



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:52 PM UTC

PDB ID : 8OVG / pdb_00008ovg
EMDB ID : EMD-17214
Title : Human Mitochondrial Lon Y186E Mutant ADP Bound
Authors : Kereiche, S.; Bauer, J.A.; Matyas, P.; Novacek, J.; Kutejova, E.
Deposited on : 2023-04-26
Resolution : 8.47 Å(reported)
Based on initial model : 7NFY

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

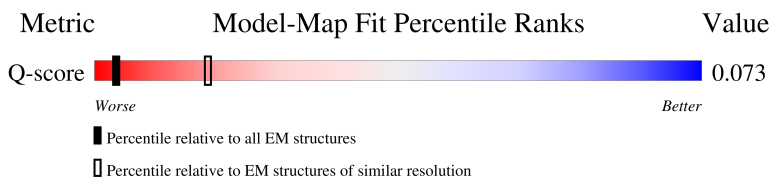
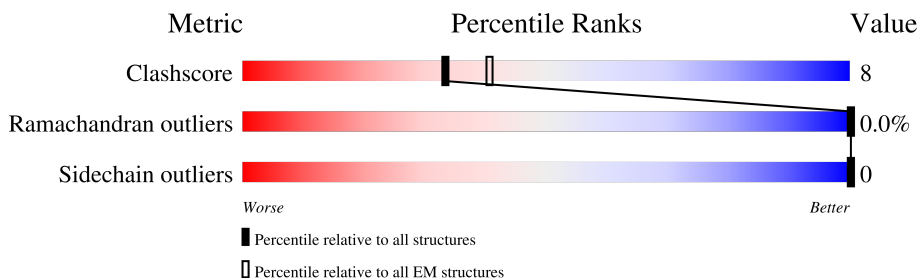
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.47 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	276 (7.99 - 8.96)

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

Mol	Chain	Length	Quality of chain
1	A	869	30% 73% 16% 11%
1	B	869	25% 72% 17% 11%
1	C	869	22% 72% 17% 11%
1	D	869	23% 73% 16% 11%

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Mol	Chain	Length	Quality of chain
1	E	869	23% 75% 14% 11%
1	F	869	75% 71% 18% 11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 74676 atoms, of which 37758 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 Lon protease homolog, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	777	Total	C	H	N	O	S	0	0
			12446	3903	6293	1067	1156	27		
1	B	777	Total	C	H	N	O	S	0	0
			12446	3903	6293	1067	1156	27		
1	C	777	Total	C	H	N	O	S	0	0
			12446	3903	6293	1067	1156	27		
1	D	777	Total	C	H	N	O	S	0	0
			12446	3903	6293	1067	1156	27		
1	E	777	Total	C	H	N	O	S	0	0
			12446	3903	6293	1067	1156	27		
1	F	777	Total	C	H	N	O	S	0	0
			12446	3903	6293	1067	1156	27		

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	MET	-	initiating methionine	UNP P36776
A	92	GLY	-	expression tag	UNP P36776
A	93	HIS	-	expression tag	UNP P36776
A	94	HIS	-	expression tag	UNP P36776
A	95	HIS	-	expression tag	UNP P36776
A	96	HIS	-	expression tag	UNP P36776
A	97	HIS	-	expression tag	UNP P36776
A	98	HIS	-	expression tag	UNP P36776
A	99	ASP	-	expression tag	UNP P36776
A	100	TYR	-	expression tag	UNP P36776
A	101	ASP	-	expression tag	UNP P36776
A	102	ILE	-	expression tag	UNP P36776
A	103	PRO	-	expression tag	UNP P36776
A	104	THR	-	expression tag	UNP P36776
A	105	THR	-	expression tag	UNP P36776
A	106	GLU	-	expression tag	UNP P36776
A	107	ASN	-	expression tag	UNP P36776
A	108	LEU	-	expression tag	UNP P36776

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Chain	Residue	Modelled	Actual	Comment	Reference
A	109	TYR	-	expression tag	UNP P36776
A	110	PHE	-	expression tag	UNP P36776
A	111	GLN	-	expression tag	UNP P36776
A	112	GLY	-	expression tag	UNP P36776
A	113	ALA	-	expression tag	UNP P36776
A	114	HIS	-	expression tag	UNP P36776
A	186	1PA	TYR	conflict	UNP P36776
B	91	MET	-	initiating methionine	UNP P36776
B	92	GLY	-	expression tag	UNP P36776
B	93	HIS	-	expression tag	UNP P36776
B	94	HIS	-	expression tag	UNP P36776
B	95	HIS	-	expression tag	UNP P36776
B	96	HIS	-	expression tag	UNP P36776
B	97	HIS	-	expression tag	UNP P36776
B	98	HIS	-	expression tag	UNP P36776
B	99	ASP	-	expression tag	UNP P36776
B	100	TYR	-	expression tag	UNP P36776
B	101	ASP	-	expression tag	UNP P36776
B	102	ILE	-	expression tag	UNP P36776
B	103	PRO	-	expression tag	UNP P36776
B	104	THR	-	expression tag	UNP P36776
B	105	THR	-	expression tag	UNP P36776
B	106	GLU	-	expression tag	UNP P36776
B	107	ASN	-	expression tag	UNP P36776
B	108	LEU	-	expression tag	UNP P36776
B	109	TYR	-	expression tag	UNP P36776
B	110	PHE	-	expression tag	UNP P36776
B	111	GLN	-	expression tag	UNP P36776
B	112	GLY	-	expression tag	UNP P36776
B	113	ALA	-	expression tag	UNP P36776
B	114	HIS	-	expression tag	UNP P36776
B	186	1PA	TYR	conflict	UNP P36776
C	91	MET	-	initiating methionine	UNP P36776
C	92	GLY	-	expression tag	UNP P36776
C	93	HIS	-	expression tag	UNP P36776
C	94	HIS	-	expression tag	UNP P36776
C	95	HIS	-	expression tag	UNP P36776
C	96	HIS	-	expression tag	UNP P36776
C	97	HIS	-	expression tag	UNP P36776
C	98	HIS	-	expression tag	UNP P36776
C	99	ASP	-	expression tag	UNP P36776
C	100	TYR	-	expression tag	UNP P36776

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Chain	Residue	Modelled	Actual	Comment	Reference
C	101	ASP	-	expression tag	UNP P36776
C	102	ILE	-	expression tag	UNP P36776
C	103	PRO	-	expression tag	UNP P36776
C	104	THR	-	expression tag	UNP P36776
C	105	THR	-	expression tag	UNP P36776
C	106	GLU	-	expression tag	UNP P36776
C	107	ASN	-	expression tag	UNP P36776
C	108	LEU	-	expression tag	UNP P36776
C	109	TYR	-	expression tag	UNP P36776
C	110	PHE	-	expression tag	UNP P36776
C	111	GLN	-	expression tag	UNP P36776
C	112	GLY	-	expression tag	UNP P36776
C	113	ALA	-	expression tag	UNP P36776
C	114	HIS	-	expression tag	UNP P36776
C	186	1PA	TYR	conflict	UNP P36776
D	91	MET	-	initiating methionine	UNP P36776
D	92	GLY	-	expression tag	UNP P36776
D	93	HIS	-	expression tag	UNP P36776
D	94	HIS	-	expression tag	UNP P36776
D	95	HIS	-	expression tag	UNP P36776
D	96	HIS	-	expression tag	UNP P36776
D	97	HIS	-	expression tag	UNP P36776
D	98	HIS	-	expression tag	UNP P36776
D	99	ASP	-	expression tag	UNP P36776
D	100	TYR	-	expression tag	UNP P36776
D	101	ASP	-	expression tag	UNP P36776
D	102	ILE	-	expression tag	UNP P36776
D	103	PRO	-	expression tag	UNP P36776
D	104	THR	-	expression tag	UNP P36776
D	105	THR	-	expression tag	UNP P36776
D	106	GLU	-	expression tag	UNP P36776
D	107	ASN	-	expression tag	UNP P36776
D	108	LEU	-	expression tag	UNP P36776
D	109	TYR	-	expression tag	UNP P36776
D	110	PHE	-	expression tag	UNP P36776
D	111	GLN	-	expression tag	UNP P36776
D	112	GLY	-	expression tag	UNP P36776
D	113	ALA	-	expression tag	UNP P36776
D	114	HIS	-	expression tag	UNP P36776
D	186	1PA	TYR	conflict	UNP P36776
E	91	MET	-	initiating methionine	UNP P36776
E	92	GLY	-	expression tag	UNP P36776

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Chain	Residue	Modelled	Actual	Comment	Reference
E	93	HIS	-	expression tag	UNP P36776
E	94	HIS	-	expression tag	UNP P36776
E	95	HIS	-	expression tag	UNP P36776
E	96	HIS	-	expression tag	UNP P36776
E	97	HIS	-	expression tag	UNP P36776
E	98	HIS	-	expression tag	UNP P36776
E	99	ASP	-	expression tag	UNP P36776
E	100	TYR	-	expression tag	UNP P36776
E	101	ASP	-	expression tag	UNP P36776
E	102	ILE	-	expression tag	UNP P36776
E	103	PRO	-	expression tag	UNP P36776
E	104	THR	-	expression tag	UNP P36776
E	105	THR	-	expression tag	UNP P36776
E	106	GLU	-	expression tag	UNP P36776
E	107	ASN	-	expression tag	UNP P36776
E	108	LEU	-	expression tag	UNP P36776
E	109	TYR	-	expression tag	UNP P36776
E	110	PHE	-	expression tag	UNP P36776
E	111	GLN	-	expression tag	UNP P36776
E	112	GLY	-	expression tag	UNP P36776
E	113	ALA	-	expression tag	UNP P36776
E	114	HIS	-	expression tag	UNP P36776
E	186	1PA	TYR	conflict	UNP P36776
F	91	MET	-	initiating methionine	UNP P36776
F	92	GLY	-	expression tag	UNP P36776
F	93	HIS	-	expression tag	UNP P36776
F	94	HIS	-	expression tag	UNP P36776
F	95	HIS	-	expression tag	UNP P36776
F	96	HIS	-	expression tag	UNP P36776
F	97	HIS	-	expression tag	UNP P36776
F	98	HIS	-	expression tag	UNP P36776
F	99	ASP	-	expression tag	UNP P36776
F	100	TYR	-	expression tag	UNP P36776
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F	102	ILE	-	expression tag	UNP P36776
F	103	PRO	-	expression tag	UNP P36776
F	104	THR	-	expression tag	UNP P36776
F	105	THR	-	expression tag	UNP P36776
F	106	GLU	-	expression tag	UNP P36776
F	107	ASN	-	expression tag	UNP P36776
F	108	LEU	-	expression tag	UNP P36776
F	109	TYR	-	expression tag	UNP P36776

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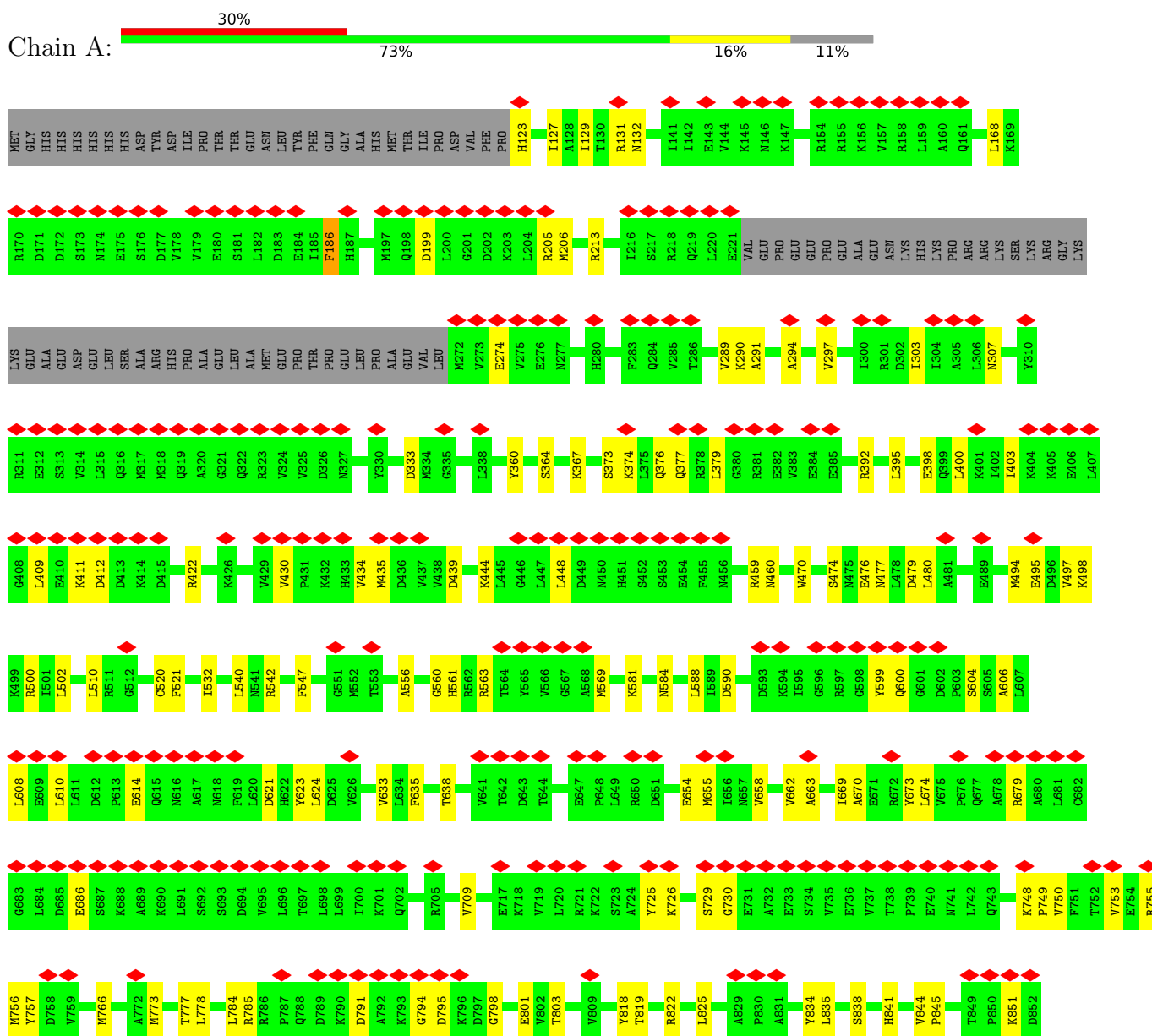
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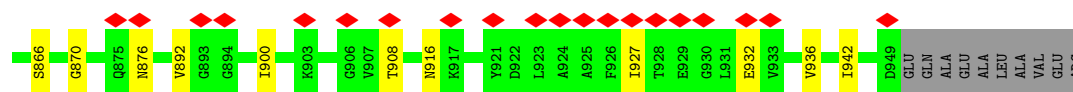
Chain	Residue	Modelled	Actual	Comment	Reference
F	110	PHE	-	expression tag	UNP P36776
F	111	GLN	-	expression tag	UNP P36776
F	112	GLY	-	expression tag	UNP P36776
F	113	ALA	-	expression tag	UNP P36776
F	114	HIS	-	expression tag	UNP P36776
F	186	1PA	TYR	conflict	UNP P36776

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: Lon protease homolog, mitochondrial



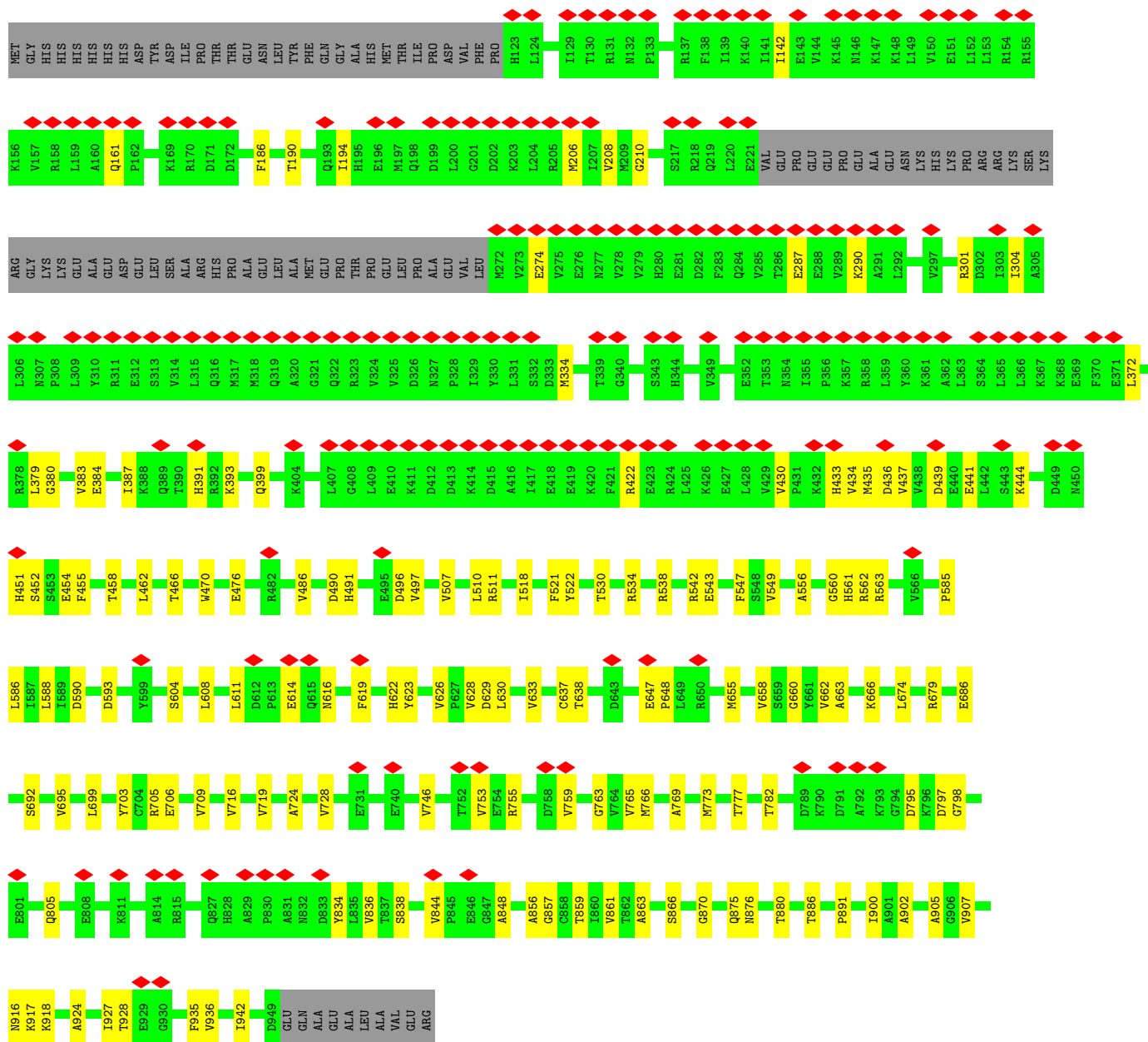


- Molecule 1: Lon protease homolog, mitochondrial

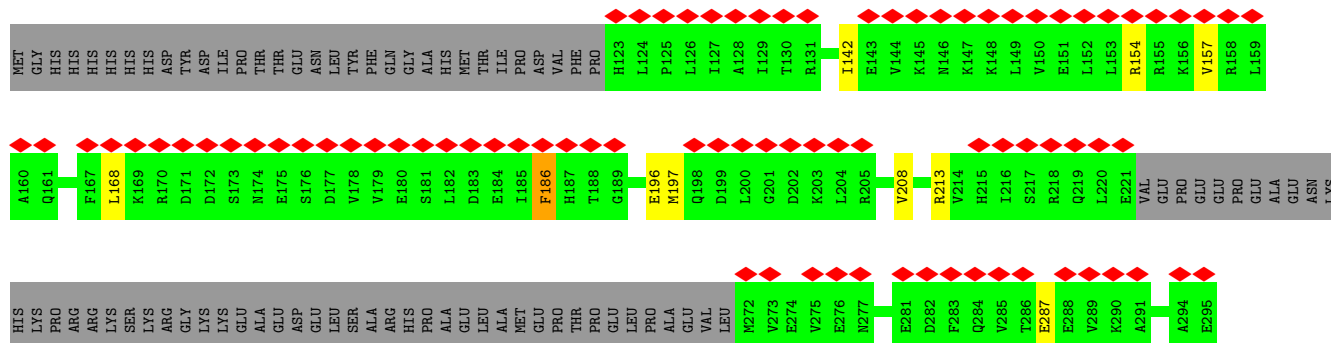
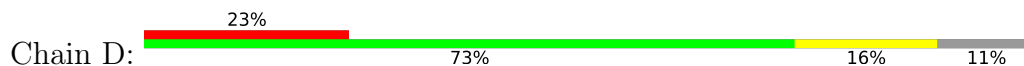


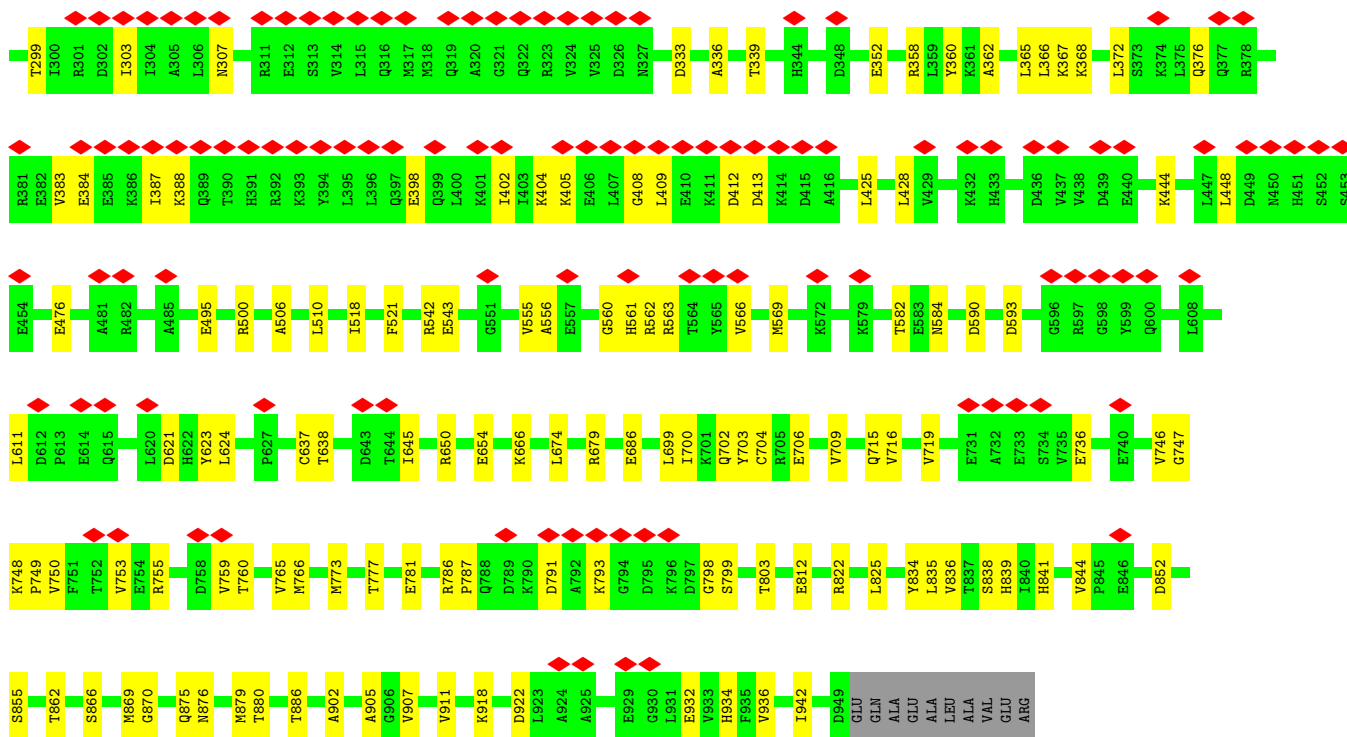
- Molecule 1: Lon protease homolog, mitochondrial



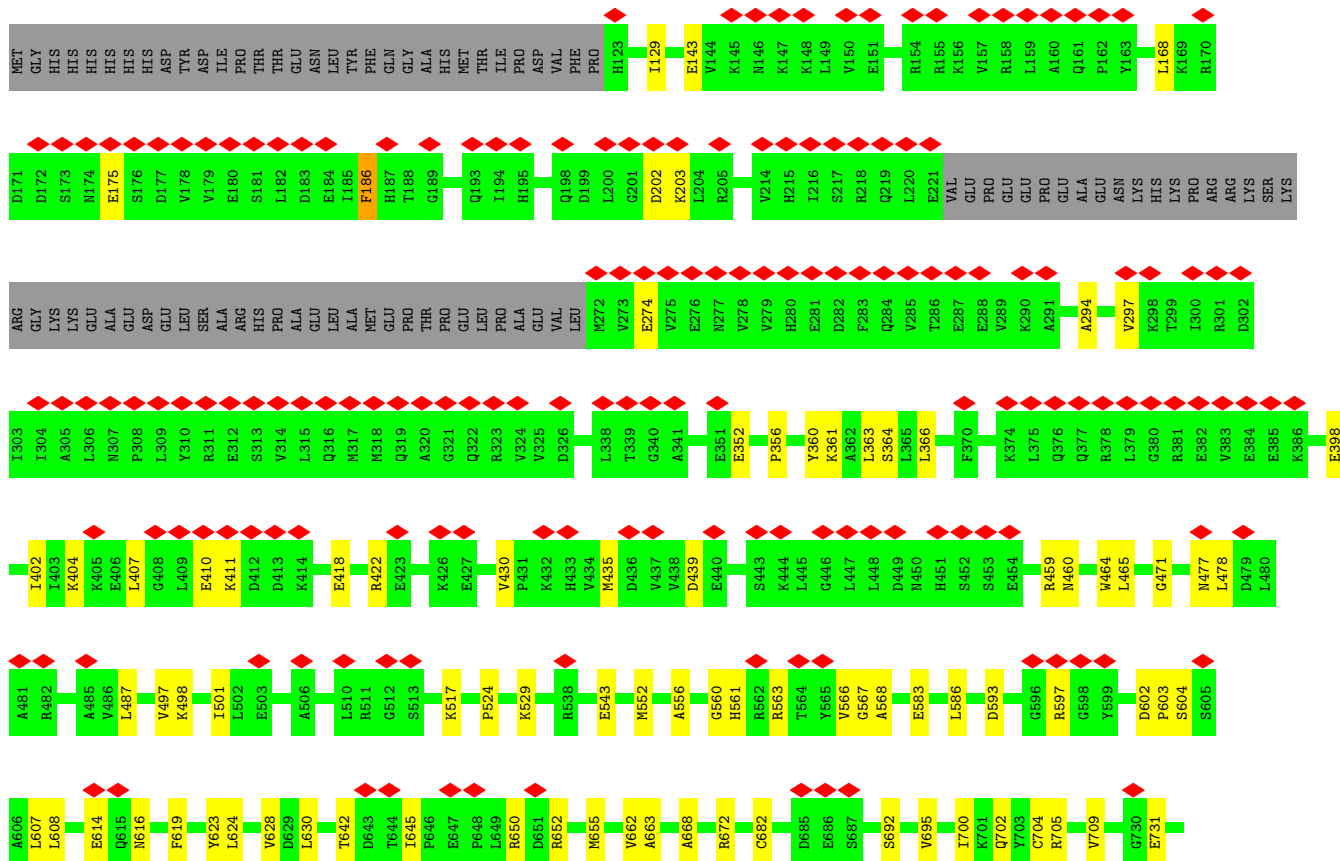
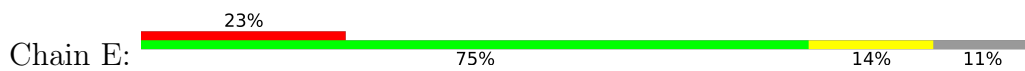


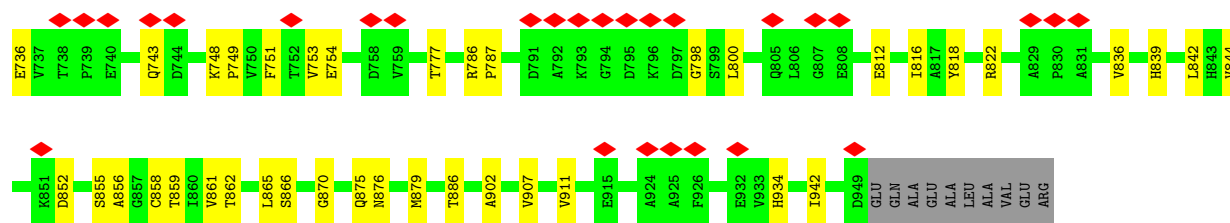
● Molecule 1: Lon protease homolog, mitochondrial



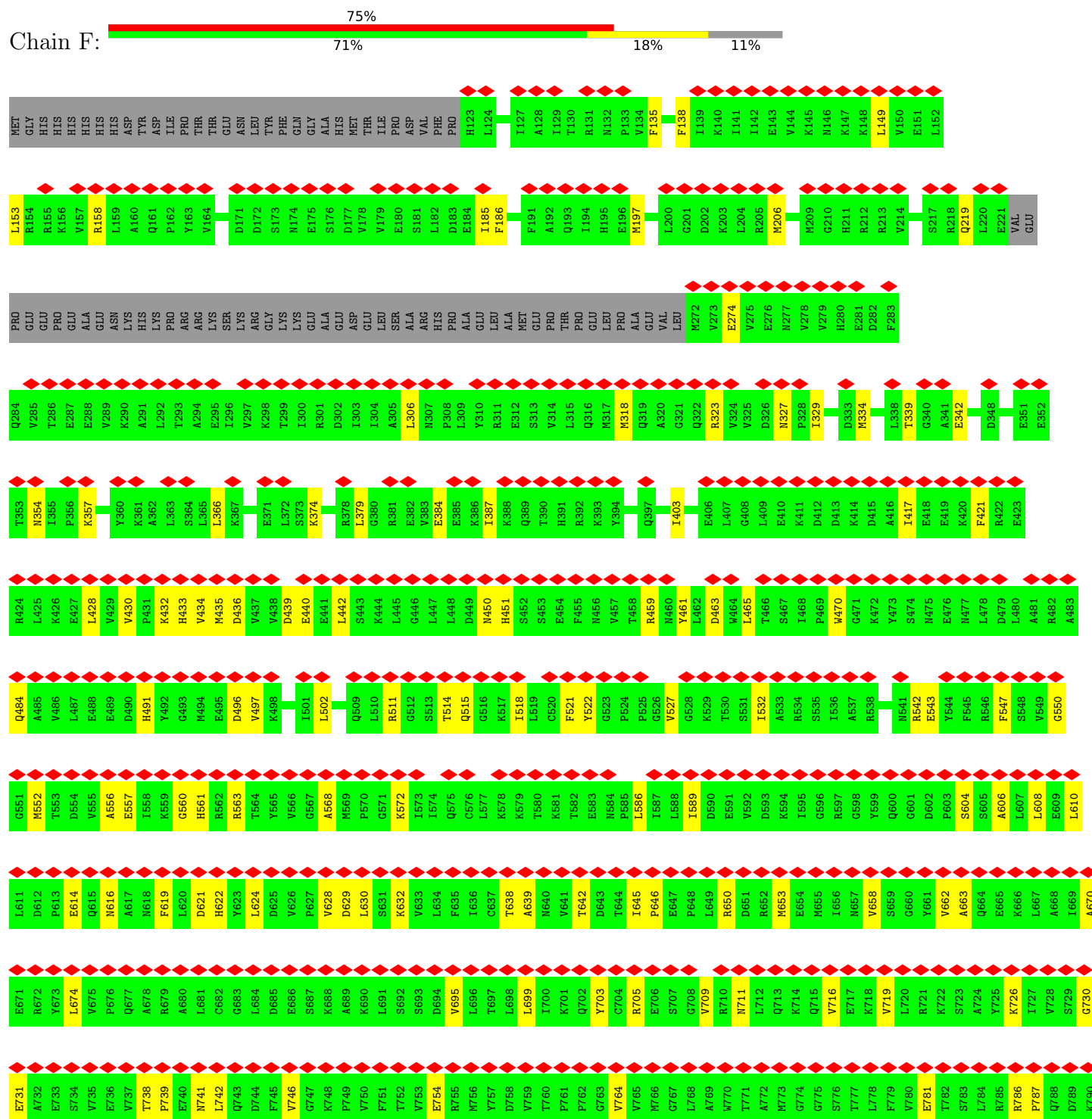


- Molecule 1: Lon protease homolog, mitochondrial





- Molecule 1: Lon protease homolog, mitochondrial



D791	A792	K793	G794	D795	K796	D797	G798	S799	L800	E801	V802	T803	G804	Q805	L806	G807	E808	V809	M810	K811	E812	S813	A814	R815	I816	A817	F820	A821	R822	A823	F824	L825	M826	Q827	H828	A829	P830	A831	N832	D833	Y834	L835	V836	T837	S838	H839	I840	H841	L842	H843	V844	P845	E846	G847	A848	T849	P850	K851																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
D852	G853	P854	S855	A856	G857	C858	T859	I860	V861	T862	A863	L864	L865	S866	L867	A868	M869	G870	R871	P872	V873	R874	Q875	N876	L877	A878	M879	T880	G881	E882	L885	T886	G887	K888	I889	L890	P891	V892	G893	G894	I895	K896	E897	K898	T899	I900	A901	A902	K903	R904	A905	G906	V907	T908	C909	I910	V911	L912																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
P913	A914	E915	N916	K917	K918	D919	F920	Y921	D922	L923	A924	A925	F926	I927	T928	E929	G930	L931	E932	V933	H934	F935	V936	E937	H938	Y939	R940	E941	I942	F943	D944	I945	A946	F947	P948	D949	GLU	GLN	ALA	GLU	ALA	LEU	ALA	VAL	GLU	ARG																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23915	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.509	Depositor
Minimum map value	-2.917	Depositor
Average map value	-0.007	Depositor
Map value standard deviation	0.210	Depositor
Recommended contour level	1.684	Depositor
Map size ($\text{\AA}$)	512.4, 512.4, 512.4	wwPDB
Map dimensions	210, 210, 210	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.44, 2.44, 2.44	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1PA

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	0.11	0/6238	0.29	0/8419
1	B	0.11	0/6238	0.28	0/8419
1	C	0.11	0/6238	0.29	0/8419
1	D	0.12	0/6238	0.28	0/8419
1	E	0.11	0/6238	0.28	0/8419
1	F	0.11	0/6238	0.28	0/8419
All	All	0.11	0/37428	0.28	0/50514

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6153	6293	6291	119	0
1	B	6153	6293	6291	110	0
1	C	6153	6293	6291	122	0
1	D	6153	6293	6291	112	0
1	E	6153	6293	6291	93	0
1	F	6153	6293	6291	124	0
All	All	36918	37758	37746	617	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 (617) 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:C:679:ARG:NH1	1:C:686:GLU:OE1	2.09	0.86
1:C:666:LYS:NZ	1:C:706:GLU:O	2.09	0.85
1:D:404:LYS:O	1:D:408:GLY:N	2.13	0.82
1:A:476:GLU:OE1	1:A:542:ARG:NH2	2.13	0.82
1:D:911:VAL:HG22	1:D:934:HIS:HB2	1.61	0.80
1:F:459:ARG:NH1	1:F:463:ASP:OD1	2.16	0.79
1:F:556:ALA:O	1:F:560:GLY:N	2.16	0.78
1:A:876:ASN:OD1	1:A:908:THR:OG1	2.02	0.78
1:F:274:GLU:N	1:F:274:GLU:OE1	2.17	0.78
1:B:556:ALA:O	1:B:560:GLY:N	2.17	0.77
1:A:556:ALA:O	1:A:560:GLY:N	2.18	0.77
1:B:147:LYS:NZ	1:B:151:GLU:OE2	2.19	0.75
1:B:666:LYS:NZ	1:B:706:GLU:O	2.18	0.75
1:C:274:GLU:OE1	1:C:274:GLU:N	2.19	0.75
1:F:153:LEU:HD13	1:F:206:MET:HE3	1.69	0.74
1:E:556:ALA:O	1:E:560:GLY:N	2.20	0.74
1:F:542:ARG:NH2	1:F:632:LYS:O	2.20	0.74
1:C:561:HIS:O	1:C:623:TYR:N	2.20	0.74
1:C:798:GLY:N	1:C:836:VAL:O	2.22	0.73
1:A:725:TYR:O	1:A:729:SER:OG	2.06	0.72
1:A:409:LEU:HD21	1:F:442:LEU:HB2	1.70	0.72
1:A:679:ARG:NH1	1:A:686:GLU:OE1	2.23	0.72
1:C:562:ARG:NH1	1:C:622:HIS:O	2.23	0.71
1:D:213:ARG:NH2	1:D:333:ASP:OD2	2.23	0.71
1:D:834:TYR:O	1:D:838:SER:OG	2.06	0.71
1:D:476:GLU:OE1	1:D:542:ARG:NH2	2.23	0.71
1:A:500:ARG:NH2	1:A:654:GLU:OE2	2.23	0.71
1:B:489:GLU:OE2	1:B:538:ARG:NH2	2.24	0.71
1:B:474:SER:N	1:B:584:ASN:OD1	2.24	0.71
1:E:645:ILE:O	1:E:650:ARG:NH2	2.24	0.70
1:F:738:THR:O	1:F:742:LEU:N	2.24	0.70
1:C:490:ASP:O	1:C:491:HIS:ND1	2.25	0.70
1:F:547:PHE:HB3	1:F:589:ILE:HD13	1.74	0.70
1:D:932:GLU:OE1	1:D:934:HIS:NE2	2.25	0.70
1:A:395:LEU:HD23	1:D:387:ILE:HD12	1.74	0.69
1:A:364:SER:CA	1:C:387:ILE:HD11	2.22	0.69
1:A:434:VAL:HG23	1:A:435:MET:HE2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:799:SER:HG	1:D:839:HIS:HD1	1.36	0.69
1:E:736:GLU:N	1:E:736:GLU:OE1	2.26	0.69
1:C:434:VAL:HG12	1:C:626:VAL:HG11	1.74	0.69
1:E:524:PRO:O	1:E:529:LYS:NZ	2.26	0.69
1:C:436:ASP:OD1	1:C:437:VAL:N	2.26	0.69
1:D:556:ALA:O	1:D:560:GLY:N	2.26	0.69
1:A:409:LEU:HD23	1:F:439:ASP:O	1.93	0.68
1:A:460:ASN:OD1	1:A:623:TYR:OH	2.11	0.68
1:A:798:GLY:O	1:A:818:TYR:OH	2.11	0.68
1:F:798:GLY:N	1:F:836:VAL:O	2.27	0.68
1:C:724:ALA:O	1:C:728:VAL:HG23	1.93	0.68
1:D:154:ARG:NH2	1:D:157:VAL:HG21	2.09	0.68
1:A:364:SER:HB3	1:C:387:ILE:HD11	1.76	0.68
1:F:153:LEU:HD13	1:F:206:MET:CE	2.22	0.68
1:F:871:ARG:NH2	1:F:949:ASP:O	2.26	0.68
1:E:430:VAL:HG11	1:E:435:MET:HE3	1.75	0.67
1:C:430:VAL:HG11	1:C:435:MET:HE3	1.75	0.67
1:D:703:TYR:OH	1:D:747:GLY:O	2.13	0.66
1:C:590:ASP:OD1	1:C:638:THR:OG1	2.13	0.66
1:F:484:GLN:OE1	1:F:502:LEU:HD11	1.95	0.66
1:E:561:HIS:O	1:E:623:TYR:N	2.29	0.66
1:B:755:ARG:NH1	1:B:905:ALA:O	2.29	0.66
1:B:616:ASN:ND2	1:B:630:LEU:O	2.29	0.65
1:A:459:ARG:NH2	1:F:440:GLU:OE2	2.30	0.65
1:A:364:SER:CB	1:C:387:ILE:HD11	2.26	0.65
1:B:876:ASN:OD1	1:B:908:THR:OG1	2.14	0.65
1:C:728:VAL:HG22	1:D:510:LEU:HG	1.80	0.64
1:A:123:HIS:O	1:A:123:HIS:ND1	2.30	0.64
1:C:705:ARG:NH2	1:C:753:VAL:O	2.31	0.64
1:E:604:SER:O	1:E:608:LEU:HD23	1.98	0.64
1:B:731:GLU:OE1	1:B:731:GLU:N	2.30	0.64
1:C:507:VAL:O	1:C:511:ARG:N	2.30	0.64
1:D:368:LYS:HZ3	1:F:387:ILE:HD12	1.62	0.64
1:D:645:ILE:O	1:D:650:ARG:NH2	2.31	0.64
1:F:803:THR:OG1	1:F:841:HIS:NE2	2.31	0.63
1:D:799:SER:OG	1:D:839:HIS:ND1	2.29	0.63
1:E:464:TRP:CD1	1:E:623:TYR:HH	2.16	0.63
1:B:866:SER:O	1:B:870:GLY:N	2.33	0.62
1:D:679:ARG:NH1	1:D:686:GLU:OE1	2.30	0.62
1:E:616:ASN:ND2	1:E:630:LEU:O	2.32	0.62
1:A:474:SER:N	1:A:584:ASN:OD1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:ASP:OD1	1:A:624:LEU:N	2.29	0.62
1:A:908:THR:O	1:A:932:GLU:N	2.30	0.62
1:C:647:GLU:HG3	1:C:648:PRO:HD3	1.81	0.62
1:E:410:GLU:OE1	1:E:410:GLU:N	2.33	0.62
1:B:274:GLU:N	1:B:274:GLU:OE1	2.31	0.61
1:E:460:ASN:OD1	1:E:464:TRP:NE1	2.33	0.61
1:A:803:THR:OG1	1:A:841:HIS:NE2	2.20	0.61
1:B:875:GLN:N	1:B:875:GLN:OE1	2.34	0.61
1:E:628:VAL:HG23	1:E:630:LEU:CD1	2.30	0.60
1:D:590:ASP:OD1	1:D:638:THR:OG1	2.18	0.60
1:A:834:TYR:O	1:A:838:SER:OG	2.18	0.60
1:C:430:VAL:CG1	1:C:435:MET:HE3	2.32	0.60
1:A:199:ASP:OD1	1:A:205:ARG:N	2.35	0.60
1:F:695:VAL:O	1:F:699:LEU:HD23	2.02	0.60
1:B:785:ARG:O	1:B:786:ARG:HG3	2.01	0.60
1:E:642:THR:HG22	1:E:642:THR:O	2.01	0.59
1:C:834:TYR:O	1:C:838:SER:OG	2.19	0.59
1:E:274:GLU:OE1	1:E:274:GLU:N	2.34	0.59
1:A:606:ALA:O	1:A:610:LEU:HD23	2.02	0.59
1:E:786:ARG:HB3	1:E:839:HIS:HB2	1.84	0.59
1:A:131:ARG:O	1:A:131:ARG:NH1	2.35	0.59
1:F:866:SER:O	1:F:870:GLY:N	2.35	0.59
1:C:616:ASN:ND2	1:C:630:LEU:O	2.36	0.59
1:B:563:ARG:O	1:B:563:ARG:NE	2.29	0.58
1:A:614:GLU:OE1	1:A:614:GLU:N	2.34	0.58
1:F:738:THR:OG1	1:F:741:ASN:OD1	2.20	0.58
1:C:604:SER:O	1:C:608:LEU:HD23	2.04	0.58
1:C:918:LYS:HB2	1:E:748:LYS:HD3	1.85	0.58
1:D:412:ASP:OD1	1:D:413:ASP:N	2.36	0.58
1:C:728:VAL:HG21	1:D:506:ALA:HB1	1.85	0.58
1:A:364:SER:HA	1:C:387:ILE:HD11	1.85	0.58
1:B:738:THR:O	1:B:742:LEU:N	2.34	0.58
1:C:434:VAL:CG1	1:C:626:VAL:HG11	2.33	0.58
1:E:705:ARG:NH1	1:E:753:VAL:O	2.36	0.58
1:F:606:ALA:O	1:F:610:LEU:HD23	2.02	0.58
1:E:856:ALA:O	1:E:859:THR:OG1	2.21	0.58
1:A:213:ARG:NH2	1:A:333:ASP:OD2	2.37	0.57
1:A:654:GLU:N	1:A:654:GLU:OE1	2.37	0.57
1:E:862:THR:HG21	1:E:879:MET:SD	2.44	0.57
1:F:497:VAL:HG21	1:F:658:VAL:HG22	1.86	0.57
1:C:628:VAL:HG23	1:C:630:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:699:LEU:HD12	1:D:703:TYR:HD2	1.69	0.57
1:D:621:ASP:OD1	1:D:624:LEU:N	2.33	0.57
1:B:565:TYR:HE1	1:D:566:VAL:HG22	1.69	0.56
1:D:368:LYS:NZ	1:F:387:ILE:HD12	2.20	0.56
1:A:604:SER:O	1:A:608:LEU:HD23	2.05	0.56
1:B:647:GLU:OE1	1:B:650:ARG:NH1	2.39	0.56
1:C:763:GLY:O	1:C:782:THR:OG1	2.13	0.56
1:C:902:ALA:HB1	1:C:907:VAL:CG1	2.36	0.56
1:D:773:MET:HE3	1:D:773:MET:O	2.05	0.56
1:F:604:SER:O	1:F:608:LEU:HD23	2.06	0.56
1:A:434:VAL:HG23	1:A:435:MET:CE	2.35	0.56
1:A:547:PHE:N	1:A:588:LEU:O	2.37	0.56
1:F:433:HIS:O	1:F:436:ASP:OD1	2.22	0.56
1:F:563:ARG:HD2	1:F:563:ARG:O	2.04	0.56
1:A:168:LEU:HB3	1:A:186:1PA:HD2	1.88	0.56
1:E:614:GLU:N	1:E:614:GLU:OE1	2.37	0.56
1:F:859:THR:N	1:F:879:MET:HE1	2.20	0.56
1:F:511:ARG:NE	1:F:515:GLN:OE1	2.40	0.55
1:F:731:GLU:N	1:F:731:GLU:OE1	2.40	0.55
1:B:472:LYS:O	1:B:583:GLU:N	2.39	0.55
1:B:933:VAL:HG21	1:B:935:PHE:CZ	2.41	0.55
1:D:755:ARG:NH2	1:D:905:ALA:O	2.39	0.55
1:E:911:VAL:HG12	1:E:934:HIS:HB2	1.88	0.55
1:F:918:LYS:O	1:F:922:ASP:N	2.37	0.55
1:C:773:MET:HE3	1:C:773:MET:O	2.06	0.55
1:F:428:LEU:HD13	1:F:470:TRP:HB2	1.87	0.55
1:E:143:GLU:N	1:E:143:GLU:OE1	2.38	0.55
1:E:798:GLY:N	1:E:836:VAL:O	2.38	0.55
1:E:800:LEU:HD11	1:E:842:LEU:HD23	1.87	0.55
1:E:422:ARG:NH1	1:E:439:ASP:OD1	2.38	0.55
1:C:301:ARG:HD2	1:C:304:ILE:HD11	1.89	0.55
1:D:709:VAL:HG12	1:D:709:VAL:O	2.06	0.55
1:F:339:THR:HG22	1:F:366:LEU:HD23	1.89	0.55
1:B:825:LEU:O	1:B:829:ALA:N	2.36	0.55
1:A:360:TYR:CE1	1:C:379:LEU:HD21	2.42	0.54
1:D:142:ILE:HD12	1:D:208:VAL:HG11	1.88	0.54
1:C:476:GLU:OE1	1:C:542:ARG:NH2	2.41	0.54
1:D:703:TYR:HE1	1:D:749:PRO:HA	1.72	0.54
1:E:642:THR:HG23	1:E:655:MET:HE2	1.88	0.54
1:F:674:LEU:CD2	1:F:716:VAL:HG11	2.37	0.54
1:F:527:VAL:HG11	1:F:658:VAL:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:ASP:OD2	1:A:794:GLY:N	2.41	0.54
1:D:798:GLY:N	1:D:836:VAL:O	2.41	0.54
1:E:202:ASP:OD1	1:E:203:LYS:N	2.40	0.54
1:F:616:ASN:ND2	1:F:630:LEU:O	2.41	0.54
1:E:175:GLU:N	1:E:175:GLU:OE1	2.41	0.54
1:A:495:GLU:OE1	1:A:495:GLU:N	2.35	0.54
1:C:399:GLN:HB3	1:E:407:LEU:HD21	1.89	0.54
1:D:699:LEU:HD11	1:D:715:GLN:HB3	1.89	0.54
1:D:777:THR:O	1:D:777:THR:HG23	2.08	0.54
1:D:786:ARG:HG2	1:D:787:PRO:HD2	1.90	0.54
1:B:422:ARG:NH1	1:B:439:ASP:OD1	2.41	0.53
1:D:844:VAL:O	1:D:844:VAL:HG23	2.08	0.53
1:E:471:GLY:N	1:E:583:GLU:OE1	2.42	0.53
1:F:621:ASP:OD1	1:F:624:LEU:N	2.40	0.53
1:B:413:ASP:O	1:B:414:LYS:CB	2.56	0.53
1:D:352:GLU:O	1:D:358:ARG:NH2	2.38	0.53
1:D:372:LEU:O	1:D:376:GLN:HG3	2.09	0.53
1:A:561:HIS:O	1:A:623:TYR:N	2.41	0.53
1:B:367:LYS:O	1:B:371:GLU:OE1	2.27	0.53
1:B:825:LEU:HD12	1:B:835:LEU:HD12	1.91	0.53
1:E:886:THR:O	1:E:886:THR:HG22	2.09	0.53
1:B:557:GLU:O	1:B:572:LYS:N	2.42	0.52
1:E:748:LYS:HB2	1:E:749:PRO:HD2	1.90	0.52
1:F:645:ILE:O	1:F:650:ARG:NH2	2.42	0.52
1:F:739:PRO:HA	1:F:742:LEU:HB3	1.90	0.52
1:A:658:VAL:HG13	1:A:658:VAL:O	2.10	0.52
1:D:336:ALA:O	1:D:339:THR:OG1	2.19	0.52
1:D:748:LYS:HD2	1:D:748:LYS:C	2.34	0.52
1:A:785:ARG:O	1:F:822:ARG:NH1	2.37	0.52
1:A:590:ASP:OD1	1:A:638:THR:OG1	2.27	0.52
1:B:739:PRO:HA	1:B:742:LEU:HB3	1.91	0.52
1:A:819:THR:HG21	1:B:841:HIS:ND1	2.25	0.52
1:B:520:CYS:HB3	1:B:655:MET:SD	2.50	0.52
1:B:856:ALA:O	1:B:859:THR:OG1	2.28	0.52
1:D:561:HIS:O	1:D:623:TYR:N	2.43	0.52
1:E:477:ASN:OD1	1:E:478:LEU:N	2.43	0.52
1:E:543:GLU:O	1:E:586:LEU:N	2.39	0.52
1:A:757:TYR:HE1	1:F:888:LYS:HB2	1.75	0.51
1:C:161:GLN:OE1	1:F:158:ARG:NH1	2.43	0.51
1:C:430:VAL:HG12	1:C:434:VAL:HG23	1.92	0.51
1:C:866:SER:O	1:C:870:GLY:N	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:197:MET:HE3	1:F:197:MET:HA	1.92	0.51
1:B:304:ILE:HD12	1:B:312:GLU:OE1	2.10	0.51
1:F:135:PHE:HB2	1:F:138:PHE:CD1	2.45	0.51
1:A:400:LEU:HA	1:A:403:ILE:HD12	1.92	0.51
1:D:852:ASP:O	1:D:855:SER:OG	2.26	0.51
1:F:803:THR:HG22	1:F:804:GLY:N	2.26	0.51
1:A:497:VAL:HG13	1:A:521:PHE:CE1	2.45	0.51
1:D:444:LYS:O	1:D:448:LEU:N	2.39	0.51
1:F:764:VAL:HG23	1:F:781:GLU:HG3	1.93	0.51
1:D:495:GLU:OE1	1:D:495:GLU:N	2.43	0.50
1:F:786:ARG:HG2	1:F:787:PRO:HD2	1.93	0.50
1:B:674:LEU:HD11	1:B:709:VAL:CG1	2.42	0.50
1:A:748:LYS:O	1:F:918:LYS:HE3	2.11	0.50
1:C:430:VAL:CG1	1:C:434:VAL:HG23	2.41	0.50
1:D:902:ALA:HB1	1:D:907:VAL:CG1	2.41	0.50
1:A:599:TYR:O	1:A:600:GLN:HG3	2.11	0.50
1:C:287:GLU:O	1:C:290:LYS:NZ	2.41	0.50
1:B:918:LYS:CG	1:D:748:LYS:HE2	2.42	0.50
1:C:556:ALA:O	1:C:560:GLY:N	2.44	0.50
1:B:154:ARG:O	1:B:157:VAL:HG22	2.10	0.50
1:E:852:ASP:O	1:E:855:SER:OG	2.27	0.50
1:B:759:VAL:O	1:B:875:GLN:NE2	2.44	0.50
1:C:142:ILE:HD12	1:C:208:VAL:HG11	1.94	0.50
1:E:356:PRO:O	1:E:360:TYR:CD2	2.65	0.50
1:B:819:THR:HG22	1:B:822:ARG:HH21	1.77	0.50
1:D:703:TYR:CE2	1:D:746:VAL:HG11	2.47	0.50
1:F:703:TYR:CE2	1:F:746:VAL:HG21	2.47	0.50
1:D:825:LEU:HD21	1:D:869:MET:SD	2.52	0.50
1:F:421:PHE:HZ	1:F:459:ARG:NH1	2.10	0.50
1:A:373:SER:O	1:A:376:GLN:N	2.45	0.49
1:B:929:GLU:N	1:B:929:GLU:OE1	2.45	0.49
1:D:368:LYS:CE	1:F:384:GLU:HA	2.41	0.49
1:D:425:LEU:HD12	1:D:428:LEU:HD12	1.93	0.49
1:F:435:MET:SD	1:F:436:ASP:N	2.85	0.49
1:B:206:MET:HE1	1:B:208:VAL:HG12	1.94	0.49
1:A:498:LYS:O	1:A:502:LEU:HD23	2.12	0.49
1:A:757:TYR:OH	1:F:886:THR:HB	2.12	0.49
1:D:699:LEU:HD12	1:D:703:TYR:CD2	2.46	0.49
1:A:379:LEU:CD1	1:E:402:ILE:HG21	2.43	0.49
1:D:866:SER:O	1:D:870:GLY:N	2.46	0.49
1:A:563:ARG:HD2	1:A:563:ARG:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:ILE:O	1:A:673:TYR:N	2.44	0.49
1:D:518:ILE:HG21	1:D:611:LEU:HD23	1.94	0.49
1:D:703:TYR:CE1	1:D:749:PRO:HA	2.48	0.49
1:E:294:ALA:O	1:E:297:VAL:HG22	2.12	0.49
1:C:422:ARG:NH1	1:C:439:ASP:OD1	2.43	0.49
1:C:510:LEU:HD22	1:E:682:CYS:O	2.12	0.49
1:E:731:GLU:OE1	1:E:731:GLU:N	2.41	0.49
1:F:527:VAL:CG1	1:F:658:VAL:HG12	2.42	0.49
1:F:543:GLU:O	1:F:586:LEU:N	2.32	0.49
1:A:373:SER:O	1:A:377:GLN:OE1	2.31	0.49
1:A:773:MET:HE3	1:A:773:MET:O	2.13	0.49
1:C:797:ASP:OD2	1:E:786:ARG:NH2	2.46	0.49
1:C:765:VAL:HG12	1:C:863:ALA:HB2	1.95	0.49
1:D:521:PHE:N	1:D:637:CYS:O	2.46	0.49
1:D:759:VAL:O	1:D:760:THR:OG1	2.28	0.49
1:B:336:ALA:O	1:B:339:THR:OG1	2.24	0.48
1:A:291:ALA:HB2	1:C:372:LEU:HD21	1.94	0.48
1:A:866:SER:O	1:A:870:GLY:N	2.43	0.48
1:B:561:HIS:O	1:B:623:TYR:N	2.46	0.48
1:C:728:VAL:HG22	1:D:510:LEU:CG	2.44	0.48
1:C:454:GLU:OE2	1:E:459:ARG:NH1	2.45	0.48
1:F:318:MET:SD	1:F:318:MET:C	2.95	0.48
1:C:562:ARG:HD2	1:C:622:HIS:HB3	1.95	0.48
1:C:755:ARG:NH1	1:C:905:ALA:O	2.39	0.48
1:C:844:VAL:HG23	1:C:844:VAL:O	2.13	0.48
1:A:367:LYS:CD	1:C:384:GLU:HG2	2.44	0.48
1:C:593:ASP:OD1	1:C:593:ASP:N	2.47	0.48
1:F:149:LEU:O	1:F:153:LEU:HG	2.13	0.48
1:F:642:THR:O	1:F:642:THR:HG22	2.14	0.48
1:A:709:VAL:HG12	1:A:709:VAL:O	2.13	0.48
1:F:825:LEU:O	1:F:829:ALA:N	2.39	0.48
1:E:858:CYS:SG	1:E:942:ILE:HD13	2.54	0.48
1:F:432:LYS:O	1:F:435:MET:HG3	2.12	0.48
1:D:299:THR:O	1:D:303:ILE:HG12	2.14	0.48
1:E:866:SER:O	1:E:870:GLY:N	2.47	0.48
1:F:491:HIS:CD2	1:F:532:ILE:HD13	2.49	0.48
1:C:856:ALA:O	1:C:859:THR:OG1	2.27	0.48
1:E:517:LYS:NZ	1:E:652:ARG:O	2.45	0.48
1:D:367:LYS:NZ	1:F:384:GLU:OE2	2.36	0.48
1:F:614:GLU:OE1	1:F:614:GLU:N	2.45	0.48
1:F:879:MET:SD	1:F:879:MET:C	2.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ALA:O	1:A:297:VAL:HG22	2.14	0.47
1:A:825:LEU:HD12	1:A:835:LEU:HD12	1.95	0.47
1:B:759:VAL:O	1:B:760:THR:OG1	2.29	0.47
1:E:705:ARG:NE	1:E:754:GLU:OE1	2.47	0.47
1:F:709:VAL:HG12	1:F:709:VAL:O	2.13	0.47
1:C:399:GLN:CB	1:E:407:LEU:HD21	2.44	0.47
1:C:547:PHE:N	1:C:588:LEU:O	2.47	0.47
1:F:552:MET:HG3	1:F:557:GLU:OE2	2.14	0.47
1:B:562:ARG:O	1:B:563:ARG:HB3	2.15	0.47
1:B:918:LYS:CB	1:D:748:LYS:HE2	2.44	0.47
1:D:365:LEU:CD2	1:F:387:ILE:HD13	2.44	0.47
1:B:764:VAL:HG23	1:B:781:GLU:HG3	1.96	0.47
1:E:404:LYS:HG2	1:E:410:GLU:OE1	2.15	0.47
1:B:810:MET:HE1	1:B:853:GLY:C	2.39	0.47
1:C:430:VAL:HG11	1:C:435:MET:CE	2.43	0.47
1:D:879:MET:SD	1:D:911:VAL:HB	2.54	0.47
1:F:834:TYR:O	1:F:838:SER:OG	2.30	0.47
1:A:784:LEU:O	1:F:826:MET:HE1	2.14	0.47
1:A:844:VAL:HG23	1:A:844:VAL:O	2.15	0.47
1:B:458:THR:O	1:B:462:LEU:HG	2.14	0.47
1:B:642:THR:HG23	1:B:655:MET:HE2	1.96	0.47
1:C:658:VAL:HG23	1:C:658:VAL:O	2.14	0.47
1:C:876:ASN:C	1:C:907:VAL:HG23	2.40	0.47
1:D:736:GLU:OE1	1:D:736:GLU:N	2.48	0.47
1:E:422:ARG:NH2	1:E:439:ASP:OD1	2.45	0.47
1:A:795:ASP:O	1:B:786:ARG:NH2	2.48	0.47
1:F:138:PHE:CZ	1:F:334:MET:HA	2.50	0.47
1:E:603:PRO:O	1:E:607:LEU:HD23	2.15	0.47
1:F:844:VAL:O	1:F:844:VAL:HG13	2.15	0.47
1:A:725:TYR:HE1	1:F:502:LEU:HD13	1.81	0.46
1:B:918:LYS:HD2	1:B:919:ASP:N	2.30	0.46
1:C:543:GLU:O	1:C:586:LEU:N	2.47	0.46
1:D:555:VAL:HG22	1:D:555:VAL:O	2.15	0.46
1:E:566:VAL:HG23	1:E:566:VAL:O	2.15	0.46
1:F:908:THR:O	1:F:932:GLU:N	2.41	0.46
1:B:399:GLN:O	1:B:403:ILE:HG12	2.16	0.46
1:E:404:LYS:HG2	1:E:410:GLU:CD	2.41	0.46
1:B:573:ILE:O	1:B:577:LEU:HD23	2.15	0.46
1:B:744:ASP:OD1	1:B:745:PHE:N	2.48	0.46
1:D:875:GLN:O	1:D:876:ASN:OD1	2.33	0.46
1:E:777:THR:HG23	1:E:777:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:557:GLU:O	1:F:572:LYS:N	2.48	0.46
1:F:646:PRO:O	1:F:650:ARG:N	2.47	0.46
1:F:670:ALA:HA	1:F:674:LEU:HB3	1.97	0.46
1:C:562:ARG:O	1:C:563:ARG:HB3	2.15	0.46
1:C:917:LYS:HA	1:C:935:PHE:CE1	2.51	0.46
1:F:879:MET:HG2	1:F:911:VAL:HB	1.96	0.46
1:B:917:LYS:HA	1:B:935:PHE:CE1	2.51	0.46
1:D:197:MET:N	1:D:197:MET:HE2	2.30	0.46
1:E:410:GLU:HG2	1:E:411:LYS:HG3	1.97	0.46
1:E:798:GLY:O	1:E:818:TYR:OH	2.26	0.46
1:B:516:GLY:N	1:B:631:SER:O	2.40	0.46
1:C:444:LYS:HE3	1:E:459:ARG:HH22	1.81	0.46
1:C:695:VAL:O	1:C:699:LEU:HD13	2.16	0.46
1:A:131:ARG:O	1:A:131:ARG:CZ	2.63	0.46
1:A:662:VAL:HG22	1:A:663:ALA:H	1.80	0.46
1:A:766:MET:HE3	1:A:777:THR:OG1	2.16	0.46
1:B:865:LEU:O	1:B:869:MET:HE3	2.15	0.46
1:C:334:MET:SD	1:C:334:MET:C	2.99	0.46
1:E:352:GLU:OE2	1:E:361:LYS:NZ	2.37	0.46
1:F:450:ASN:OD1	1:F:451:HIS:N	2.49	0.46
1:F:892:VAL:N	1:F:916:ASN:OD1	2.43	0.46
1:A:274:GLU:N	1:A:274:GLU:OE1	2.49	0.46
1:A:444:LYS:O	1:A:448:LEU:N	2.37	0.46
1:B:185:ILE:O	1:B:219:GLN:NE2	2.43	0.46
1:B:777:THR:HG23	1:B:777:THR:O	2.15	0.46
1:C:585:PRO:HD2	1:C:633:VAL:HG12	1.97	0.46
1:E:709:VAL:O	1:E:709:VAL:HG12	2.15	0.46
1:E:875:GLN:O	1:E:876:ASN:OD1	2.34	0.46
1:A:479:ASP:OD1	1:A:480:LEU:N	2.49	0.46
1:B:562:ARG:NH2	1:D:569:MET:SD	2.85	0.46
1:D:287:GLU:HG2	1:F:342:GLU:HB3	1.98	0.46
1:B:182:LEU:O	1:B:219:GLN:NE2	2.49	0.46
1:E:662:VAL:HG12	1:E:663:ALA:N	2.30	0.46
1:A:367:LYS:HD3	1:C:384:GLU:HB3	1.98	0.45
1:B:590:ASP:OD1	1:B:638:THR:OG1	2.35	0.45
1:B:709:VAL:HG12	1:B:709:VAL:O	2.16	0.45
1:B:757:TYR:HB2	1:B:779:PHE:CE2	2.51	0.45
1:D:911:VAL:HG22	1:D:934:HIS:CB	2.38	0.45
1:E:743:GLN:OE1	1:E:748:LYS:HA	2.16	0.45
1:F:619:PHE:O	1:F:628:VAL:HG22	2.16	0.45
1:A:422:ARG:NH2	1:A:439:ASP:OD1	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:VAL:HG23	1:B:658:VAL:O	2.17	0.45
1:B:884:SER:O	1:D:781:GLU:OE1	2.33	0.45
1:E:435:MET:HE2	1:E:435:MET:HA	1.98	0.45
1:C:518:ILE:HG21	1:C:611:LEU:HD23	1.99	0.45
1:D:303:ILE:O	1:D:307:ASN:N	2.45	0.45
1:F:876:ASN:C	1:F:907:VAL:HG23	2.41	0.45
1:A:129:ILE:HG22	1:A:132:ASN:H	1.81	0.45
1:A:367:LYS:HD3	1:C:384:GLU:HG2	1.98	0.45
1:B:304:ILE:HG13	1:B:305:ALA:N	2.32	0.45
1:C:629:ASP:C	1:C:630:LEU:HD12	2.42	0.45
1:D:154:ARG:HA	1:D:154:ARG:NE	2.32	0.45
1:A:748:LYS:HB3	1:A:749:PRO:HD2	1.98	0.45
1:F:716:VAL:HA	1:F:719:VAL:HG12	1.98	0.45
1:B:304:ILE:CD1	1:B:312:GLU:OE1	2.65	0.45
1:B:642:THR:HG22	1:B:642:THR:O	2.17	0.45
1:D:398:GLU:O	1:D:402:ILE:HG12	2.16	0.45
1:D:543:GLU:HG2	1:D:582:THR:HG21	1.99	0.45
1:D:700:ILE:O	1:D:704:CYS:O	2.35	0.45
1:A:303:ILE:O	1:A:307:ASN:N	2.35	0.45
1:A:403:ILE:HD13	1:F:403:ILE:HG23	1.98	0.45
1:A:430:VAL:HG23	1:A:470:TRP:CG	2.52	0.45
1:B:403:ILE:O	1:B:407:LEU:HD23	2.17	0.45
1:B:786:ARG:HB2	1:B:839:HIS:HB2	1.98	0.45
1:C:521:PHE:N	1:C:637:CYS:O	2.49	0.45
1:E:818:TYR:OH	1:E:822:ARG:NH2	2.50	0.45
1:E:902:ALA:HB1	1:E:907:VAL:CG1	2.46	0.45
1:F:357:LYS:N	1:F:357:LYS:CD	2.80	0.45
1:A:364:SER:OG	1:C:383:VAL:CG1	2.64	0.45
1:B:844:VAL:HG13	1:B:844:VAL:O	2.17	0.45
1:C:562:ARG:HG3	1:E:567:GLY:HA2	1.98	0.45
1:A:569:MET:HG2	1:F:622:HIS:HE1	1.82	0.45
1:E:736:GLU:O	1:E:736:GLU:HG2	2.17	0.45
1:E:861:VAL:O	1:E:865:LEU:HD13	2.17	0.45
1:A:900:ILE:CG2	1:A:927:ILE:HD11	2.48	0.44
1:F:522:TYR:HA	1:F:639:ALA:O	2.17	0.44
1:F:742:LEU:O	1:F:746:VAL:HG22	2.17	0.44
1:A:662:VAL:HG22	1:A:663:ALA:N	2.32	0.44
1:A:803:THR:HG1	1:A:841:HIS:CE1	2.22	0.44
1:B:886:THR:O	1:B:886:THR:HG22	2.17	0.44
1:C:194:ILE:HG12	1:C:206:MET:HE2	1.98	0.44
1:C:430:VAL:HG22	1:C:470:TRP:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:ASP:OD1	1:C:497:VAL:N	2.50	0.44
1:D:666:LYS:NZ	1:D:706:GLU:O	2.33	0.44
1:A:395:LEU:CD2	1:D:384:GLU:HA	2.47	0.44
1:C:562:ARG:HG3	1:E:567:GLY:CA	2.47	0.44
1:E:398:GLU:O	1:E:402:ILE:HG12	2.18	0.44
1:E:692:SER:OG	1:E:695:VAL:HG23	2.17	0.44
1:F:430:VAL:HG22	1:F:434:VAL:CG1	2.47	0.44
1:F:858:CYS:C	1:F:879:MET:HE1	2.43	0.44
1:A:510:LEU:HG	1:B:728:VAL:HG22	2.00	0.44
1:A:748:LYS:HB2	1:F:918:LYS:HB2	2.00	0.44
1:C:190:THR:HG21	1:C:210:GLY:HA2	2.00	0.44
1:A:822:ARG:NH1	1:B:785:ARG:O	2.45	0.44
1:B:304:ILE:HD12	1:B:312:GLU:CD	2.43	0.44
1:C:766:MET:SD	1:C:777:THR:OG1	2.75	0.44
1:E:597:ARG:HA	1:E:603:PRO:HD2	1.99	0.44
1:F:726:LYS:O	1:F:730:GLY:N	2.50	0.44
1:F:822:ARG:O	1:F:826:MET:HG2	2.18	0.44
1:A:477:ASN:N	1:A:540:LEU:O	2.39	0.44
1:B:164:VAL:HG21	1:B:206:MET:HE2	1.99	0.44
1:C:614:GLU:OE1	1:C:614:GLU:N	2.42	0.44
1:D:822:ARG:HA	1:D:835:LEU:HD23	2.00	0.44
1:E:812:GLU:O	1:E:816:ILE:HG12	2.18	0.44
1:A:480:LEU:HD12	1:B:729:SER:HB3	2.00	0.44
1:C:674:LEU:HD11	1:C:709:VAL:CG1	2.48	0.44
1:F:662:VAL:HG22	1:F:663:ALA:H	1.83	0.44
1:F:306:LEU:HB3	1:F:374:LYS:HZ1	1.83	0.43
1:B:641:VAL:HG12	1:B:643:ASP:H	1.83	0.43
1:C:805:GLN:NE2	1:D:812:GLU:OE1	2.50	0.43
1:A:494:MET:HG2	1:A:658:VAL:HG23	2.01	0.43
1:A:633:VAL:HG21	1:A:635:PHE:CE1	2.53	0.43
1:B:857:GLY:O	1:B:861:VAL:HG23	2.17	0.43
1:C:886:THR:HG22	1:C:886:THR:O	2.19	0.43
1:C:936:VAL:HG21	1:C:942:ILE:HD11	1.99	0.43
1:F:662:VAL:HG22	1:F:663:ALA:N	2.34	0.43
1:C:619:PHE:O	1:C:628:VAL:N	2.46	0.43
1:C:924:ALA:O	1:C:927:ILE:HG22	2.18	0.43
1:D:886:THR:HG22	1:D:886:THR:O	2.17	0.43
1:F:327:ASN:OD1	1:F:329:ILE:HG22	2.18	0.43
1:A:892:VAL:O	1:A:916:ASN:ND2	2.51	0.43
1:B:599:TYR:O	1:B:600:GLN:HG3	2.18	0.43
1:C:857:GLY:O	1:C:861:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:748:LYS:HZ2	1:D:750:VAL:HA	1.83	0.43
1:D:918:LYS:O	1:D:922:ASP:N	2.51	0.43
1:A:430:VAL:CG2	1:A:435:MET:HE3	2.49	0.43
1:A:430:VAL:CG1	1:A:435:MET:HE3	2.48	0.43
1:A:750:VAL:HA	1:F:918:LYS:HD3	2.00	0.43
1:C:709:VAL:HG12	1:C:709:VAL:O	2.18	0.43
1:D:339:THR:HG22	1:D:366:LEU:HA	2.01	0.43
1:A:900:ILE:HG22	1:A:927:ILE:HD11	2.00	0.43
1:B:815:ARG:O	1:B:819:THR:HG23	2.19	0.43
1:B:859:THR:O	1:B:860:ILE:C	2.62	0.43
1:C:875:GLN:O	1:C:876:ASN:OD1	2.37	0.43
1:A:127:ILE:HG21	1:A:206:MET:HE1	1.99	0.43
1:B:359:LEU:O	1:B:363:LEU:HD13	2.19	0.43
1:C:301:ARG:HD2	1:C:301:ARG:HA	1.90	0.43
1:D:500:ARG:NE	1:D:654:GLU:OE1	2.40	0.43
1:E:902:ALA:O	1:E:907:VAL:HG12	2.19	0.43
1:A:753:VAL:HG12	1:A:755:ARG:O	2.18	0.43
1:D:674:LEU:HD11	1:D:709:VAL:HG11	2.00	0.43
1:D:702:GLN:OE1	1:D:749:PRO:HB3	2.19	0.43
1:D:753:VAL:HG22	1:D:755:ARG:O	2.19	0.43
1:A:373:SER:C	1:A:377:GLN:OE1	2.61	0.43
1:A:494:MET:SD	1:A:532:ILE:HD12	2.59	0.43
1:C:462:LEU:O	1:C:466:THR:HG23	2.19	0.43
1:D:793:LYS:HD2	1:D:793:LYS:O	2.19	0.43
1:E:168:LEU:HB3	1:E:186:1PA:HD1	2.01	0.43
1:F:138:PHE:HZ	1:F:334:MET:HA	1.83	0.43
1:F:197:MET:SD	1:F:206:MET:CE	3.06	0.43
1:C:380:GLY:O	1:C:384:GLU:HG3	2.19	0.42
1:C:716:VAL:HA	1:C:719:VAL:HG12	2.01	0.42
1:C:777:THR:O	1:C:777:THR:HG23	2.19	0.42
1:D:562:ARG:O	1:D:563:ARG:HB3	2.19	0.42
1:E:465:LEU:HD13	1:E:624:LEU:HD11	2.00	0.42
1:E:702:GLN:O	1:E:751:PHE:N	2.46	0.42
1:F:354:ASN:HB2	1:F:357:LYS:HD3	2.01	0.42
1:F:816:ILE:HG23	1:F:885:LEU:HB2	2.01	0.42
1:B:629:ASP:C	1:B:630:LEU:HD12	2.44	0.42
1:B:785:ARG:HD3	1:B:841:HIS:HB2	2.01	0.42
1:C:703:TYR:CE2	1:C:746:VAL:HG11	2.54	0.42
1:F:417:ILE:HD12	1:F:459:ARG:HH21	1.83	0.42
1:F:417:ILE:HD12	1:F:459:ARG:NH2	2.33	0.42
1:F:430:VAL:CG2	1:F:434:VAL:HG11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ILE:O	1:B:307:ASN:N	2.42	0.42
1:B:445:LEU:HD22	1:B:462:LEU:HD11	2.01	0.42
1:C:662:VAL:HG22	1:C:663:ALA:H	1.85	0.42
1:D:674:LEU:HD11	1:D:709:VAL:CG1	2.49	0.42
1:B:918:LYS:HG2	1:D:748:LYS:NZ	2.34	0.42
1:C:430:VAL:CG1	1:C:434:VAL:CG2	2.98	0.42
1:C:452:SER:HB3	1:C:455:PHE:CB	2.49	0.42
1:C:795:ASP:OD1	1:C:795:ASP:N	2.51	0.42
1:D:880:THR:O	1:D:880:THR:HG23	2.20	0.42
1:B:796:LYS:HD2	1:B:796:LYS:C	2.45	0.42
1:C:436:ASP:OD1	1:C:436:ASP:C	2.62	0.42
1:D:936:VAL:HG21	1:D:942:ILE:HD11	2.01	0.42
1:E:602:ASP:N	1:E:603:PRO:CD	2.82	0.42
1:E:668:ALA:O	1:E:672:ARG:HG2	2.20	0.42
1:E:844:VAL:HG23	1:E:844:VAL:O	2.19	0.42
1:C:430:VAL:HG22	1:C:470:TRP:CB	2.50	0.42
1:C:452:SER:HB3	1:C:455:PHE:HB3	2.01	0.42
1:C:769:ALA:HB1	1:C:848:ALA:HB2	2.02	0.42
1:F:918:LYS:HG3	1:F:919:ASP:N	2.34	0.42
1:A:289:VAL:HG23	1:A:290:LYS:N	2.34	0.42
1:C:549:VAL:HG22	1:C:549:VAL:O	2.20	0.42
1:C:629:ASP:O	1:C:630:LEU:HD12	2.20	0.42
1:E:593:ASP:N	1:E:593:ASP:OD1	2.53	0.42
1:F:484:GLN:OE1	1:F:502:LEU:HD21	2.20	0.42
1:B:544:TYR:O	1:B:579:LYS:NZ	2.53	0.42
1:D:593:ASP:OD1	1:D:593:ASP:N	2.52	0.42
1:F:514:THR:HG23	1:F:514:THR:O	2.20	0.42
1:A:936:VAL:HG21	1:A:942:ILE:HD11	2.02	0.42
1:B:384:GLU:HA	1:B:387:ILE:HD12	2.02	0.42
1:C:486:VAL:HG13	1:C:538:ARG:NH1	2.35	0.42
1:E:407:LEU:O	1:E:407:LEU:HG	2.20	0.42
1:E:700:ILE:O	1:E:704:CYS:O	2.37	0.42
1:F:323:ARG:HA	1:F:323:ARG:NE	2.34	0.42
1:F:518:ILE:HG23	1:F:653:MET:CB	2.50	0.42
1:A:709:VAL:O	1:A:709:VAL:CG1	2.68	0.41
1:B:387:ILE:HD13	1:E:364:SER:HA	2.02	0.41
1:E:563:ARG:HA	1:E:568:ALA:HB3	2.01	0.41
1:F:628:VAL:HG23	1:F:630:LEU:HD13	2.01	0.41
1:B:168:LEU:HB3	1:B:186:1PA:HD2	2.01	0.41
1:C:522:TYR:CE1	1:C:655:MET:HB3	2.55	0.41
1:C:900:ILE:HG13	1:C:927:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:LEU:HB3	1:D:186:1PA:HD1	2.02	0.41
1:D:716:VAL:HA	1:D:719:VAL:HG12	2.02	0.41
1:D:765:VAL:HG11	1:D:862:THR:HG23	2.02	0.41
1:A:756:MET:HE2	1:A:757:TYR:CZ	2.55	0.41
1:B:761:PRO:O	1:B:764:VAL:HG12	2.20	0.41
1:D:368:LYS:HD3	1:F:387:ILE:HG21	2.01	0.41
1:D:706:GLU:N	1:D:706:GLU:OE1	2.53	0.41
1:D:803:THR:OG1	1:D:841:HIS:NE2	2.44	0.41
1:B:562:ARG:O	1:B:562:ARG:CG	2.68	0.41
1:B:716:VAL:HA	1:B:719:VAL:HG12	2.01	0.41
1:D:154:ARG:HH12	1:D:197:MET:HG3	1.84	0.41
1:E:876:ASN:C	1:E:907:VAL:HG23	2.46	0.41
1:F:817:ALA:HB1	1:F:861:VAL:HG23	2.02	0.41
1:A:801:GLU:OE1	1:A:841:HIS:CD2	2.74	0.41
1:B:462:LEU:O	1:B:466:THR:HG23	2.20	0.41
1:C:391:HIS:O	1:C:393:LYS:N	2.53	0.41
1:C:875:GLN:OE1	1:C:875:GLN:N	2.52	0.41
1:E:497:VAL:O	1:E:501:ILE:HG12	2.21	0.41
1:A:435:MET:HE2	1:A:435:MET:N	2.36	0.41
1:C:530:THR:HG22	1:C:534:ARG:CZ	2.51	0.41
1:C:692:SER:OG	1:C:695:VAL:HG23	2.21	0.41
1:C:759:VAL:O	1:C:875:GLN:NE2	2.53	0.41
1:E:363:LEU:HA	1:E:366:LEU:HD12	2.01	0.41
1:A:444:LYS:O	1:A:448:LEU:HD13	2.21	0.41
1:E:619:PHE:O	1:E:628:VAL:HG22	2.21	0.41
1:F:561:HIS:HB2	1:F:568:ALA:HB1	2.03	0.41
1:F:674:LEU:HD21	1:F:716:VAL:HG11	2.02	0.41
1:A:373:SER:O	1:A:374:LYS:C	2.63	0.41
1:B:697:THR:O	1:B:701:LYS:HG2	2.21	0.41
1:C:441:GLU:OE2	1:C:458:THR:HG23	2.20	0.41
1:C:902:ALA:HB1	1:C:907:VAL:HG11	2.03	0.41
1:C:928:THR:O	1:C:928:THR:HG22	2.20	0.41
1:E:129:ILE:HD12	1:E:129:ILE:H	1.85	0.41
1:E:786:ARG:CG	1:E:787:PRO:HD2	2.51	0.41
1:F:800:LEU:HD21	1:F:842:LEU:HD21	2.02	0.41
1:A:777:THR:HG23	1:A:777:THR:O	2.21	0.41
1:B:858:CYS:SG	1:B:942:ILE:CD1	3.09	0.41
1:C:880:THR:O	1:C:880:THR:HG23	2.20	0.41
1:D:196:GLU:C	1:D:197:MET:HE2	2.46	0.41
1:E:487:LEU:O	1:E:498:LYS:NZ	2.54	0.41
1:F:461:TYR:CZ	1:F:465:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:629:ASP:C	1:F:630:LEU:HD12	2.46	0.41
1:A:726:LYS:O	1:A:730:GLY:N	2.54	0.41
1:B:887:GLY:O	1:B:939:TYR:N	2.52	0.41
1:D:388:LYS:HE2	1:D:388:LYS:HA	2.02	0.41
1:D:405:LYS:HG2	1:D:409:LEU:HD12	2.02	0.41
1:D:876:ASN:C	1:D:907:VAL:HG23	2.46	0.41
1:D:911:VAL:HG11	1:D:942:ILE:HG12	2.02	0.41
1:F:496:ASP:OD1	1:F:497:VAL:N	2.52	0.41
1:A:392:ARG:HA	1:A:395:LEU:HD12	2.03	0.40
1:A:670:ALA:HA	1:A:674:LEU:HB2	2.03	0.40
1:B:485:ALA:O	1:B:489:GLU:HG3	2.21	0.40
1:B:615:GLN:NE2	1:B:618:ASN:OD1	2.49	0.40
1:B:798:GLY:N	1:B:836:VAL:O	2.54	0.40
1:B:915:GLU:OE1	1:B:915:GLU:N	2.46	0.40
1:C:433:HIS:O	1:C:436:ASP:OD1	2.39	0.40
1:D:336:ALA:HB2	1:D:362:ALA:HB1	2.03	0.40
1:D:542:ARG:NH1	1:D:584:ASN:O	2.49	0.40
1:F:521:PHE:O	1:F:638:THR:HA	2.21	0.40
1:A:581:LYS:O	1:A:581:LYS:HG3	2.21	0.40
1:A:748:LYS:HD3	1:A:748:LYS:N	2.35	0.40
1:B:292:LEU:HD11	1:B:363:LEU:HD21	2.04	0.40
1:B:430:VAL:HG11	1:B:435:MET:SD	2.62	0.40
1:B:927:ILE:HG23	1:B:928:THR:HG23	2.03	0.40
1:C:451:HIS:CE1	1:D:448:LEU:HG	2.56	0.40
1:D:360:TYR:CD2	1:F:379:LEU:HD23	2.55	0.40
1:D:791:ASP:N	1:D:791:ASP:OD1	2.54	0.40
1:E:418:GLU:O	1:E:422:ARG:HG2	2.21	0.40
1:F:550:GLY:O	1:F:552:MET:HE2	2.22	0.40
1:F:703:TYR:O	1:F:711:ASN:ND2	2.54	0.40
1:A:778:LEU:HD13	1:A:845:PRO:O	2.21	0.40
1:A:851:LYS:O	1:A:851:LYS:HD2	2.21	0.40
1:B:359:LEU:O	1:B:363:LEU:CD1	2.70	0.40
1:B:422:ARG:NH2	1:B:439:ASP:OD1	2.51	0.40
1:B:565:TYR:CE1	1:D:566:VAL:HG22	2.53	0.40
1:B:840:ILE:CG2	1:B:841:HIS:N	2.84	0.40
1:C:660:GLY:HA3	1:C:900:ILE:HD13	2.03	0.40
1:D:709:VAL:O	1:D:709:VAL:CG1	2.68	0.40
1:F:705:ARG:HH12	1:F:754:GLU:HG2	1.85	0.40
1:A:398:GLU:OE1	1:D:383:VAL:HG22	2.22	0.40
1:A:520:CYS:SG	1:A:655:MET:HE3	2.61	0.40
1:F:461:TYR:CG	1:F:563:ARG:NH1	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:LYS:O	1:A:412:ASP:C	2.63	0.40
1:B:301:ARG:O	1:B:304:ILE:HG12	2.22	0.40
1:C:891:PRO:HA	1:C:916:ASN:OD1	2.21	0.40
1:D:755:ARG:NH1	1:D:766:MET:SD	2.95	0.40
1:E:552:MET:C	1:E:552:MET:SD	3.04	0.40
1:F:185:ILE:O	1:F:219:GLN:NE2	2.43	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	772/869 (89%)	738 (96%)	34 (4%)	0	100	100
1	B	772/869 (89%)	749 (97%)	22 (3%)	1 (0%)	48	83
1	C	772/869 (89%)	749 (97%)	23 (3%)	0	100	100
1	D	772/869 (89%)	738 (96%)	34 (4%)	0	100	100
1	E	772/869 (89%)	743 (96%)	29 (4%)	0	100	100
1	F	772/869 (89%)	747 (97%)	25 (3%)	0	100	100
All	All	4632/5214 (89%)	4464 (96%)	167 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	414	LYS

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	675/754 (90%)	675 (100%)	0	100	100
1	B	675/754 (90%)	675 (100%)	0	100	100
1	C	675/754 (90%)	675 (100%)	0	100	100
1	D	675/754 (90%)	675 (100%)	0	100	100
1	E	675/754 (90%)	675 (100%)	0	100	100
1	F	675/754 (90%)	675 (100%)	0	100	100
All	All	4050/4524 (90%)	4050 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	319	GLN
1	A	451	HIS
1	B	354	ASN
1	B	456	ASN
1	B	711	ASN
1	B	828	HIS
1	C	211	HIS
1	C	397	GLN
1	C	664	GLN
1	D	561	HIS
1	E	187	HIS
1	E	211	HIS
1	E	515	GLN
1	E	828	HIS
1	F	280	HIS
1	F	354	ASN
1	F	460	ASN
1	F	491	HIS
1	F	622	HIS
1	F	711	ASN
1	F	715	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	1PA	E	186	1	14,15,16	0.91	1 (7%)	14,19,21	0.76	0
1	1PA	F	186	1	14,15,16	0.91	1 (7%)	14,19,21	0.72	0
1	1PA	C	186	1	14,15,16	0.91	1 (7%)	14,19,21	0.74	0
1	1PA	B	186	1	14,15,16	0.92	1 (7%)	14,19,21	0.71	0
1	1PA	D	186	1	14,15,16	0.92	1 (7%)	14,19,21	0.74	0
1	1PA	A	186	1	14,15,16	0.93	1 (7%)	14,19,21	0.95	1 (7%)

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
1	1PA	E	186	1	-	4/9/10/12	0/1/1/1
1	1PA	F	186	1	-	4/9/10/12	0/1/1/1
1	1PA	C	186	1	-	2/9/10/12	0/1/1/1
1	1PA	B	186	1	-	3/9/10/12	0/1/1/1
1	1PA	D	186	1	-	4/9/10/12	0/1/1/1
1	1PA	A	186	1	-	4/9/10/12	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	186	1PA	CH-CO	2.29	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	186	1PA	CH-CO	2.28	1.55	1.51
1	B	186	1PA	CH-CO	2.24	1.55	1.51
1	C	186	1PA	CH-CO	2.24	1.55	1.51
1	F	186	1PA	CH-CO	2.22	1.55	1.51
1	A	186	1PA	CH-CO	2.21	1.55	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	1PA	O2-CO-CH	-2.58	115.15	122.94

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	186	1PA	O-C-CA-CB
1	F	186	1PA	CO-CH-CZ-CE1
1	F	186	1PA	CO-CH-CZ-CE2
1	E	186	1PA	CO-CH-CZ-CE1
1	D	186	1PA	CO-CH-CZ-CE1
1	E	186	1PA	CO-CH-CZ-CE2
1	B	186	1PA	CO-CH-CZ-CE1
1	D	186	1PA	CO-CH-CZ-CE2
1	B	186	1PA	CO-CH-CZ-CE2
1	C	186	1PA	CO-CH-CZ-CE1
1	C	186	1PA	CO-CH-CZ-CE2
1	A	186	1PA	CA-CB-CG-CD1
1	A	186	1PA	CA-CB-CG-CD2
1	F	186	1PA	N-CA-CB-CG
1	F	186	1PA	C-CA-CB-CG
1	D	186	1PA	CZ-CH-CO-O1
1	A	186	1PA	CO-CH-CZ-CE1
1	A	186	1PA	CO-CH-CZ-CE2
1	D	186	1PA	CZ-CH-CO-O2
1	B	186	1PA	C-CA-CB-CG
1	E	186	1PA	C-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	186	1PA	1	0
1	B	186	1PA	1	0
1	D	186	1PA	1	0
1	A	186	1PA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

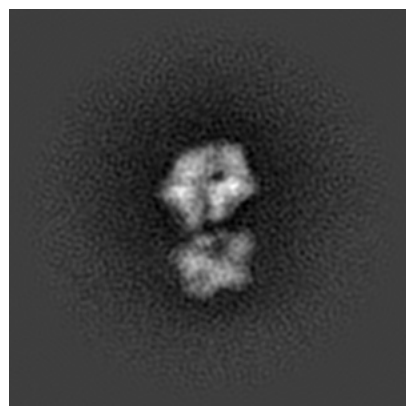
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17214. These allow visual inspection of the internal detail of the map and identification of artifacts.

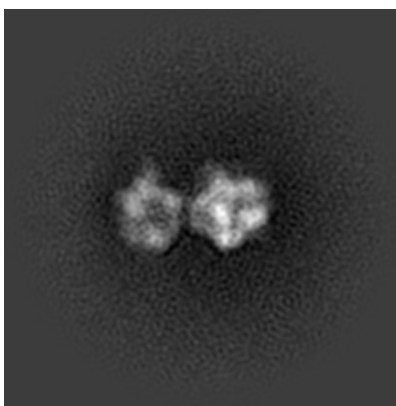
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

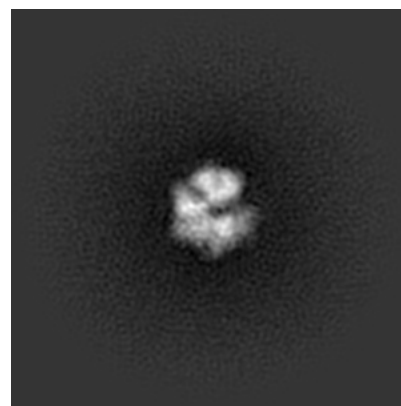
6.1.1 Primary map



X

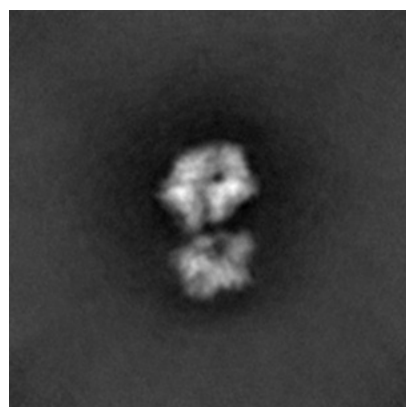


Y

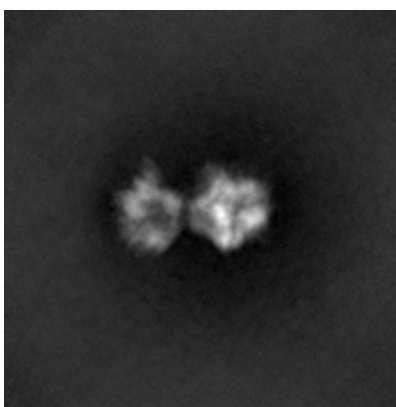


Z

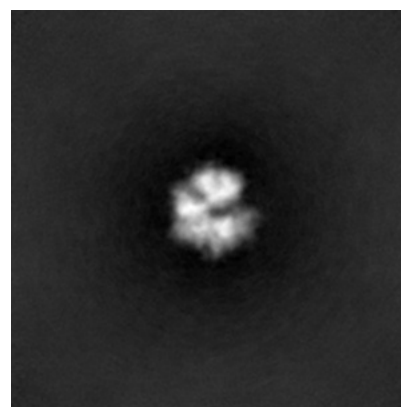
6.1.2 Raw map



X



Y

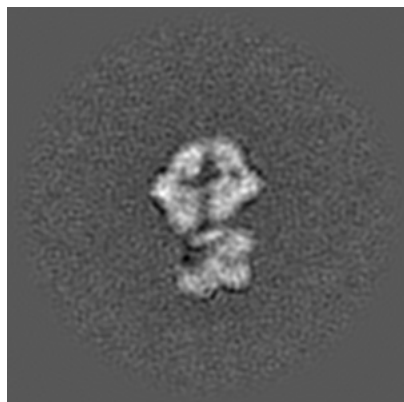


Z

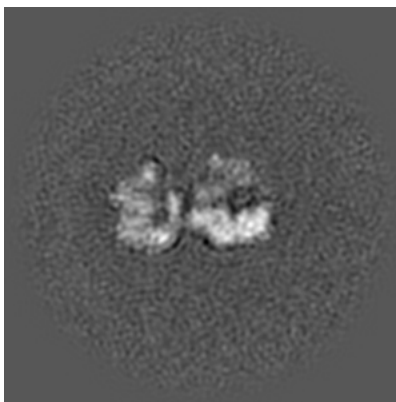
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

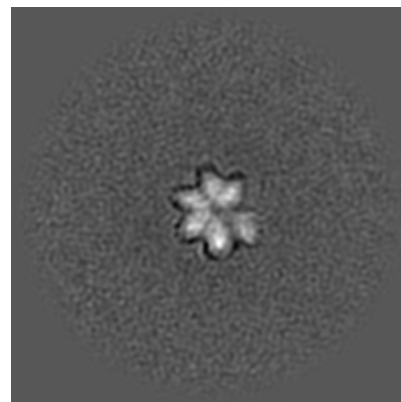
6.2.1 Primary map



X Index: 105

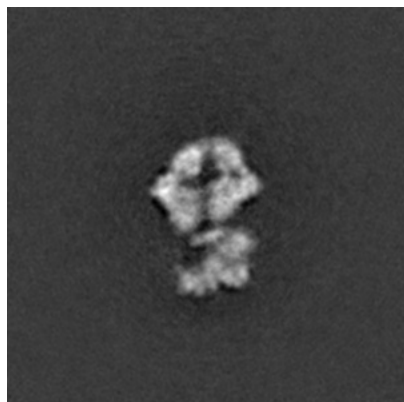


Y Index: 105

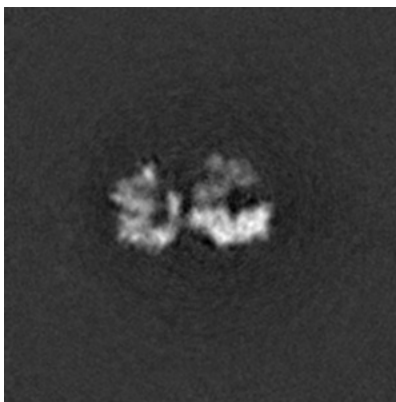


Z Index: 105

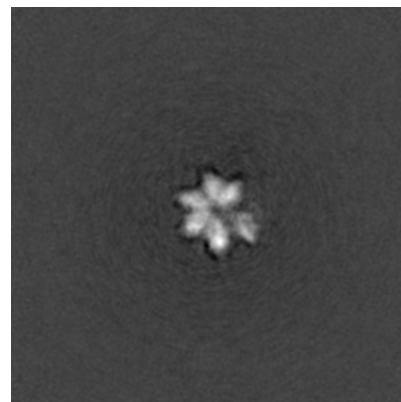
6.2.2 Raw map



X Index: 105



Y Index: 105

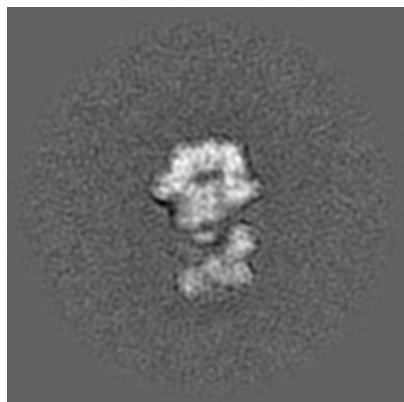


Z Index: 105

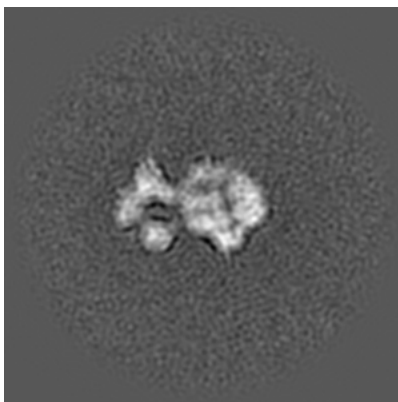
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

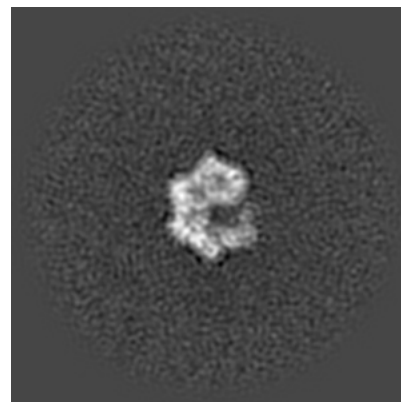
6.3.1 Primary map



X Index: 101

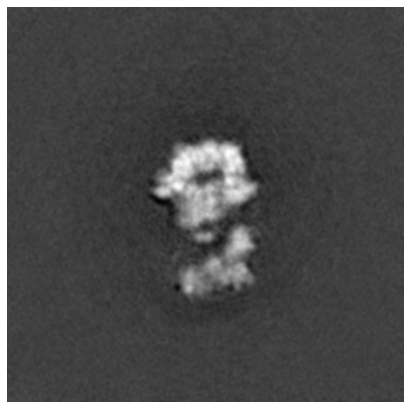


Y Index: 95

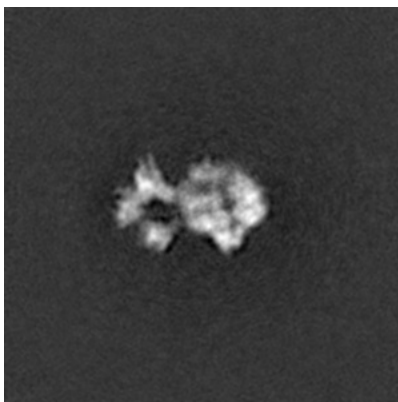


Z Index: 115

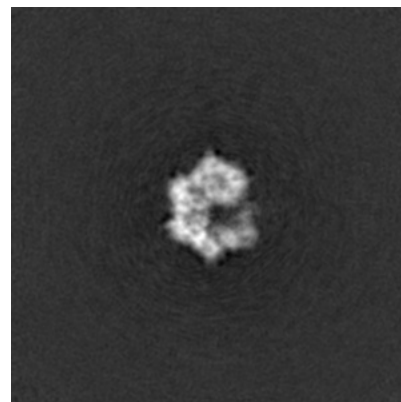
6.3.2 Raw map



X Index: 101



Y Index: 95

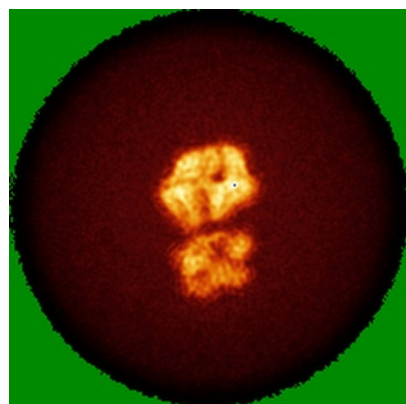


Z Index: 115

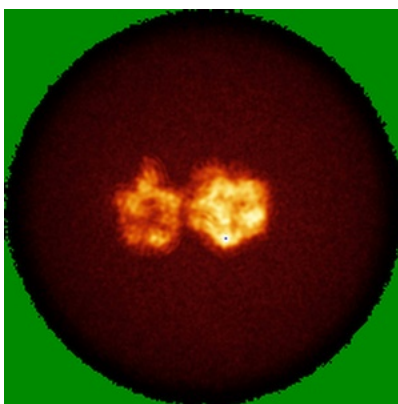
The images above show the largest variance slices of the map in three orthogonal directions.

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

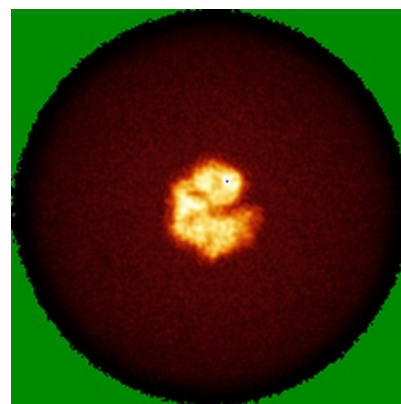
6.4.1 Primary map



X

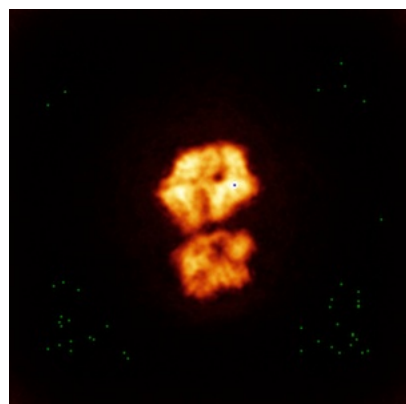


Y

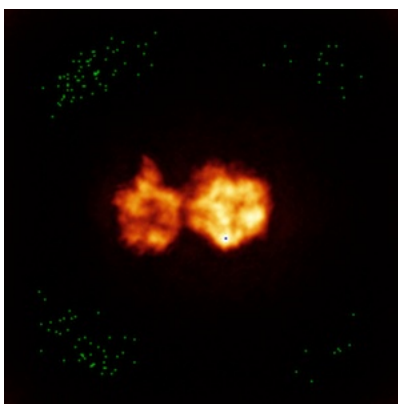


Z

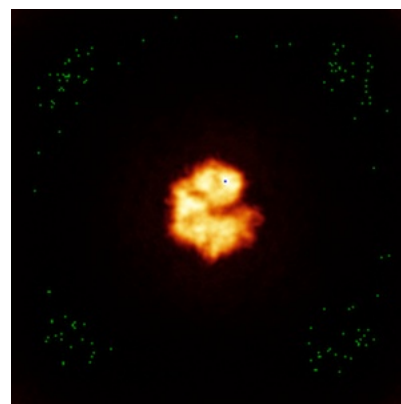
6.4.2 Raw map



X



Y

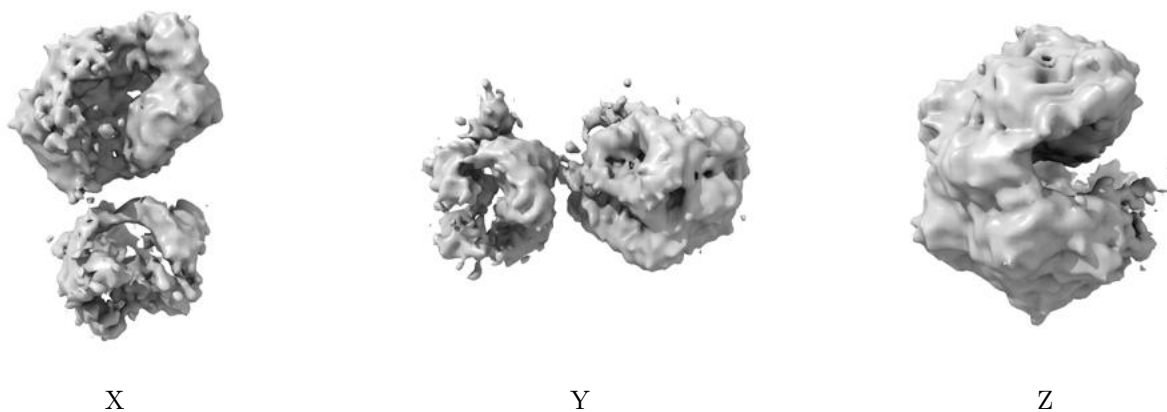


Z

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.

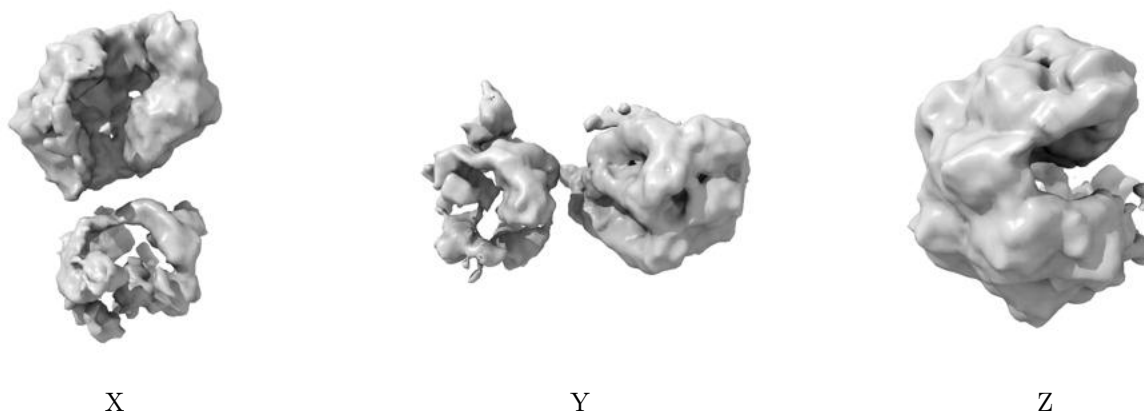
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.684. 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.

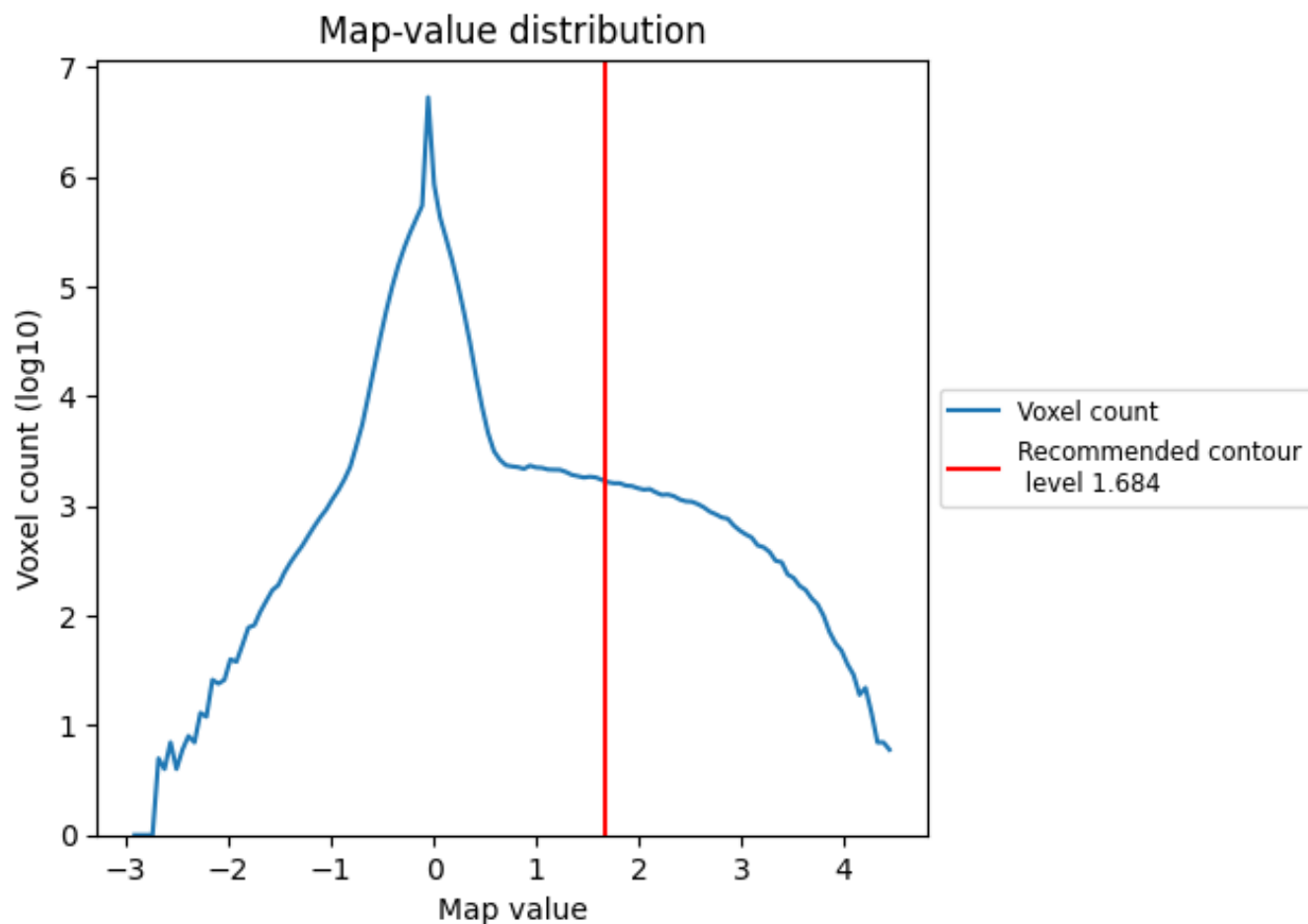
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

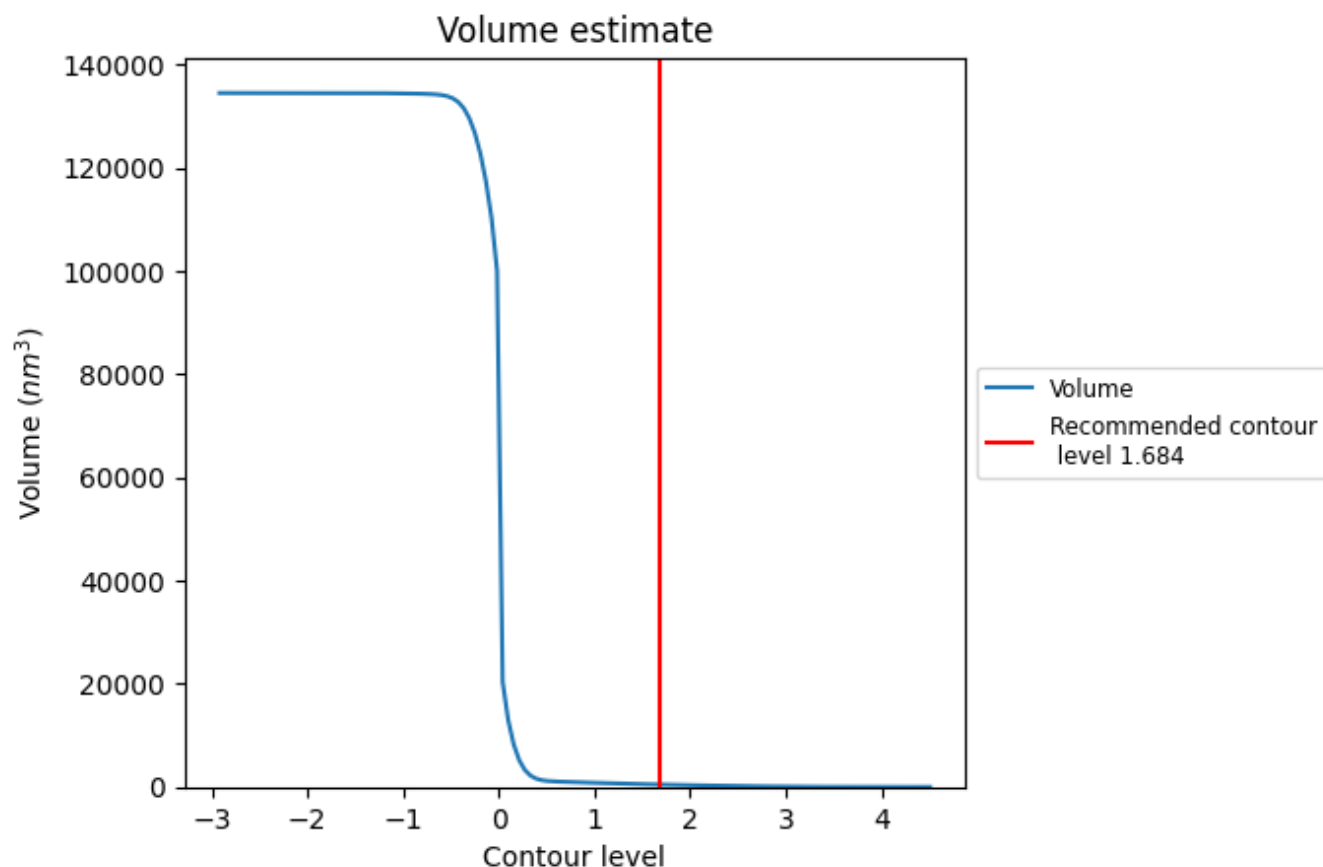
This section contains the results of statistical analysis of the map.

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.

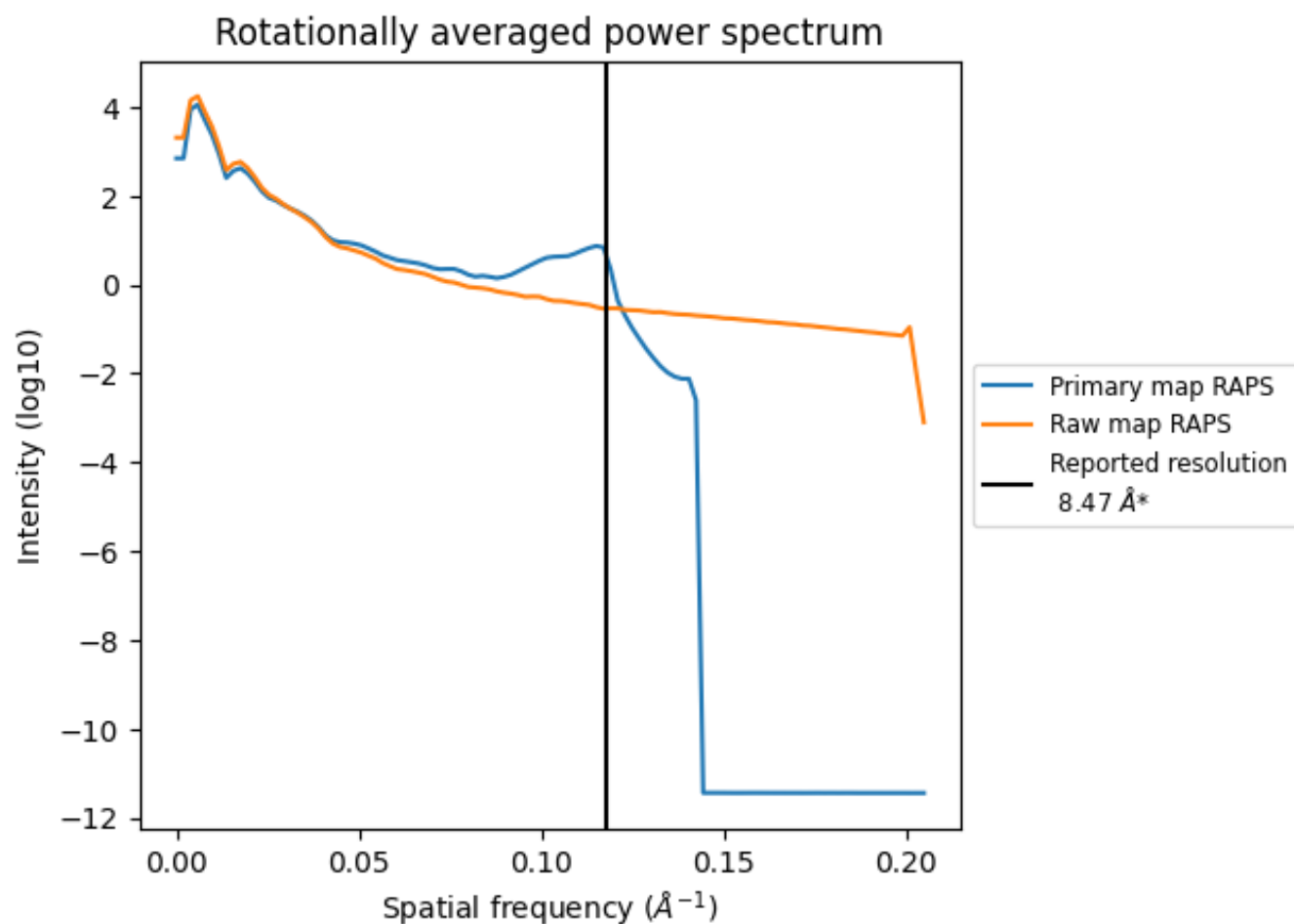
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 468 nm³; this corresponds to an approximate mass of 422 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 ⓘ

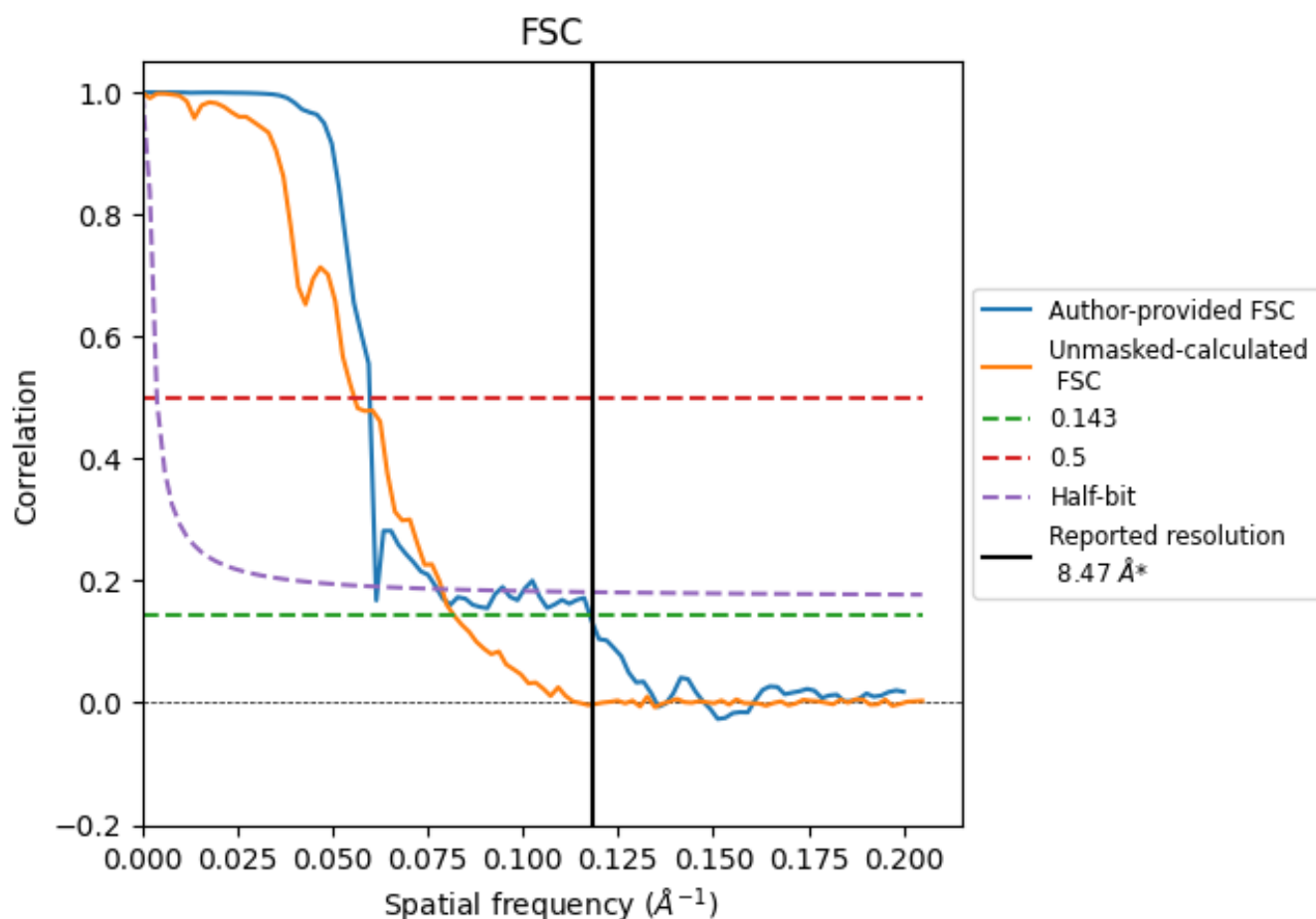


*Reported resolution corresponds to spatial frequency of 0.118 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.118 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.47	-	-
Author-provided FSC curve	8.50	16.72	16.29
Unmasked-calculated*	12.21	17.92	12.71

*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 12.21 differs from the reported value 8.47 by more than 10 %

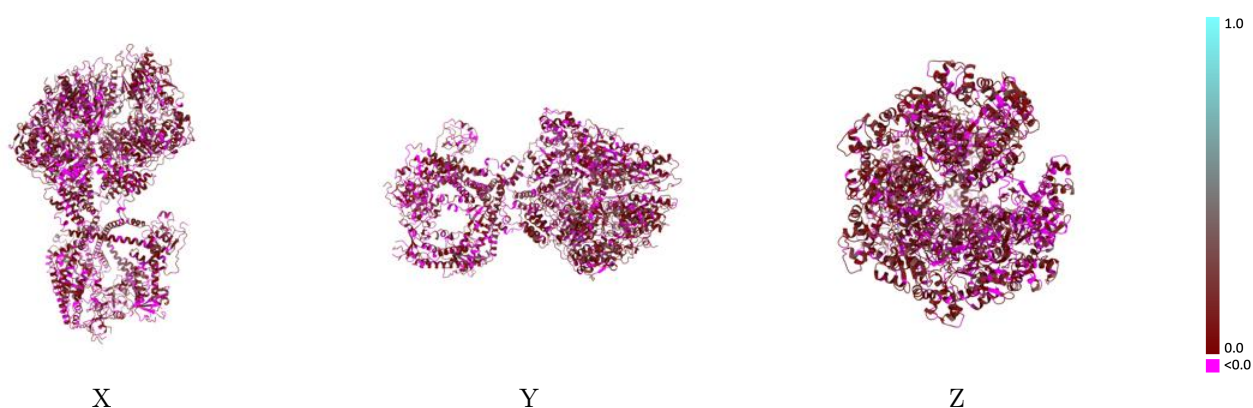
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17214 and PDB model 8OVG. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

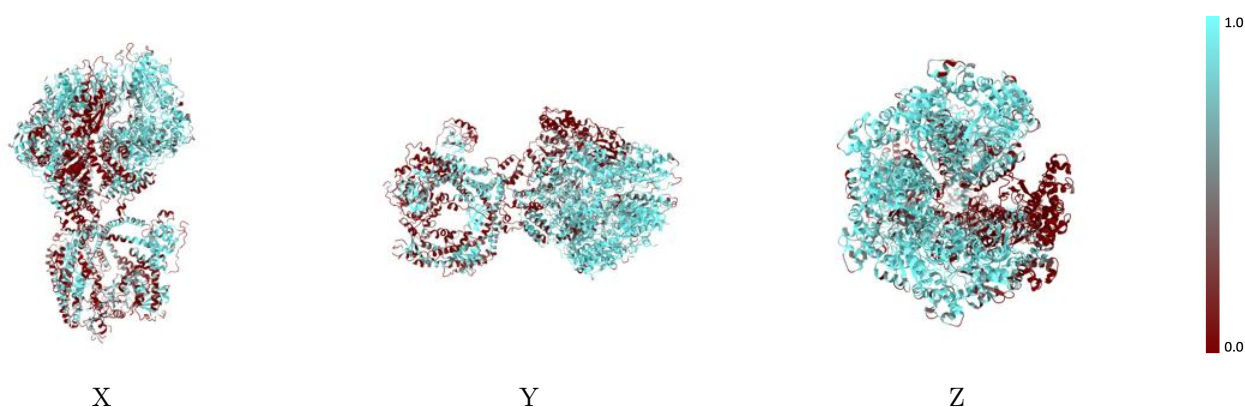
This section was not generated.

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



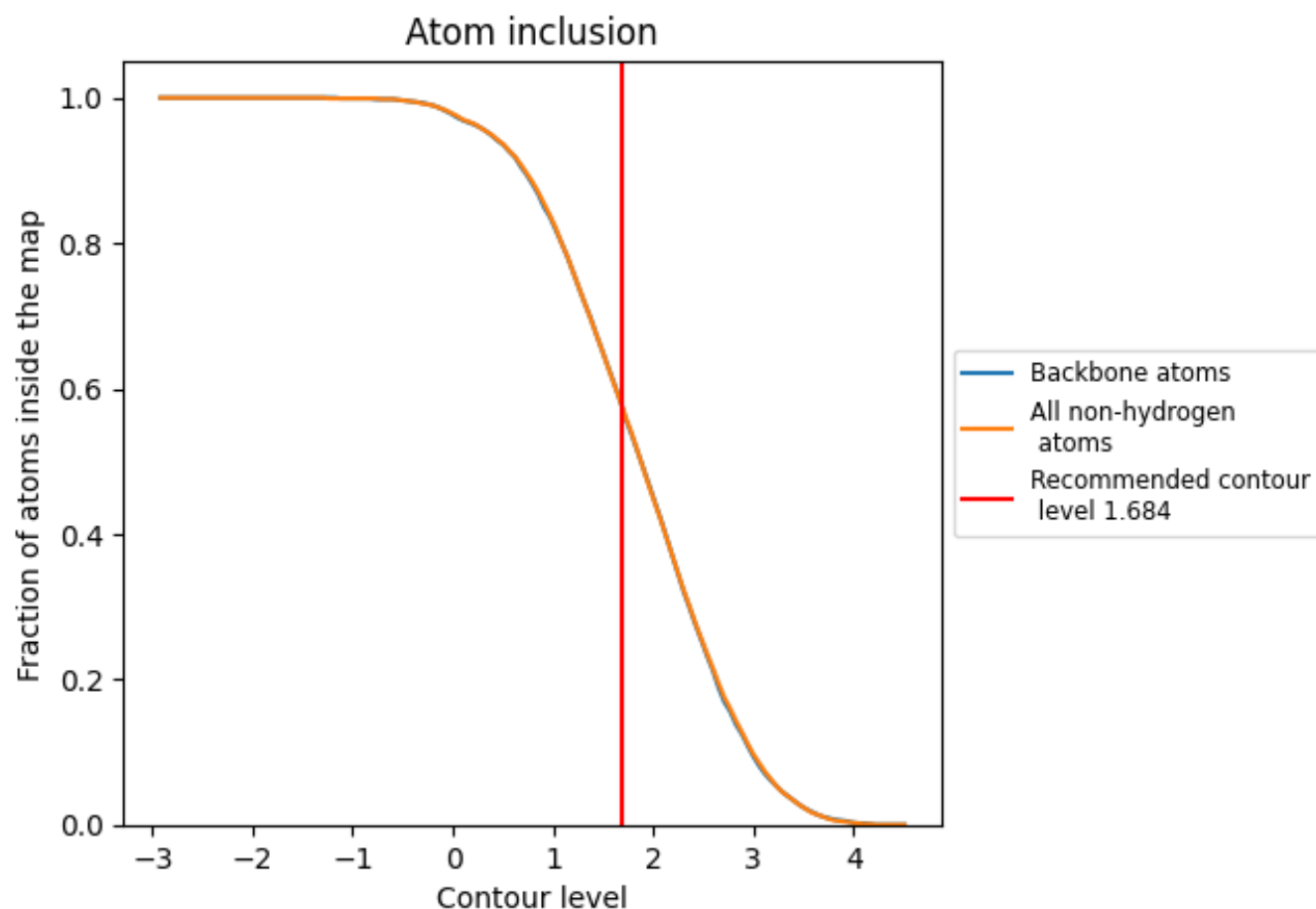
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.684).

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 58% 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 (1.684) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5780	0.0730
A	0.6200	0.0740
B	0.6730	0.0840
C	0.6930	0.0810
D	0.6840	0.0830
E	0.6880	0.0790
F	0.1540	0.0380

1.0

0.0

<0.0