



## Full wwPDB EM Validation Report ⓘ

Jun 16, 2025 – 09:22 PM JST

PDB ID : 8XKV / pdb\_00008xkv  
EMDB ID : EMD-38428  
Title : Cryo-EM structure of the Ycf2-FtsHi motor complex from Arabidopsis in Apo state  
Authors : Liang, K.; Zhan, X.; Xu, Q.; Wu, J.; Yan, Z.  
Deposited on : 2023-12-25  
Resolution : 3.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.dev118  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
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) : 2.44

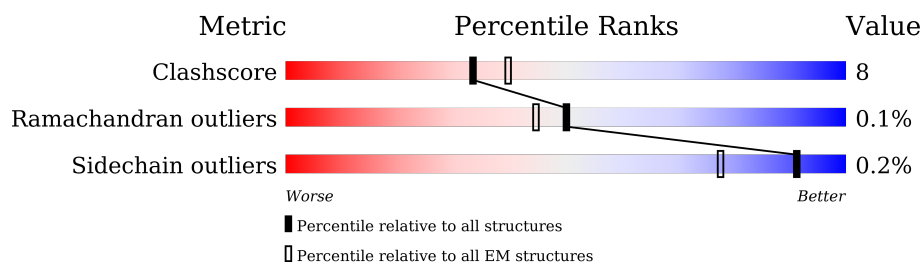
# 1 Overall quality at a glance

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	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	855	
2	B	1008	
3	C	1320	
4	D	2294	
5	E	946	
6	F	876	
7	G	396	
8	H	348	

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Mol	Chain	Length	Quality of chain
9	I	403	
9	J	403	
10	K	80	
11	L	18	
12	M	11	
13	N	37	
14	O	17	
15	P	19	
16	R	328	

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 45453 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 Probable inactive ATP-dependent zinc metalloprotease FTSHI 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	730	Total	C	N	O	S	0	0
			5841	3718	1000	1103	20		

- Molecule 2 is a protein called ATP-dependent zinc metalloprotease FTSH 12, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	841	Total	C	N	O	S	0	0
			6849	4388	1191	1241	29		

- Molecule 3 is a protein called Probable inactive ATP-dependent zinc metalloprotease FTSHI 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	921	Total	C	N	O	S	0	0
			7494	4775	1299	1386	34		

- Molecule 4 is a protein called Protein Ycf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	805	Total	C	N	O	S	0	0
			6659	4314	1145	1173	27		

- Molecule 5 is a protein called Probable inactive ATP-dependent zinc metalloprotease FTSHI 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	498	Total	C	N	O	S	0	0
			3884	2454	690	729	11		

- Molecule 6 is a protein called Probable inactive ATP-dependent zinc metalloprotease FTSHI 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	478	Total	C	N	O	S	0	0
			3744	2356	667	701	20		

- Molecule 7 is a protein called AtTam46.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	285	Total	C	N	O	S	0	0
			2375	1615	370	379	11		

- Molecule 8 is a protein called At4g28210.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	54	Total	C	N	O	S	0	0
			459	310	76	72	1		

- Molecule 9 is a protein called Malate dehydrogenase, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	317	Total	C	N	O	S	0	0
			2363	1503	396	457	7		
9	J	317	Total	C	N	O	S	0	0
			2363	1503	396	457	7		

- Molecule 10 is a protein called Aspartyl/glutamyl-tRNA (Asn/Gln) amidotransferase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	67	Total	C	N	O	S	0	0
			555	359	98	97	1		

- Molecule 11 is a protein called UNK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	18	Total	C	N	O	S	0	0
			131	89	21	20	1		

- Molecule 12 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	11	Total	C	N	O	0	0
			84	59	13	12		

- Molecule 13 is a protein called UNK.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	37	Total	C	N	O	S	0	0
			246	159	45	41	1		

- Molecule 14 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	17	Total	C	N	O	0	0
			132	89	25	18		

- Molecule 15 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	P	19	Total	C	N	O	0	0
			95	57	19	19		

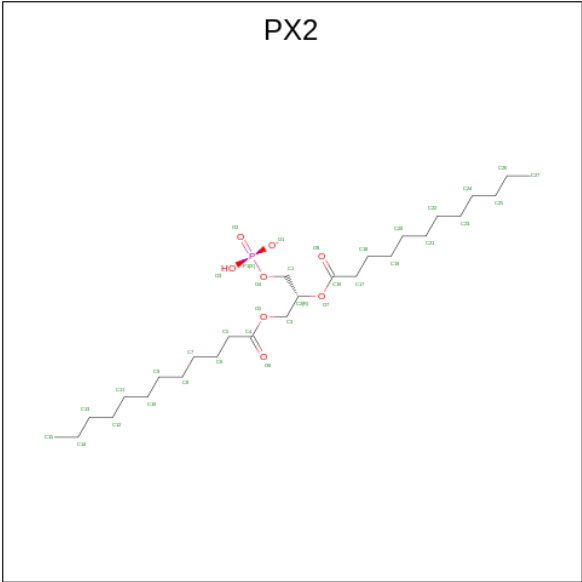
- Molecule 16 is a protein called Embryo defective 2737.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	267	Total	C	N	O	S	0	0
			2151	1371	367	397	16		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	B	1	Total	Zn	0
			1	1	
17	R	2	Total	Zn	0
			2	2	

- Molecule 18 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula: C<sub>27</sub>H<sub>52</sub>O<sub>8</sub>P).

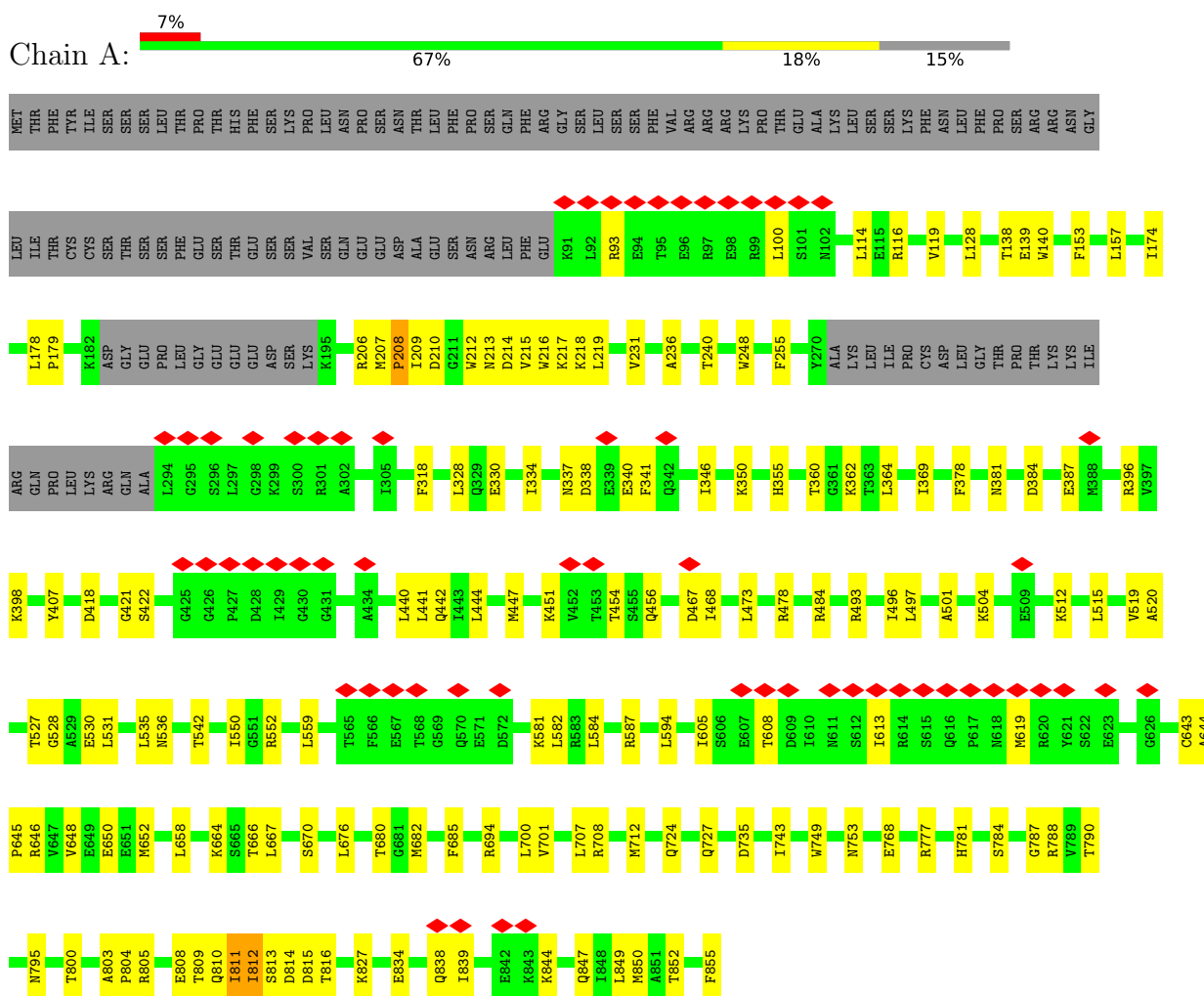


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
18	G	1	25	16	8	1	0

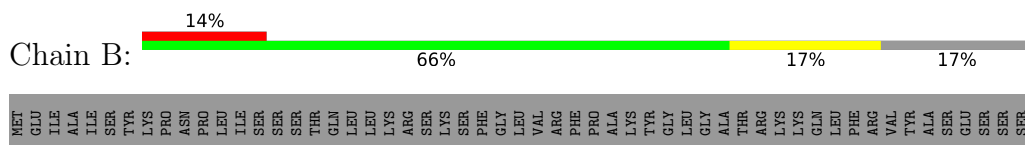
### 3 Residue-property plots

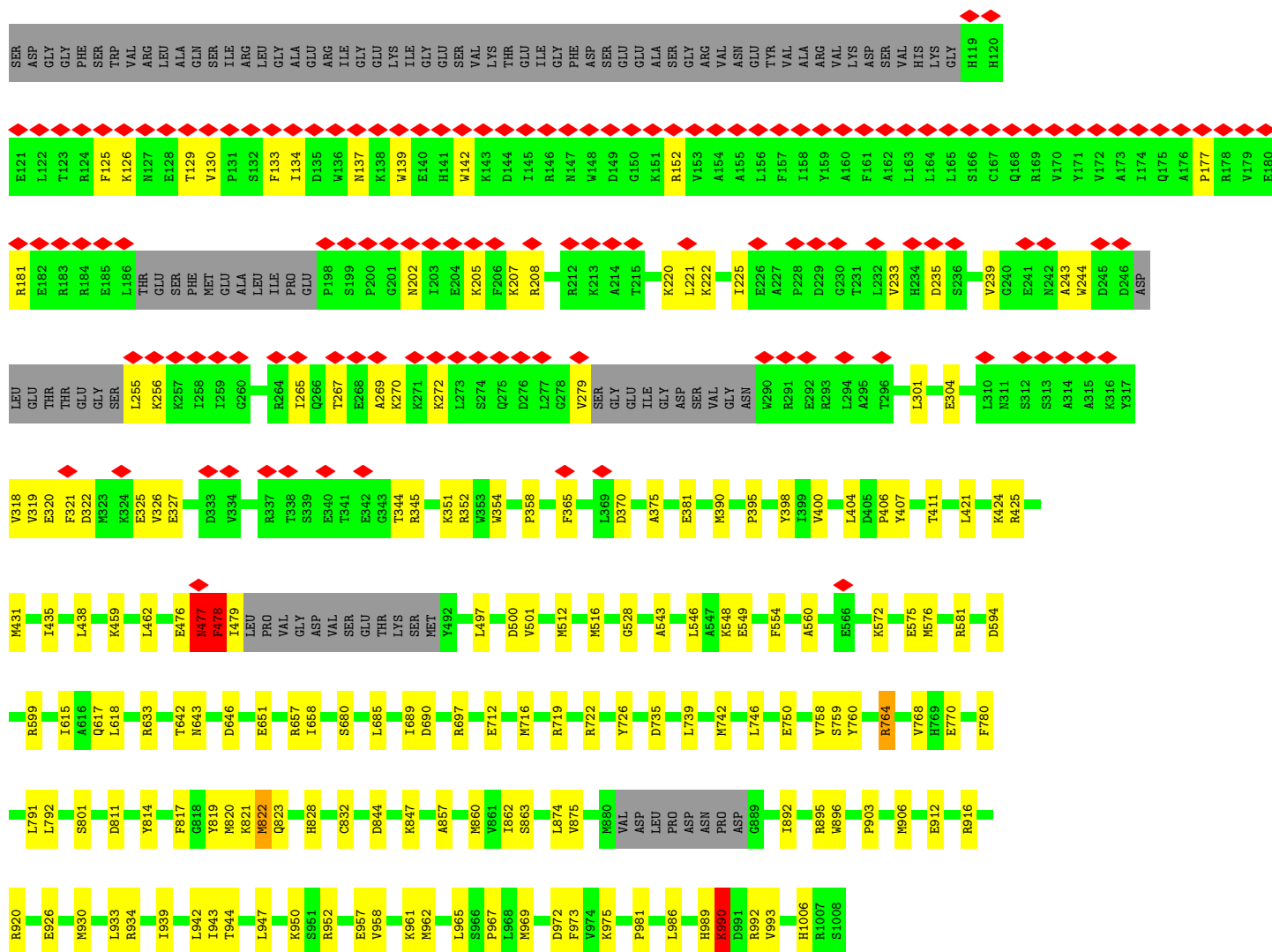
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Probable inactive ATP-dependent zinc metalloprotease FTSHI 4, chloroplastic

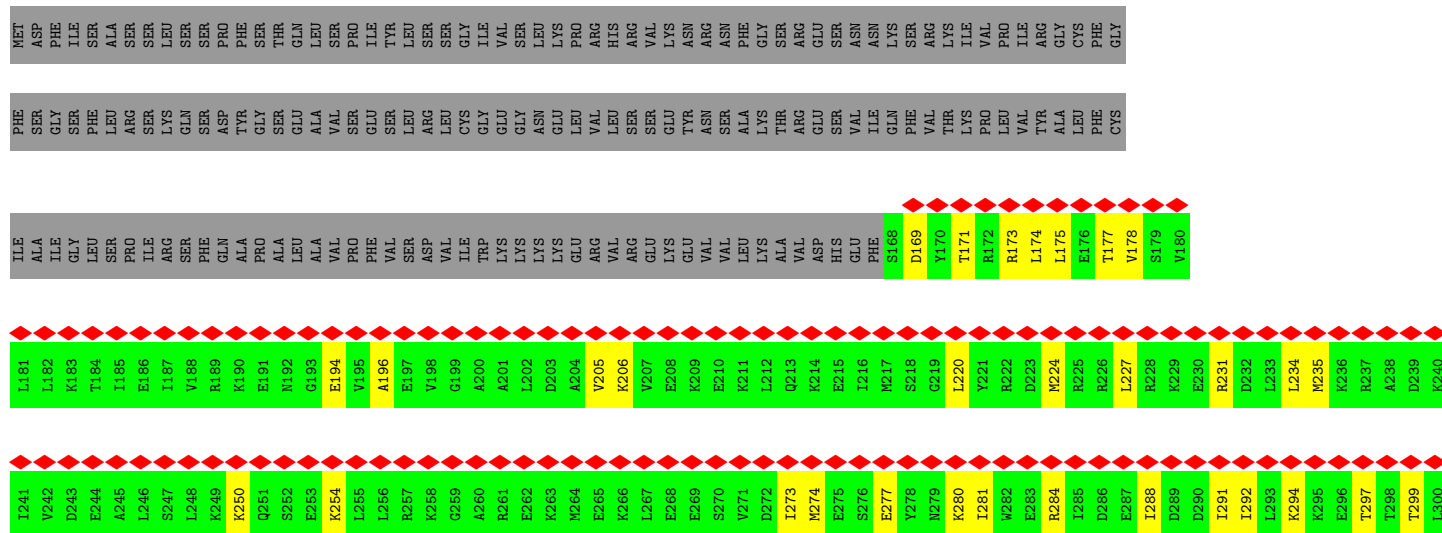
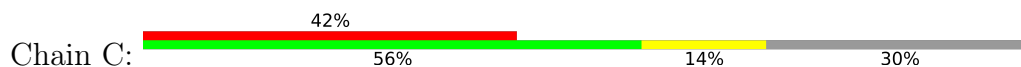


- Molecule 2: ATP-dependent zinc metalloprotease FTSH 12, chloroplastic



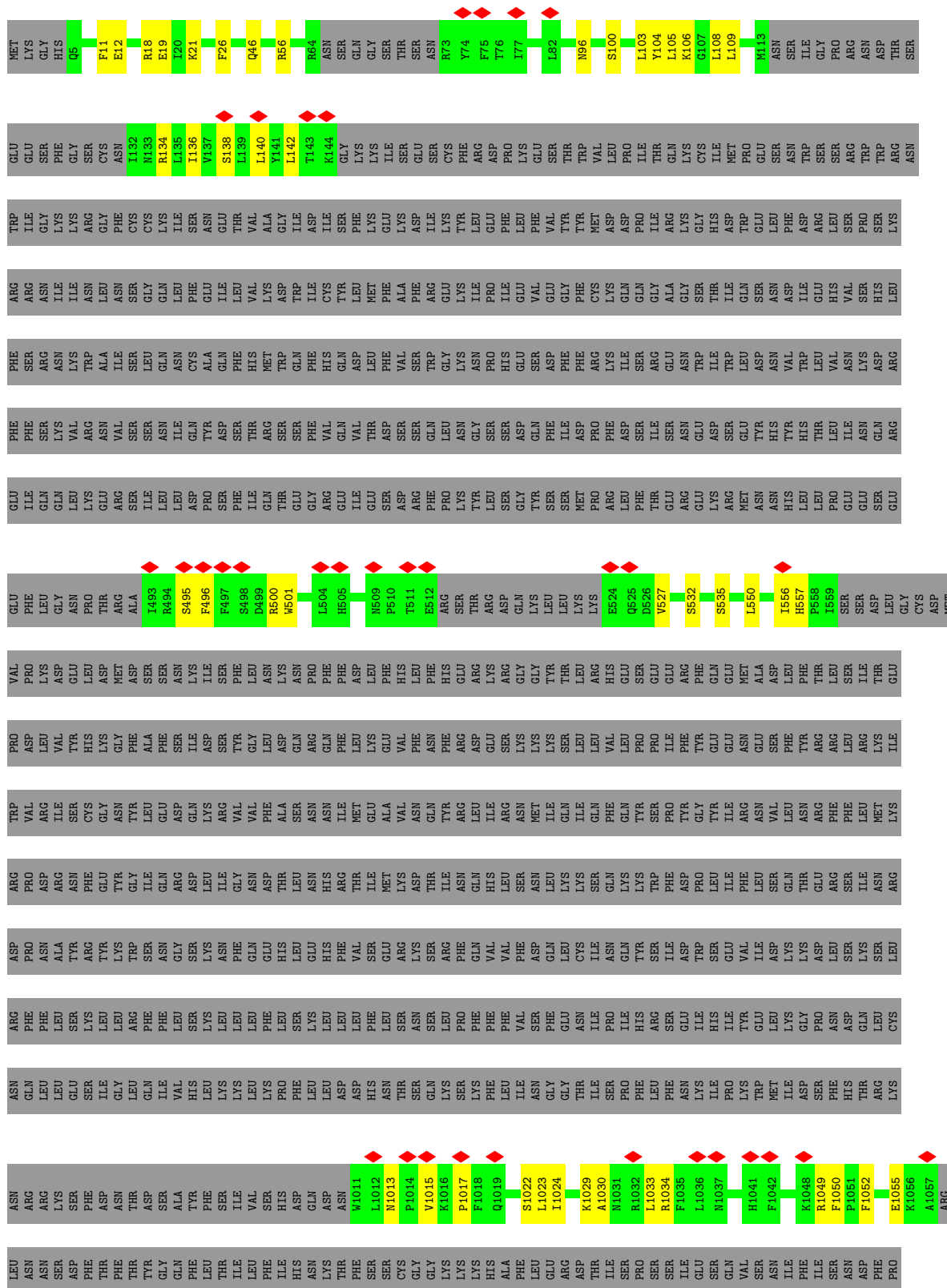


- Molecule 3: Probable inactive ATP-dependent zinc metalloprotease FTSHI 5, chloroplastic



L1239	R1104	V977	V846	F766	LEU	GLU	V606	A543	K482	K421	MET
A1244	L1109	D978	N847	A767	LEU	ILE	V607	L544	Q483	T422	ILE
L1248	D1115	I908	V848	S788	TYR	GLN	S608	K545	Y484	P423	PRO
L1255	R983	N909	E849	I789	GLY	THR	R609	G546	I485	E424	ASN
E1256	E987	E987	A850	E790	PRO	VAL	V610	D547	A486	G425	VAL
K1257	T990	M792	E852	S791	PHE	GLY	F611	D548	Q487	A426	LEU
E1261	L912	R793	L853	R793	ARG	SER	N612	K549	R488	A427	GLU
L1273	V913	E794	E854	E795	ASP	THR	A613	E550	Q489	V428	GLU
P1288	E914	E795	A855	I796	ASN	TYR	L614	F551	E490	K429	VAL
F1289	D916	N797	G856	N797	VAL	GLN	R615	D554	Q491	G430	ASP
F1290	G917	E798	L857	E798	ARG	TRP	K616	I555	V492	F431	PRO
L1291	F918	V799	W858	V799	PHE	GLN	T617	K556	L493	P432	PHE
S1292	F918	W859	V860	W800	TRP	GLU	GLN	E557	L494	E433	ASP
M1295	D922	G860	A801	A801	ARG	ALA	VAL	Y558	D495	A434	
L1300	G923	V861	P802	P802	VAL	GLU	VAL	E559	R496	E435	
SER	V924	S862	L803	L803	SER	MET	ASN	M560	D497	V436	
ARG	V925	Q804	Q804	Q804	LYS	PHE	LYS	E563	R498	K437	
ASP	L926	N805	N805	N805	ASP	SER	ASP	K564	V499	W438	
THR	N927	A864	A864	A864	THR	ARG	THR	F565	V500	M439	
PRO	A928	N865	N865	N865	ARG	ASN	VAL	G566	S501	F440	
GLY	T929	R867	R867	R867	LYS	THR	LEU	G567	K502	G441	
ALA	T930	E868	E868	E868	ARG	GLU	GLY	E568	T503	E442	
THR	R931	L869	L869	L869	ILE	PHE	ILE	F569	W504	K443	
ARG	N932	F870	F870	F870	LYS	TRP	ASN	A570	N506	E444	
ASN	H933	T871	T871	T871	GLN	PHE	ASN	L571	E507	V445	
LEU	K934	T872	T872	T872	LYS	TRP	ASP	V572	D508	V447	
LEU	Q935	A873	A873	A873	ALA	PHE	ASP	L573	K509	P448	
LEU	I936	R874	R874	R874	GLY	ILE	MET	K574	S510	K449	
LEU	D937	D875	D875	D875	ILE	ILE	MET	M575	E512	A450	
ALA	E938	L876	L876	L876	ARG	ARG	ALA	L576	E513	I451	
ALA	A939	A877	A877	A877	SER	SER	VAL	A577	M514	K396	
THR	L940	F878	F878	F878	VAL	THR	VAL	C578	D515	L397	
THR	R941	V879	V879	V879	ILE	ILE	PHE	G579	P515	Q398	
THR	P942	I881	I881	I881	GLY	GLY	PRO	P581	M517	R399	
THR	P943	F882	F882	F882	VAL	PHE	VAL	T582	A518	D400	
THR	G944	V883	V883	V883	VAL	VAL	GLY	S583	V519	L401	
THR	R945	E884	E884	E884	TYR	TYR	PHE	V584	P520	Q402	
THR	M946	D885	D885	D885	HIS	HIS	ILE	H585	A522	N403	
THR	D947	G827	G827	G827	VAL	VAL	PRO	L586	V523	R404	
THR	R948	T828	T828	T828	PHE	PHE	TYR	M587	S524	I405	
THR	D887	G829	G829	G829	ARG	ARG	GLN	W589	R525	R406	
THR	L888	K830	K830	K830	LYS	LYS	ARG	F590	I528	K407	
THR	F889	T831	T831	T831	LYS	LYS	ARG	M591	D529	M408	
THR	A890	G891	G891	G891	VAL	VAL	GLY	E593	K410	M409	
THR	V892	S832	S832	S832	PRO	PRO	MET	L594	K411	K410	
THR	R893	L833	L833	L833	ALA	ALA	TRP	Q597	F412	F412	
THR	Q894	L835	L835	L835	PRO	PRO	PRO	Q599	G413	G413	
THR	F896	T837	T837	T837	ARG	ARG	GLU	F600	E414	E414	
THR	H898	A838	A838	A838	LYS	LYS	ARG	Q599	K471	K471	
THR	T899	R839	R839	R839	LYS	LYS	ARG	Q599	K473	K473	
THR	F899	L836	L836	L836	VAL	VAL	GLY	F600	L474	L474	
THR	R899	T837	T837	T837	PRO	PRO	PRO	L602	L475	L475	
THR	H899	A839	A839	A839	ARG	ARG	GLU	Q599	E476	E476	
THR	T899	E840	E840	E840	LYS	LYS	ARG	F600	D477	D477	
THR	F899	A841	A841	A841	VAL	VAL	GLY	L602	V478	V478	
THR	R899	L836	L836	L836	PRO	PRO	PRO	V603	F480	F480	
THR	F899	T837	T837	T837	ARG	ARG	GLU	T604	G481	G481	
THR	H899	A839	A839	A839	LYS	LYS	ARG	R605			
THR	T899	E840	E840	E840	VAL	VAL	GLY				
THR	F899	A841	A841	A841	PRO	PRO	PRO				
THR	R899	L836	L836	L836	ARG	ARG	GLU				
THR	F899	T837	T837	T837	LYS	LYS	ARG				
THR	H899	A839	A839	A839	VAL	VAL	GLY				
THR	T899	E840	E840	E840	PRO	PRO	PRO				
THR	F899	A841	A841	A841	ARG	ARG	GLU				
THR	R899	L836	L836	L836	LYS	LYS	ARG				
THR	F899	T837	T837	T837	VAL	VAL	GLY				
THR	H899	A839	A839	A839	PRO	PRO	PRO				
THR	T899	E840	E840	E840	ARG	ARG	GLU				
THR	F899	A841	A841	A841	LYS	LYS	ARG				
THR	R899	L836	L836	L836	VAL	VAL	GLY				
THR	F899	T837	T837	T837	PRO	PRO	PRO				
THR	H899	A839	A839	A839	ARG	ARG	GLU				
THR	T899	E840	E840	E840	LYS	LYS	ARG				
THR	F899	A841	A841	A841	VAL	VAL	GLY				
THR	R899	L836	L836	L836	PRO	PRO	PRO				
THR	F899	T837	T837	T837	ARG	ARG	GLU				
THR	H899	A839	A839	A839	LYS	LYS	ARG				
THR	T899	E840	E840	E840	VAL	VAL	GLY				
THR	F899	A841	A841	A841	PRO	PRO	PRO				
THR	R899	L836	L836	L836	ARG	ARG	GLU				
THR	F899	T837	T837	T837	LYS	LYS	ARG				
THR	H899	A839	A839	A839	VAL	VAL	GLY				
THR	T899	E840	E840	E840	PRO	PRO	PRO				
THR	F899	A841	A841	A841	ARG	ARG	GLU				
THR	R899	L836	L836	L836	LYS	LYS	ARG				
THR	F899	T837	T837	T837	VAL	VAL	GLY				
THR	H899	A839	A839	A839	PRO	PRO	PRO				
THR	T899	E840	E840	E840	ARG	ARG	GLU				
THR	F899	A841	A841	A841	LYS	LYS	ARG				
THR	R899	L836	L836	L836	VAL	VAL	GLY				
THR	F899	T837	T837	T837	PRO	PRO	PRO				
THR	H899	A839	A839	A839	ARG	ARG	GLU				
THR	T899	E840	E840	E840	LYS	LYS	ARG				
THR	F899	A841	A841	A841	VAL	VAL	GLY				
THR	R899	L836	L836	L836	PRO	PRO	PRO				
THR	F899	T837	T837	T837	ARG	ARG	GLU				
THR	H899	A839	A839	A839	LYS	LYS	ARG				
THR	T899	E840	E840	E840	VAL	VAL	GLY				
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THR	R899	L836	L836	L836	ARG	ARG	GLU				
THR	F899	T837	T837	T837	LYS	LYS	ARG				
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THR	T899	E840	E840	E840	PRO	PRO	PRO				
THR	F899	A841	A841	A841	ARG	ARG	GLU				
THR	R899	L836	L836	L836	LYS	LYS	ARG				
THR	F899	T837	T837	T837	VAL	VAL	GLY				
THR	H899	A839	A839	A839	PRO	PRO	PRO				
THR	T899	E840	E840	E840	ARG	ARG	GLU				
THR	F899	A841	A841	A841	LYS	LYS	ARG				
THR	R899	L836	L836	L836	VAL	VAL	GLY				
THR	F899	T837	T837	T837	PRO	PRO	PRO				
THR	H899	A839	A839	A839	ARG	ARG	GLU				
THR	T899	E840	E840	E840	LYS	LYS	ARG				
THR	F899	A841	A841	A841	VAL	VAL	GLY				
THR	R899	L836	L836	L836	PRO	PRO	PRO				
THR	F899	T837	T837	T837	ARG	ARG	GLU				
THR	H899	A839	A839	A839	LYS	LYS	ARG				
THR	T899	E840	E840	E840	VAL	VAL	GLY				
THR	F899	A841	A841	A841	PRO	PRO	PRO				
THR	R899	L836	L836	L836	ARG	ARG	GLU				
THR	F899	T837	T837	T837	LYS	LYS	ARG				
THR	H899	A839	A839	A839	VAL	VAL	GLY				
THR	T899	E840	E840	E840	PRO	PRO	PRO				
THR	F899	A841	A841	A841	ARG	ARG	GLU				
THR	R899	L836	L836	L836	LYS	LYS	ARG				
THR	F899	T837	T837	T837	VAL	VAL	GLY				
THR	H899	A839	A839	A839	PRO	PRO	PRO				
THR	T899	E840	E840	E840	ARG	ARG	GLU				
THR	F899	A841	A841	A841	LYS	LYS	ARG				
THR	R899	L836	L836	L836	VAL	VAL	GLY				
THR	F899	T837	T837	T837	PRO	PRO	PRO				
THR	H899	A839	A839	A839	ARG	ARG	GLU				
THR	T899	E840	E840	E840	LYS	LYS	ARG				
THR	F899	A841	A841	A841	VAL	VAL	GLY				
THR	R899	L836	L836	L836	PRO	PRO	PRO				
THR	F899	T837	T837	T837	ARG	ARG	GLU				
THR	H899	A839	A839	A839	LYS	LYS	ARG				
THR	T899	E840	E840	E840	VAL	VAL	GLY				
THR	F899	A841	A841	A841	PRO	PRO	PRO				
THR	R899	L836	L836	L836	ARG	ARG	GLU				
THR	F899	T837	T837	T837	LYS	LYS	ARG				
THR	H899	A839	A839	A839	VAL	VAL	GLY				
THR	T899	E840	E840	E840	PRO	PRO	PRO				
THR	F899	A841	A841	A841	ARG	ARG	GLU				
THR	R899	L836	L836	L836	LYS	LYS	ARG				
THR	F899	T837	T837	T837	VAL	VAL	GLY				
THR	H899	A839	A839	A839	PRO	PRO	PRO				
THR	T899	E840	E840	E840							

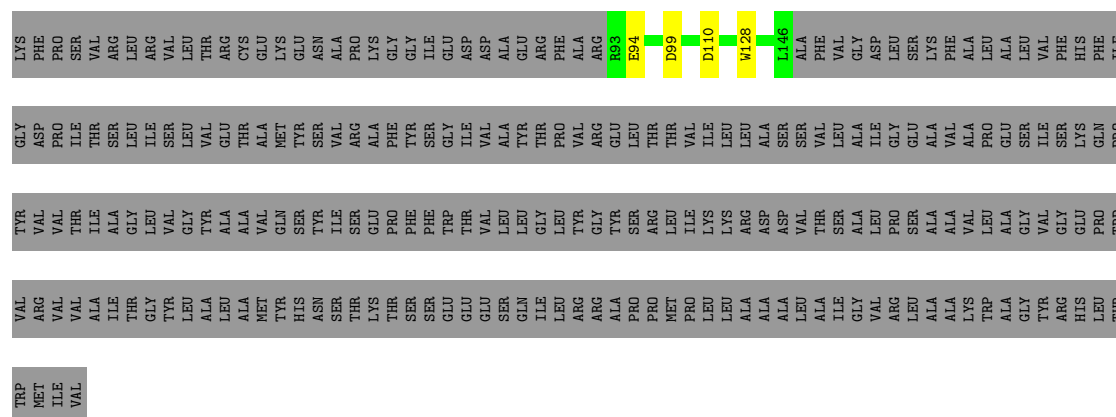
Chain D:  28% 7% 65%





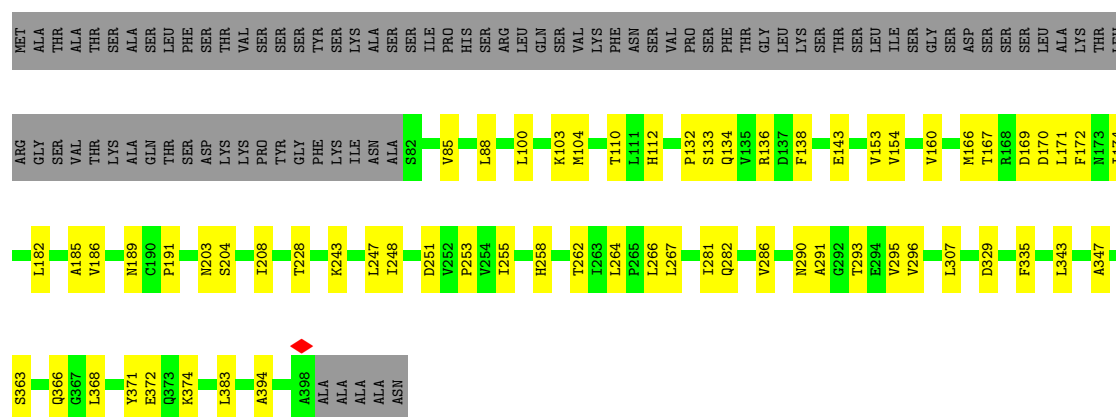






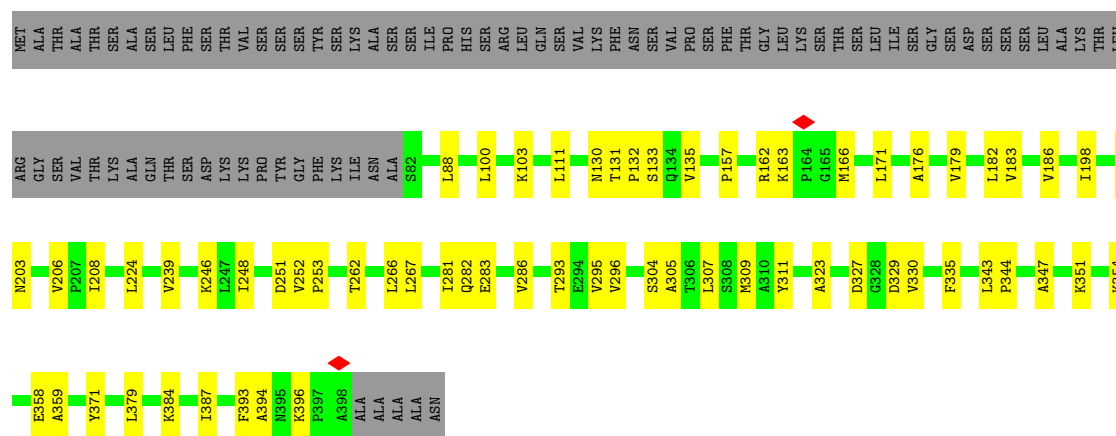
• Molecule 9: Malate dehydrogenase, chloroplastic

Chain I: 63% 16% 21%



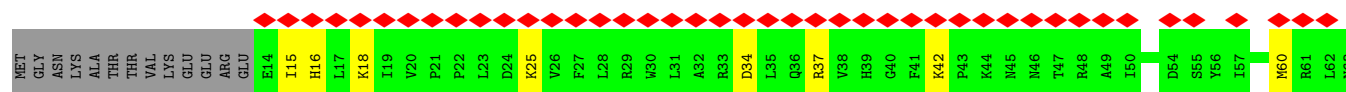
• Molecule 9: Malate dehydrogenase, chloroplastic

Chain J: 63% 16% 21%

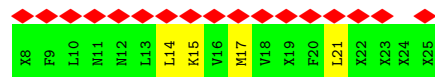
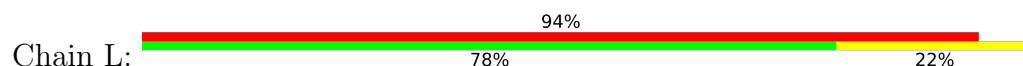


• Molecule 10: Aspartyl/glutamyl-tRNA (Asn/Gln) amidotransferase subunit B

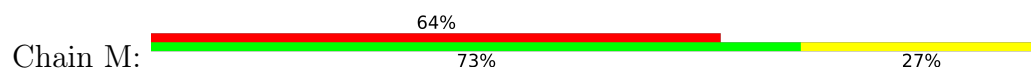
Chain K: 75% 69% 15% 16%



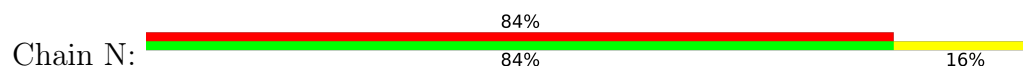
• Molecule 11: UNK



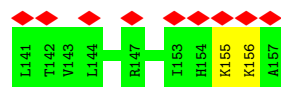
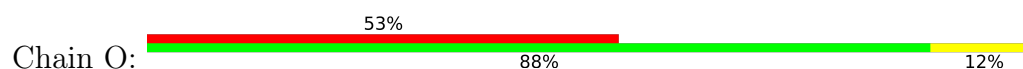
• Molecule 12: UNK



• Molecule 13: UNK



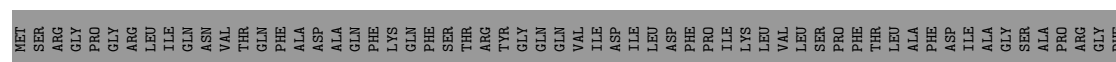
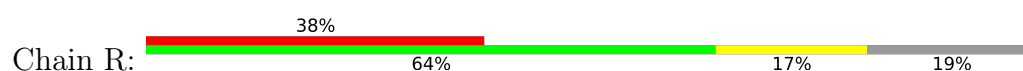
• Molecule 14: UNK

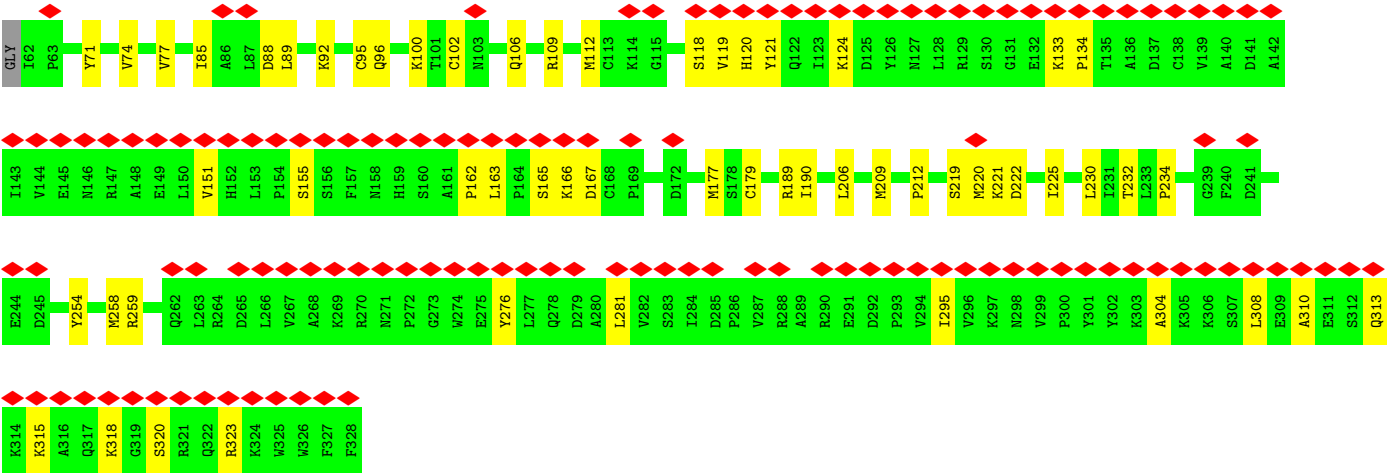


• Molecule 15: UNK



• Molecule 16: Embryo defective 2737





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	340640	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.960	Depositor
Minimum map value	-2.634	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.086	Depositor
Recommended contour level	0.3	Depositor
Map size ( $\text{\AA}$ )	391.32, 391.32, 391.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.087, 1.087, 1.087	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, PX2

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	0.17	0/5952	0.45	0/8038
2	B	0.18	0/6992	0.53	2/9419 (0.0%)
3	C	0.16	0/7627	0.43	1/10262 (0.0%)
4	D	0.17	0/6804	0.50	0/9177
5	E	0.33	2/3956 (0.1%)	0.51	3/5361 (0.1%)
6	F	0.15	0/3798	0.43	0/5115
7	G	0.37	3/2470 (0.1%)	0.66	5/3375 (0.1%)
8	H	0.19	0/477	0.44	0/651
9	I	0.23	1/2399 (0.0%)	0.55	3/3261 (0.1%)
9	J	0.15	0/2399	0.41	0/3261
10	K	0.16	0/570	0.47	0/772
11	L	0.16	0/101	0.44	0/133
12	M	0.17	0/74	0.72	0/99
13	N	0.13	0/142	0.42	0/179
14	O	0.25	0/132	0.71	0/175
16	R	0.20	0/2206	0.52	1/2986 (0.0%)
All	All	0.21	6/46099 (0.0%)	0.49	15/62264 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	4
4	D	0	2
5	E	0	1
All	All	0	8

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	523	PRO	CG-CD	-15.88	1.08	1.51
7	G	198	PRO	CG-CD	-11.49	1.11	1.50
5	E	523	PRO	N-CD	7.17	1.57	1.47
7	G	198	PRO	N-CD	6.04	1.56	1.47
7	G	198	PRO	N-CA	-5.49	1.43	1.47
9	I	191	PRO	CG-CD	-5.22	1.33	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	523	PRO	N-CD-CG	-17.39	82.93	103.80
9	I	191	PRO	CA-N-CD	-12.65	94.29	112.00
7	G	198	PRO	CA-N-CD	-12.62	94.34	112.00
7	G	198	PRO	N-CD-CG	-12.11	85.03	103.20
5	E	523	PRO	CA-N-CD	-12.02	94.67	111.50
9	I	191	PRO	N-CD-CG	-8.17	90.94	103.20
7	G	198	PRO	CA-CB-CG	-7.26	90.70	104.50
5	E	523	PRO	CA-CB-CG	-6.55	91.55	104.00
7	G	198	PRO	CB-CA-C	5.72	116.21	109.92
2	B	764	ARG	CA-CB-CG	5.37	124.85	114.10
2	B	822	MET	CA-CB-CG	5.31	124.72	114.10
16	R	220	MET	CA-CB-CG	5.15	124.40	114.10
9	I	191	PRO	N-CA-CB	-5.11	98.37	103.48
7	G	198	PRO	N-CA-CB	-5.08	97.56	101.83
3	C	1170	MET	N-CA-CB	5.06	118.09	110.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	811	ILE	Peptide
2	B	476	GLU	Peptide
2	B	477	ASN	Peptide
2	B	478	PHE	Peptide
2	B	990	LYS	Peptide
4	D	1982	VAL	Peptide
4	D	495	SER	Peptide
5	E	803	ASN	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5841	0	5859	119	0
2	B	6849	0	6890	133	0
3	C	7494	0	7625	116	0
4	D	6659	0	6763	121	0
5	E	3884	0	3935	68	0
6	F	3744	0	3823	89	0
7	G	2375	0	2353	56	0
8	H	459	0	455	4	0
9	I	2363	0	2437	39	0
9	J	2363	0	2437	44	0
10	K	555	0	561	9	0
11	L	131	0	122	5	0
12	M	84	0	98	3	0
13	N	246	0	174	4	0
14	O	132	0	161	2	0
15	P	95	0	21	0	0
16	R	2151	0	2123	47	0
17	B	1	0	0	0	0
17	R	2	0	0	0	0
18	G	25	0	23	10	0
All	All	45453	0	45860	741	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 8.

All (741) 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)
7:G:199:ALA:CB	18:G:401:PX2:H7	2.06	0.85
2:B:764:ARG:HH21	2:B:768:VAL:HB	1.48	0.78
7:G:199:ALA:HB1	18:G:401:PX2:C4	2.15	0.77
9:I:166:MET:HE1	9:I:171:LEU:HB3	1.67	0.77
5:E:759:LEU:HG	5:E:861:MET:HE1	1.68	0.76
7:G:199:ALA:O	18:G:401:PX2:H4	1.86	0.75
1:A:838:GLN:HG2	1:A:839:ILE:HG12	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:926:GLU:HG3	2:B:930:MET:HE2	1.70	0.72
16:R:120:HIS:HB3	16:R:163:LEU:HB2	1.72	0.72
7:G:199:ALA:HB1	18:G:401:PX2:C5	2.18	0.72
3:C:489:GLN:NE2	11:L:17:MET:SD	2.63	0.71
5:E:759:LEU:HD13	5:E:791:LEU:HD23	1.73	0.71
1:A:784:SER:HB3	9:J:251:ASP:HB3	1.73	0.70
1:A:381:ASN:HB3	1:A:384:ASP:HB2	1.74	0.70
2:B:406:PRO:HG3	16:R:209:MET:HB3	1.73	0.70
1:A:811:ILE:HD12	4:D:2255:GLU:HG3	1.73	0.69
2:B:370:ASP:OD1	2:B:411:THR:OG1	2.11	0.69
2:B:404:LEU:HB3	16:R:209:MET:HE1	1.75	0.68
4:D:1034:ARG:HH12	16:R:219:SER:HB2	1.57	0.68
1:A:214:ASP:O	1:A:217:LYS:HB3	1.92	0.68
5:E:800:ASN:ND2	5:E:805:MET:SD	2.67	0.68
1:A:670:SER:HA	1:A:712:MET:HE1	1.77	0.67
3:C:1096:PRO:HB3	3:C:1178:ASN:HD21	1.60	0.67
5:E:807:ILE:HG22	5:E:846:MET:HE1	1.75	0.67
4:D:557:HIS:O	4:D:1052:PHE:HA	1.94	0.67
1:A:207:MET:SD	1:A:207:MET:N	2.66	0.67
3:C:972:MET:O	3:C:974:ARG:NH1	2.28	0.67
4:D:2006:LEU:HD13	4:D:2249:ARG:HB3	1.77	0.66
3:C:792:MET:HE3	3:C:796:ILE:HD11	1.78	0.66
16:R:222:ASP:HB3	16:R:225:ILE:HB	1.77	0.66
6:F:595:LYS:HG3	6:F:596:LYS:HE3	1.78	0.66
3:C:194:GLU:HG3	3:C:196:ALA:H	1.61	0.66
2:B:972:ASP:HB3	2:B:975:LYS:HD3	1.78	0.65
3:C:499:VAL:HG21	3:C:522:ALA:HB2	1.76	0.65
1:A:418:ASP:HB2	1:A:468:ILE:HD11	1.77	0.65
1:A:504:LYS:HE3	1:A:535:LEU:HB3	1.77	0.65
3:C:224:MET:HE1	3:C:292:ILE:HG23	1.78	0.65
7:G:158:ALA:O	7:G:192:TRP:NE1	2.31	0.64
3:C:851:GLN:NE2	4:D:1764:TYR:O	2.30	0.64
4:D:2006:LEU:HB3	4:D:2249:ARG:HD2	1.78	0.64
16:R:96:GLN:O	16:R:189:ARG:NH1	2.31	0.64
2:B:139:TRP:HE1	16:R:304:ALA:HB3	1.63	0.63
2:B:222:LYS:HG2	2:B:318:VAL:HB	1.79	0.63
7:G:199:ALA:CB	18:G:401:PX2:C5	2.74	0.63
4:D:2274:MET:HE1	4:D:2284:LEU:HD11	1.80	0.63
7:G:247:THR:HB	7:G:252:ARG:HD3	1.79	0.63
1:A:255:PHE:HB3	16:R:74:VAL:HG12	1.81	0.63
2:B:581:ARG:NH2	2:B:617:GLN:OE1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:R:102:CYS:SG	16:R:179:CYS:CB	2.87	0.63
1:A:694:ARG:NH2	2:B:896:TRP:O	2.33	0.62
4:D:1852:MET:HE3	4:D:1925:PRO:HG3	1.80	0.62
3:C:844:PRO:HG2	3:C:879:VAL:HG12	1.81	0.62
1:A:138:THR:HG23	1:A:140:TRP:H	1.64	0.62
4:D:1838:GLU:HB3	4:D:1841:MET:HE1	1.82	0.62
9:I:85:VAL:HG22	9:I:153:VAL:HB	1.82	0.62
2:B:177:PRO:HB2	2:B:181:ARG:HH21	1.65	0.61
2:B:351:LYS:NZ	7:G:206:GLU:OE1	2.32	0.61
7:G:362:ASN:OD1	7:G:390:LYS:NZ	2.34	0.61
1:A:504:LYS:HD3	6:F:438:ARG:HH22	1.65	0.61
16:R:221:LYS:HG2	16:R:258:MET:HE1	1.81	0.61
4:D:1755:HIS:HB2	4:D:1797:LYS:HD3	1.82	0.61
5:E:435:ILE:HG22	5:E:438:ALA:HB3	1.82	0.61
5:E:445:LEU:HD21	5:E:466:VAL:HG21	1.82	0.61
2:B:395:PRO:HB3	7:G:151:LEU:HD21	1.81	0.61
4:D:1013:ASN:ND2	4:D:1015:VAL:O	2.33	0.60
6:F:630:MET:SD	6:F:630:MET:N	2.73	0.60
2:B:344:THR:HG22	4:D:527:VAL:HB	1.83	0.60
4:D:1841:MET:SD	4:D:1841:MET:N	2.74	0.60
7:G:388:ARG:O	7:G:388:ARG:NH1	2.34	0.60
9:I:343:LEU:HD13	9:I:383:LEU:HD23	1.84	0.60
4:D:1597:CYS:SG	4:D:1598:LEU:N	2.73	0.60
2:B:375:ALA:H	2:B:390:MET:HA	1.67	0.60
9:I:282:GLN:OE1	9:I:371:TYR:OH	2.20	0.60
1:A:724:GLN:HA	1:A:727:GLN:HG2	1.84	0.60
3:C:976:LEU:HD12	3:C:979:LEU:HD13	1.84	0.60
2:B:354:TRP:CZ2	18:G:401:PX2:C16	2.84	0.60
3:C:1209:VAL:HG21	5:E:785:LEU:HB3	1.82	0.60
3:C:1244:ALA:O	3:C:1248:LEU:HB2	2.02	0.60
7:G:199:ALA:HB1	18:G:401:PX2:O5	2.02	0.60
16:R:102:CYS:SG	16:R:179:CYS:HB2	2.42	0.60
5:E:720:GLU:OE2	5:E:758:ARG:NH1	2.35	0.59
2:B:791:LEU:HD11	2:B:947:LEU:HB3	1.84	0.59
9:I:132:PRO:O	9:I:134:GLN:NE2	2.35	0.59
2:B:770:GLU:OE1	2:B:801:SER:OG	2.19	0.59
5:E:720:GLU:HA	5:E:742:LEU:HD21	1.84	0.59
9:J:343:LEU:HD22	9:J:387:ILE:HD12	1.83	0.59
1:A:787:GLY:HA2	1:A:800:THR:O	2.01	0.59
3:C:523:VAL:HG21	3:C:575:MET:HE1	1.83	0.59
3:C:174:LEU:HD21	3:C:310:ILE:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:18:ARG:HA	4:D:21:LYS:HE3	1.84	0.59
4:D:1642:ARG:NH1	4:D:1778:CYS:O	2.36	0.59
3:C:571:LEU:HD12	3:C:575:MET:HE3	1.85	0.59
16:R:112:MET:SD	16:R:112:MET:N	2.75	0.59
2:B:516:MET:HE1	4:D:11:PHE:HA	1.85	0.58
1:A:808:GLU:OE1	4:D:2035:ARG:NH2	2.37	0.58
7:G:392:ILE:HB	7:G:395:VAL:HB	1.85	0.58
6:F:629:ASN:ND2	6:F:642:ASP:OD1	2.32	0.58
1:A:341:PHE:HB3	1:A:346:ILE:HB	1.86	0.58
1:A:536:ASN:ND2	6:F:441:LYS:O	2.36	0.58
2:B:322:ASP:O	2:B:325:GLU:N	2.36	0.58
5:E:499:PHE:O	5:E:557:ARG:NH2	2.37	0.58
1:A:542:THR:HG21	1:A:550:ILE:HA	1.86	0.58
2:B:875:VAL:HG12	2:B:903:PRO:HA	1.86	0.58
1:A:608:THR:OG1	1:A:619:MET:SD	2.62	0.57
1:A:850:MET:SD	1:A:852:THR:OG1	2.61	0.57
6:F:793:LEU:HD23	6:F:794:ARG:HH12	1.68	0.57
9:J:282:GLN:OE1	9:J:371:TYR:OH	2.22	0.57
6:F:652:ARG:HH22	6:F:699:ARG:HH11	1.50	0.57
1:A:749:TRP:O	1:A:753:ASN:ND2	2.37	0.57
1:A:114:LEU:HD13	4:D:550:LEU:HD11	1.86	0.57
1:A:213:ASN:ND2	16:R:209:MET:O	2.38	0.57
2:B:208:ARG:HG2	2:B:243:ALA:HA	1.85	0.57
4:D:138:SER:HA	4:D:142:LEU:HD13	1.86	0.57
5:E:476:LYS:HG2	5:E:605:VAL:HG21	1.86	0.57
1:A:338:ASP:OD1	1:A:338:ASP:N	2.36	0.57
6:F:592:HIS:O	6:F:595:LYS:NZ	2.38	0.57
7:G:326:ARG:NH1	7:G:369:GLU:OE1	2.35	0.57
2:B:528:GLY:HA3	2:B:658:ILE:HD13	1.87	0.57
4:D:2278:LEU:HD13	4:D:2284:LEU:HD22	1.85	0.57
7:G:258:GLY:HA3	7:G:356:VAL:HG21	1.87	0.57
4:D:1380:GLN:O	16:R:71:TYR:OH	2.22	0.57
6:F:415:LEU:HB3	6:F:419:ARG:HB2	1.87	0.57
6:F:616:GLY:HA2	6:F:619:LEU:HD12	1.86	0.57
16:R:206:LEU:HA	16:R:209:MET:HE3	1.87	0.57
2:B:615:ILE:HD11	2:B:657:ARG:HD3	1.87	0.57
2:B:863:SER:HA	2:B:895:ARG:HH22	1.70	0.57
2:B:722:ARG:HD3	2:B:726:TYR:CE1	2.41	0.56
5:E:763:LEU:HD13	5:E:862:TYR:HD1	1.71	0.56
2:B:497:LEU:HD22	2:B:501:VAL:HG11	1.86	0.56
1:A:100:LEU:HD13	2:B:265:ILE:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1008:ALA:HA	3:C:1066:VAL:HG21	1.87	0.56
4:D:1584:HIS:NE2	4:D:1785:ASN:O	2.39	0.56
6:F:793:LEU:O	6:F:797:ASN:ND2	2.39	0.56
9:J:262:THR:HA	9:J:379:LEU:HB2	1.88	0.56
9:I:100:LEU:HD13	9:J:307:LEU:HB3	1.86	0.56
4:D:1805:PRO:O	4:D:1809:ASN:ND2	2.39	0.56
4:D:2234:GLN:NE2	6:F:786:ASN:OD1	2.32	0.56
16:R:118:SER:O	16:R:155:SER:OG	2.24	0.56
3:C:227:LEU:HD12	3:C:288:ILE:HG23	1.88	0.55
3:C:514:MET:SD	3:C:515:ASP:N	2.79	0.55
4:D:1654:ARG:NH2	4:D:1753:ASN:OD1	2.38	0.55
4:D:1734:ILE:HB	4:D:1769:LEU:HD22	1.88	0.55
6:F:747:SER:OG	6:F:748:THR:N	2.38	0.55
2:B:134:ILE:HG12	16:R:162:PRO:HD2	1.87	0.55
3:C:1217:SER:OG	3:C:1218:ALA:N	2.38	0.55
4:D:2216:ARG:NH2	6:F:759:SER:OG	2.39	0.55
2:B:989:HIS:HD2	4:D:1977:LEU:HB3	1.72	0.55
1:A:708:ARG:O	1:A:712:MET:HG2	2.06	0.55
2:B:735:ASP:OD2	2:B:952:ARG:NH2	2.27	0.55
3:C:828:THR:HG22	3:C:993:ARG:HG2	1.89	0.55
1:A:652:MET:SD	1:A:652:MET:N	2.80	0.55
2:B:479:ILE:HB	2:B:554:PHE:HB3	1.89	0.55
7:G:262:GLY:HA3	7:G:353:LEU:HD13	1.88	0.55
3:C:521:TYR:O	3:C:524:SER:OG	2.22	0.55
7:G:310:VAL:HG12	7:G:311:VAL:HG23	1.89	0.55
9:J:293:THR:HA	9:J:296:VAL:HG22	1.89	0.55
1:A:519:VAL:HG23	1:A:559:LEU:HD11	1.88	0.54
1:A:813:SER:HB2	1:A:815:ASP:H	1.72	0.54
4:D:1754:ILE:HD12	4:D:1754:ILE:H	1.72	0.54
6:F:692:THR:OG1	6:F:694:ASN:ND2	2.40	0.54
7:G:203:GLY:O	18:G:401:PX2:O8	2.26	0.54
9:J:103:LYS:HZ2	9:J:131:THR:HB	1.70	0.54
9:J:103:LYS:NZ	9:J:133:SER:O	2.40	0.54
4:D:1754:ILE:HD11	4:D:1790:ALA:HB1	1.90	0.54
9:J:203:ASN:HD21	9:J:262:THR:HG21	1.71	0.54
1:A:501:ALA:O	1:A:512:LYS:NZ	2.41	0.54
9:J:183:VAL:HA	9:J:186:VAL:HG22	1.89	0.54
1:A:664:LYS:HG3	1:A:667:LEU:HD22	1.90	0.54
2:B:739:LEU:HA	2:B:742:MET:HE2	1.89	0.54
10:K:60:MET:SD	10:K:65:SER:OG	2.65	0.54
1:A:682:MET:SD	1:A:682:MET:N	2.78	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:329:ASP:OD1	9:I:329:ASP:N	2.41	0.54
1:A:178:LEU:HD12	1:A:179:PRO:HD2	1.88	0.53
4:D:2233:ARG:NH1	6:F:779:PHE:O	2.36	0.53
3:C:234:LEU:HD22	3:C:281:ILE:HG23	1.91	0.53
3:C:408:ARG:HB3	3:C:409:MET:HE2	1.89	0.53
4:D:2285:PHE:N	4:D:2288:GLU:OE1	2.40	0.53
5:E:568:LEU:HB3	5:E:598:ARG:HG2	1.90	0.53
9:I:247:LEU:HD13	9:J:132:PRO:HB3	1.91	0.53
3:C:384:SER:HB2	16:R:276:TYR:HD2	1.73	0.53
6:F:438:ARG:HG3	6:F:440:VAL:HG23	1.89	0.53
1:A:608:THR:HB	1:A:743:ILE:HG13	1.91	0.53
4:D:1648:GLY:HA3	4:D:1814:ILE:HB	1.90	0.53
3:C:220:LEU:HD21	3:C:299:THR:HG21	1.91	0.53
6:F:654:MET:SD	6:F:654:MET:N	2.76	0.53
6:F:755:ASP:HA	6:F:758:ARG:HG2	1.90	0.53
1:A:527:THR:HG22	1:A:530:GLU:HG2	1.90	0.53
2:B:134:ILE:HD12	2:B:137:ASN:HB3	1.91	0.53
4:D:1596:SER:OG	4:D:1597:CYS:N	2.41	0.53
7:G:139:ASP:HB3	7:G:142:PHE:HB3	1.91	0.53
2:B:354:TRP:HE1	7:G:154:PRO:HG3	1.74	0.53
6:F:431:HIS:HB3	6:F:434:MET:HE3	1.91	0.53
3:C:484:TYR:OH	3:C:488:ARG:NH1	2.41	0.53
3:C:820:VAL:HG12	3:C:948:ARG:HB2	1.90	0.53
2:B:651:GLU:O	2:B:657:ARG:NH1	2.40	0.52
5:E:460:ILE:HD11	6:F:628:ILE:HG22	1.91	0.52
5:E:711:LEU:HD13	5:E:757:HIS:HB3	1.90	0.52
6:F:828:THR:OG1	6:F:829:LYS:N	2.43	0.52
9:I:167:THR:HG23	9:I:169:ASP:H	1.73	0.52
1:A:387:GLU:HA	6:F:485:GLY:HA3	1.90	0.52
2:B:916:ARG:NH2	9:J:327:ASP:OD2	2.42	0.52
1:A:248:TRP:HZ3	16:R:77:VAL:HG13	1.75	0.52
1:A:735:ASP:OD1	6:F:853:ARG:NH2	2.42	0.52
3:C:866:VAL:HG11	3:C:907:PHE:HE1	1.75	0.52
5:E:620:HIS:HA	5:E:623:LYS:HZ3	1.74	0.52
5:E:848:ASP:O	5:E:852:HIS:ND1	2.42	0.52
7:G:334:MET:HE1	7:G:358:LEU:HD23	1.91	0.52
2:B:758:VAL:HG21	2:B:792:LEU:HD22	1.90	0.52
2:B:823:GLN:HG3	2:B:892:ILE:HD11	1.91	0.52
4:D:136:ILE:HD11	16:R:234:PRO:HG2	1.91	0.52
2:B:697:ARG:NH1	2:B:735:ASP:OD1	2.43	0.52
2:B:992:ARG:NH1	4:D:2258:GLN:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1201:TRP:NE1	5:E:777:THR:OG1	2.43	0.52
1:A:384:ASP:O	1:A:396:ARG:NH1	2.42	0.52
9:I:88:LEU:HD13	9:I:182:LEU:HD22	1.91	0.52
3:C:829:GLY:O	3:C:833:LEU:N	2.40	0.52
9:I:112:HIS:HA	9:I:136:ARG:O	2.10	0.52
2:B:990:LYS:NZ	4:D:1976:ASP:O	2.43	0.51
9:I:208:ILE:HG12	9:I:394:ALA:HB2	1.92	0.51
4:D:1561:LYS:HB2	7:G:230:LEU:HG	1.92	0.51
1:A:501:ALA:HA	1:A:504:LYS:HG3	1.93	0.51
2:B:126:LYS:HE3	16:R:165:SER:H	1.76	0.51
3:C:1190:GLU:OE2	3:C:1194:ARG:NH1	2.44	0.51
4:D:1850:ILE:HG21	4:D:1884:ARG:HH21	1.75	0.51
6:F:585:ARG:NH2	6:F:612:ASP:OD1	2.44	0.51
1:A:800:THR:HG21	1:A:805:ARG:HG2	1.93	0.51
3:C:1046:MET:HE3	3:C:1050:LEU:HD12	1.93	0.51
4:D:46:GLN:NE2	7:G:225:SER:OG	2.44	0.51
4:D:1328:MET:HB2	16:R:100:LYS:HD3	1.93	0.51
4:D:1584:HIS:HD2	4:D:1787:LEU:HD23	1.74	0.51
5:E:565:LEU:HB2	5:E:598:ARG:HH11	1.74	0.51
1:A:330:GLU:HG3	2:B:719:ARG:HH11	1.75	0.51
2:B:950:LYS:NZ	2:B:957:GLU:OE1	2.33	0.51
5:E:640:PRO:HG3	5:E:741:ARG:HD3	1.91	0.51
3:C:1288:PRO:HG2	3:C:1290:PHE:HE2	1.75	0.51
1:A:550:ILE:HD11	6:F:438:ARG:HE	1.74	0.51
2:B:221:LEU:HD13	2:B:319:VAL:HG12	1.92	0.51
16:R:95:CYS:SG	16:R:96:GLN:N	2.83	0.51
16:R:133:LYS:HG2	16:R:134:PRO:HD2	1.91	0.51
2:B:256:LYS:HZ3	2:B:279:VAL:HG11	1.76	0.51
3:C:1167:ALA:HA	3:C:1170:MET:HE3	1.93	0.51
16:R:315:LYS:HA	16:R:318:LYS:HD2	1.93	0.51
1:A:338:ASP:OD2	1:A:456:GLN:NE2	2.37	0.51
2:B:989:HIS:CD2	4:D:1977:LEU:HB3	2.45	0.51
3:C:845:VAL:HG12	3:C:880:ILE:HB	1.92	0.51
6:F:689:GLU:HA	6:F:829:LYS:HB2	1.92	0.51
1:A:795:ASN:O	9:J:130:ASN:ND2	2.44	0.50
2:B:125:PHE:O	2:B:129:THR:OG1	2.23	0.50
3:C:1171:LEU:HD11	3:C:1255:LEU:HG	1.93	0.50
4:D:2219:ILE:HB	4:D:2222:THR:HG23	1.92	0.50
16:R:89:LEU:HA	16:R:92:LYS:NZ	2.26	0.50
4:D:1017:PRO:HG2	4:D:1033:LEU:HD21	1.94	0.50
7:G:247:THR:O	7:G:252:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:TRP:HA	1:A:215:VAL:HB	1.93	0.50
2:B:939:ILE:HG12	2:B:965:LEU:HD13	1.91	0.50
3:C:803:LEU:HD22	3:C:843:VAL:HG21	1.92	0.50
13:N:7:UNK:HA	13:N:10:LEU:HB3	1.93	0.50
3:C:1115:ASP:HB3	3:C:1137:LYS:HA	1.94	0.50
7:G:357:CYS:O	7:G:361:TYR:HB2	2.12	0.50
9:J:295:VAL:HG11	9:J:305:ALA:HB2	1.93	0.50
4:D:496:PHE:HE2	13:N:24:ARG:HD3	1.76	0.50
10:K:74:ASP:OD1	10:K:74:ASP:N	2.44	0.50
1:A:206:ARG:NH2	16:R:106:GLN:O	2.42	0.50
3:C:587:MET:HA	3:C:587:MET:HE2	1.92	0.50
4:D:532:SER:O	4:D:535:SER:OG	2.28	0.50
2:B:857:ALA:O	2:B:860:MET:HB3	2.11	0.50
16:R:119:VAL:O	16:R:165:SER:HA	2.12	0.50
1:A:328:LEU:HD13	1:A:369:ILE:HD11	1.94	0.50
5:E:442:LEU:HD13	5:E:483:ILE:HD11	1.94	0.50
5:E:800:ASN:HD21	5:E:806:VAL:H	1.60	0.50
3:C:960:ARG:NH2	3:C:990:THR:O	2.45	0.49
9:J:88:LEU:HD13	9:J:182:LEU:HD22	1.94	0.49
16:R:121:TYR:OH	16:R:167:ASP:O	2.30	0.49
6:F:447:LEU:HD11	6:F:555:THR:HG23	1.94	0.49
1:A:587:ARG:HD3	1:A:645:PRO:HB3	1.94	0.49
2:B:930:MET:O	2:B:934:ARG:HG2	2.12	0.49
5:E:462:PRO:HD2	5:E:573:THR:HB	1.94	0.49
6:F:413:ALA:HB1	6:F:587:GLU:HG3	1.95	0.49
6:F:693:ILE:HG23	6:F:821:LEU:HD22	1.93	0.49
1:A:444:LEU:HD22	1:A:478:ARG:HD3	1.95	0.49
1:A:777:ARG:HD3	2:B:912:GLU:HG3	1.93	0.49
2:B:633:ARG:NH2	4:D:12:GLU:OE2	2.45	0.49
9:J:335:PHE:HA	9:J:347:ALA:HA	1.95	0.49
3:C:386:ARG:HA	3:C:389:LYS:HD3	1.94	0.49
6:F:678:VAL:HG13	6:F:729:VAL:HG22	1.93	0.49
9:J:351:LYS:NZ	9:J:358:GLU:OE2	2.35	0.49
2:B:973:PHE:HA	4:D:1986:LYS:HD3	1.95	0.49
5:E:861:MET:HA	5:E:864:LYS:HD3	1.93	0.49
1:A:236:ALA:O	1:A:240:THR:HG23	2.11	0.49
2:B:425:ARG:NH1	4:D:96:ASN:OD1	2.45	0.49
4:D:2282:ARG:NH2	8:H:99:ASP:OD1	2.38	0.49
5:E:725:VAL:HG22	5:E:737:VAL:HG23	1.93	0.49
2:B:972:ASP:O	2:B:975:LYS:NZ	2.39	0.49
4:D:557:HIS:NE2	4:D:1055:GLU:OE1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1029:LYS:O	4:D:1029:LYS:NZ	2.37	0.49
2:B:780:PHE:CD1	2:B:822:MET:HE1	2.47	0.49
9:I:203:ASN:HD21	9:I:262:THR:HG21	1.78	0.49
1:A:334:ILE:HG12	1:A:341:PHE:HD2	1.77	0.49
1:A:643:CYS:HB2	1:A:666:THR:HG22	1.94	0.49
1:A:650:GLU:HG3	1:A:658:LEU:HD21	1.95	0.49
2:B:920:ARG:HH21	9:J:354:LYS:HZ3	1.60	0.49
5:E:699:THR:HG23	5:E:772:ILE:HD12	1.95	0.49
1:A:497:LEU:HD21	1:A:520:ALA:HB2	1.95	0.48
3:C:1226:GLU:HA	3:C:1229:MET:HE2	1.94	0.48
6:F:585:ARG:NH2	6:F:608:ALA:O	2.40	0.48
1:A:318:PHE:HB2	1:A:364:LEU:HG	1.95	0.48
1:A:809:THR:HG22	1:A:810:GLN:H	1.78	0.48
4:D:1768:GLY:O	4:D:1772:ASN:ND2	2.46	0.48
5:E:515:PHE:O	5:E:519:LYS:HG2	2.13	0.48
1:A:581:LYS:HE3	1:A:581:LYS:HA	1.95	0.48
1:A:790:THR:OG1	1:A:805:ARG:NH1	2.46	0.48
3:C:1195:MET:HB3	3:C:1201:TRP:HB2	1.96	0.48
9:J:111:LEU:HD23	9:J:135:VAL:HG22	1.95	0.48
4:D:2226:HIS:HE1	6:F:778:ASN:HB3	1.78	0.48
5:E:874:THR:HG21	5:E:905:THR:HG23	1.95	0.48
6:F:421:GLU:O	6:F:424:GLU:HB2	2.13	0.48
1:A:216:TRP:HA	1:A:219:LEU:HB2	1.95	0.48
1:A:788:ARG:HB3	2:B:1006:HIS:CE1	2.48	0.48
2:B:759:SER:OG	2:B:760:TYR:N	2.46	0.48
9:J:323:ALA:HB2	9:J:330:VAL:HG11	1.96	0.48
3:C:773:MET:SD	3:C:775:ARG:NH1	2.87	0.48
2:B:811:ASP:HB3	4:D:1899:ARG:HD3	1.96	0.48
4:D:1734:ILE:HD12	4:D:1769:LEU:HB2	1.96	0.48
6:F:674:ALA:HA	6:F:814:MET:HE1	1.95	0.48
6:F:585:ARG:HD2	6:F:619:LEU:HD21	1.95	0.48
9:J:351:LYS:HB3	9:J:359:ALA:HB3	1.95	0.48
16:R:254:TYR:CZ	16:R:258:MET:HE3	2.49	0.48
1:A:337:ASN:ND2	1:A:340:GLU:OE1	2.47	0.48
3:C:1193:THR:HG21	4:D:2048:GLY:HA3	1.96	0.48
1:A:451:LYS:HB2	1:A:454:THR:HG22	1.96	0.47
3:C:983:ARG:O	3:C:987:GLU:HG2	2.14	0.47
4:D:2269:THR:O	4:D:2273:ARG:HG2	2.13	0.47
5:E:466:VAL:HG13	5:E:601:ARG:HB3	1.96	0.47
5:E:713:ARG:NH2	5:E:899:ASP:OD1	2.47	0.47
6:F:450:GLY:O	6:F:556:ASN:ND2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:847:GLN:O	7:G:227:ARG:NH2	2.42	0.47
6:F:730:GLN:HB2	6:F:757:ALA:HB2	1.95	0.47
9:J:166:MET:HE3	9:J:171:LEU:HD22	1.97	0.47
13:N:21:UNK:O	13:N:24:ARG:NH2	2.46	0.47
2:B:685:LEU:HB3	2:B:689:ILE:HG21	1.95	0.47
6:F:727:ILE:HG23	6:F:757:ALA:HB1	1.95	0.47
9:J:246:LYS:HZ2	9:J:248:ILE:HB	1.80	0.47
9:J:343:LEU:HD21	9:J:384:LYS:HA	1.97	0.47
1:A:496:ILE:HD12	1:A:528:GLY:HA2	1.96	0.47
2:B:381:GLU:OE2	2:B:424:LYS:N	2.46	0.47
4:D:1985:GLU:HB3	4:D:1988:ARG:HD2	1.95	0.47
6:F:621:ASN:O	6:F:625:ILE:HG12	2.14	0.47
7:G:261:VAL:O	7:G:265:LEU:HB2	2.15	0.47
2:B:943:ILE:HD11	2:B:962:MET:HE1	1.95	0.47
2:B:993:VAL:HG12	4:D:1976:ASP:HB3	1.96	0.47
3:C:416:LYS:HB3	3:C:439:MET:HB2	1.95	0.47
3:C:534:ARG:HD3	3:C:541:TYR:HE1	1.80	0.47
4:D:2286:SER:O	4:D:2289:MET:HB2	2.15	0.47
9:I:172:PHE:HE2	9:I:204:SER:HB2	1.79	0.47
9:J:163:LYS:H	9:J:166:MET:HE2	1.79	0.47
2:B:319:VAL:HG22	12:M:7:VAL:HG22	1.96	0.47
2:B:345:ARG:HH22	2:B:375:ALA:HB1	1.80	0.47
2:B:462:LEU:HD21	4:D:1386:ILE:HD13	1.96	0.47
2:B:942:LEU:HD21	2:B:961:LYS:HE3	1.96	0.47
3:C:231:ARG:O	3:C:235:MET:HG3	2.15	0.47
3:C:312:ARG:HA	3:C:315:VAL:HG22	1.97	0.47
3:C:546:GLY:HA2	11:L:15:LYS:HZ2	1.79	0.47
3:C:799:VAL:HG21	3:C:820:VAL:HG11	1.96	0.47
3:C:886:PHE:HB3	3:C:930:THR:HG22	1.96	0.47
4:D:1646:VAL:HG13	4:D:1791:SER:HB2	1.97	0.47
7:G:192:TRP:HA	7:G:196:VAL:HB	1.97	0.47
8:H:128:TRP:H	8:H:128:TRP:CD1	2.32	0.47
1:A:116:ARG:HA	1:A:119:VAL:HG22	1.96	0.47
1:A:209:ILE:HG22	1:A:210:ASP:HB3	1.95	0.47
1:A:360:THR:HG22	1:A:362:LYS:HE2	1.97	0.47
3:C:308:ILE:O	3:C:312:ARG:HG2	2.15	0.47
4:D:1561:LYS:HG3	4:D:1568:MET:HE2	1.97	0.47
5:E:680:VAL:HG11	5:E:736:GLN:HE22	1.80	0.47
5:E:703:GLY:HA3	5:E:768:ALA:HB2	1.97	0.47
1:A:613:ILE:HG21	6:F:715:GLU:HB3	1.97	0.47
2:B:202:ASN:HA	2:B:205:LYS:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:ASP:HB3	4:D:1894:LEU:HD12	1.97	0.47
3:C:1191:ILE:HG22	3:C:1195:MET:HE1	1.96	0.47
6:F:790:VAL:O	6:F:794:ARG:HG2	2.14	0.47
1:A:138:THR:OG1	1:A:139:GLU:OE1	2.30	0.47
3:C:291:ILE:HA	3:C:294:LYS:HG2	1.97	0.47
3:C:294:LYS:HA	3:C:297:THR:HG22	1.96	0.47
1:A:816:THR:HB	4:D:1959:PHE:HE2	1.80	0.46
2:B:594:ASP:OD1	2:B:594:ASP:N	2.48	0.46
2:B:599:ARG:NH2	2:B:646:ASP:O	2.47	0.46
2:B:847:LYS:HE2	2:B:847:LYS:HB3	1.75	0.46
3:C:500:VAL:HG23	11:L:21:LEU:HD12	1.97	0.46
3:C:602:LEU:O	3:C:605:ARG:HG3	2.15	0.46
3:C:812:MET:HE3	3:C:814:ALA:HB3	1.97	0.46
7:G:208:TRP:CD2	7:G:343:ALA:HB1	2.51	0.46
7:G:343:ALA:O	7:G:345:ARG:NH1	2.47	0.46
1:A:174:ILE:HG12	1:A:207:MET:HE3	1.97	0.46
2:B:642:THR:OG1	2:B:643:ASN:N	2.47	0.46
2:B:819:TYR:O	2:B:823:GLN:HG2	2.14	0.46
4:D:2214:TYR:OH	6:F:672:GLU:OE2	2.30	0.46
7:G:328:PRO:O	7:G:332:SER:OG	2.23	0.46
9:J:393:PHE:HA	9:J:396:LYS:HE3	1.96	0.46
1:A:441:LEU:HD22	2:B:560:ALA:HB1	1.98	0.46
2:B:142:TRP:CG	2:B:152:ARG:HE	2.33	0.46
3:C:819:GLY:O	3:C:947:ASP:N	2.48	0.46
4:D:1783:THR:O	4:D:1783:THR:OG1	2.31	0.46
5:E:442:LEU:HD23	5:E:445:LEU:HD13	1.97	0.46
5:E:827:PHE:HD2	5:E:828:GLU:HG2	1.80	0.46
2:B:207:LYS:HB3	2:B:239:VAL:HG21	1.97	0.46
2:B:969:MET:HE3	2:B:969:MET:HA	1.96	0.46
3:C:517:MET:HE3	3:C:517:MET:O	2.15	0.46
3:C:1219:LEU:O	3:C:1221:MET:HG2	2.16	0.46
6:F:611:THR:HG21	6:F:622:ILE:HD11	1.97	0.46
9:I:170:ASP:O	9:I:174:ILE:HG22	2.16	0.46
3:C:536:ASP:H	4:D:1323:LEU:HD23	1.81	0.46
3:C:1207:PRO:HG2	5:E:858:ILE:HG22	1.98	0.46
4:D:1649:SER:HB3	4:D:1793:HIS:HB3	1.96	0.46
6:F:627:ALA:HA	6:F:630:MET:HE1	1.98	0.46
14:O:155:LYS:HG3	14:O:156:LYS:H	1.81	0.46
1:A:231:VAL:HG21	14:O:155:LYS:HA	1.98	0.46
1:A:467:ASP:N	1:A:467:ASP:OD1	2.49	0.46
2:B:267:THR:HA	2:B:270:LYS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:548:LYS:HD3	2:B:549:GLU:HG3	1.97	0.46
3:C:1109:LEU:HD11	3:C:1273:LEU:HB3	1.97	0.46
4:D:1879:ASP:OD1	4:D:1879:ASP:N	2.39	0.46
6:F:521:ILE:HG22	6:F:529:ARG:HH22	1.81	0.46
6:F:691:LEU:HD13	6:F:704:VAL:HG12	1.96	0.46
9:I:267:LEU:HD12	9:I:281:ILE:HG23	1.97	0.46
1:A:504:LYS:NZ	6:F:439:GLY:O	2.48	0.46
3:C:171:THR:O	3:C:175:LEU:HB2	2.15	0.46
3:C:206:LYS:HD2	3:C:206:LYS:HA	1.71	0.46
3:C:1177:GLU:HB2	4:D:1958:LYS:HB2	1.97	0.46
4:D:56:ARG:HH21	4:D:1588:LEU:HD23	1.81	0.46
1:A:645:PRO:HA	1:A:648:VAL:HG12	1.98	0.46
4:D:1049:ARG:HD2	4:D:1050:PHE:HB2	1.98	0.46
4:D:2226:HIS:CE1	6:F:778:ASN:HB3	2.50	0.46
5:E:538:ARG:NE	5:E:558:GLU:OE1	2.46	0.46
6:F:585:ARG:HG2	6:F:619:LEU:HD11	1.98	0.46
9:I:293:THR:HA	9:I:296:VAL:HG22	1.98	0.46
1:A:515:LEU:HD21	1:A:552:ARG:HG2	1.98	0.46
2:B:981:PRO:HA	4:D:2279:LEU:HD13	1.97	0.46
3:C:978:ASP:OD2	3:C:978:ASP:N	2.41	0.46
4:D:556:ILE:HG22	4:D:1052:PHE:HD2	1.81	0.46
1:A:676:LEU:O	1:A:680:THR:OG1	2.28	0.45
2:B:365:PHE:HB2	2:B:400:VAL:HG21	1.98	0.45
4:D:1365:VAL:HG21	16:R:89:LEU:HD13	1.97	0.45
4:D:1984:ASP:OD1	4:D:1984:ASP:N	2.47	0.45
5:E:625:LYS:HG3	5:E:665:SER:HA	1.97	0.45
7:G:123:LEU:O	7:G:127:THR:OG1	2.33	0.45
1:A:157:LEU:HD11	1:A:219:LEU:HD12	1.97	0.45
3:C:1000:VAL:HG13	3:C:1004:LEU:HD23	1.97	0.45
3:C:1104:ARG:HG3	3:C:1164:SER:HB3	1.98	0.45
16:R:310:ALA:O	16:R:313:GLN:HG3	2.16	0.45
1:A:418:ASP:O	1:A:422:SER:OG	2.32	0.45
1:A:849:LEU:HG	7:G:182:GLN:HB3	1.97	0.45
6:F:507:PHE:HD1	6:F:552:ILE:HG23	1.81	0.45
1:A:827:LYS:HG2	4:D:1919:VAL:HA	1.98	0.45
2:B:130:VAL:HA	2:B:133:PHE:HB3	1.98	0.45
3:C:942:ARG:HE	3:C:945:ARG:HD3	1.81	0.45
9:I:138:PHE:HB3	9:I:143:GLU:HB2	1.97	0.45
16:R:124:LYS:HD3	16:R:151:VAL:HG21	1.97	0.45
4:D:100:SER:HB2	4:D:103:LEU:HB3	1.98	0.45
1:A:128:LEU:HD11	7:G:138:LEU:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2279:LEU:HD23	4:D:2279:LEU:HA	1.82	0.45
9:I:291:ALA:O	9:I:295:VAL:HG23	2.17	0.45
9:I:363:SER:HA	9:I:366:GLN:HE22	1.81	0.45
1:A:213:ASN:HD21	16:R:212:PRO:HD3	1.81	0.45
2:B:321:PHE:HB3	2:B:326:VAL:HG21	1.97	0.45
2:B:512:MET:O	2:B:512:MET:HE3	2.17	0.45
3:C:496:ARG:NH1	11:L:14:LEU:HD22	2.32	0.45
4:D:1365:VAL:HG11	16:R:89:LEU:HD11	1.99	0.45
9:J:305:ALA:HB3	9:J:309:MET:HG3	1.98	0.45
2:B:220:LYS:HG2	2:B:244:TRP:CD1	2.51	0.45
6:F:469:VAL:HB	6:F:504:SER:HA	1.98	0.45
9:I:255:ILE:HD11	9:I:264:LEU:HD23	1.99	0.45
5:E:606:ARG:HG2	5:E:607:PRO:HD2	1.98	0.45
6:F:661:SER:OG	6:F:662:LEU:N	2.49	0.45
1:A:157:LEU:HD23	1:A:218:LYS:HD2	1.98	0.45
3:C:177:THR:HG22	3:C:205:VAL:HG22	1.99	0.45
5:E:787:ASP:OD1	5:E:816:LYS:NZ	2.44	0.45
7:G:263:HIS:CE1	7:G:353:LEU:HD21	2.52	0.45
9:J:162:ARG:NE	9:J:304:SER:OG	2.47	0.45
2:B:958:VAL:O	2:B:962:MET:HE3	2.18	0.44
4:D:1677:PHE:HE1	4:D:1737:GLN:HE22	1.65	0.44
5:E:611:LYS:HA	5:E:611:LYS:HD2	1.87	0.44
7:G:192:TRP:CE3	7:G:196:VAL:HG11	2.52	0.44
9:J:176:ALA:HA	9:J:179:VAL:HG12	1.99	0.44
1:A:646:ARG:NH1	6:F:768:GLY:O	2.50	0.44
2:B:817:PHE:HA	2:B:820:MET:HG3	1.99	0.44
3:C:308:ILE:HD13	4:D:1319:LEU:HA	1.99	0.44
5:E:420:ARG:NH1	5:E:493:GLN:OE1	2.50	0.44
16:R:281:LEU:HD12	16:R:295:ILE:HD11	1.99	0.44
1:A:444:LEU:HD21	1:A:473:LEU:HG	1.99	0.44
2:B:690:ASP:OD1	2:B:690:ASP:N	2.50	0.44
3:C:273:ILE:HG23	3:C:274:MET:HE2	1.99	0.44
3:C:1205:ASP:OD2	3:C:1295:ASN:ND2	2.49	0.44
6:F:445:GLY:HA3	6:F:571:PHE:HA	2.00	0.44
10:K:25:LYS:HA	10:K:25:LYS:HD2	1.84	0.44
1:A:421:GLY:HA2	1:A:440:LEU:HD12	1.99	0.44
2:B:139:TRP:HA	2:B:142:TRP:HB2	1.99	0.44
2:B:615:ILE:HD12	2:B:618:LEU:HD12	1.99	0.44
5:E:587:ASP:N	5:E:587:ASP:OD1	2.48	0.44
6:F:417:LYS:O	6:F:420:LEU:HB2	2.17	0.44
6:F:685:MET:HG2	6:F:706:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:280:LYS:HE2	3:C:284:ARG:HG3	2.00	0.44
2:B:680:SER:O	2:B:680:SER:OG	2.31	0.44
3:C:534:ARG:HH12	3:C:589:ILE:HB	1.83	0.44
6:F:481:GLU:OE2	6:F:490:ARG:NH1	2.50	0.44
9:I:307:LEU:HD22	9:J:100:LEU:HD22	1.99	0.44
9:J:329:ASP:N	9:J:329:ASP:OD1	2.50	0.44
10:K:42:LYS:H	10:K:42:LYS:HG2	1.55	0.44
2:B:920:ARG:HE	9:J:354:LYS:HZ1	1.66	0.44
3:C:916:ASP:CG	3:C:945:ARG:HE	2.25	0.44
5:E:766:ARG:HA	5:E:766:ARG:HD3	1.79	0.44
6:F:628:ILE:O	6:F:632:ARG:NH1	2.51	0.44
9:I:251:ASP:OD1	9:I:251:ASP:N	2.49	0.44
10:K:18:LYS:HA	10:K:18:LYS:HD2	1.66	0.44
16:R:118:SER:HB3	16:R:165:SER:HB3	1.98	0.44
1:A:814:ASP:OD1	1:A:814:ASP:N	2.42	0.44
2:B:962:MET:HE2	2:B:962:MET:HB3	1.89	0.44
3:C:1064:GLU:HA	3:C:1067:VAL:HG22	1.99	0.44
6:F:865:LEU:O	6:F:869:MET:HG3	2.18	0.44
9:J:157:PRO:HA	9:J:198:ILE:HB	1.99	0.44
9:J:343:LEU:HD23	9:J:344:PRO:HD2	1.99	0.44
7:G:161:LEU:HD11	7:G:192:TRP:CD1	2.53	0.44
9:J:253:PRO:HB2	9:J:266:LEU:HB2	2.00	0.44
1:A:157:LEU:HD12	1:A:157:LEU:HA	1.83	0.43
1:A:398:LYS:HB3	1:A:442:GLN:HE21	1.82	0.43
1:A:844:LYS:HB3	7:G:235:TYR:CZ	2.53	0.43
3:C:391:LEU:O	3:C:395:LYS:HG3	2.18	0.43
4:D:1817:LEU:HD23	4:D:1822:GLN:HG2	2.00	0.43
7:G:240:ASP:HB3	7:G:243:TRP:HD1	1.82	0.43
9:I:368:LEU:HB3	9:I:372:GLU:HB2	2.00	0.43
12:M:9:VAL:HG11	16:R:222:ASP:HB2	2.00	0.43
1:A:594:LEU:HD12	1:A:644:ALA:HB2	2.01	0.43
3:C:823:VAL:HG23	3:C:951:HIS:HA	1.99	0.43
4:D:1022:SER:OG	4:D:1023:LEU:N	2.51	0.43
6:F:438:ARG:HD2	6:F:438:ARG:O	2.17	0.43
9:I:253:PRO:HB2	9:I:266:LEU:HB2	1.98	0.43
10:K:15:ILE:O	10:K:16:HIS:ND1	2.51	0.43
1:A:708:ARG:HH22	6:F:779:PHE:HA	1.83	0.43
2:B:225:ILE:HB	2:B:233:VAL:HG13	1.99	0.43
2:B:225:ILE:HD11	2:B:235:ASP:HB2	2.00	0.43
2:B:906:MET:N	4:D:2240:ASN:OD1	2.39	0.43
3:C:994:PRO:HA	3:C:997:LEU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:185:ALA:O	9:I:189:ASN:ND2	2.31	0.43
9:I:335:PHE:HA	9:I:347:ALA:HA	2.00	0.43
1:A:550:ILE:HD11	6:F:438:ARG:NE	2.34	0.43
2:B:822:MET:HA	2:B:822:MET:HE2	1.99	0.43
6:F:810:ASN:O	6:F:814:MET:HB2	2.18	0.43
2:B:572:LYS:O	2:B:576:MET:HB2	2.18	0.43
3:C:313:GLU:O	3:C:316:GLU:HG2	2.19	0.43
3:C:573:LEU:HD23	3:C:573:LEU:HA	1.88	0.43
4:D:1980:LEU:HA	4:D:1981:PRO:HD2	1.88	0.43
5:E:914:GLN:H	5:E:914:GLN:HG3	1.67	0.43
6:F:472:PHE:HB3	6:F:474:ILE:HD11	2.00	0.43
6:F:599:ALA:HB2	6:F:637:GLU:HG3	2.01	0.43
16:R:190:ILE:HD12	16:R:190:ILE:HA	1.88	0.43
2:B:764:ARG:HH22	2:B:944:THR:HG21	1.82	0.43
3:C:564:LYS:HE3	3:C:564:LYS:HB2	1.83	0.43
16:R:320:SER:HA	16:R:323:ARG:HG2	2.00	0.43
3:C:943:PRO:HG2	5:E:656:LEU:HD13	2.00	0.43
5:E:646:LYS:O	5:E:649:GLN:HG2	2.18	0.43
6:F:865:LEU:HD12	6:F:869:MET:HE2	2.00	0.43
2:B:381:GLU:HA	2:B:421:LEU:HD11	2.00	0.43
3:C:485:ILE:HG13	10:K:70:LEU:HD21	2.01	0.43
4:D:1565:GLY:HA2	4:D:1824:LYS:HG2	2.01	0.43
9:J:208:ILE:HA	9:J:394:ALA:HB2	2.01	0.43
1:A:497:LEU:HB3	1:A:531:LEU:HD23	2.00	0.43
3:C:273:ILE:O	3:C:277:GLU:HG2	2.18	0.43
9:I:228:THR:HG22	9:I:258:HIS:HB2	2.01	0.43
10:K:34:ASP:OD1	10:K:37:ARG:NH1	2.52	0.43
1:A:493:ARG:O	1:A:497:LEU:HG	2.19	0.43
2:B:220:LYS:HG2	2:B:244:TRP:HD1	1.84	0.43
4:D:1841:MET:HB3	4:D:1847:PHE:HB3	2.00	0.43
5:E:496:GLY:HA2	5:E:499:PHE:HD2	1.84	0.43
5:E:522:LYS:HE2	5:E:575:LYS:HD3	2.01	0.43
5:E:539:GLN:HG3	5:E:541:ILE:H	1.83	0.43
2:B:862:ILE:HA	2:B:874:LEU:HD13	2.01	0.42
5:E:630:VAL:HG13	5:E:635:TYR:HE2	1.84	0.42
2:B:746:LEU:HG	2:B:750:GLU:HG3	2.02	0.42
3:C:1239:LEU:HD21	3:C:1292:SER:HB3	2.01	0.42
4:D:134:ARG:HG3	4:D:501:TRP:HZ2	1.84	0.42
5:E:721:ARG:O	5:E:740:HIS:ND1	2.52	0.42
5:E:762:LEU:HD11	5:E:825:LEU:HD21	2.01	0.42
5:E:804:PRO:HG2	5:E:853:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:691:LEU:HG	6:F:821:LEU:HD21	2.00	0.42
6:F:748:THR:O	6:F:748:THR:OG1	2.34	0.42
9:I:286:VAL:O	9:I:290:ASN:ND2	2.39	0.42
9:J:267:LEU:HD12	9:J:281:ILE:HG23	2.01	0.42
11:L:21:LEU:HD23	11:L:21:LEU:HA	1.86	0.42
2:B:222:LYS:NZ	2:B:320:GLU:HG2	2.34	0.42
2:B:438:LEU:HD12	2:B:438:LEU:HA	1.88	0.42
2:B:780:PHE:CE1	2:B:822:MET:HE1	2.54	0.42
2:B:933:LEU:HD23	2:B:933:LEU:HA	1.90	0.42
3:C:250:LYS:O	3:C:254:LYS:HG2	2.19	0.42
3:C:979:LEU:HD23	3:C:1060:LYS:HB2	2.01	0.42
3:C:1058:LEU:HD12	3:C:1058:LEU:HA	1.83	0.42
3:C:1190:GLU:OE1	4:D:2055:GLN:NE2	2.53	0.42
4:D:500:ARG:HA	4:D:500:ARG:HD3	1.73	0.42
4:D:1582:ASP:HA	4:D:1585:LYS:HE2	2.02	0.42
6:F:434:MET:HB2	6:F:437:ARG:HH21	1.83	0.42
6:F:572:ASP:OD1	6:F:572:ASP:N	2.44	0.42
6:F:678:VAL:HG11	6:F:729:VAL:HA	2.01	0.42
10:K:66:LEU:HD23	10:K:66:LEU:H	1.84	0.42
1:A:208:PRO:HG2	16:R:109:ARG:HG3	2.02	0.42
1:A:584:LEU:HD11	1:A:613:ILE:HD13	2.01	0.42
2:B:821:LYS:NZ	4:D:1984:ASP:O	2.52	0.42
5:E:614:LEU:O	5:E:618:LYS:HG2	2.19	0.42
5:E:803:ASN:OD1	6:F:734:ARG:NH2	2.36	0.42
6:F:615:VAL:HG13	6:F:617:ALA:H	1.85	0.42
7:G:224:VAL:O	7:G:228:LYS:HG2	2.20	0.42
1:A:93:ARG:NE	2:B:255:LEU:O	2.52	0.42
1:A:834:GLU:O	1:A:838:GLN:HB3	2.20	0.42
2:B:459:LYS:HE2	2:B:459:LYS:HB2	1.86	0.42
5:E:450:LYS:HG3	5:E:451:ASN:OD1	2.19	0.42
5:E:664:ASN:OD1	5:E:664:ASN:N	2.53	0.42
6:F:605:MET:HA	6:F:605:MET:HE2	2.02	0.42
7:G:192:TRP:CE2	7:G:196:VAL:HG21	2.55	0.42
7:G:327:HIS:HD2	7:G:390:LYS:HG2	1.83	0.42
9:I:335:PHE:HD1	9:I:347:ALA:HB2	1.84	0.42
3:C:169:ASP:O	3:C:173:ARG:HG3	2.19	0.42
6:F:412:VAL:HG11	6:F:459:LEU:HD23	2.01	0.42
7:G:366:LYS:HD3	7:G:366:LYS:HA	1.93	0.42
9:J:202:VAL:HG22	9:J:206:VAL:HG23	2.01	0.42
1:A:350:LYS:HB3	1:A:447:MET:HE1	2.02	0.42
2:B:352:ARG:HA	2:B:354:TRP:CE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:234:LEU:HA	3:C:234:LEU:HD23	1.80	0.42
3:C:303:GLY:O	3:C:307:LEU:HG	2.19	0.42
3:C:305:ARG:HG3	3:C:586:LEU:HD11	2.01	0.42
4:D:105:LEU:HD23	4:D:108:LEU:HD12	2.00	0.42
9:I:248:ILE:HD12	9:I:248:ILE:H	1.85	0.42
16:R:308:LEU:HD23	16:R:308:LEU:HA	1.91	0.42
1:A:735:ASP:OD2	6:F:857:ARG:NH1	2.52	0.42
2:B:572:LYS:HA	2:B:575:GLU:HG2	2.02	0.42
3:C:401:LEU:HD12	3:C:401:LEU:HA	1.81	0.42
3:C:586:LEU:HD13	4:D:1318:SER:HA	2.01	0.42
7:G:199:ALA:CB	18:G:401:PX2:C4	2.90	0.42
7:G:216:TYR:HE1	7:G:336:LEU:HD22	1.84	0.42
2:B:407:TYR:O	2:B:411:THR:HG22	2.20	0.42
3:C:175:LEU:HA	3:C:178:VAL:HG22	2.02	0.42
3:C:1195:MET:HG3	3:C:1201:TRP:HE3	1.85	0.42
5:E:433:ALA:HB1	5:E:615:ASP:HB3	2.01	0.42
7:G:190:PHE:O	7:G:194:THR:OG1	2.33	0.42
7:G:216:TYR:CE1	7:G:336:LEU:HD22	2.54	0.42
9:J:283:GLU:HA	9:J:286:VAL:HG12	2.01	0.42
1:A:355:HIS:CE1	1:A:484:ARG:HB3	2.55	0.42
6:F:512:ASP:N	6:F:512:ASP:OD1	2.52	0.42
16:R:85:ILE:HA	16:R:88:ASP:HB3	2.02	0.42
1:A:701:VAL:HG13	6:F:780:TRP:HB3	2.01	0.41
2:B:269:ALA:HA	2:B:272:LYS:HD2	2.01	0.41
2:B:716:MET:N	2:B:716:MET:SD	2.93	0.41
2:B:967:PRO:HG2	2:B:969:MET:SD	2.59	0.41
3:C:540:MET:HG2	3:C:555:ILE:HD11	2.01	0.41
3:C:1030:SER:HA	3:C:1033:VAL:HG22	2.02	0.41
5:E:725:VAL:HG13	5:E:737:VAL:HB	2.01	0.41
4:D:1569:ILE:HD12	4:D:1569:ILE:HA	1.91	0.41
4:D:1609:GLN:HE21	4:D:1613:TYR:HD2	1.67	0.41
9:J:103:LYS:NZ	9:J:133:SER:OG	2.50	0.41
1:A:153:PHE:HZ	1:A:219:LEU:HD11	1.83	0.41
1:A:378:PHE:HZ	1:A:407:TYR:HD1	1.67	0.41
2:B:814:TYR:HE2	4:D:1933:MET:HE1	1.84	0.41
3:C:288:ILE:HD13	3:C:288:ILE:HA	1.90	0.41
4:D:1030:ALA:HB1	12:M:5:VAL:HG11	2.02	0.41
4:D:1562:ASN:OD1	7:G:237:ARG:NH2	2.53	0.41
5:E:460:ILE:HA	6:F:627:ALA:HB1	2.01	0.41
5:E:554:THR:O	5:E:558:GLU:HG2	2.21	0.41
7:G:389:HIS:CD2	7:G:394:PHE:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:109:LEU:HD23	4:D:109:LEU:HA	1.76	0.41
7:G:131:LYS:HE3	7:G:131:LYS:HB2	1.77	0.41
2:B:431:MET:O	2:B:435:ILE:HG12	2.20	0.41
3:C:880:ILE:HA	3:C:925:VAL:O	2.21	0.41
3:C:1184:GLU:O	3:C:1187:LYS:HB2	2.19	0.41
5:E:749:PHE:HE1	6:F:664:THR:HG23	1.84	0.41
6:F:700:GLU:H	6:F:700:GLU:HG2	1.63	0.41
8:H:110:ASP:OD1	8:H:110:ASP:N	2.47	0.41
2:B:358:PRO:HG2	2:B:398:TYR:CD2	2.56	0.41
2:B:828:HIS:HB3	2:B:832:CYS:SG	2.61	0.41
4:D:1024:ILE:HD12	4:D:1024:ILE:HA	1.85	0.41
6:F:602:LEU:HD21	6:F:604:TYR:CZ	2.56	0.41
8:H:94:GLU:H	8:H:94:GLU:HG2	1.67	0.41
9:I:243:LYS:HD3	9:I:243:LYS:HA	1.84	0.41
1:A:680:THR:HB	1:A:682:MET:HE1	2.02	0.41
5:E:639:LEU:HD12	5:E:642:TRP:CE2	2.55	0.41
7:G:145:TYR:HA	7:G:148:TRP:HB2	2.03	0.41
9:I:110:THR:HG23	9:I:134:GLN:HB2	2.03	0.41
9:I:154:VAL:HG11	9:I:186:VAL:HG21	2.03	0.41
9:J:239:VAL:HG21	9:J:252:VAL:HG21	2.02	0.41
13:N:13:UNK:O	16:R:259:ARG:NH1	2.53	0.41
1:A:605:ILE:H	1:A:605:ILE:HG12	1.73	0.41
1:A:803:ALA:HA	1:A:804:PRO:HD3	1.92	0.41
1:A:855:PHE:OXT	7:G:364:LYS:NZ	2.54	0.41
2:B:543:ALA:O	2:B:546:LEU:HB3	2.21	0.41
2:B:712:GLU:O	2:B:716:MET:HG2	2.21	0.41
4:D:1731:ARG:HB2	4:D:1765:LEU:HD21	2.02	0.41
5:E:711:LEU:HD12	5:E:761:VAL:HG23	2.02	0.41
7:G:388:ARG:HH12	7:G:390:LYS:HB2	1.85	0.41
2:B:301:LEU:HA	2:B:304:GLU:HG3	2.03	0.41
2:B:354:TRP:HZ2	18:G:401:PX2:C16	2.34	0.41
3:C:598:GLN:O	3:C:602:LEU:HG	2.20	0.41
4:D:140:LEU:HD21	16:R:230:LEU:HD21	2.03	0.41
4:D:1023:LEU:HD12	4:D:1023:LEU:H	1.85	0.41
4:D:1970:ALA:HA	4:D:2260:LEU:HD13	2.03	0.41
5:E:477:THR:OG1	5:E:529:ASP:OD2	2.38	0.41
5:E:749:PHE:CE1	6:F:664:THR:HG23	2.55	0.41
6:F:565:LEU:HD23	6:F:565:LEU:HA	1.89	0.41
7:G:354:LEU:HD23	7:G:354:LEU:HA	1.92	0.41
9:I:103:LYS:NZ	9:I:133:SER:O	2.52	0.41
9:I:170:ASP:OD2	9:I:171:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:203:ASN:ND2	9:J:262:THR:HG21	2.36	0.41
4:D:2055:GLN:O	4:D:2059:TYR:HB2	2.21	0.41
4:D:2206:GLN:NE2	4:D:2216:ARG:O	2.54	0.41
6:F:820:LYS:HA	6:F:820:LYS:HD2	1.89	0.41
7:G:368:GLU:O	7:G:372:MET:HE3	2.20	0.41
9:J:206:VAL:HG13	9:J:224:LEU:HD21	2.03	0.41
2:B:142:TRP:CD1	2:B:152:ARG:HE	2.39	0.40
4:D:105:LEU:HD23	4:D:105:LEU:HA	1.93	0.40
4:D:106:LYS:HD2	4:D:106:LYS:HA	1.88	0.40
4:D:2213:ILE:HG22	6:F:675:MET:HE2	2.02	0.40
5:E:621:ALA:HB1	5:E:626:MET:HG3	2.03	0.40
1:A:707:LEU:HD21	1:A:768:GLU:HB3	2.02	0.40
2:B:477:ASN:O	2:B:478:PHE:HB2	2.21	0.40
3:C:592:SER:OG	3:C:593:GLU:OE2	2.32	0.40
7:G:289:ILE:HA	7:G:292:THR:HG22	2.03	0.40
9:I:104:MET:HE1	9:J:311:TYR:CD2	2.56	0.40
1:A:812:ILE:H	1:A:812:ILE:HG13	1.61	0.40
2:B:844:ASP:HB2	2:B:847:LYS:HG3	2.03	0.40
4:D:19:GLU:HG2	4:D:26:PHE:HE2	1.86	0.40
4:D:1351:LEU:HD12	4:D:1351:LEU:HA	1.94	0.40
6:F:472:PHE:HB2	6:F:506:VAL:HG12	2.03	0.40
6:F:610:MET:HG2	6:F:644:LEU:HD13	2.03	0.40
1:A:685:PHE:CZ	1:A:700:LEU:HB3	2.57	0.40
2:B:986:LEU:HD22	4:D:2273:ARG:NH2	2.36	0.40
3:C:615:ARG:HD2	3:C:615:ARG:HA	1.78	0.40
3:C:866:VAL:HA	3:C:869:LEU:HB2	2.02	0.40
4:D:103:LEU:HD23	4:D:104:TYR:HD2	1.86	0.40
5:E:721:ARG:HB3	5:E:740:HIS:HD1	1.87	0.40
9:I:160:VAL:HG11	9:I:174:ILE:HD13	2.03	0.40
1:A:440:LEU:O	1:A:444:LEU:HG	2.21	0.40
1:A:811:ILE:HD11	4:D:2251:ASN:HB3	2.03	0.40
2:B:327:GLU:HG3	16:R:232:THR:HG21	2.03	0.40
3:C:568:PHE:HD1	3:C:571:LEU:HD23	1.87	0.40
3:C:605:ARG:HH11	3:C:609:ARG:HD2	1.86	0.40
3:C:1257:LYS:O	3:C:1261:GLU:HG2	2.20	0.40
9:I:371:TYR:HA	9:I:374:LYS:NZ	2.37	0.40
16:R:121:TYR:CE2	16:R:166:LYS:HB2	2.57	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	724/855 (85%)	693 (96%)	29 (4%)	2 (0%)	37	66
2	B	829/1008 (82%)	789 (95%)	38 (5%)	2 (0%)	44	71
3	C	911/1320 (69%)	888 (98%)	23 (2%)	0	100	100
4	D	775/2294 (34%)	712 (92%)	63 (8%)	0	100	100
5	E	494/946 (52%)	473 (96%)	21 (4%)	0	100	100
6	F	476/876 (54%)	462 (97%)	14 (3%)	0	100	100
7	G	283/396 (72%)	275 (97%)	8 (3%)	0	100	100
8	H	52/348 (15%)	48 (92%)	4 (8%)	0	100	100
9	I	315/403 (78%)	312 (99%)	3 (1%)	0	100	100
9	J	315/403 (78%)	312 (99%)	3 (1%)	0	100	100
10	K	65/80 (81%)	60 (92%)	5 (8%)	0	100	100
11	L	12/18 (67%)	11 (92%)	1 (8%)	0	100	100
12	M	8/11 (73%)	6 (75%)	2 (25%)	0	100	100
13	N	17/37 (46%)	15 (88%)	2 (12%)	0	100	100
14	O	15/17 (88%)	10 (67%)	5 (33%)	0	100	100
16	R	265/328 (81%)	255 (96%)	10 (4%)	0	100	100
All	All	5556/9340 (60%)	5321 (96%)	231 (4%)	4 (0%)	50	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	PRO
2	B	477	ASN
2	B	478	PHE
1	A	812	ILE

### 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	628/744 (84%)	626 (100%)	2 (0%)	91	94
2	B	730/872 (84%)	729 (100%)	1 (0%)	92	96
3	C	817/1177 (69%)	814 (100%)	3 (0%)	89	93
4	D	753/2151 (35%)	751 (100%)	2 (0%)	91	94
5	E	423/817 (52%)	423 (100%)	0	100	100
6	F	399/757 (53%)	399 (100%)	0	100	100
7	G	246/347 (71%)	246 (100%)	0	100	100
8	H	46/287 (16%)	46 (100%)	0	100	100
9	I	261/332 (79%)	261 (100%)	0	100	100
9	J	261/332 (79%)	261 (100%)	0	100	100
10	K	62/73 (85%)	62 (100%)	0	100	100
11	L	12/12 (100%)	12 (100%)	0	100	100
12	M	9/9 (100%)	9 (100%)	0	100	100
13	N	16/16 (100%)	15 (94%)	1 (6%)	15	41
14	O	14/15 (93%)	14 (100%)	0	100	100
16	R	236/286 (82%)	235 (100%)	1 (0%)	89	93
All	All	4913/8227 (60%)	4903 (100%)	10 (0%)	91	95

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

Mol	Chain	Res	Type
1	A	582	LEU
1	A	781	HIS
2	B	990	LYS
3	C	417	LEU
3	C	845	VAL
3	C	949	VAL
4	D	1560	SER
4	D	1852	MET

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Mol	Chain	Res	Type
13	N	34	ASN
16	R	177	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	ASN
1	A	337	ASN
1	A	517	GLN
1	A	533	ASN
1	A	570	GLN
1	A	692	ASN
2	B	120	HIS
2	B	262	ASN
2	B	467	ASN
2	B	517	GLN
2	B	711	ASN
2	B	727	GLN
3	C	326	ASN
3	C	398	GLN
3	C	402	GLN
3	C	805	ASN
3	C	1065	ASN
3	C	1178	ASN
3	C	1189	GLN
3	C	1225	HIS
3	C	1270	HIS
4	D	133	ASN
4	D	1380	GLN
4	D	1558	HIS
4	D	1609	GLN
4	D	2055	GLN
4	D	2206	GLN
4	D	2251	ASN
5	E	443	GLN
5	E	649	GLN
5	E	736	GLN
5	E	800	ASN
5	E	915	ASN
6	F	496	GLN
6	F	501	ASN
6	F	535	GLN

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Mol	Chain	Res	Type
6	F	726	HIS
9	I	134	GLN
9	I	200	ASN
9	I	355	ASN
9	J	112	HIS
9	J	200	ASN
9	J	275	ASN
9	J	395	ASN
10	K	39	HIS
16	R	187	GLN
16	R	298	ASN
16	R	322	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	PX2	G	401	-	24,24,35	1.97	7 (29%)	28,29,40	2.65	14 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	PX2	G	401	-	-	9/26/26/37	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	401	PX2	O5-C4	4.56	1.46	1.33
18	G	401	PX2	O7-C2	-4.23	1.36	1.46
18	G	401	PX2	O8-C16	-4.10	1.10	1.22
18	G	401	PX2	P1-O3	-3.07	1.43	1.54
18	G	401	PX2	O6-C4	-2.74	1.14	1.22
18	G	401	PX2	C17-C16	-2.26	1.44	1.50
18	G	401	PX2	P1-O1	-2.22	1.46	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	401	PX2	O7-C16-C17	4.70	121.64	111.50
18	G	401	PX2	C19-C18-C17	-4.59	96.67	113.19
18	G	401	PX2	O5-C4-C5	4.57	126.25	111.91
18	G	401	PX2	C3-O5-C4	4.02	132.02	117.12
18	G	401	PX2	O1-P1-O4	-3.73	96.82	106.73
18	G	401	PX2	O7-C16-O8	-3.67	114.84	123.70
18	G	401	PX2	O5-C4-O6	-3.64	114.41	123.59
18	G	401	PX2	O7-C2-C3	-3.60	95.35	108.40
18	G	401	PX2	O4-P1-O2	3.38	115.94	106.47
18	G	401	PX2	C8-C7-C6	-2.88	99.80	114.42
18	G	401	PX2	C7-C6-C5	-2.67	103.58	113.19
18	G	401	PX2	C2-O7-C16	2.65	124.31	117.79
18	G	401	PX2	P1-O4-C1	2.48	125.12	118.30
18	G	401	PX2	O1-P1-O2	2.37	119.97	110.68

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	G	401	PX2	C1-O4-P1-O1
18	G	401	PX2	C1-O4-P1-O2

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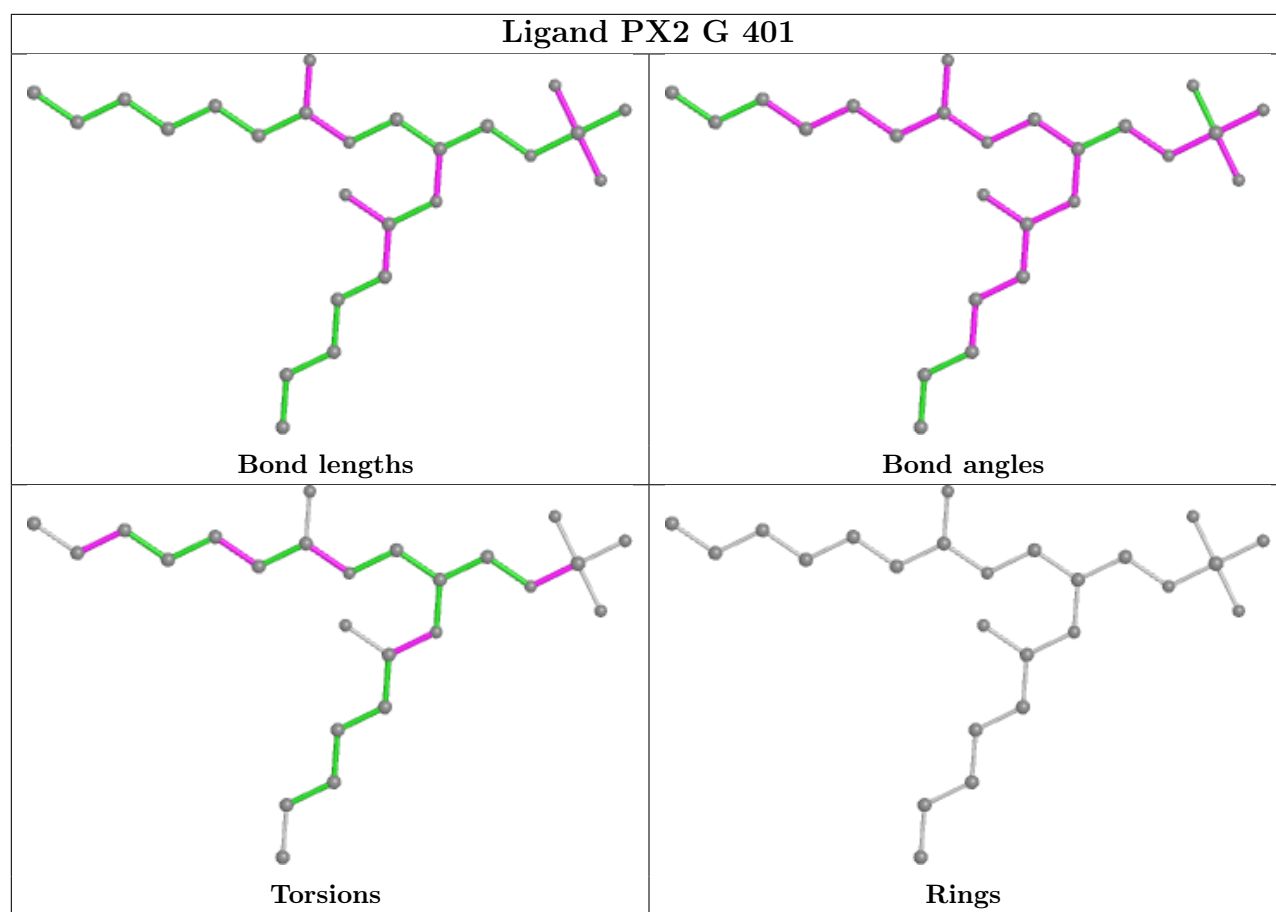
Mol	Chain	Res	Type	Atoms
18	G	401	PX2	C1-O4-P1-O3
18	G	401	PX2	C4-C5-C6-C7
18	G	401	PX2	O8-C16-O7-C2
18	G	401	PX2	C17-C16-O7-C2
18	G	401	PX2	C7-C8-C9-C10
18	G	401	PX2	O6-C4-O5-C3
18	G	401	PX2	C5-C4-O5-C3

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	G	401	PX2	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

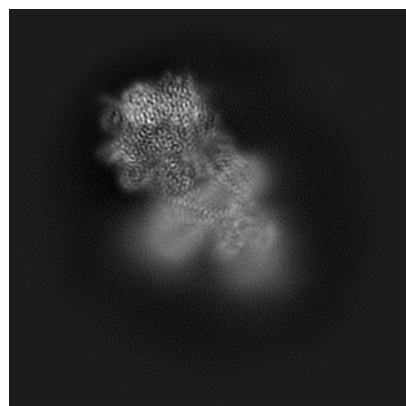
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38428. These allow visual inspection of the internal detail of the map and identification of artifacts.

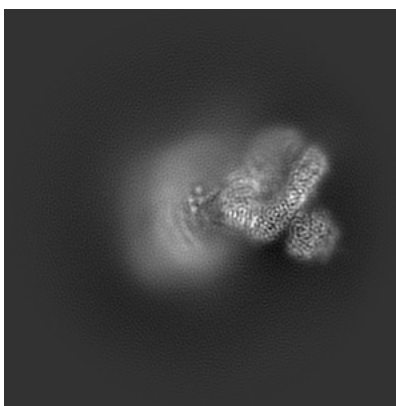
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

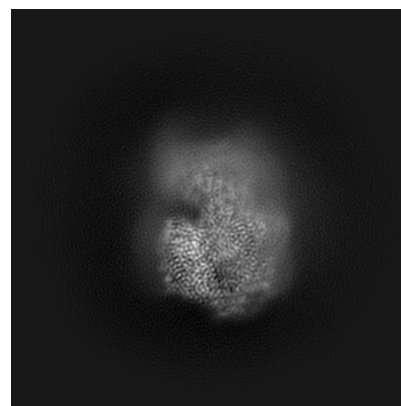
#### 6.1.1 Primary map



X

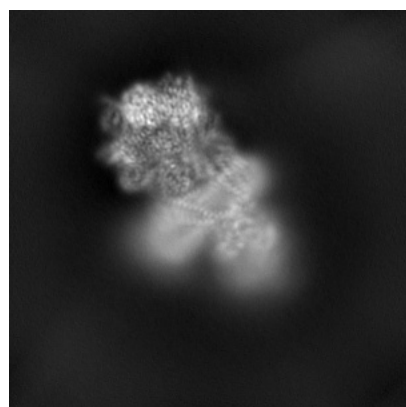


Y

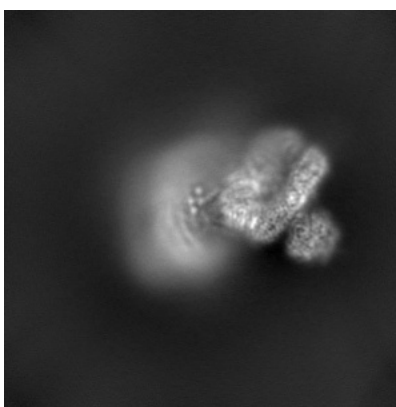


Z

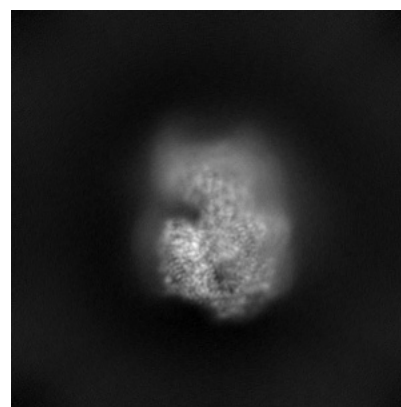
#### 6.1.2 Raw map



X



Y

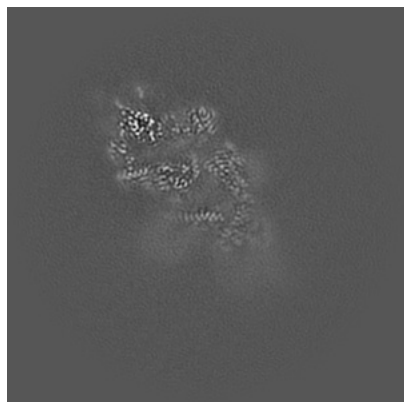


Z

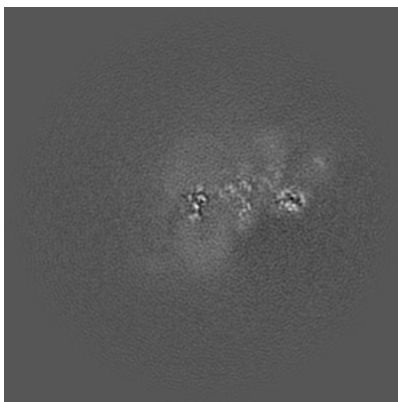
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

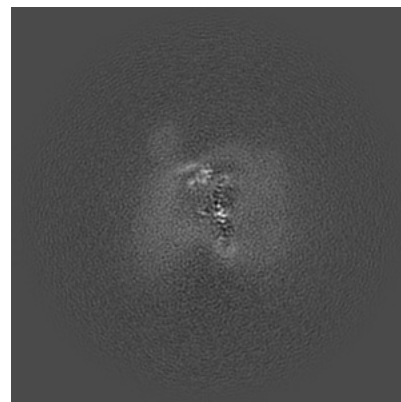
### 6.2.1 Primary map



X Index: 180

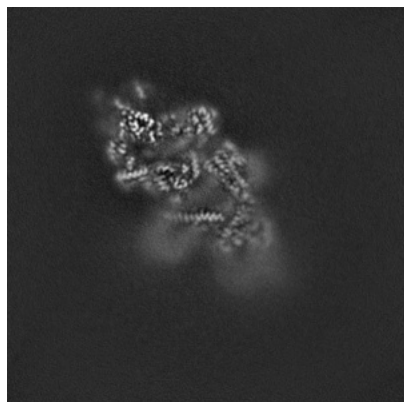


Y Index: 180

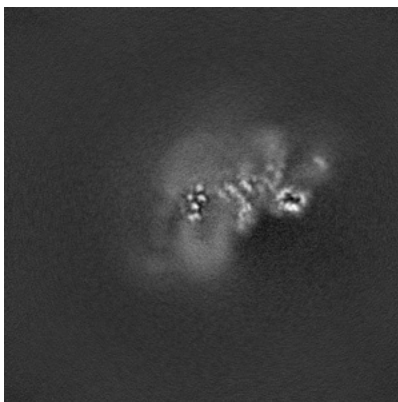


Z Index: 180

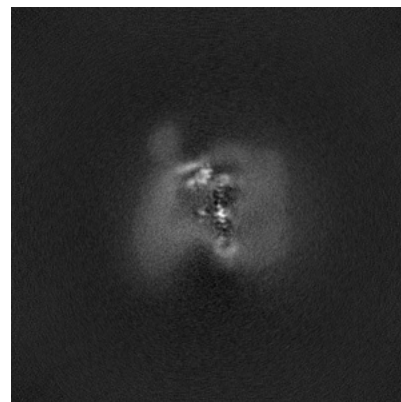
### 6.2.2 Raw map



X Index: 180



Y Index: 180

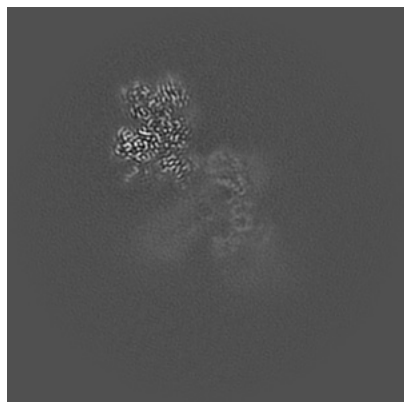


Z Index: 180

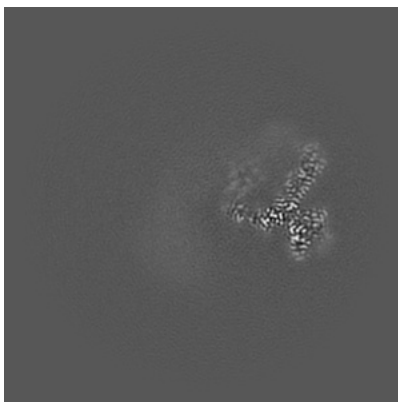
The images above show central slices of the map in three orthogonal directions.

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

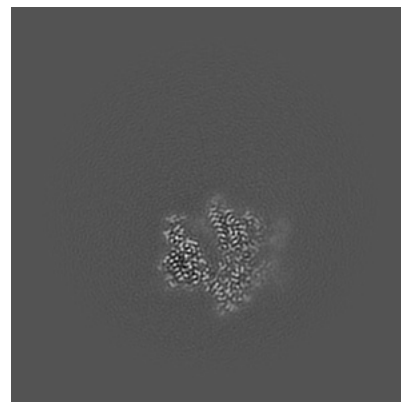
### 6.3.1 Primary map



X Index: 167

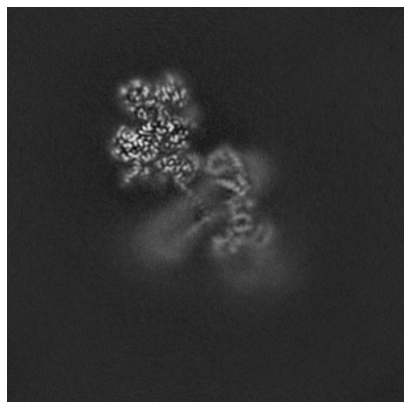


Y Index: 125

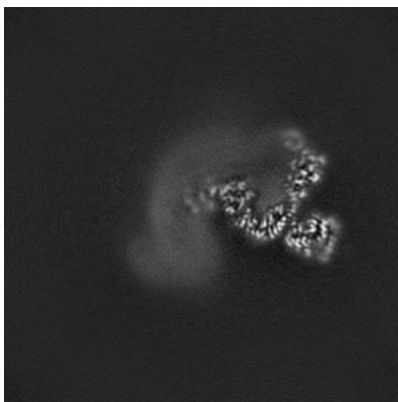


Z Index: 266

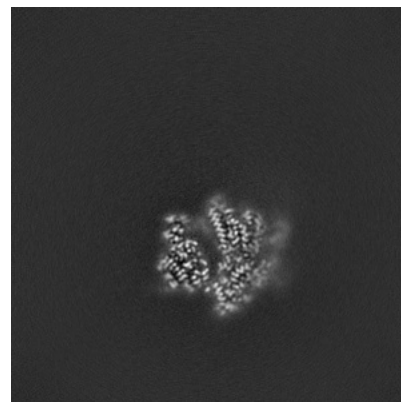
### 6.3.2 Raw map



X Index: 168



Y Index: 149

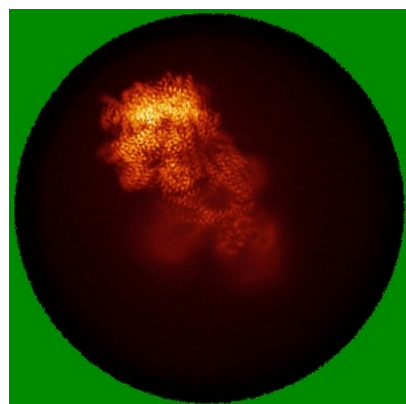


Z Index: 267

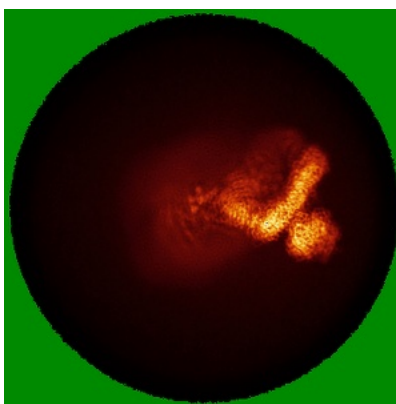
The images above show the largest variance slices of the map in three orthogonal directions.

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

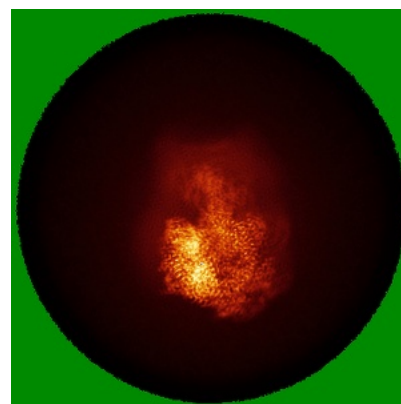
### 6.4.1 Primary map



X

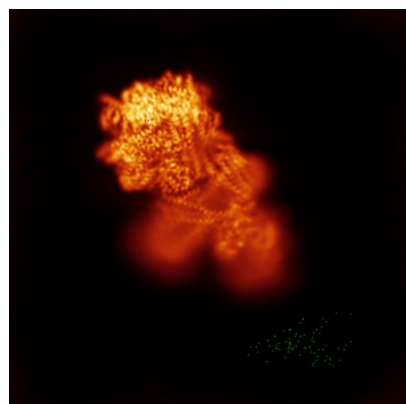


Y

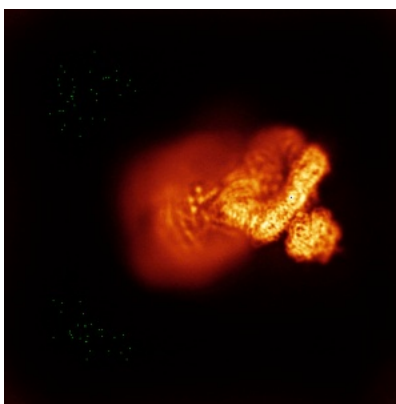


Z

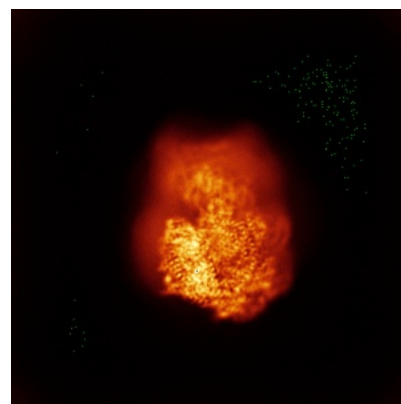
### 6.4.2 Raw map



X



Y

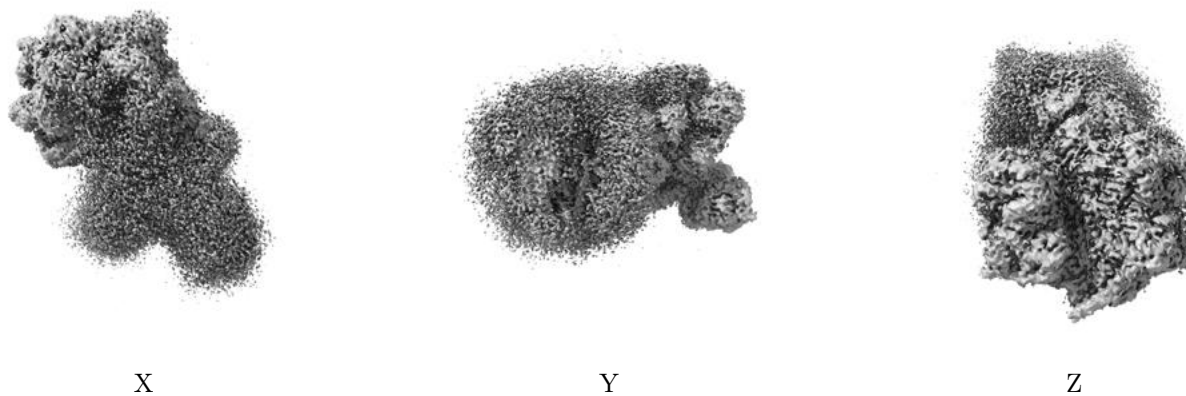


Z

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.

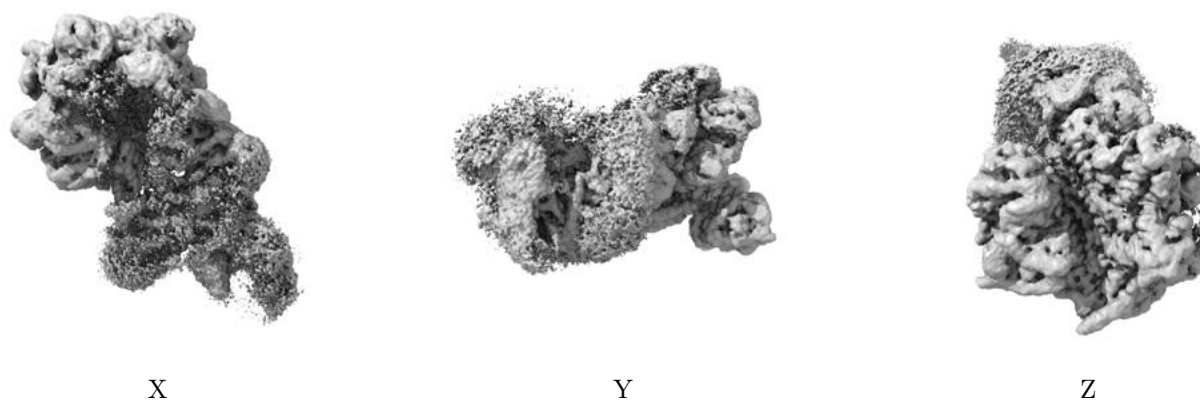
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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



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.

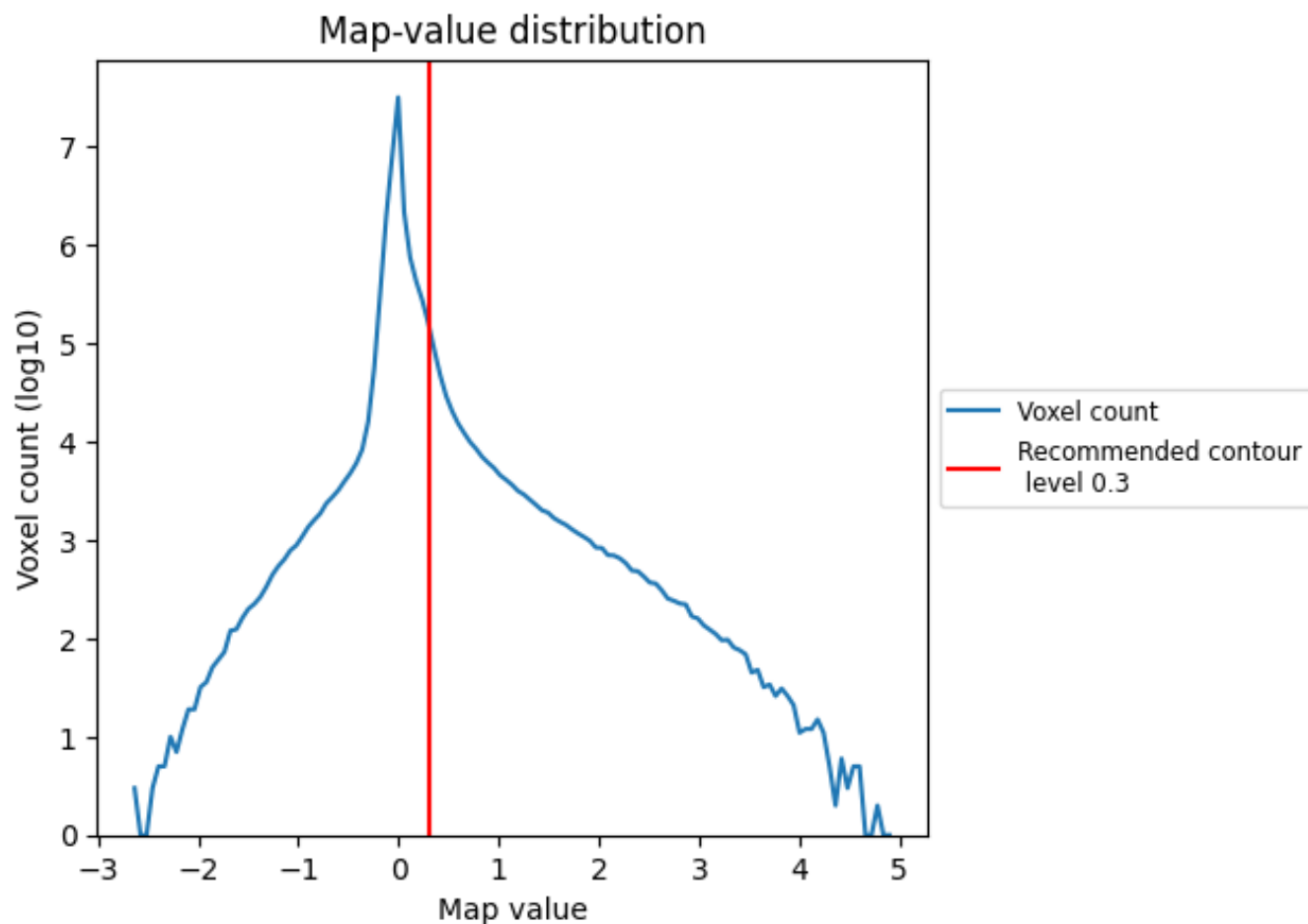
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

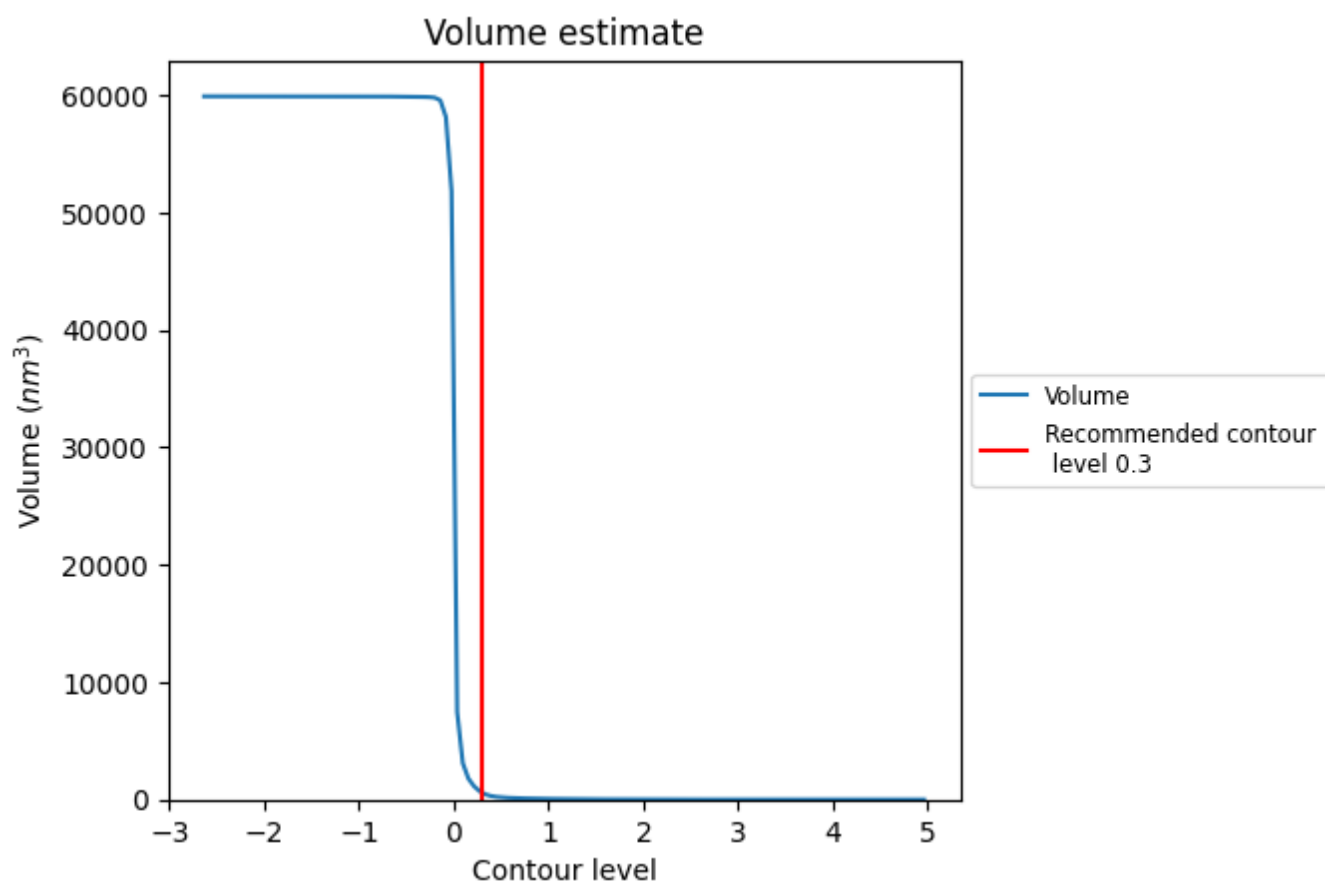
This section contains the results of statistical analysis of the map.

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



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

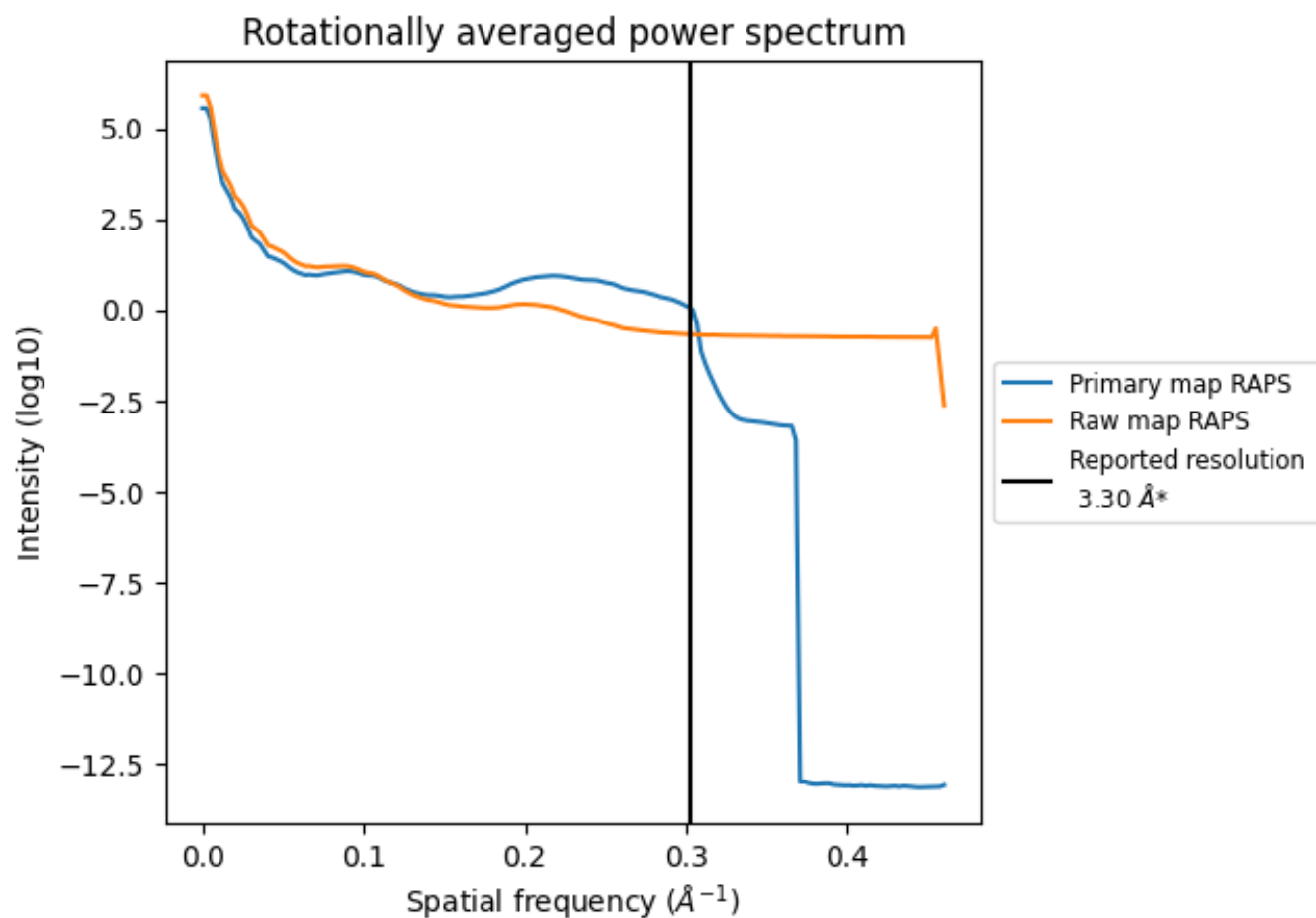
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 591 nm<sup>3</sup>; this corresponds to an approximate mass of 534 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 ⓘ

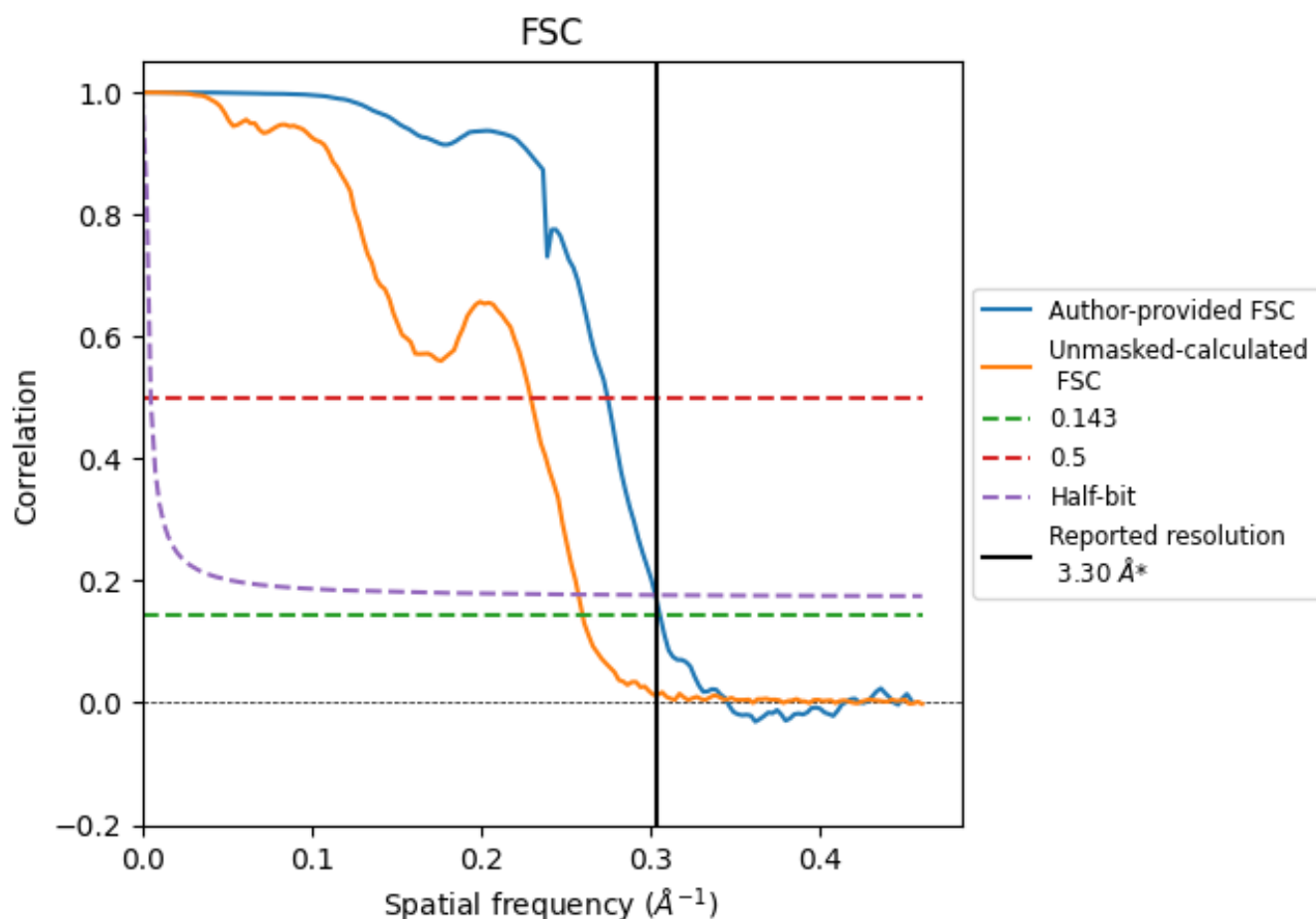


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

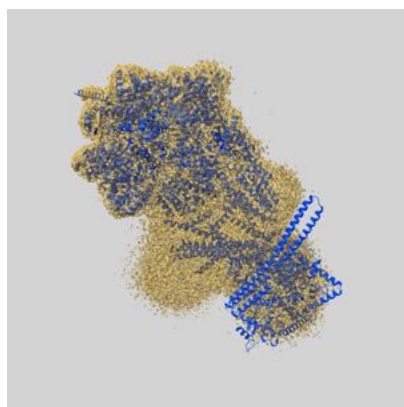
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.64	3.30
Unmasked-calculated*	3.85	4.36	3.89

\*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 3.85 differs from the reported value 3.3 by more than 10 %

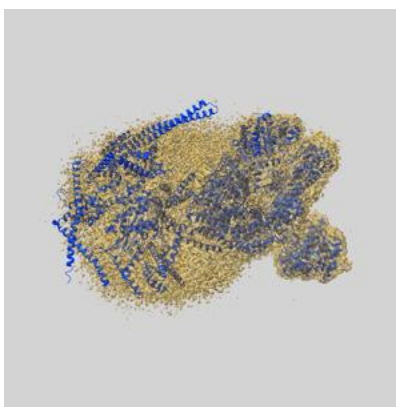
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38428 and PDB model 8XKV. Per-residue inclusion information can be found in section [3](#) on page [8](#).

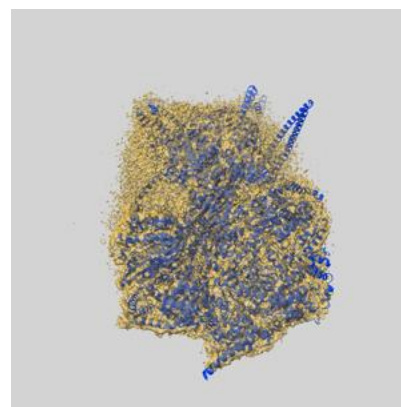
### 9.1 Map-model overlay [i](#)



X



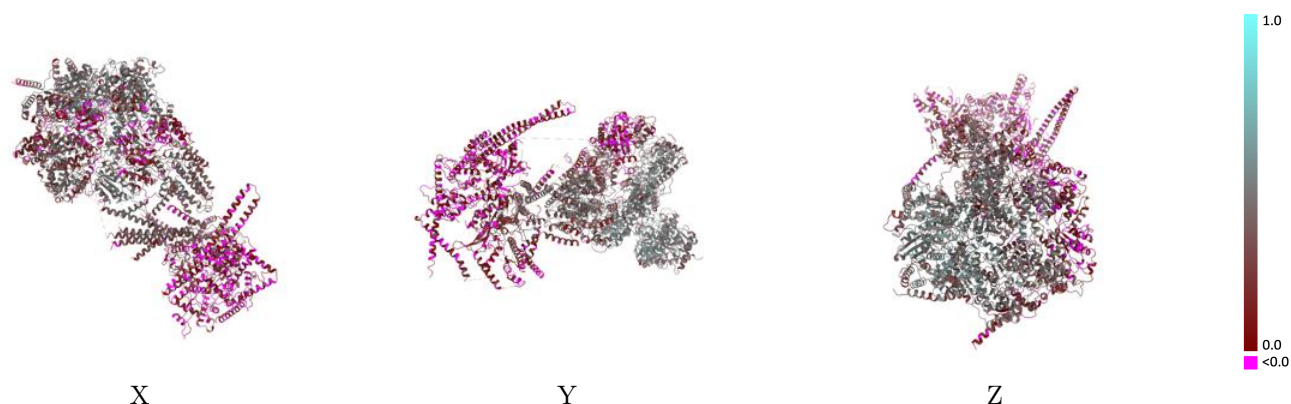
Y



Z

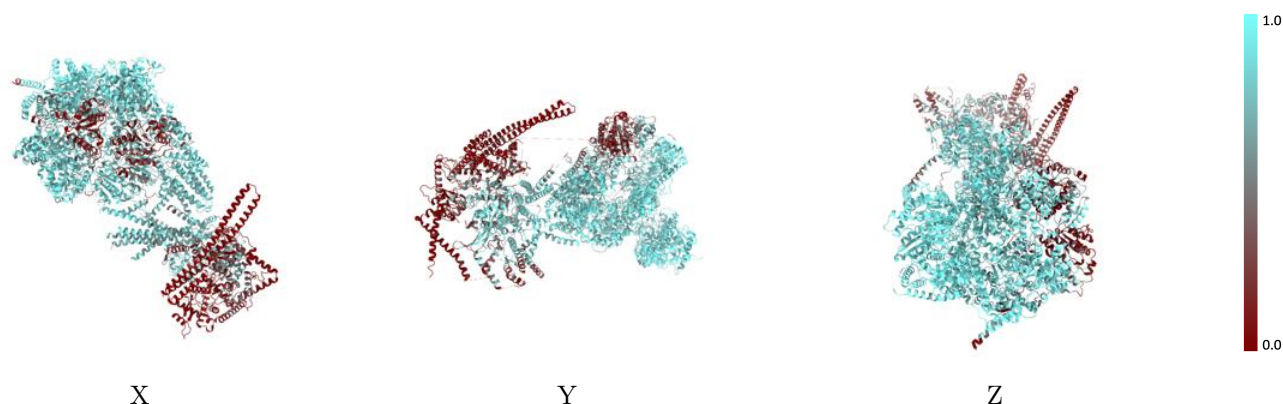
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



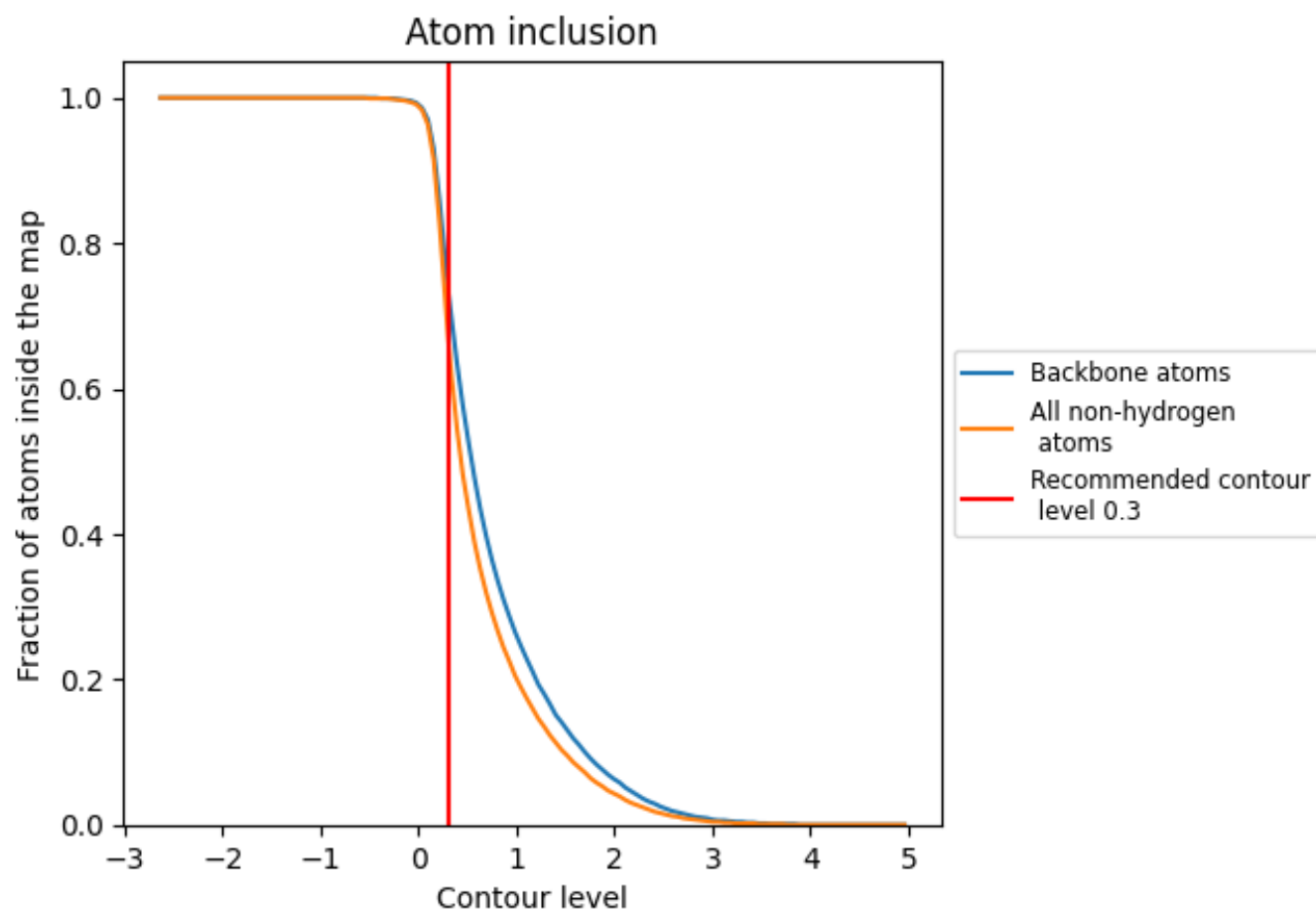
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).





































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 74% of all backbone atoms, 67% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6720	 0.2920
A	 0.7950	 0.3270
B	 0.7310	 0.3420
C	 0.3880	 0.1760
D	 0.7380	 0.3150
E	 0.5840	 0.2760
F	 0.7820	 0.3230
G	 0.8130	 0.3060
H	 0.8190	 0.3520
I	 0.9110	 0.4420
J	 0.9300	 0.4600
K	 0.1660	 0.0530
L	 0.0530	 -0.0090
M	 0.3610	 0.0180
N	 0.2510	 0.0370
O	 0.4230	 0.1250
P	 0.0530	 0.0960
R	 0.4310	 0.1050

