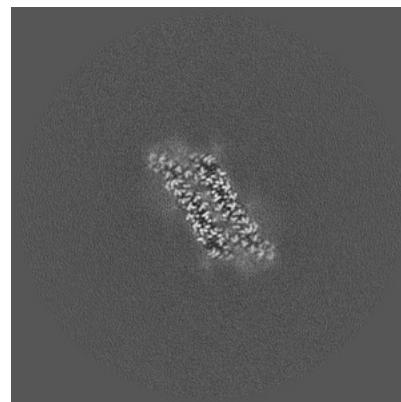
### 6.3.2 Raw map



X Index: 182



Y Index: 227

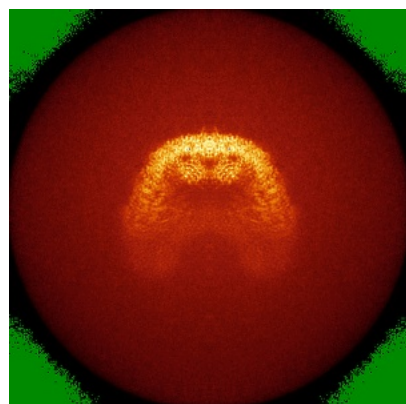


Z Index: 236

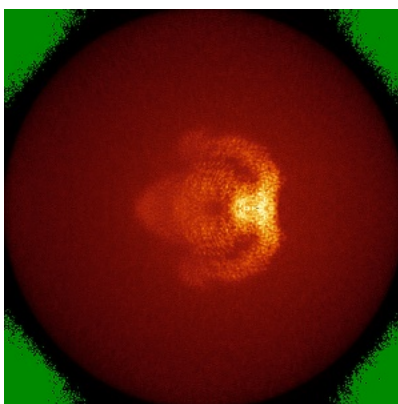
The images above show the largest variance slices of the map in three orthogonal directions.

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

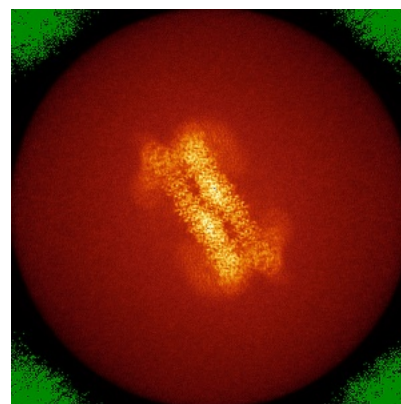
### 6.4.1 Primary map



X

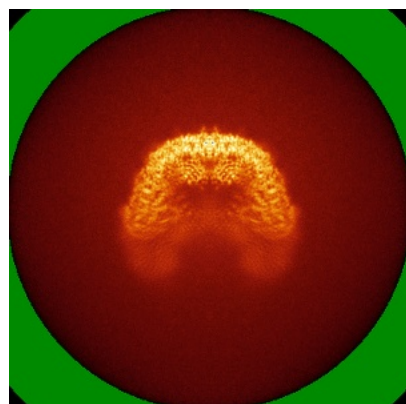


Y

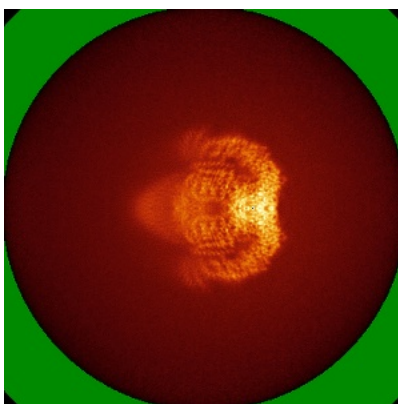


Z

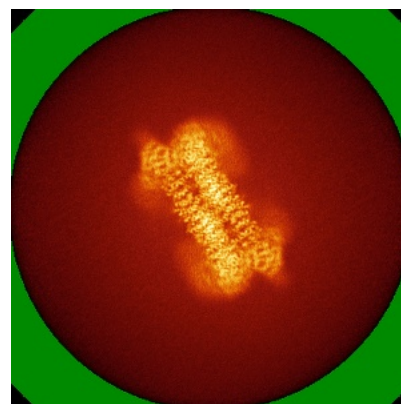
### 6.4.2 Raw map



X



Y



Z

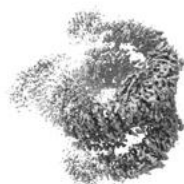
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



Y



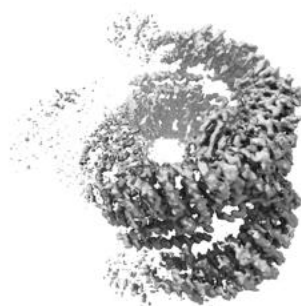
Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

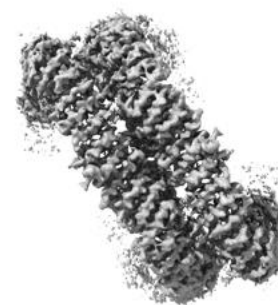
### 6.5.2 Raw map



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.

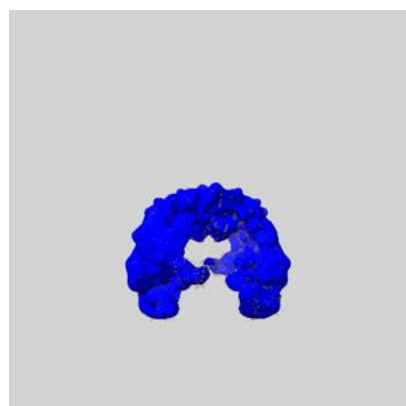
## 6.6 Mask visualisation [i](#)

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

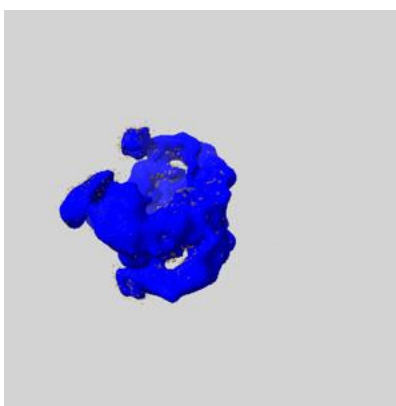
A mask typically either:

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

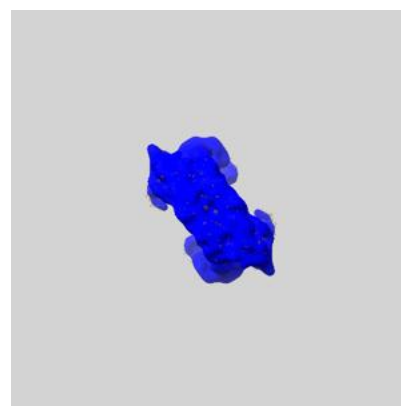
### 6.6.1 emd\_15663\_msk\_1.map [i](#)



X



Y



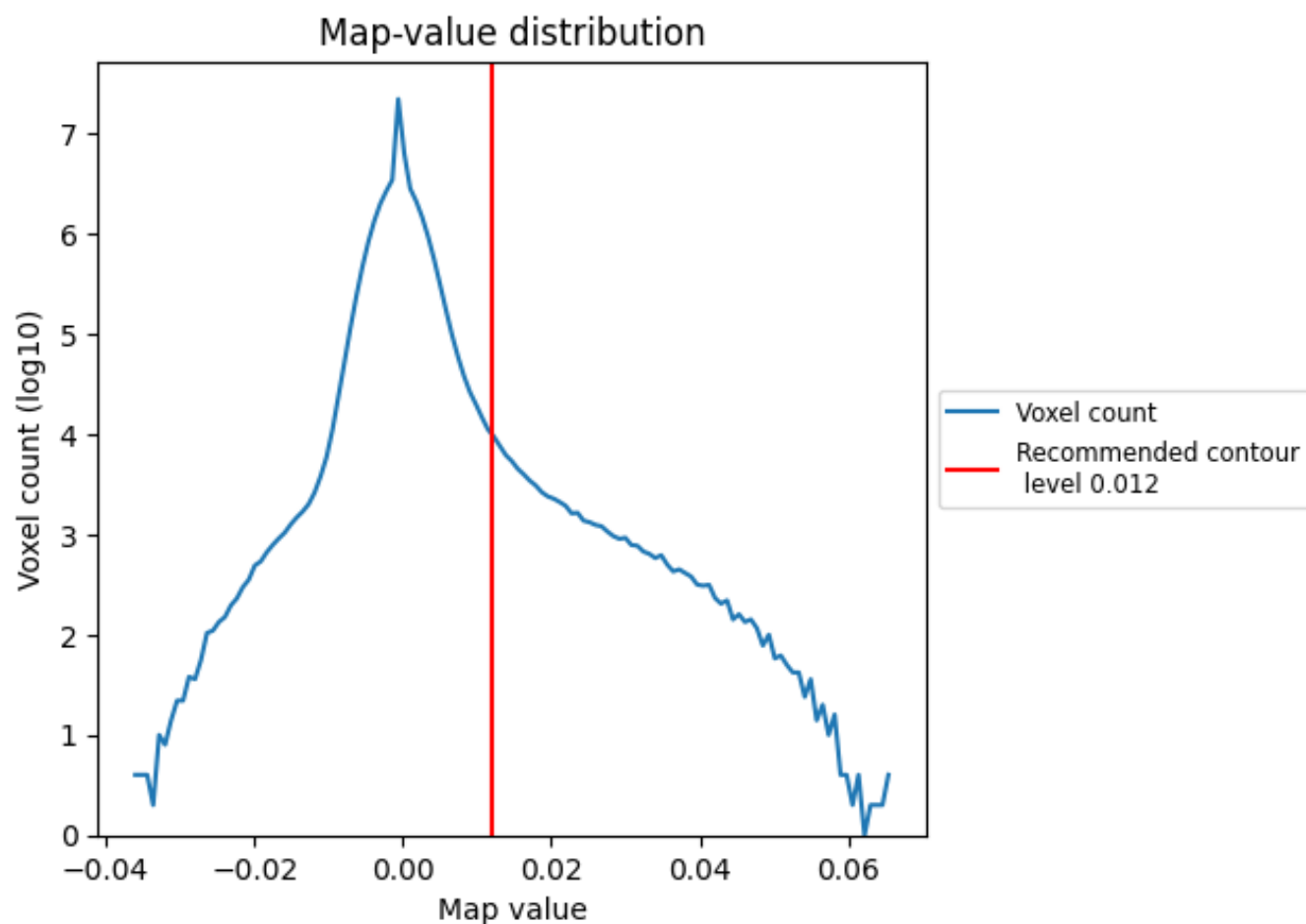
Z



## 7 Map analysis [i](#)

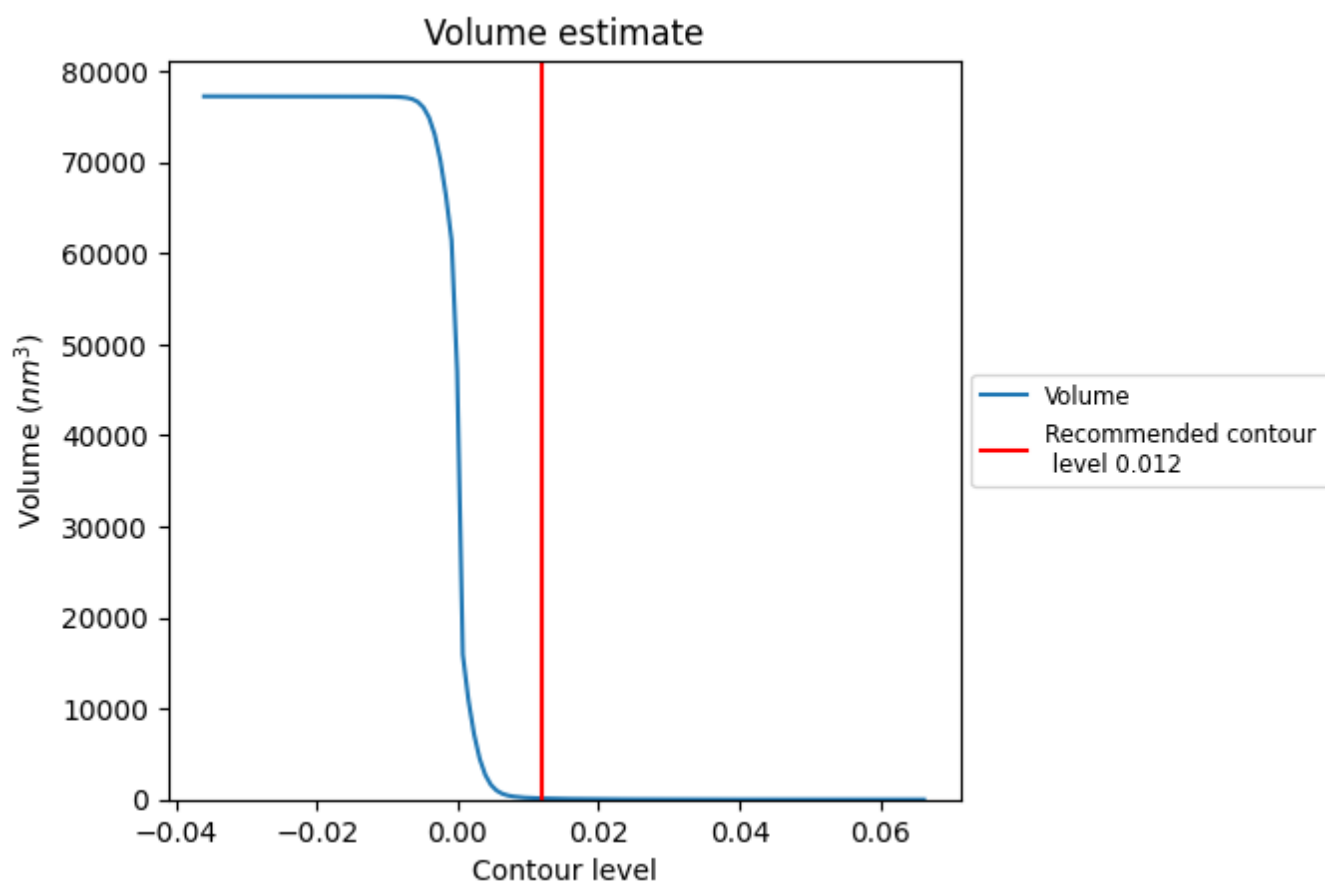
This section contains the results of statistical analysis of the map.

### 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.

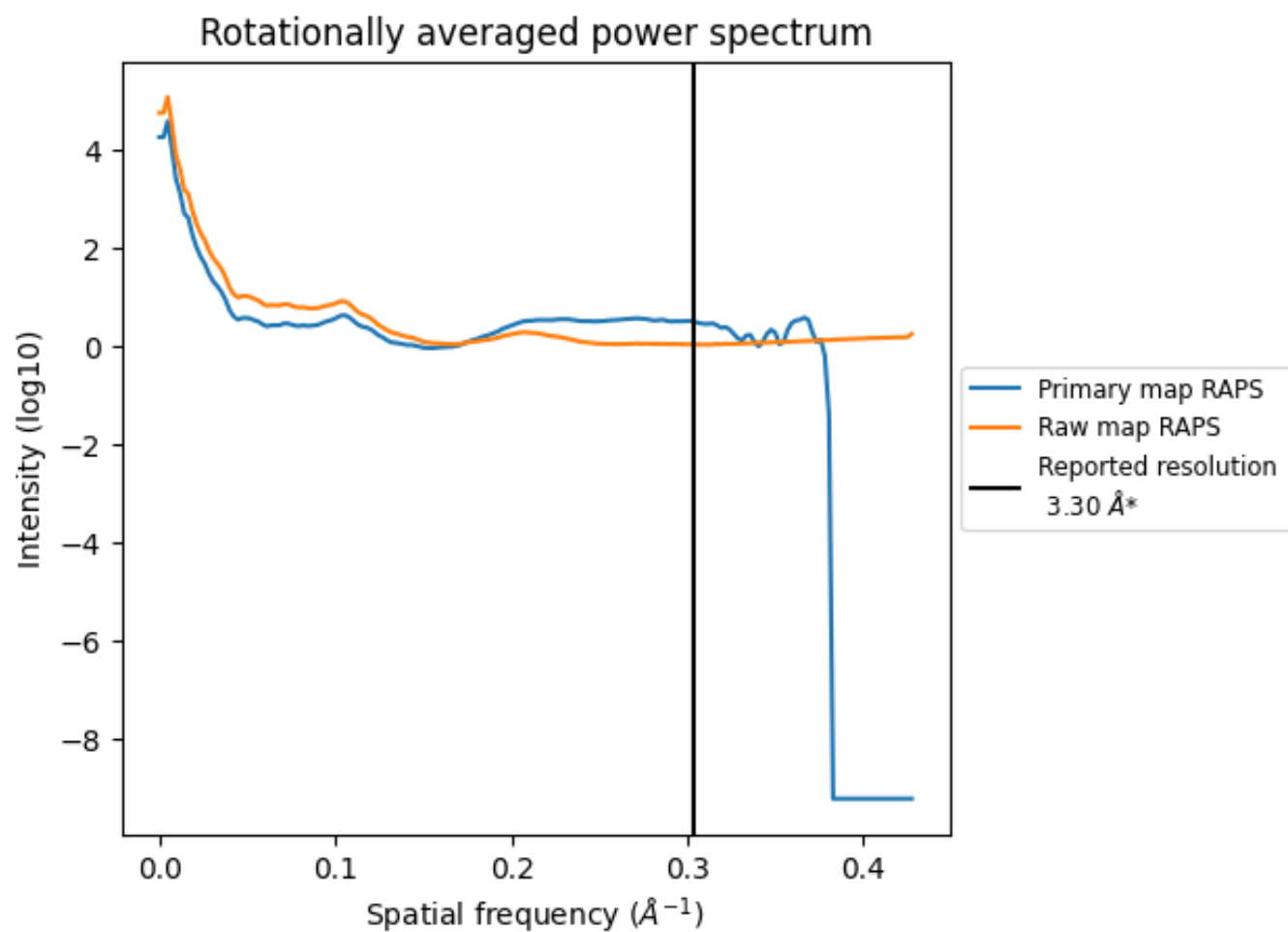
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 128 nm<sup>3</sup>; this corresponds to an approximate mass of 116 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 ⓘ



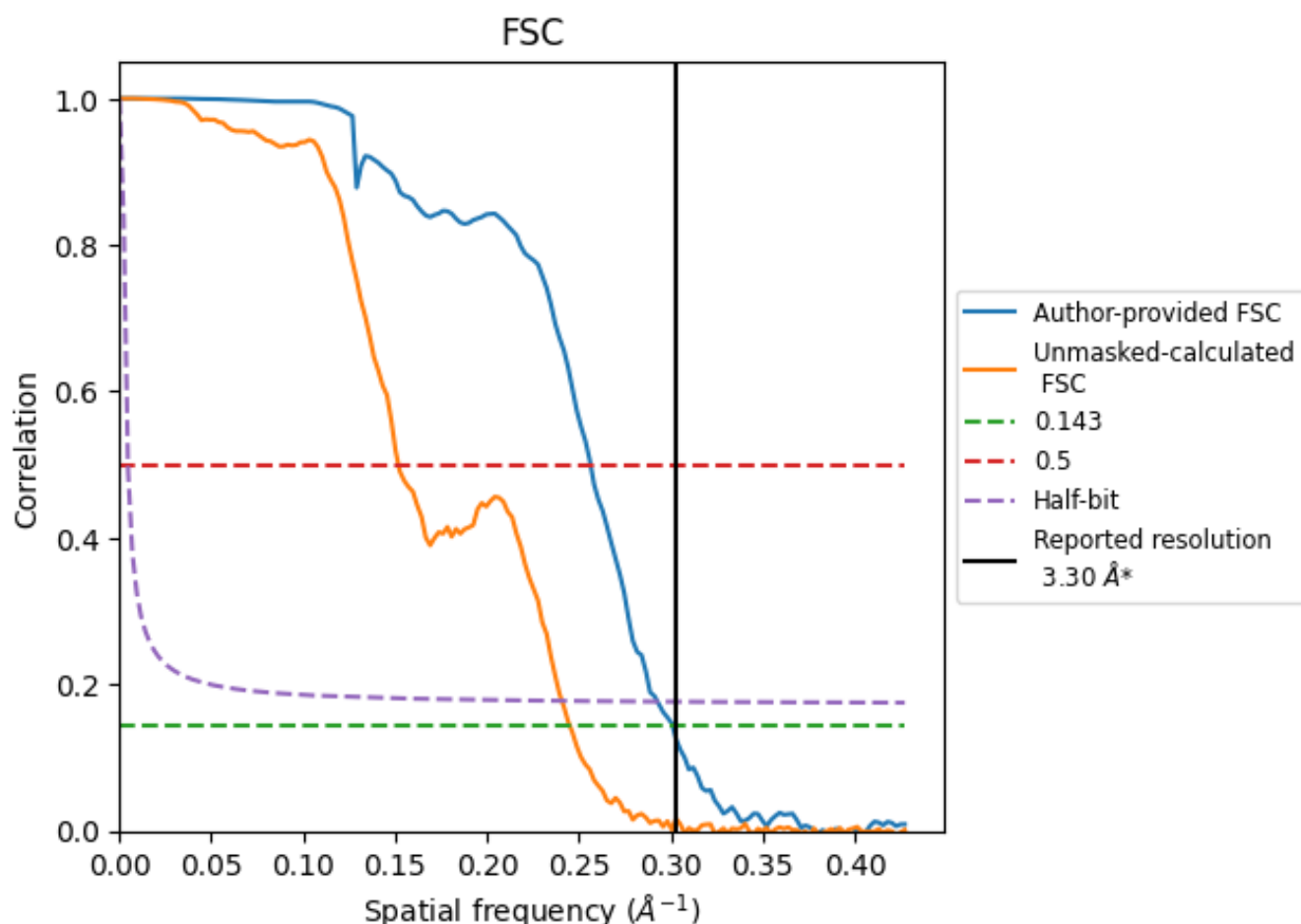
\*Reported resolution corresponds to spatial frequency of 0.303  $\text{\AA}^{-1}$



## 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 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

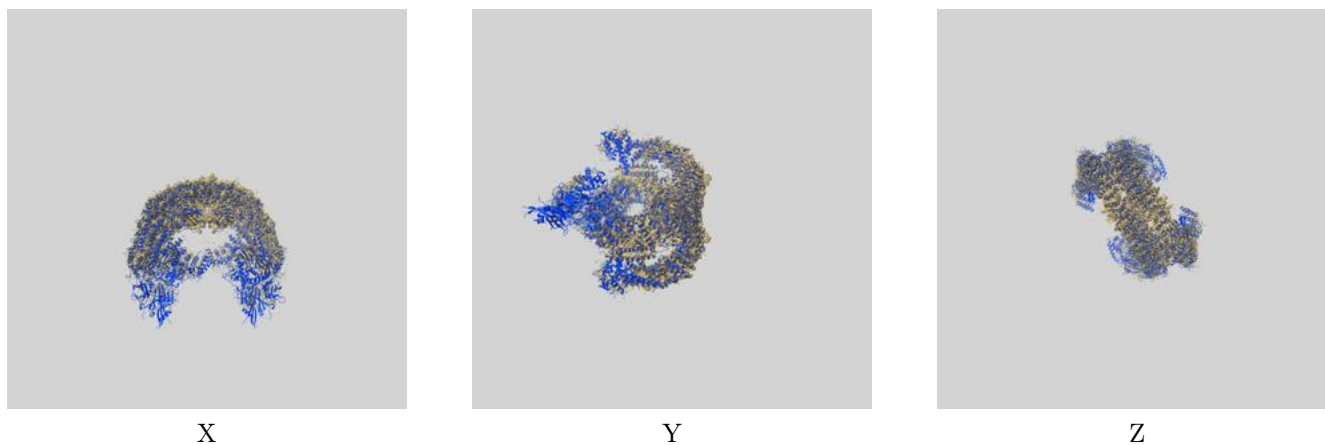
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.90	3.42
Unmasked-calculated*	4.08	6.59	4.15

\*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 4.08 differs from the reported value 3.3 by more than 10 %

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

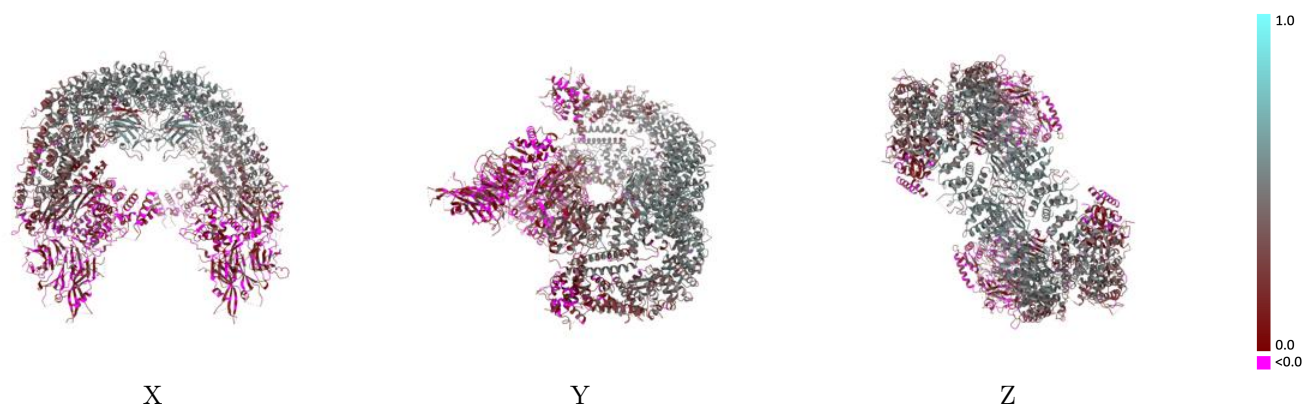
This section contains information regarding the fit between EMDB map EMD-15663 and PDB model 8ATU. Per-residue inclusion information can be found in section [3](#) on page [5](#).

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



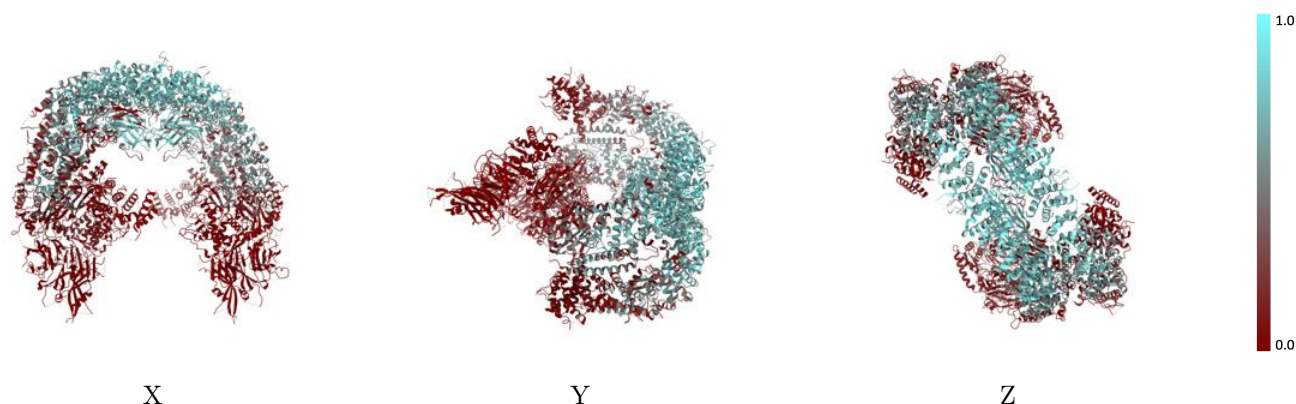
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



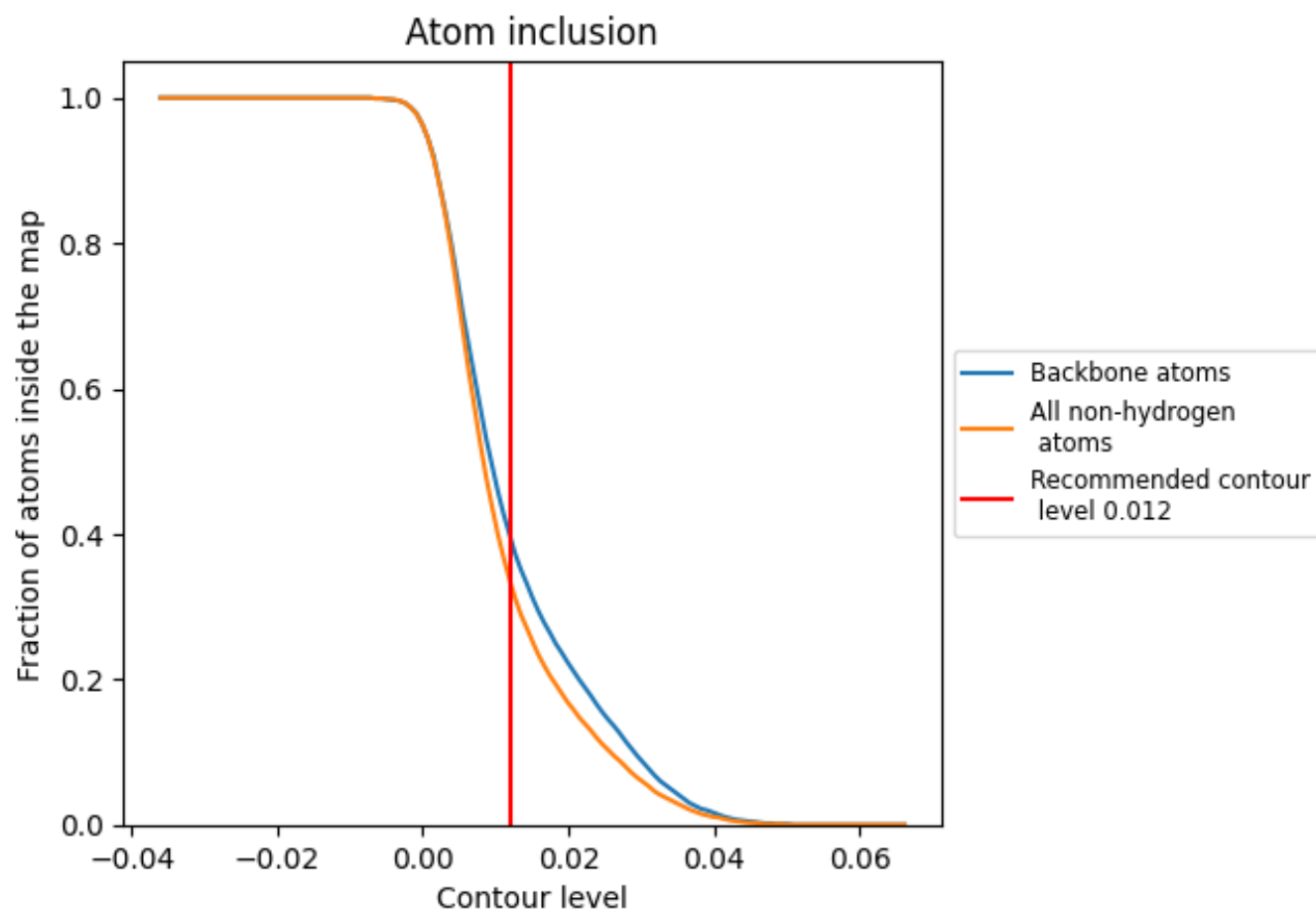
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 40% of all backbone atoms, 34% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3350	<div></div> 0.3010
A	<div></div> 0.3350	<div></div> 0.3010
B	<div></div> 0.3350	<div></div> 0.3010

