



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:10 PM UTC

PDB ID : 8K95 / pdb_00008k95
EMDB ID : EMD-36975
Title : CryoEM structure of LonC protease open Hexamer, AGS
Authors : Li, M.; Hsieh, K.; Liu, H.; Zhang, S.; Gao, Y.; Gong, Q.; Zhang, K.; Chang, C.; Li, S.
Deposited on : 2023-07-31
Resolution : 3.05 Å(reported)

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<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
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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

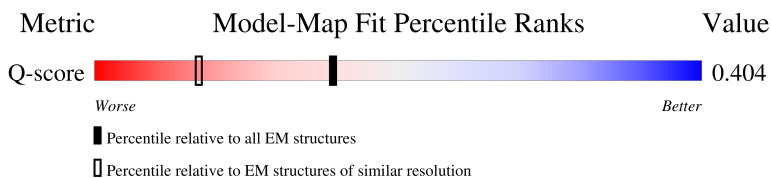
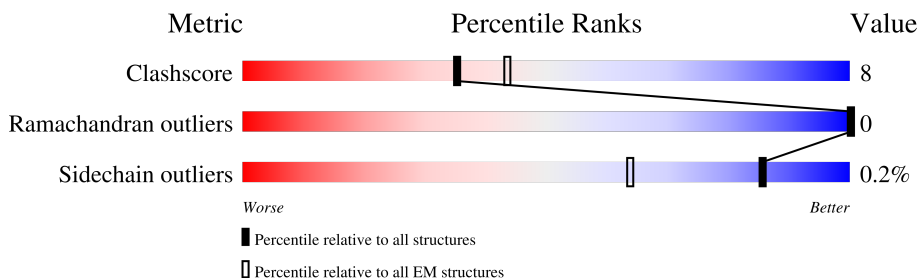
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.05 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	13971 (2.55 - 3.55)

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	732	34% 79% 19% .
1	B	732	11% 77% 21% .
1	C	732	5% 77% 21% .
1	D	732	. 81% 17% .

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Mol	Chain	Length	Quality of chain
1	E	732	6% 80% 18%
1	F	732	53% 77% 21%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 33481 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 endopeptidase La.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	719	Total	C	N	O	S	0	0
			5576	3525	1000	1044	7		
1	B	719	Total	C	N	O	S	0	0
			5576	3525	1000	1044	7		
1	C	719	Total	C	N	O	S	0	0
			5576	3525	1000	1044	7		
1	D	719	Total	C	N	O	S	0	0
			5576	3525	1000	1044	7		
1	E	719	Total	C	N	O	S	0	0
			5576	3525	1000	1044	7		
1	F	719	Total	C	N	O	S	0	0
			5576	3525	1000	1044	7		

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	720	LYS	-	expression tag	UNP C9DRU9
A	721	LEU	-	expression tag	UNP C9DRU9
A	722	ALA	-	expression tag	UNP C9DRU9
A	723	ALA	-	expression tag	UNP C9DRU9
A	724	ALA	-	expression tag	UNP C9DRU9
A	725	LEU	-	expression tag	UNP C9DRU9
A	726	GLU	-	expression tag	UNP C9DRU9
A	727	HIS	-	expression tag	UNP C9DRU9
A	728	HIS	-	expression tag	UNP C9DRU9
A	729	HIS	-	expression tag	UNP C9DRU9
A	730	HIS	-	expression tag	UNP C9DRU9
A	731	HIS	-	expression tag	UNP C9DRU9
A	732	HIS	-	expression tag	UNP C9DRU9
B	720	LYS	-	expression tag	UNP C9DRU9
B	721	LEU	-	expression tag	UNP C9DRU9
B	722	ALA	-	expression tag	UNP C9DRU9
B	723	ALA	-	expression tag	UNP C9DRU9
B	724	ALA	-	expression tag	UNP C9DRU9

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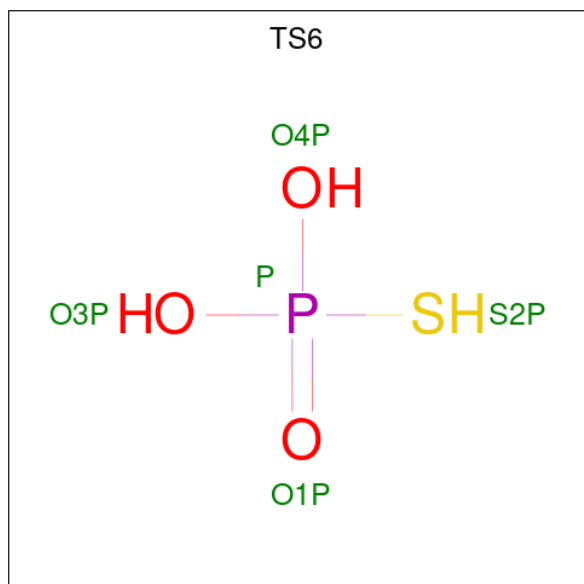
Chain	Residue	Modelled	Actual	Comment	Reference
B	725	LEU	-	expression tag	UNP C9DRU9
B	726	GLU	-	expression tag	UNP C9DRU9
B	727	HIS	-	expression tag	UNP C9DRU9
B	728	HIS	-	expression tag	UNP C9DRU9
B	729	HIS	-	expression tag	UNP C9DRU9
B	730	HIS	-	expression tag	UNP C9DRU9
B	731	HIS	-	expression tag	UNP C9DRU9
B	732	HIS	-	expression tag	UNP C9DRU9
C	720	LYS	-	expression tag	UNP C9DRU9
C	721	LEU	-	expression tag	UNP C9DRU9
C	722	ALA	-	expression tag	UNP C9DRU9
C	723	ALA	-	expression tag	UNP C9DRU9
C	724	ALA	-	expression tag	UNP C9DRU9
C	725	LEU	-	expression tag	UNP C9DRU9
C	726	GLU	-	expression tag	UNP C9DRU9
C	727	HIS	-	expression tag	UNP C9DRU9
C	728	HIS	-	expression tag	UNP C9DRU9
C	729	HIS	-	expression tag	UNP C9DRU9
C	730	HIS	-	expression tag	UNP C9DRU9
C	731	HIS	-	expression tag	UNP C9DRU9
C	732	HIS	-	expression tag	UNP C9DRU9
D	720	LYS	-	expression tag	UNP C9DRU9
D	721	LEU	-	expression tag	UNP C9DRU9
D	722	ALA	-	expression tag	UNP C9DRU9
D	723	ALA	-	expression tag	UNP C9DRU9
D	724	ALA	-	expression tag	UNP C9DRU9
D	725	LEU	-	expression tag	UNP C9DRU9
D	726	GLU	-	expression tag	UNP C9DRU9
D	727	HIS	-	expression tag	UNP C9DRU9
D	728	HIS	-	expression tag	UNP C9DRU9
D	729	HIS	-	expression tag	UNP C9DRU9
D	730	HIS	-	expression tag	UNP C9DRU9
D	731	HIS	-	expression tag	UNP C9DRU9
D	732	HIS	-	expression tag	UNP C9DRU9
E	720	LYS	-	expression tag	UNP C9DRU9
E	721	LEU	-	expression tag	UNP C9DRU9
E	722	ALA	-	expression tag	UNP C9DRU9
E	723	ALA	-	expression tag	UNP C9DRU9
E	724	ALA	-	expression tag	UNP C9DRU9
E	725	LEU	-	expression tag	UNP C9DRU9
E	726	GLU	-	expression tag	UNP C9DRU9
E	727	HIS	-	expression tag	UNP C9DRU9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	728	HIS	-	expression tag	UNP C9DRU9
E	729	HIS	-	expression tag	UNP C9DRU9
E	730	HIS	-	expression tag	UNP C9DRU9
E	731	HIS	-	expression tag	UNP C9DRU9
E	732	HIS	-	expression tag	UNP C9DRU9
F	720	LYS	-	expression tag	UNP C9DRU9
F	721	LEU	-	expression tag	UNP C9DRU9
F	722	ALA	-	expression tag	UNP C9DRU9
F	723	ALA	-	expression tag	UNP C9DRU9
F	724	ALA	-	expression tag	UNP C9DRU9
F	725	LEU	-	expression tag	UNP C9DRU9
F	726	GLU	-	expression tag	UNP C9DRU9
F	727	HIS	-	expression tag	UNP C9DRU9
F	728	HIS	-	expression tag	UNP C9DRU9
F	729	HIS	-	expression tag	UNP C9DRU9
F	730	HIS	-	expression tag	UNP C9DRU9
F	731	HIS	-	expression tag	UNP C9DRU9
F	732	HIS	-	expression tag	UNP C9DRU9

- Molecule 2 is Monothiophosphate (CCD ID: TS6) (formula: $\text{H}_3\text{O}_3\text{PS}$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	O	P	S	0
			5	3	1	1	
2	B	1	Total	O	P	S	0
			5	3	1	1	

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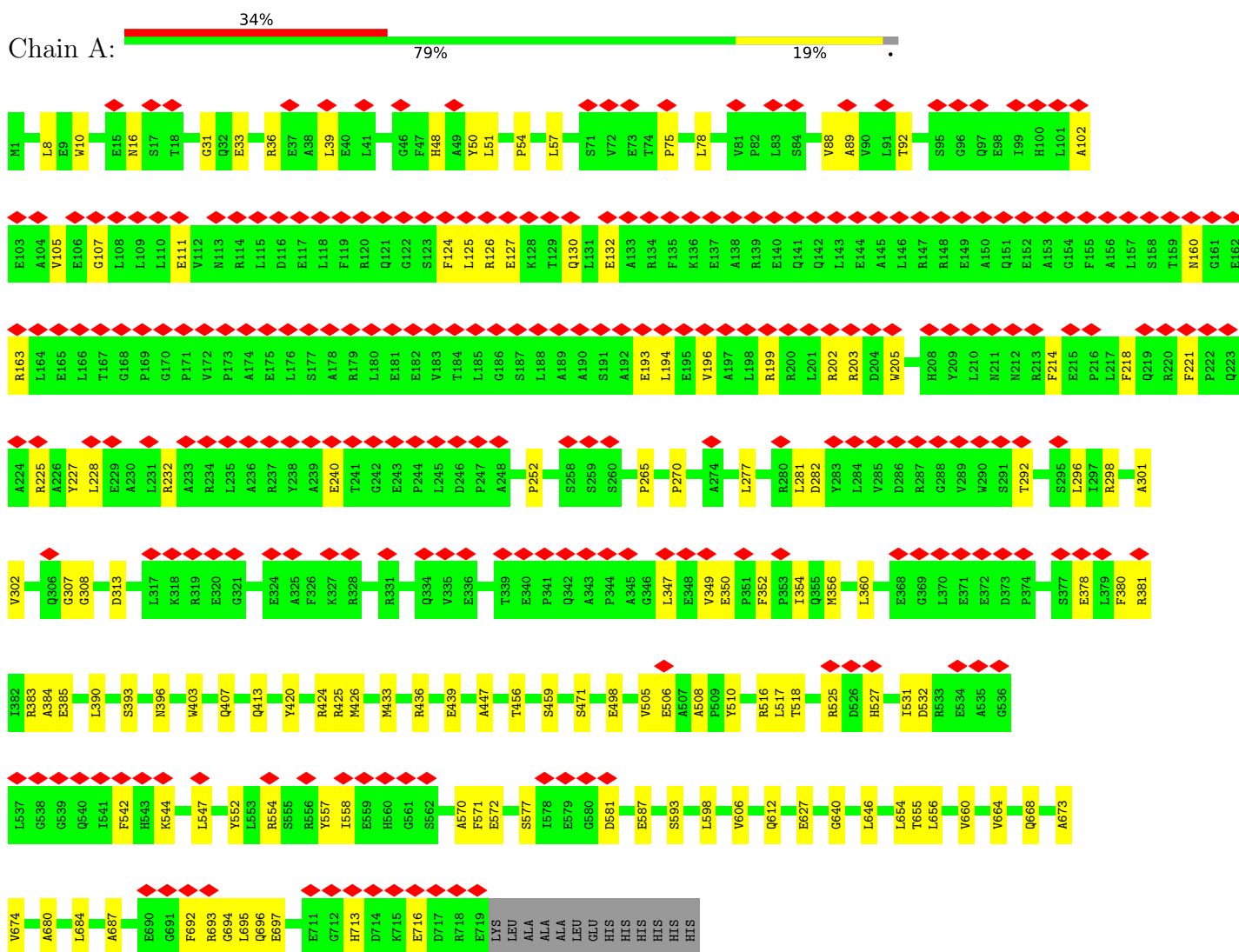
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Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	O	P	S	0
			5	3	1	1	
2	D	1	Total	O	P	S	0
			5	3	1	1	
2	E	1	Total	O	P	S	0
			5	3	1	1	

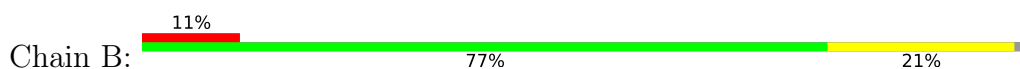
3 Residue-property plots [i](#)

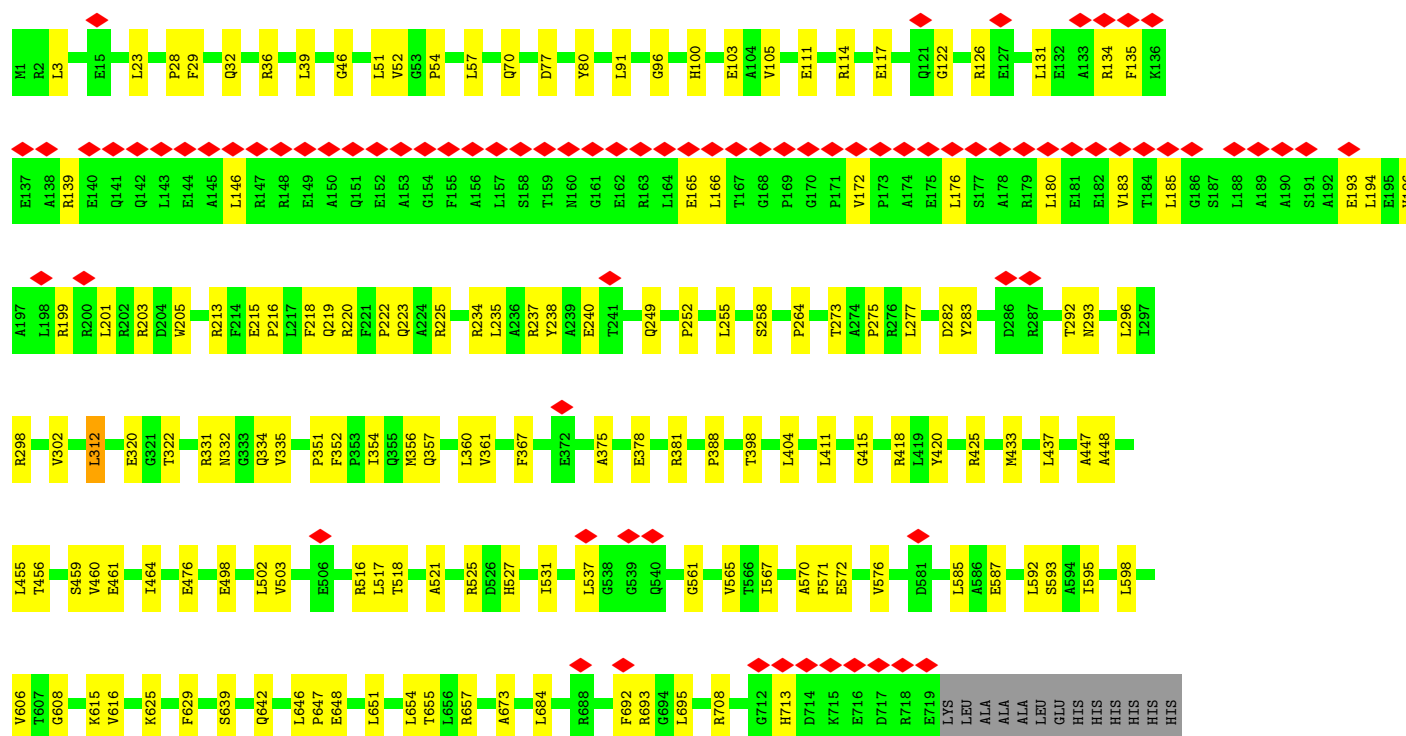
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: endopeptidase La

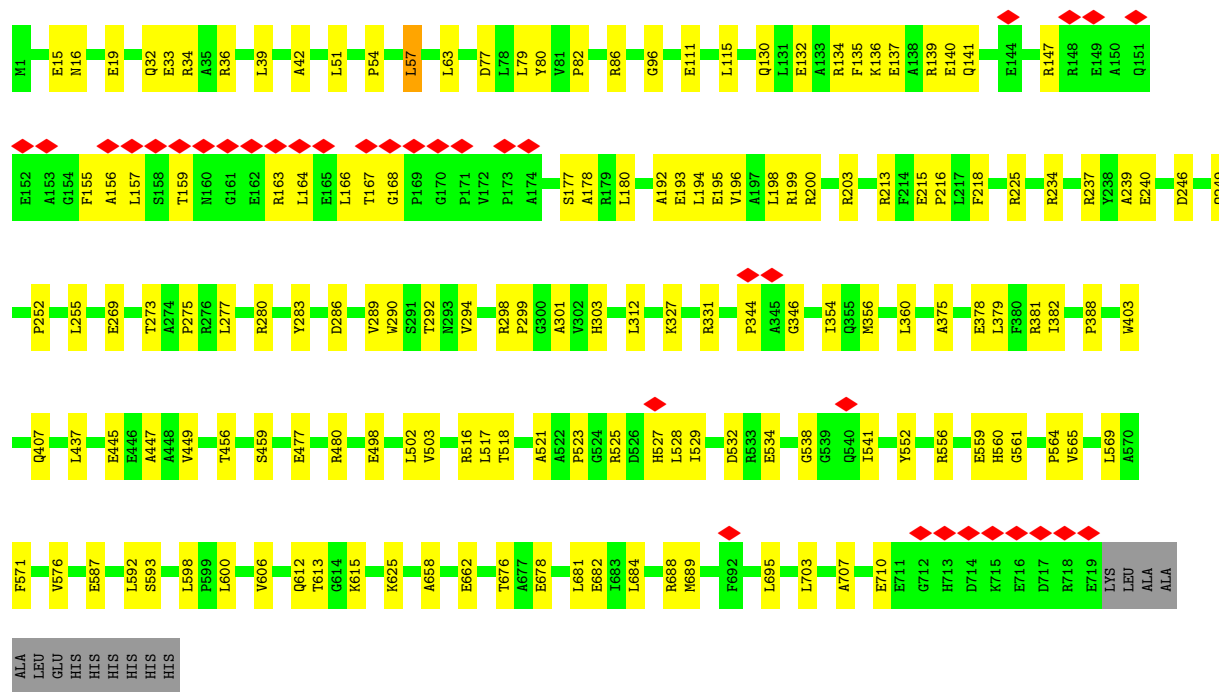
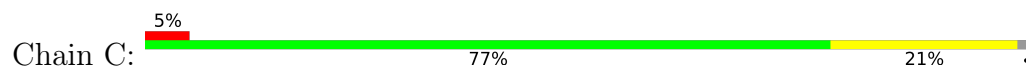


• Molecule 1: endopeptidase La

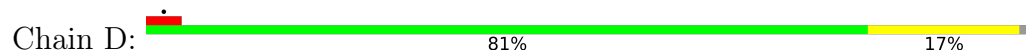


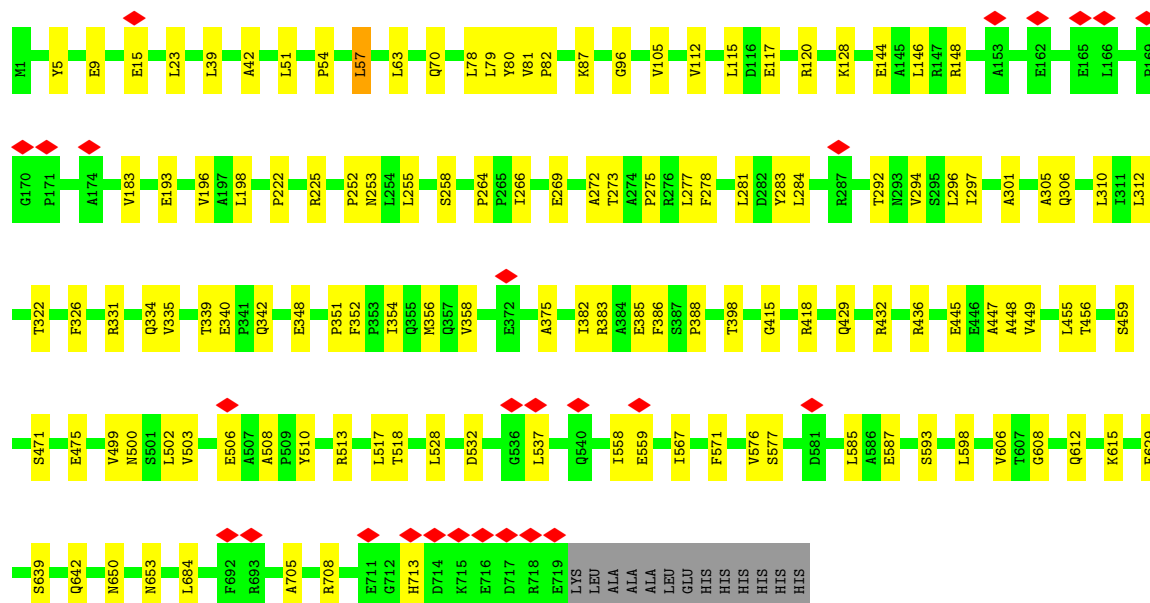


• Molecule 1: endopeptidase La

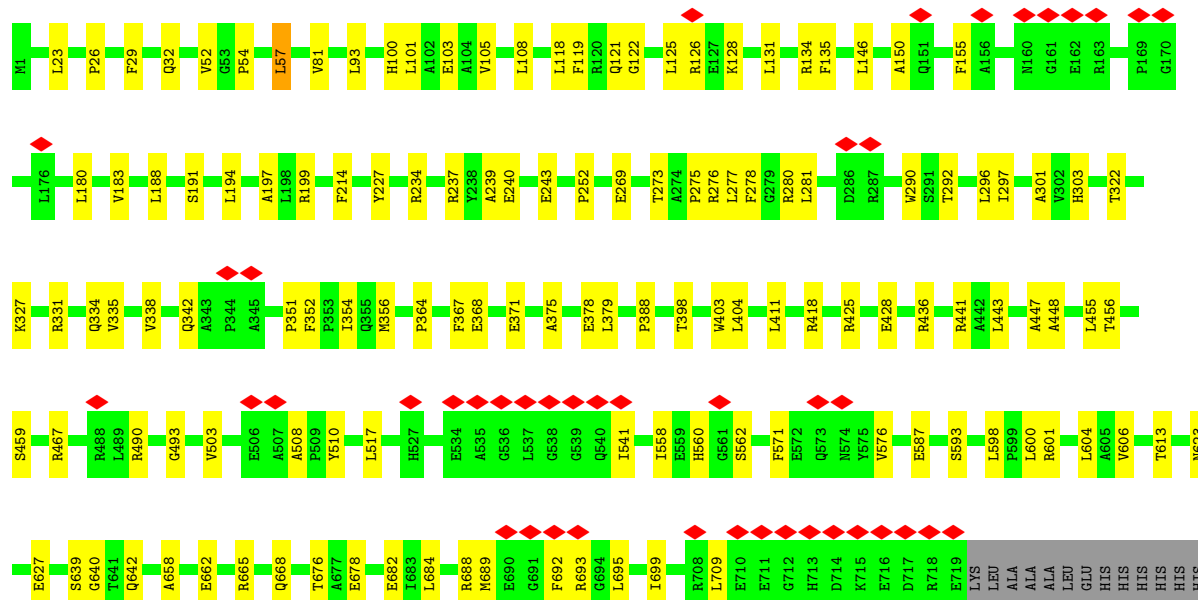
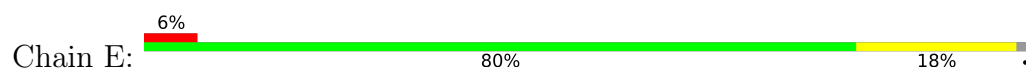


• Molecule 1: endopeptidase La

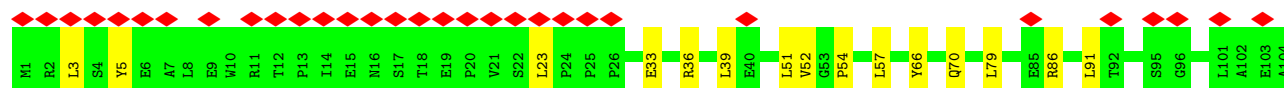
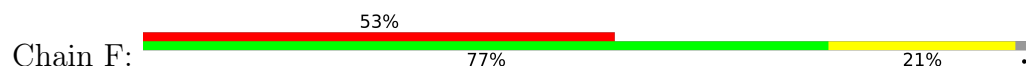




• Molecule 1: endopeptidase La



• Molecule 1: endopeptidase La



E678	E679	L681	E682	L683	L684	A685	G686	A687	R688	R689	E690	A691	E692	R693	G694	L695	Q696	E697	K698	L699	R700	A701	G702	L703	E704	A705	F706	A707	R708	L709	E710	E711	G712	H713	D714	K715	E716	D717	R718	E719	LYS	LEU	ALA	ALA	LEU	GLU	HIS	HIS	HIS	HIS	HIS								
A605	V606	T607	G608	A609	K615	V616	L617	A618	V619	G620	A621	A624	K625	V626	E627	G628	R631	V632	C633	K634	A635	L636	G637	A701	G639	G640	T641	Q642	G643	L646	A649	R650	L651	L654	T655	L656	R657	A658	E659	V660	L661	E662	A663	V664	R665	A666	G667	Q668	F669	H670	I671	Y672	A673						
K544	A545	V546	L547	T548	L549	A550	G551	Y552	S555	R556	Y557	I558	E559	H560	G561	S562	L563	P564	V565	T566	I567	S568	L569	A570	F571	E572	Q573	N574	Y575	V576	S577	T578	E579	G580	D581	S582	A583	G584	L585	A586	L588	V589	A590	A591	L592	S593	A594	T595	G596	N597	L598	P599	L600	R601	Q602	D603	L604		
E484	G485	V486	T487	R488	L489	R490	T491	T492	G493	R494	A495	V496	G497	E498	V499	N500	S501	L502	V503	V504	V505	E506	A507	A508	P509	Y510	Y511	G512	R513	P514	A515	R516	L517	T518	A519	R520	A521	A522	P523	G524	R525	D526	H469	L528	T529	S530	T531	D532	R533	E534	A535	G536	L537	G538	G539	Y540	T541	F542	H543
L411	T412	Q413	G414	C415	L416	T417	R418	L419	Y420	R424	R432	M433	T440	R441	A442	L443	A444	E445	E446	A447	A448	V449	L450	C451	C452	C453	L454	L455	T456	A457	E458	S459	V460	E461	Q462	A463	L464	A465	A466	R467	E468	H469	R470	S471	F472	L473	S474	E475	E476	E477	F478	L479	R480	A481	V482	Q483			
R331	N332	G333	Q334	T339	E340	F341	Q342	A343	P344	A345	G346	L347	E348	I354	Q355	K356	Q357	V358	V361	E365	E368	G369	L370	E371	E372	E378	L379	F380	R381	I382	R383	F386	S387	P388	T389	P394	E395	N396	C397	T398	A399	W403	L404	L405	A406	Q407	G408	F409	Q410										
A236	R237	Y238	A239	E240	T241	G242	E243	P244	P247	W250	R251	P252	N253	S260	G261	T262	A272	T273	A274	P275	R276	L277	F278	G279	R280	L281	D282	Y283	L284	V285	D286	R287	G288	V289	W290	S291	T292	R293	V294	S295	L296	T297	R298	A301	L310	L315	K318	R319	L228	E229	A230	L231	A232	R233	R234	L235			
E165	L166	T167	G168	P169	G170	P171	V172	P173	A174	E175	R179	L180	E181	R182	V183	T184	L185	G186	S187	A190	S191	A192	E193	L194	E195	V196	A197	L198	R199	R200	L201	R202	R203	D204	W205	W206	L207	N212	E215	P216	L217	F218	Q219	Q223	A224	L228	E229	A230	L231	A232	R233	R234	L235						
V105	E106	G107	L108	L109	L110	E111	V112	N113	R114	L115	D116	E117	L118	F119	R120	Q121	G122	S123	F124	L125	R126	E127	K128	T129	Q130	L131	E132	A133	R134	F135	K136	E137	A138	R139	E140	Q141	Q142	L143	E144	A145	L146	R147	R148	E149	A150	Q151	E152	G154	F155	A156	L157	S158	T159	N160	G161	E162	R163	L164	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118741	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.334	Depositor
Minimum map value	-0.687	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	275.52, 275.52, 275.52	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	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: TS6

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/5687	0.42	1/7721 (0.0%)
1	B	0.32	0/5687	0.47	0/7721
1	C	0.35	0/5687	0.48	0/7721
1	D	0.35	0/5687	0.48	3/7721 (0.0%)
1	E	0.30	0/5687	0.45	0/7721
1	F	0.17	0/5687	0.36	0/7721
All	All	0.29	0/34122	0.45	4/46326 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	PRO	N-CA-C	-5.94	105.27	113.53
1	D	559	GLU	N-CA-C	-5.42	105.33	113.89
1	D	266	ILE	CA-C-N	-5.16	115.82	122.99
1	D	266	ILE	C-N-CA	-5.16	115.82	122.99

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	5576	0	5589	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5576	0	5589	104	0
1	C	5576	0	5589	106	0
1	D	5576	0	5589	81	0
1	E	5576	0	5589	83	0
1	F	5576	0	5589	94	0
2	A	5	0	1	0	0
2	B	5	0	1	0	0
2	C	5	0	1	0	0
2	D	5	0	1	0	0
2	E	5	0	1	0	0
All	All	33481	0	33539	531	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 (531) 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:E:54:PRO:HG2	1:E:388:PRO:HB3	1.51	0.92
1:C:155:PHE:HE2	1:C:166:LEU:HB3	1.34	0.92
1:D:54:PRO:HG2	1:D:388:PRO:HB3	1.54	0.90
1:C:54:PRO:HG2	1:C:388:PRO:HB3	1.53	0.89
1:C:137:GLU:HG2	1:C:141:GLN:HE22	1.38	0.88
1:C:130:GLN:HB3	1:C:134:ARG:HH12	1.41	0.83
1:E:331:ARG:HH22	1:E:378:GLU:HB2	1.41	0.83
1:F:356:MET:HE2	1:F:358:VAL:HG22	1.62	0.82
1:C:498:GLU:OE2	1:C:516:ARG:NE	2.14	0.80
1:C:155:PHE:CE2	1:C:166:LEU:HB3	2.16	0.80
1:C:82:PRO:HB3	1:C:294:VAL:HG21	1.63	0.80
1:F:199:ARG:HB3	1:F:240:GLU:HG3	1.63	0.79
1:B:54:PRO:HG2	1:B:388:PRO:HB3	1.65	0.78
1:D:78:LEU:HD12	1:D:306:GLN:HG3	1.65	0.78
1:A:531:ILE:HD12	1:A:570:ALA:HB2	1.67	0.77
1:A:199:ARG:HB3	1:A:240:GLU:HG3	1.69	0.74
1:F:86:ARG:NH1	1:F:346:GLY:O	2.20	0.74
1:E:273:THR:HG22	1:E:275:PRO:HD2	1.67	0.74
1:A:203:ARG:HB2	1:A:240:GLU:HB2	1.69	0.74
1:B:713:HIS:HB2	1:C:561:GLY:H	1.54	0.73
1:D:713:HIS:CE1	1:E:562:SER:H	2.07	0.72
1:C:137:GLU:O	1:C:141:GLN:NE2	2.23	0.72
1:E:606:VAL:HG21	1:E:684:LEU:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:ARG:HG3	1:F:236:ALA:HB1	1.72	0.70
1:C:115:LEU:HD21	1:C:239:ALA:HB2	1.72	0.70
1:E:23:LEU:HD22	1:E:398:THR:HG23	1.74	0.69
1:A:692:PHE:O	1:A:693:ARG:HD3	1.93	0.69
1:C:273:THR:HG22	1:C:275:PRO:HD2	1.73	0.68
1:E:662:GLU:OE1	1:E:665:ARG:NH2	2.27	0.68
1:A:593:SER:OG	1:A:598:LEU:O	2.11	0.68
1:C:86:ARG:NH1	1:C:346:GLY:O	2.27	0.67
1:C:606:VAL:HG21	1:C:684:LEU:HD11	1.76	0.67
1:D:475:GLU:OE2	1:D:513:ARG:NH2	2.28	0.67
1:F:331:ARG:HH22	1:F:378:GLU:HB2	1.60	0.67
1:E:689:MET:HG2	1:E:695:LEU:HB2	1.77	0.67
1:B:502:LEU:HD21	1:B:629:PHE:HB2	1.76	0.66
1:A:378:GLU:OE1	1:A:381:ARG:NH2	2.29	0.66
1:A:221:PHE:O	1:A:225:ARG:NH1	2.25	0.66
1:D:281:LEU:HD12	1:D:339:THR:HG22	1.78	0.66
1:C:130:GLN:HB3	1:C:134:ARG:NH1	2.11	0.65
1:F:54:PRO:HG2	1:F:388:PRO:HB3	1.79	0.65
1:C:163:ARG:NH1	1:C:164:LEU:O	2.29	0.65
1:A:694:GLY:N	1:A:697:GLU:OE2	2.25	0.65
1:F:571:PHE:HB3	1:F:576:VAL:HG11	1.79	0.64
1:A:50:TYR:HB3	1:A:360:LEU:HB2	1.80	0.64
1:B:503:VAL:HG21	1:B:576:VAL:HG22	1.80	0.64
1:B:593:SER:OG	1:B:598:LEU:O	2.15	0.64
1:E:125:LEU:HD23	1:E:128:LYS:HD3	1.80	0.64
1:E:571:PHE:HB3	1:E:576:VAL:HG11	1.80	0.64
1:D:354:ILE:HG23	1:D:356:MET:HG2	1.79	0.63
1:F:511:TRP:HA	1:F:624:ALA:HB1	1.79	0.63
1:E:428:GLU:OE2	1:E:623:ASN:ND2	2.28	0.63
1:F:465:ALA:O	1:F:469:HIS:ND1	2.31	0.63
1:B:418:ARG:NH1	1:B:461:GLU:OE2	2.31	0.63
1:C:147:ARG:CZ	1:C:157:LEU:HB2	2.28	0.63
1:B:54:PRO:HD2	1:B:57:LEU:HD11	1.80	0.62
1:D:593:SER:OG	1:D:598:LEU:O	2.15	0.62
1:B:215:GLU:HG3	1:B:216:PRO:HD3	1.82	0.62
1:B:567:ILE:HD11	1:B:595:ILE:HD11	1.81	0.62
1:E:639:SER:OG	1:E:642:GLN:NE2	2.33	0.62
1:F:354:ILE:HG23	1:F:356:MET:HG2	1.81	0.62
1:A:447:ALA:O	1:A:459:SER:OG	2.19	0.61
1:A:716:GLU:OE2	1:B:708:ARG:NH2	2.34	0.61
1:C:525:ARG:HH11	1:C:527:HIS:HB3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:VAL:HG11	1:B:252:PRO:HD3	1.81	0.61
1:A:506:GLU:HG2	1:A:577:SER:HB3	1.81	0.61
1:C:286:ASP:HB3	1:C:289:VAL:HB	1.83	0.61
1:F:282:ASP:OD2	1:F:298:ARG:NE	2.30	0.61
1:A:606:VAL:HG21	1:A:684:LEU:HD11	1.83	0.60
1:E:105:VAL:HG11	1:E:252:PRO:HD3	1.83	0.60
1:C:203:ARG:HG3	1:C:240:GLU:HB2	1.82	0.60
1:B:517:LEU:HB2	1:B:571:PHE:CE1	2.36	0.60
1:C:593:SER:OG	1:C:598:LEU:O	2.20	0.59
1:A:51:LEU:HA	1:A:384:ALA:HB3	1.85	0.59
1:D:518:THR:HG21	1:E:613:THR:HB	1.85	0.59
1:D:383:ARG:NE	1:D:385:GLU:OE2	2.33	0.59
1:B:517:LEU:HB2	1:B:571:PHE:HE1	1.67	0.59
1:D:105:VAL:HG11	1:D:252:PRO:HD3	1.84	0.59
1:C:516:ARG:HH12	1:D:615:LYS:HD3	1.68	0.59
1:F:456:THR:HG23	1:F:459:SER:H	1.67	0.59
1:F:5:TYR:HE1	1:F:661:LEU:HB3	1.68	0.59
1:F:404:LEU:HB2	1:F:411:LEU:HD11	1.84	0.59
1:F:640:GLY:HA2	1:F:668:GLN:HA	1.85	0.59
1:A:424:ARG:HA	1:A:433:MET:HA	1.85	0.58
1:A:456:THR:HG23	1:A:459:SER:H	1.67	0.58
1:E:640:GLY:HA2	1:E:668:GLN:HA	1.83	0.58
1:A:10:TRP:O	1:A:424:ARG:NH2	2.35	0.58
1:C:111:GLU:OE2	1:C:213:ARG:NH2	2.37	0.58
1:F:164:LEU:HB3	1:F:180:LEU:HD11	1.86	0.58
1:A:78:LEU:HG	1:A:92:THR:HG22	1.86	0.57
1:B:606:VAL:HG21	1:B:684:LEU:HD11	1.85	0.57
1:B:525:ARG:HG3	1:B:527:HIS:H	1.69	0.57
1:B:334:GLN:HB3	1:B:351:PRO:HB2	1.86	0.57
1:C:552:TYR:OH	1:C:678:GLU:OE2	2.23	0.57
1:C:77:ASP:OD2	1:C:96:GLY:N	2.36	0.57
1:A:426:MET:HE1	1:A:439:GLU:HB3	1.87	0.57
1:F:378:GLU:HA	1:F:381:ARG:HH21	1.70	0.57
1:F:114:ARG:NH2	1:F:117:GLU:OE2	2.34	0.57
1:C:137:GLU:HG2	1:C:141:GLN:NE2	2.16	0.56
1:A:516:ARG:HH12	1:B:615:LYS:HD3	1.71	0.56
1:B:131:LEU:HD21	1:B:201:LEU:HD22	1.88	0.56
1:C:556:ARG:NH1	1:C:678:GLU:OE2	2.38	0.56
1:E:57:LEU:HD12	1:E:436:ARG:HG2	1.87	0.56
1:C:516:ARG:NH1	1:D:615:LYS:HD3	2.20	0.56
1:B:456:THR:HG23	1:B:459:SER:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:354:ILE:HG23	1:E:356:MET:HG2	1.87	0.56
1:B:23:LEU:HD22	1:B:398:THR:HG23	1.88	0.56
1:C:177:SER:O	1:C:180:LEU:HG	2.05	0.56
1:C:456:THR:HG23	1:C:459:SER:H	1.70	0.56
1:F:525:ARG:HG2	1:F:527:HIS:H	1.71	0.56
1:B:100:HIS:HB3	1:B:220:ARG:HH12	1.70	0.56
1:B:165:GLU:HA	1:B:180:LEU:HD21	1.86	0.56
1:C:538:GLY:HA2	1:C:541:ILE:HG22	1.88	0.56
1:C:525:ARG:NH1	1:C:527:HIS:HB3	2.21	0.56
1:B:460:VAL:O	1:B:464:ILE:HG12	2.05	0.55
1:D:112:VAL:HA	1:D:115:LEU:HD12	1.87	0.55
1:D:447:ALA:O	1:D:459:SER:OG	2.25	0.55
1:B:235:LEU:O	1:B:238:TYR:HB3	2.06	0.55
1:B:531:ILE:HD12	1:B:570:ALA:HB2	1.89	0.55
1:C:200:ARG:HG2	1:C:203:ARG:HH21	1.71	0.55
1:D:585:LEU:N	1:D:608:GLY:O	2.31	0.55
1:D:606:VAL:HG21	1:D:684:LEU:HD11	1.87	0.55
1:B:302:VAL:HA	1:B:356:MET:HE1	1.87	0.55
1:C:199:ARG:HB3	1:C:240:GLU:HG3	1.88	0.55
1:A:674:VAL:HG21	1:A:680:ALA:HB2	1.88	0.55
1:B:282:ASP:OD2	1:B:298:ARG:NE	2.32	0.55
1:A:218:PHE:HA	1:A:225:ARG:NH2	2.21	0.55
1:D:146:LEU:HB2	1:D:183:VAL:HG21	1.88	0.55
1:D:713:HIS:NE2	1:E:560:HIS:HB3	2.22	0.55
1:E:447:ALA:O	1:E:459:SER:OG	2.25	0.55
1:A:471:SER:HB2	1:A:510:TYR:OH	2.07	0.54
1:E:277:LEU:HD12	1:E:322:THR:HG21	1.90	0.54
1:A:640:GLY:HA2	1:A:668:GLN:HA	1.89	0.54
1:C:678:GLU:OE1	1:C:689:MET:HE2	2.08	0.54
1:C:147:ARG:NH2	1:C:157:LEU:HB2	2.23	0.54
1:A:498:GLU:OE2	1:A:518:THR:OG1	2.23	0.54
1:E:237:ARG:NH2	1:E:243:GLU:OE2	2.35	0.54
1:A:292:THR:HA	1:A:296:LEU:HD12	1.90	0.54
1:A:687:ALA:HB3	1:A:695:LEU:HD21	1.89	0.53
1:D:117:GLU:OE2	1:D:120:ARG:NH1	2.41	0.53
1:E:275:PRO:HB3	1:E:280:ARG:HB3	1.89	0.53
1:B:335:VAL:O	1:B:352:PHE:N	2.36	0.53
1:B:447:ALA:O	1:B:459:SER:OG	2.26	0.53
1:B:598:LEU:HD13	1:B:695:LEU:HD12	1.91	0.53
1:E:118:LEU:HA	1:E:121:GLN:HG2	1.91	0.53
1:C:682:GLU:HG2	1:C:688:ARG:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:PHE:CD1	1:D:335:VAL:HG21	2.44	0.53
1:E:558:ILE:O	1:E:558:ILE:HG13	2.08	0.53
1:E:709:LEU:HD13	1:F:558:ILE:HG22	1.90	0.53
1:F:494:ARG:HG2	1:F:601:ARG:HA	1.91	0.53
1:A:127:GLU:HB2	1:A:205:TRP:HH2	1.73	0.53
1:A:552:TYR:HB2	1:A:612:GLN:HA	1.91	0.53
1:D:23:LEU:HD22	1:D:398:THR:HG23	1.90	0.53
1:A:54:PRO:HD2	1:A:57:LEU:HD11	1.91	0.53
1:B:166:LEU:HD13	1:B:176:LEU:HB3	1.91	0.53
1:E:682:GLU:OE1	1:E:688:ARG:HA	2.08	0.53
1:F:277:LEU:HA	1:F:301:ALA:HB3	1.90	0.53
1:F:420:TYR:CZ	1:F:424:ARG:HD2	2.43	0.53
1:C:136:LYS:O	1:C:140:GLU:HG2	2.09	0.53
1:A:132:GLU:HG2	1:A:194:LEU:HD11	1.91	0.52
1:E:334:GLN:HB3	1:E:351:PRO:HB2	1.90	0.52
1:F:646:LEU:HD11	1:F:654:LEU:HD11	1.90	0.52
1:A:126:ARG:HH21	1:A:130:GLN:HB2	1.73	0.52
1:B:218:PHE:HB3	1:B:225:ARG:HH11	1.73	0.52
1:D:503:VAL:HG11	1:D:576:VAL:HG13	1.90	0.52
1:D:517:LEU:HD11	1:D:587:GLU:HG2	1.92	0.52
1:C:269:GLU:HG3	1:C:301:ALA:HB2	1.91	0.52
1:F:193:GLU:HA	1:F:196:VAL:HG22	1.91	0.52
1:A:160:ASN:HB2	1:A:163:ARG:HG3	1.92	0.52
1:C:689:MET:SD	1:C:695:LEU:HB2	2.50	0.52
1:A:542:PHE:HB3	1:A:547:LEU:HD21	1.92	0.52
1:C:132:GLU:HB3	1:C:136:LYS:NZ	2.25	0.52
1:A:554:ARG:HH12	1:A:558:ILE:HG22	1.75	0.52
1:F:543:HIS:HB3	1:F:546:VAL:HG12	1.92	0.52
1:B:518:THR:O	1:C:612:GLN:NE2	2.44	0.51
1:B:234:ARG:HD2	1:B:237:ARG:HD2	1.92	0.51
1:D:284:LEU:HD23	1:D:296:LEU:HD11	1.91	0.51
1:F:231:LEU:HD23	1:F:250:TRP:HE3	1.76	0.51
1:F:446:GLU:OE1	1:F:467:ARG:NE	2.43	0.51
1:B:571:PHE:CD2	1:B:576:VAL:HG11	2.45	0.51
1:A:50:TYR:CB	1:A:360:LEU:HB2	2.40	0.51
1:B:572:GLU:OE2	1:C:615:LYS:NZ	2.44	0.51
1:A:281:LEU:HD21	1:A:347:LEU:HD13	1.93	0.51
1:C:135:PHE:HB3	1:C:139:ARG:HH12	1.75	0.51
1:B:692:PHE:C	1:B:693:ARG:HD3	2.35	0.50
1:F:310:LEU:HD23	1:F:356:MET:HE1	1.92	0.50
1:A:517:LEU:HD11	1:A:587:GLU:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:517:LEU:HD12	1:C:571:PHE:CZ	2.47	0.50
1:D:517:LEU:HD12	1:D:571:PHE:CZ	2.46	0.50
1:F:552:TYR:OH	1:F:678:GLU:OE2	2.29	0.50
1:A:88:VAL:HB	1:A:349:VAL:HG22	1.94	0.50
1:E:122:GLY:O	1:E:126:ARG:HG3	2.11	0.50
1:A:31:GLY:HA3	1:A:390:LEU:HD22	1.93	0.50
1:E:119:PHE:HZ	1:E:239:ALA:HB1	1.77	0.50
1:A:557:TYR:HE1	1:A:696:GLN:HG3	1.75	0.50
1:A:50:TYR:OH	1:A:383:ARG:NH1	2.34	0.50
1:A:125:LEU:HD11	1:B:185:LEU:HD12	1.94	0.50
1:A:517:LEU:HD12	1:A:571:PHE:CE1	2.47	0.50
1:B:425:ARG:HG2	1:B:657:ARG:HH12	1.76	0.50
1:F:39:LEU:HD21	1:F:51:LEU:HD11	1.94	0.50
1:F:146:LEU:HB2	1:F:183:VAL:HG21	1.94	0.49
1:F:480:ARG:HE	1:F:484:GLU:HG2	1.76	0.49
1:A:277:LEU:HD23	1:A:301:ALA:HB3	1.93	0.49
1:E:508:ALA:C	1:E:510:TYR:H	2.20	0.49
1:D:650:ASN:HD22	1:D:653:ASN:HD22	1.59	0.49
1:B:517:LEU:HD21	1:B:587:GLU:HA	1.94	0.49
1:C:517:LEU:HD11	1:C:587:GLU:HG2	1.94	0.49
1:E:125:LEU:HA	1:E:128:LYS:HG2	1.94	0.49
1:D:79:LEU:HD12	1:D:252:PRO:HB2	1.93	0.49
1:F:592:LEU:HD13	1:F:681:LEU:HD22	1.95	0.49
1:F:526:ASP:HA	1:F:563:LEU:HB3	1.95	0.49
1:D:713:HIS:CE1	1:E:560:HIS:HB3	2.48	0.49
1:E:278:PHE:CD1	1:E:335:VAL:HG21	2.47	0.48
1:E:676:THR:HG22	1:E:678:GLU:H	1.78	0.48
1:C:218:PHE:CD1	1:C:225:ARG:HD2	2.49	0.48
1:D:5:TYR:OH	1:D:9:GLU:OE2	2.19	0.48
1:E:100:HIS:O	1:E:103:GLU:HG2	2.12	0.48
1:E:593:SER:OG	1:E:598:LEU:O	2.26	0.48
1:B:448:ALA:HB2	1:B:455:LEU:HD11	1.95	0.48
1:B:537:LEU:H	1:C:541:ILE:HD12	1.79	0.48
1:C:447:ALA:O	1:C:459:SER:OG	2.31	0.48
1:F:52:VAL:O	1:F:386:PHE:N	2.45	0.48
1:A:203:ARG:HD3	1:A:240:GLU:OE1	2.14	0.48
1:B:354:ILE:HG23	1:B:356:MET:HG2	1.95	0.48
1:E:456:THR:HG23	1:E:459:SER:H	1.78	0.48
1:F:628:GLY:HA2	1:F:631:ARG:HE	1.78	0.48
1:A:554:ARG:NH1	1:A:558:ILE:HG22	2.28	0.48
1:C:354:ILE:HG23	1:C:356:MET:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:LEU:HD12	1:D:436:ARG:HG2	1.96	0.48
1:E:692:PHE:CE2	1:E:693:ARG:HG3	2.48	0.48
1:B:273:THR:HG22	1:B:275:PRO:HD2	1.95	0.48
1:C:445:GLU:O	1:C:449:VAL:HG23	2.14	0.48
1:E:135:PHE:HD2	1:E:194:LEU:HD12	1.78	0.48
1:E:327:LYS:HD2	1:E:375:ALA:HB3	1.96	0.48
1:F:502:LEU:HB3	1:F:625:LYS:HB3	1.95	0.48
1:B:282:ASP:HB2	1:B:296:LEU:HB3	1.95	0.48
1:C:331:ARG:HD2	1:C:379:LEU:HD21	1.95	0.48
1:C:564:PRO:HD2	1:C:703:LEU:HD22	1.96	0.48
1:D:39:LEU:HD11	1:D:51:LEU:HD11	1.95	0.48
1:E:490:ARG:HH22	1:E:493:GLY:HA3	1.78	0.48
1:B:415:GLY:HA3	1:B:455:LEU:O	2.14	0.47
1:C:534:GLU:HG3	1:C:538:GLY:HA3	1.95	0.47
1:A:75:PRO:HB3	1:A:307:GLY:HA3	1.96	0.47
1:A:544:LYS:HE3	1:A:581:ASP:HA	1.95	0.47
1:D:273:THR:HG23	1:D:275:PRO:HD2	1.96	0.47
1:D:532:ASP:OD2	1:D:571:PHE:N	2.47	0.47
1:E:503:VAL:HG21	1:E:576:VAL:HG23	1.96	0.47
1:E:695:LEU:O	1:E:699:ILE:HD12	2.15	0.47
1:F:498:GLU:HG3	1:F:518:THR:HG22	1.96	0.47
1:A:107:GLY:O	1:A:111:GLU:HG3	2.14	0.47
1:A:713:HIS:HB2	1:B:561:GLY:H	1.79	0.47
1:B:425:ARG:HA	1:B:655:THR:HG21	1.96	0.47
1:E:281:LEU:HD13	1:E:297:ILE:HG12	1.95	0.47
1:A:265:PRO:HG2	1:A:308:GLY:HA3	1.96	0.47
1:B:222:PRO:O	1:B:225:ARG:HG2	2.14	0.47
1:C:194:LEU:HD23	1:C:198:LEU:HD23	1.95	0.47
1:C:525:ARG:HH22	1:C:529:ILE:HD11	1.79	0.47
1:C:658:ALA:O	1:C:662:GLU:HG2	2.15	0.47
1:F:292:THR:HA	1:F:296:LEU:HD12	1.96	0.47
1:D:82:PRO:HG3	1:D:294:VAL:HG11	1.97	0.47
1:E:425:ARG:NH2	1:E:627:GLU:OE1	2.48	0.47
1:E:517:LEU:HD21	1:E:587:GLU:HA	1.97	0.47
1:F:593:SER:OG	1:F:598:LEU:O	2.32	0.47
1:B:122:GLY:O	1:B:126:ARG:HG2	2.15	0.47
1:D:272:ALA:O	1:D:322:THR:HG21	2.15	0.47
1:F:530:SER:HB3	1:F:533:ARG:HB2	1.94	0.47
1:B:378:GLU:O	1:B:381:ARG:NH2	2.48	0.47
1:C:477:GLU:HG2	1:C:480:ARG:NH2	2.30	0.47
1:E:93:LEU:HD11	1:E:101:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:LEU:HB2	1:B:361:VAL:HG22	1.97	0.47
1:C:156:ALA:HB3	1:C:167:THR:O	2.14	0.47
1:C:327:LYS:HD2	1:C:375:ALA:HB3	1.96	0.47
1:D:39:LEU:HD21	1:D:51:LEU:HD11	1.97	0.47
1:B:648:GLU:HA	1:B:651:LEU:HD23	1.96	0.47
1:C:299:PRO:HA	1:C:303:HIS:ND1	2.30	0.47
1:E:598:LEU:HD11	1:E:699:ILE:HD11	1.97	0.47
1:F:128:LYS:HG3	1:F:198:LEU:HD22	1.96	0.47
1:F:203:ARG:HB2	1:F:240:GLU:HB2	1.97	0.47
1:F:405:LEU:HG	1:F:411:LEU:HD12	1.97	0.47
1:F:565:VAL:HG11	1:F:595:ILE:HD13	1.96	0.47
1:B:277:LEU:HD21	1:B:312:LEU:HD21	1.96	0.46
1:C:79:LEU:HD12	1:C:252:PRO:HB2	1.97	0.46
1:D:528:LEU:CD1	1:D:567:ILE:HB	2.46	0.46
1:D:277:LEU:HD21	1:D:312:LEU:HD21	1.97	0.46
1:D:429:GLN:NE2	1:D:653:ASN:OD1	2.47	0.46
1:F:23:LEU:HD13	1:F:398:THR:HG23	1.96	0.46
1:A:302:VAL:HG13	1:A:356:MET:HE1	1.98	0.46
1:B:126:ARG:NH2	1:C:178:ALA:HB3	2.31	0.46
1:B:139:ARG:HH22	1:B:194:LEU:HD11	1.81	0.46
1:C:42:ALA:HB2	1:C:382:ILE:HG21	1.97	0.46
1:C:51:LEU:HD22	1:C:63:LEU:HD22	1.98	0.46
1:E:364:PRO:O	1:E:368:GLU:HG3	2.16	0.46
1:F:51:LEU:HB2	1:F:361:VAL:HG22	1.97	0.46
1:A:532:ASP:OD2	1:A:571:PHE:HD2	1.97	0.46
1:B:193:GLU:HA	1:B:196:VAL:HG22	1.97	0.46
1:D:96:GLY:H	1:D:258:SER:HG	1.63	0.46
1:D:310:LEU:HB2	1:D:356:MET:HE2	1.98	0.46
1:E:303:HIS:HD2	1:E:352:PHE:CD2	2.33	0.46
1:C:80:TYR:CD2	1:C:255:LEU:HD11	2.51	0.46
1:E:448:ALA:HB2	1:E:455:LEU:HD11	1.97	0.46
1:B:273:THR:OG1	1:B:320:GLU:OE1	2.26	0.46
1:D:448:ALA:HB2	1:D:455:LEU:HD11	1.98	0.46
1:E:269:GLU:HG3	1:E:301:ALA:HB2	1.98	0.46
1:E:277:LEU:HA	1:E:301:ALA:HB3	1.97	0.46
1:A:89:ALA:HA	1:A:350:GLU:HG3	1.97	0.46
1:A:420:TYR:CZ	1:A:424:ARG:HD2	2.51	0.46
1:C:32:GLN:NE2	1:C:57:LEU:HD21	2.31	0.46
1:B:111:GLU:OE2	1:B:213:ARG:NH2	2.49	0.46
1:C:195:GLU:O	1:C:198:LEU:HG	2.16	0.46
1:C:246:ASP:HB3	1:C:249:GLN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:SER:HG	1:A:396:ASN:HD22	1.63	0.45
1:E:600:LEU:HD13	1:E:684:LEU:HD13	1.97	0.45
1:A:646:LEU:O	1:A:673:ALA:HA	2.15	0.45
1:F:253:ASN:HB2	1:F:294:VAL:HG22	1.97	0.45
1:F:512:GLY:HA3	1:F:625:LYS:HG2	1.99	0.45
1:C:33:GLU:OE1	1:C:36:ARG:NH2	2.50	0.45
1:D:639:SER:OG	1:D:642:GLN:NE2	2.50	0.45
1:E:29:PHE:HB3	1:E:32:GLN:HB2	1.97	0.45
1:F:166:LEU:HG	1:F:180:LEU:HD13	1.98	0.45
1:D:51:LEU:HD22	1:D:63:LEU:HD22	1.99	0.45
1:F:528:LEU:HD23	1:F:546:VAL:HG23	1.99	0.45
1:A:193:GLU:HA	1:A:196:VAL:HG22	1.99	0.45
1:C:147:ARG:NE	1:C:147:ARG:HA	2.32	0.45
1:F:231:LEU:HD23	1:F:250:TRP:CE3	2.52	0.45
1:F:420:TYR:HE1	1:F:433:MET:HE2	1.82	0.45
1:F:33:GLU:O	1:F:36:ARG:N	2.49	0.45
1:A:78:LEU:HB3	1:A:352:PHE:HE1	1.81	0.45
1:A:124:PHE:HZ	1:A:202:ARG:HG2	1.81	0.45
1:C:528:LEU:HD21	1:C:569:LEU:HD12	1.97	0.45
1:D:269:GLU:HG3	1:D:301:ALA:HB2	1.98	0.45
1:E:146:LEU:HB2	1:E:183:VAL:HG21	1.98	0.45
1:E:273:THR:O	1:E:276:ARG:N	2.49	0.45
1:E:368:GLU:HA	1:E:371:GLU:CD	2.42	0.45
1:E:598:LEU:HD13	1:E:695:LEU:HD22	1.98	0.45
1:E:404:LEU:HB2	1:E:411:LEU:HD11	1.98	0.45
1:F:273:THR:HG22	1:F:275:PRO:HD2	1.98	0.45
1:A:16:ASN:O	1:A:413:GLN:HB3	2.17	0.44
1:A:105:VAL:HG21	1:A:227:TYR:HE2	1.82	0.44
1:A:525:ARG:HB2	1:A:527:HIS:CD2	2.53	0.44
1:B:131:LEU:HA	1:B:134:ARG:HE	1.82	0.44
1:F:331:ARG:NH2	1:F:379:LEU:HG	2.32	0.44
1:F:552:TYR:CZ	1:F:556:ARG:HD3	2.52	0.44
1:A:225:ARG:HA	1:A:225:ARG:NE	2.33	0.44
1:B:199:ARG:HB3	1:B:240:GLU:HG3	1.99	0.44
1:E:188:LEU:O	1:E:191:SER:OG	2.35	0.44
1:A:403:TRP:O	1:A:407:GLN:HG2	2.18	0.44
1:C:592:LEU:HD13	1:C:681:LEU:HD11	1.99	0.44
1:C:676:THR:HG22	1:C:678:GLU:H	1.82	0.44
1:E:275:PRO:HG3	1:E:338:VAL:HG21	2.00	0.44
1:F:501:SER:O	1:F:514:PRO:HA	2.16	0.44
1:C:378:GLU:O	1:C:381:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:LEU:HD21	1:E:180:LEU:HD12	1.99	0.44
1:E:234:ARG:O	1:E:237:ARG:HB3	2.17	0.44
1:A:102:ALA:HA	1:A:252:PRO:HG3	1.99	0.44
1:B:54:PRO:O	1:B:57:LEU:HG	2.18	0.44
1:C:39:LEU:HD11	1:C:51:LEU:HD11	1.98	0.44
1:C:502:LEU:HB3	1:C:625:LYS:HB3	1.99	0.44
1:F:66:TYR:O	1:F:70:GLN:HG2	2.18	0.44
1:F:229:GLU:HG2	1:F:232:ARG:HH21	1.82	0.44
1:B:52:VAL:HG22	1:B:367:PHE:CD2	2.53	0.44
1:C:518:THR:HG22	1:D:612:GLN:HE21	1.82	0.44
1:C:523:PRO:HD2	1:D:558:ILE:HG21	1.99	0.44
1:D:81:VAL:HG12	1:D:252:PRO:HB3	2.00	0.44
1:E:292:THR:HA	1:E:296:LEU:HD12	2.00	0.44
1:B:476:GLU:OE1	1:C:34:ARG:NH2	2.43	0.44
1:C:290:TRP:HB2	1:C:344:PRO:HD3	2.00	0.44
1:E:658:ALA:O	1:E:662:GLU:HG2	2.18	0.44
1:B:201:LEU:HG	1:B:205:TRP:HD1	1.83	0.43
1:F:79:LEU:HD12	1:F:252:PRO:HB2	1.99	0.43
1:F:107:GLY:O	1:F:111:GLU:HG2	2.18	0.43
1:F:593:SER:O	1:F:597:ASN:N	2.51	0.43
1:A:572:GLU:OE2	1:B:615:LYS:NZ	2.51	0.43
1:B:498:GLU:OE2	1:B:516:ARG:NH1	2.51	0.43
1:D:335:VAL:O	1:D:352:PHE:N	2.43	0.43
1:F:228:LEU:HA	1:F:231:LEU:HD12	2.00	0.43
1:F:609:ALA:HB3	1:F:617:LEU:HB2	2.00	0.43
1:B:216:PRO:O	1:B:219:GLN:HG3	2.18	0.43
1:B:692:PHE:O	1:B:693:ARG:HD3	2.19	0.43
1:C:280:ARG:HH11	1:C:298:ARG:HG3	1.83	0.43
1:E:199:ARG:HB3	1:E:240:GLU:HG3	1.99	0.43
1:D:506:GLU:OE1	1:D:577:SER:HB3	2.18	0.43
1:A:39:LEU:HD21	1:A:51:LEU:HD11	2.00	0.43
1:C:403:TRP:O	1:C:407:GLN:HG2	2.19	0.43
1:C:707:ALA:O	1:C:710:GLU:HG3	2.18	0.43
1:F:91:LEU:HD21	1:F:224:ALA:HB2	1.99	0.43
1:F:105:VAL:HG11	1:F:252:PRO:HD3	2.01	0.43
1:B:592:LEU:HD23	1:B:592:LEU:HA	1.83	0.43
1:B:639:SER:OG	1:B:642:GLN:NE2	2.52	0.43
1:C:521:ALA:HB1	1:C:565:VAL:HG21	2.00	0.43
1:F:609:ALA:O	1:F:617:LEU:N	2.34	0.43
1:A:57:LEU:HA	1:A:436:ARG:HA	1.99	0.43
1:B:332:ASN:C	1:B:334:GLN:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:TYR:CE1	1:B:433:MET:HE2	2.54	0.43
1:C:155:PHE:CE1	1:C:168:GLY:HA3	2.53	0.43
1:C:283:TYR:CD2	1:C:292:THR:HB	2.54	0.43
1:C:559:GLU:HG3	1:C:560:HIS:CD2	2.54	0.43
1:D:80:TYR:CD2	1:D:255:LEU:HD11	2.54	0.43
1:D:222:PRO:O	1:D:225:ARG:HB2	2.19	0.43
1:D:312:LEU:HD23	1:D:312:LEU:HA	1.86	0.43
1:D:334:GLN:HB3	1:D:351:PRO:HB2	1.99	0.43
1:F:124:PHE:HZ	1:F:202:ARG:HG2	1.84	0.43
1:B:77:ASP:OD2	1:B:96:GLY:N	2.50	0.43
1:B:114:ARG:HH21	1:B:117:GLU:CD	2.26	0.43
1:B:135:PHE:HB2	1:B:194:LEU:HD21	2.01	0.43
1:D:415:GLY:HA3	1:D:455:LEU:O	2.18	0.43
1:E:425:ARG:HH21	1:E:627:GLU:CD	2.26	0.43
1:A:8:LEU:HD12	1:A:664:VAL:HG11	1.99	0.43
1:C:192:ALA:O	1:C:195:GLU:HG2	2.18	0.43
1:C:525:ARG:NH1	1:C:527:HIS:O	2.51	0.43
1:D:456:THR:HG23	1:D:459:SER:H	1.84	0.43
1:F:195:GLU:HB3	1:F:199:ARG:HH21	1.83	0.43
1:B:249:GLN:HG2	1:B:293:ASN:HB2	2.00	0.43
1:B:293:ASN:OD1	1:B:296:LEU:HG	2.18	0.43
1:B:521:ALA:HB1	1:B:565:VAL:HG21	2.01	0.43
1:E:290:TRP:CD1	1:E:342:GLN:HB2	2.54	0.43
1:E:601:ARG:NH1	1:E:604:LEU:HD11	2.33	0.43
1:A:593:SER:HA	1:A:598:LEU:HB2	2.01	0.42
1:A:654:LEU:HD22	1:A:656:LEU:HD21	2.01	0.42
1:F:448:ALA:O	1:F:452:GLY:N	2.51	0.42
1:F:488:ARG:HB3	1:F:516:ARG:HH11	1.83	0.42
1:D:502:LEU:HD21	1:D:629:PHE:HB2	2.01	0.42
1:A:516:ARG:NH1	1:B:615:LYS:HD3	2.33	0.42
1:B:77:ASP:OD2	1:B:258:SER:OG	2.38	0.42
1:B:277:LEU:HD12	1:B:322:THR:HG21	2.01	0.42
1:A:214:PHE:CE2	1:A:232:ARG:HB2	2.55	0.42
1:B:146:LEU:HD22	1:B:183:VAL:HG21	2.02	0.42
1:C:480:ARG:HH11	1:D:432:ARG:NE	2.17	0.42
1:E:418:ARG:HD2	1:E:418:ARG:HA	1.89	0.42
1:F:3:LEU:HD11	1:F:673:ALA:HB2	2.01	0.42
1:F:530:SER:O	1:F:534:GLU:N	2.52	0.42
1:A:354:ILE:HG23	1:A:356:MET:HE2	2.02	0.42
1:B:70:GLN:O	1:B:264:PRO:HD3	2.19	0.42
1:E:443:LEU:HD13	1:E:467:ARG:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:VAL:HG21	1:F:383:ARG:HE	1.84	0.42
1:F:149:GLU:OE1	1:F:179:ARG:HG3	2.20	0.42
1:F:160:ASN:OD1	1:F:160:ASN:N	2.52	0.42
1:B:91:LEU:HD11	1:B:223:GLN:HB3	2.00	0.42
1:C:600:LEU:HD13	1:C:684:LEU:HD13	2.01	0.42
1:D:57:LEU:CD2	1:D:386:PHE:HB3	2.50	0.42
1:D:340:GLU:HB3	1:D:342:GLN:OE1	2.19	0.42
1:A:383:ARG:HG3	1:A:385:GLU:HG3	2.01	0.42
1:B:29:PHE:HB3	1:B:32:GLN:HB2	2.02	0.42
1:B:114:ARG:NH2	1:B:117:GLU:OE2	2.49	0.42
1:B:331:ARG:HD2	1:B:375:ALA:HB1	2.02	0.42
1:E:331:ARG:HH21	1:E:379:LEU:HG	1.85	0.42
1:F:118:LEU:HA	1:F:121:GLN:HG2	2.02	0.42
1:F:403:TRP:O	1:F:407:GLN:HG2	2.20	0.42
1:D:193:GLU:HA	1:D:196:VAL:HG22	2.02	0.42
1:E:639:SER:N	1:E:642:GLN:HE22	2.18	0.42
1:F:389:THR:HB	1:F:432:ARG:HB3	2.01	0.42
1:F:618:ALA:HB2	1:F:649:ALA:HB3	2.02	0.42
1:B:39:LEU:HD13	1:B:51:LEU:HD11	2.02	0.42
1:C:159:THR:HG22	1:C:164:LEU:HD22	2.00	0.42
1:C:327:LYS:HD2	1:C:375:ALA:CB	2.50	0.42
1:C:532:ASP:OD2	1:C:571:PHE:N	2.52	0.42
1:D:70:GLN:O	1:D:264:PRO:HD3	2.19	0.42
1:D:144:GLU:HG2	1:D:148:ARG:NH2	2.35	0.42
1:C:15:GLU:N	1:C:15:GLU:OE1	2.52	0.41
1:E:26:PRO:HG3	1:E:403:TRP:HB2	2.02	0.41
1:E:52:VAL:HG22	1:E:367:PHE:CD2	2.55	0.41
1:F:517:LEU:HD21	1:F:587:GLU:HA	2.02	0.41
1:A:225:ARG:NH2	1:A:228:LEU:HD12	2.35	0.41
1:C:16:ASN:ND2	1:C:19:GLU:OE2	2.53	0.41
1:D:305:ALA:HB3	1:D:356:MET:HE3	2.02	0.41
1:B:46:GLY:HA2	1:B:357:GLN:NE2	2.34	0.41
1:B:646:LEU:HD11	1:B:654:LEU:HD11	2.01	0.41
1:C:280:ARG:HG2	1:C:298:ARG:HB2	2.01	0.41
1:E:81:VAL:HB	1:E:227:TYR:CD1	2.56	0.41
1:B:28:PRO:O	1:B:36:ARG:NH1	2.53	0.41
1:B:80:TYR:CD2	1:B:255:LEU:HD11	2.55	0.41
1:D:128:LYS:HD2	1:D:198:LEU:HD11	2.02	0.41
1:D:283:TYR:CD1	1:D:292:THR:HB	2.56	0.41
1:D:705:ALA:O	1:D:708:ARG:HG2	2.19	0.41
1:E:150:ALA:O	1:E:155:PHE:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:VAL:HG23	1:A:508:ALA:H	1.85	0.41
1:C:215:GLU:N	1:C:216:PRO:HD2	2.35	0.41
1:D:445:GLU:O	1:D:449:VAL:HG23	2.20	0.41
1:D:499:VAL:HG22	1:D:500:ASN:H	1.85	0.41
1:F:234:ARG:HB2	1:F:250:TRP:CH2	2.56	0.41
1:F:656:LEU:HB3	1:F:660:VAL:HG21	2.01	0.41
1:B:404:LEU:HB2	1:B:411:LEU:HD11	2.03	0.41
1:C:193:GLU:HA	1:C:196:VAL:HG22	2.02	0.41
1:C:360:LEU:HD23	1:C:360:LEU:HA	1.91	0.41
1:E:403:TRP:HH2	1:E:441:ARG:HB2	1.85	0.41
1:F:528:LEU:HD11	1:F:567:ILE:HB	2.03	0.41
1:A:124:PHE:HA	1:A:205:TRP:CZ3	2.55	0.41
1:B:203:ARG:HD2	1:B:240:GLU:CD	2.45	0.41
1:C:503:VAL:HG11	1:C:576:VAL:HG13	2.02	0.41
1:D:42:ALA:HB2	1:D:382:ILE:HG21	2.02	0.41
1:F:123:SER:HA	1:F:126:ARG:HG2	2.03	0.41
1:F:144:GLU:O	1:F:148:ARG:HG2	2.21	0.41
1:F:412:THR:OG1	1:F:456:THR:HA	2.21	0.41
1:A:627:GLU:HG3	1:A:660:VAL:HG21	2.03	0.41
1:B:518:THR:HG21	1:C:613:THR:HB	2.03	0.41
1:D:471:SER:HB2	1:D:510:TYR:OH	2.20	0.41
1:F:332:ASN:C	1:F:334:GLN:H	2.29	0.41
1:B:100:HIS:O	1:B:103:GLU:HG2	2.21	0.41
1:C:82:PRO:HB3	1:C:294:VAL:CG2	2.44	0.41
1:D:326:PHE:HZ	1:D:358:VAL:HG21	1.85	0.41
1:D:331:ARG:HE	1:D:375:ALA:HB1	1.85	0.41
1:B:283:TYR:HD2	1:B:292:THR:HB	1.85	0.41
1:B:502:LEU:HB3	1:B:625:LYS:HB3	2.03	0.41
1:D:15:GLU:N	1:D:15:GLU:OE1	2.53	0.41
1:D:418:ARG:HD2	1:D:418:ARG:HA	1.87	0.41
1:E:131:LEU:HD21	1:E:197:ALA:HB1	2.03	0.41
1:F:448:ALA:HB2	1:F:455:LEU:HD11	2.02	0.41
1:A:420:TYR:HE1	1:A:433:MET:HE2	1.86	0.40
1:B:166:LEU:HB3	1:B:172:VAL:HG11	2.03	0.40
1:B:585:LEU:N	1:B:608:GLY:O	2.33	0.40
1:D:87:LYS:HA	1:D:348:GLU:HB3	2.04	0.40
1:D:508:ALA:C	1:D:510:TYR:H	2.29	0.40
1:E:131:LEU:HD13	1:E:134:ARG:HH21	1.85	0.40
1:A:48:HIS:O	1:A:380:PHE:HA	2.21	0.40
1:A:598:LEU:HD21	1:A:695:LEU:HB3	2.03	0.40
1:B:3:LEU:HD11	1:B:673:ALA:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ARG:CZ	1:C:237:ARG:HH21	2.34	0.40
1:D:331:ARG:HH21	1:D:375:ALA:HA	1.86	0.40
1:E:108:LEU:HD13	1:E:214:PHE:CZ	2.56	0.40
1:F:54:PRO:O	1:F:57:LEU:HD13	2.21	0.40
1:A:282:ASP:OD2	1:A:298:ARG:NE	2.54	0.40
1:B:312:LEU:HB2	1:B:360:LEU:CD2	2.52	0.40
1:B:616:VAL:HG12	1:B:647:PRO:HB3	2.03	0.40
1:C:277:LEU:HD21	1:C:312:LEU:HD21	2.02	0.40
1:D:615:LYS:HB3	1:D:615:LYS:HE2	1.92	0.40
1:A:33:GLU:O	1:A:36:ARG:N	2.55	0.40
1:A:425:ARG:NH1	1:A:655:THR:O	2.55	0.40
1:C:39:LEU:HD21	1:C:51:LEU:HD11	2.03	0.40
1:D:537:LEU:H	1:E:541:ILE:HD12	1.87	0.40
1:F:3:LEU:HD12	1:F:671:ILE:HG22	2.03	0.40
1:F:274:ALA:HB3	1:F:275:PRO:HD3	2.02	0.40
1:D:253:ASN:ND2	1:D:297:ILE:HB	2.36	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	717/732 (98%)	701 (98%)	16 (2%)	0	100	100
1	B	717/732 (98%)	699 (98%)	18 (2%)	0	100	100
1	C	717/732 (98%)	701 (98%)	16 (2%)	0	100	100
1	D	717/732 (98%)	696 (97%)	21 (3%)	0	100	100
1	E	717/732 (98%)	703 (98%)	14 (2%)	0	100	100
1	F	717/732 (98%)	705 (98%)	12 (2%)	0	100	100
All	All	4302/4392 (98%)	4205 (98%)	97 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	568/578 (98%)	567 (100%)	1 (0%)	87	87
1	B	568/578 (98%)	566 (100%)	2 (0%)	84	84
1	C	568/578 (98%)	566 (100%)	2 (0%)	84	84
1	D	568/578 (98%)	567 (100%)	1 (0%)	87	87
1	E	568/578 (98%)	567 (100%)	1 (0%)	87	87
1	F	568/578 (98%)	568 (100%)	0	100	100
All	All	3408/3468 (98%)	3401 (100%)	7 (0%)	85	87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	313	ASP
1	B	312	LEU
1	B	437	LEU
1	C	57	LEU
1	C	437	LEU
1	D	57	LEU
1	E	57	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	151	GLN
1	A	306	GLN
1	A	355	GLN
1	A	462	GLN
1	A	527	HIS
1	A	540	GLN

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Mol	Chain	Res	Type
1	A	573	GLN
1	B	113	ASN
1	B	208	HIS
1	B	355	GLN
1	B	396	ASN
1	B	429	GLN
1	B	483	GLN
1	C	141	GLN
1	C	223	GLN
1	C	332	ASN
1	C	357	GLN
1	C	653	ASN
1	D	141	GLN
1	D	208	HIS
1	D	355	GLN
1	D	413	GLN
1	D	429	GLN
1	D	540	GLN
1	D	653	ASN
1	D	696	GLN
1	D	713	HIS
1	E	151	GLN
1	E	357	GLN
1	E	602	GLN
1	E	642	GLN
1	F	97	GLN
1	F	249	GLN
1	F	355	GLN
1	F	410	GLN
1	F	500	ASN
1	F	597	ASN
1	F	679	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands 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
2	TS6	A	801	-	3,4,4	2.06	2 (66%)	3,6,6	2.77	1 (33%)
2	TS6	D	801	-	3,4,4	2.02	1 (33%)	3,6,6	2.92	2 (66%)
2	TS6	C	801	-	3,4,4	1.98	1 (33%)	3,6,6	2.99	2 (66%)
2	TS6	B	801	-	3,4,4	2.00	1 (33%)	3,6,6	2.74	2 (66%)
2	TS6	E	801	-	3,4,4	2.05	1 (33%)	3,6,6	2.83	2 (66%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	TS6	P-O3P	-2.35	1.50	1.56
2	E	801	TS6	P-O3P	-2.34	1.50	1.56
2	C	801	TS6	P-O3P	-2.33	1.50	1.56
2	B	801	TS6	P-O3P	-2.29	1.51	1.56
2	A	801	TS6	P-O3P	-2.27	1.51	1.56
2	A	801	TS6	P-O1P	2.04	1.51	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	TS6	O4P-P-O1P	-4.54	101.64	113.37
2	D	801	TS6	O4P-P-O1P	-4.37	102.08	113.37
2	E	801	TS6	O4P-P-O1P	-4.23	102.44	113.37
2	A	801	TS6	O4P-P-O1P	-4.14	102.67	113.37
2	B	801	TS6	O4P-P-O1P	-4.06	102.88	113.37
2	D	801	TS6	O3P-P-O4P	-2.19	101.70	107.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	TS6	O3P-P-O4P	-2.17	101.75	107.59
2	B	801	TS6	O3P-P-O4P	-2.08	102.01	107.59
2	E	801	TS6	O3P-P-O4P	-2.06	102.04	107.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

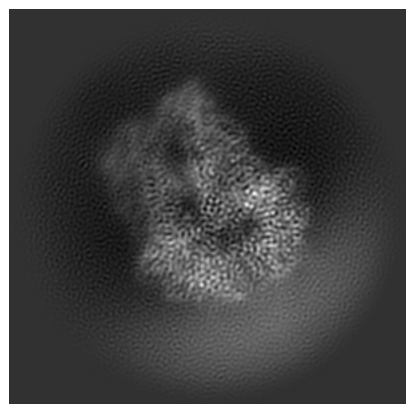
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36975. These allow visual inspection of the internal detail of the map and identification of artifacts.

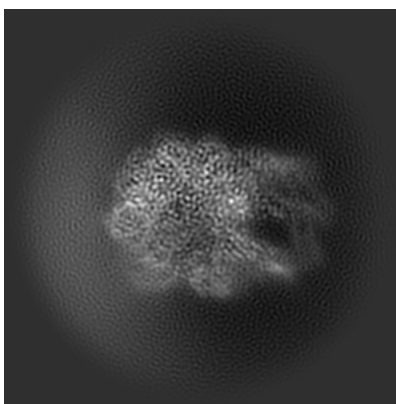
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

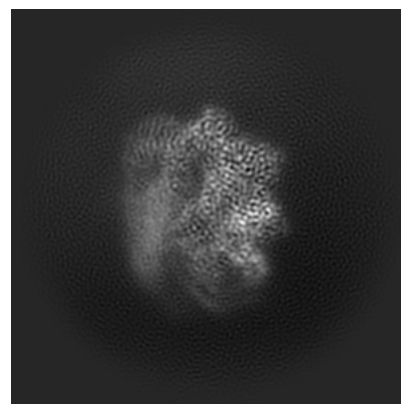
6.1.1 Primary map



X

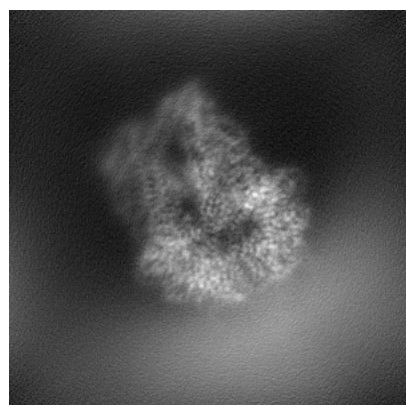


Y

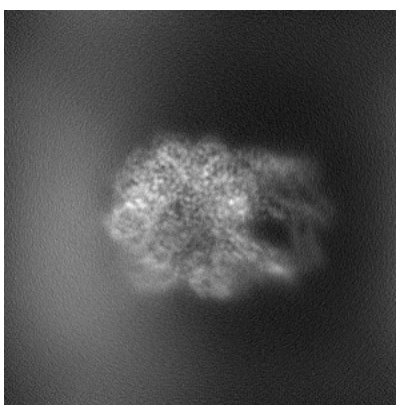


Z

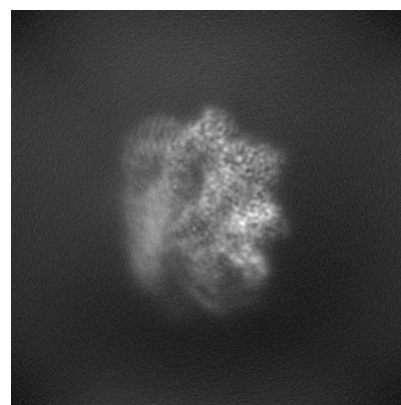
6.1.2 Raw map



X



Y

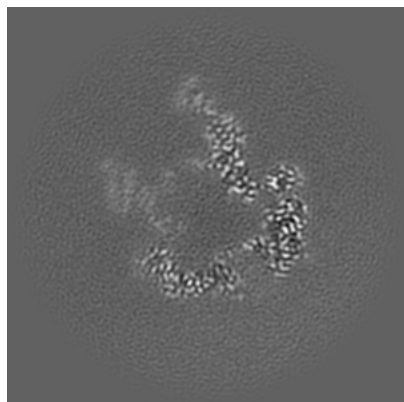


Z

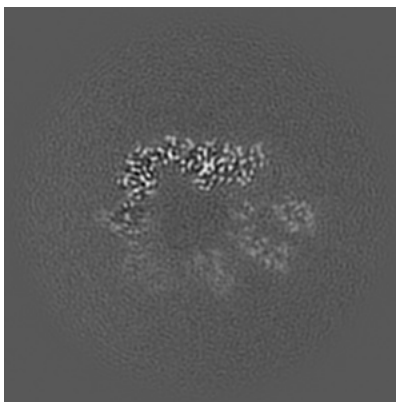
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

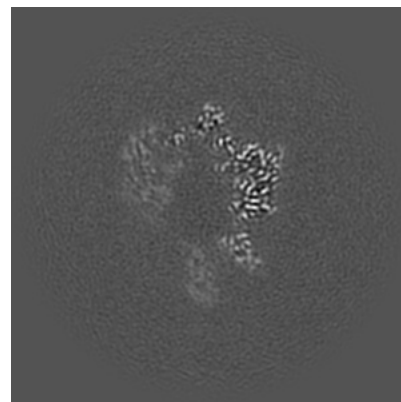
6.2.1 Primary map



X Index: 168

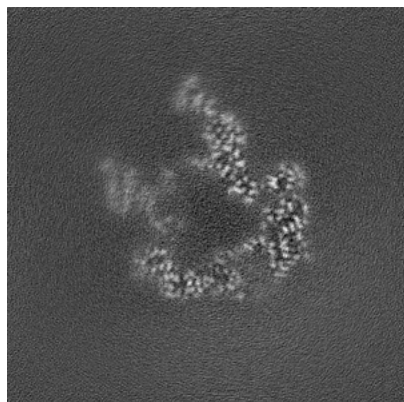


Y Index: 168

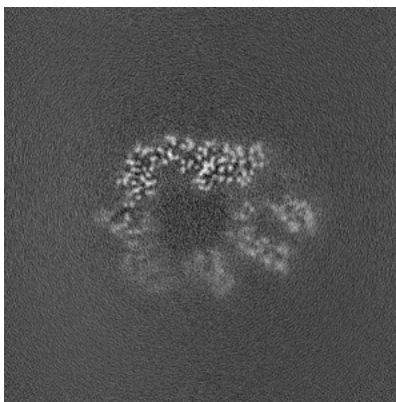


Z Index: 168

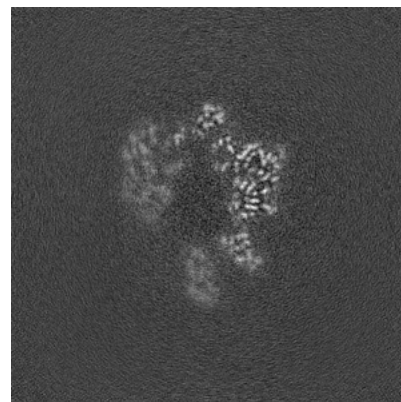
6.2.2 Raw map



X Index: 168



Y Index: 168

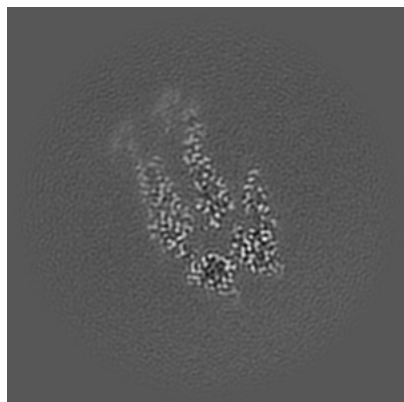


Z Index: 168

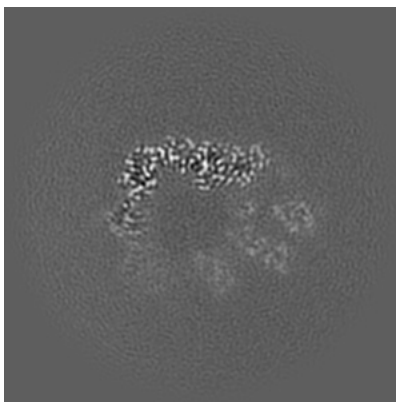
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

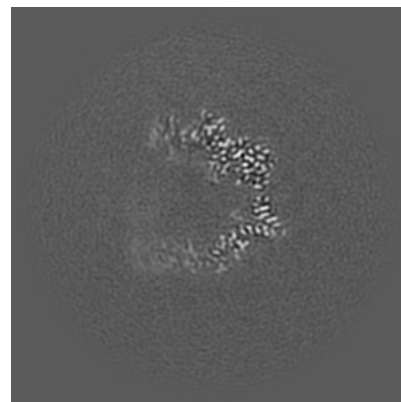
6.3.1 Primary map



X Index: 196

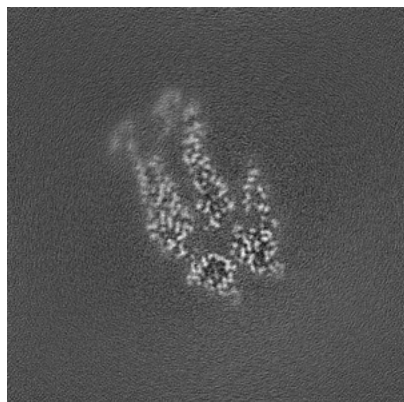


Y Index: 167

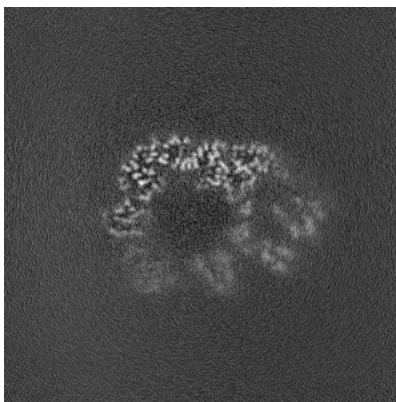


Z Index: 133

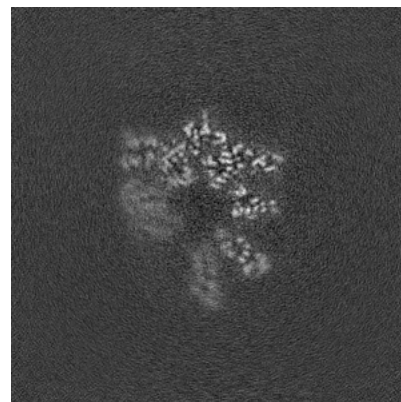
6.3.2 Raw map



X Index: 196



Y Index: 164

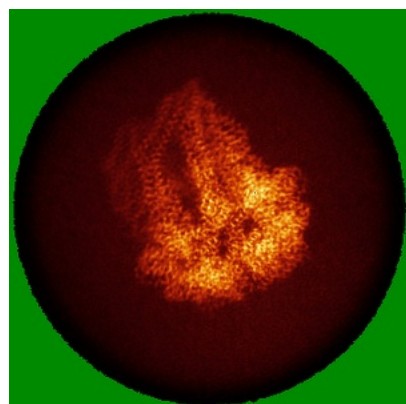


Z Index: 180

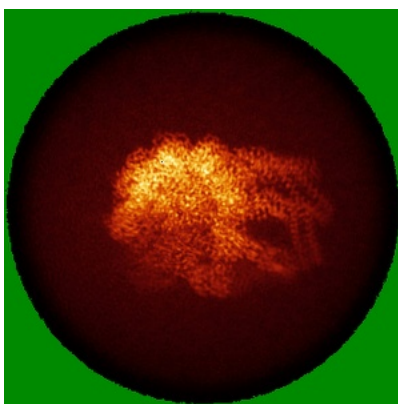
The images above show the largest variance slices of the map in three orthogonal directions.

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

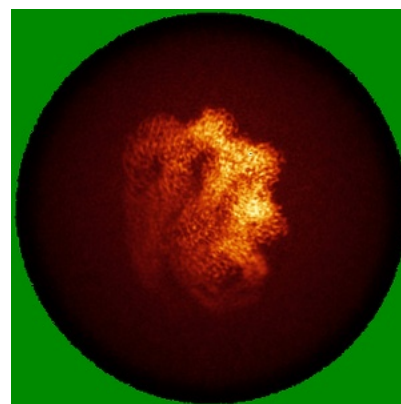
6.4.1 Primary map



X

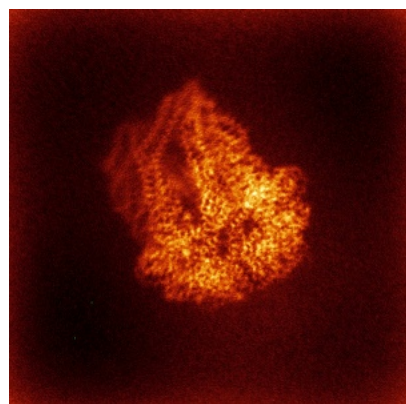


Y

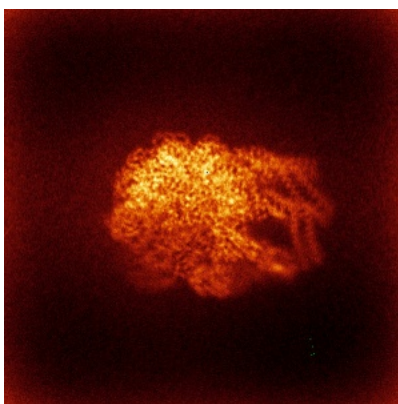


Z

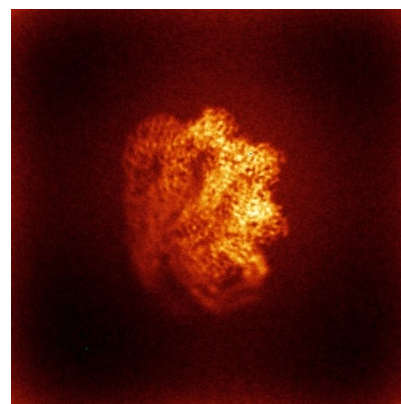
6.4.2 Raw map



X



Y

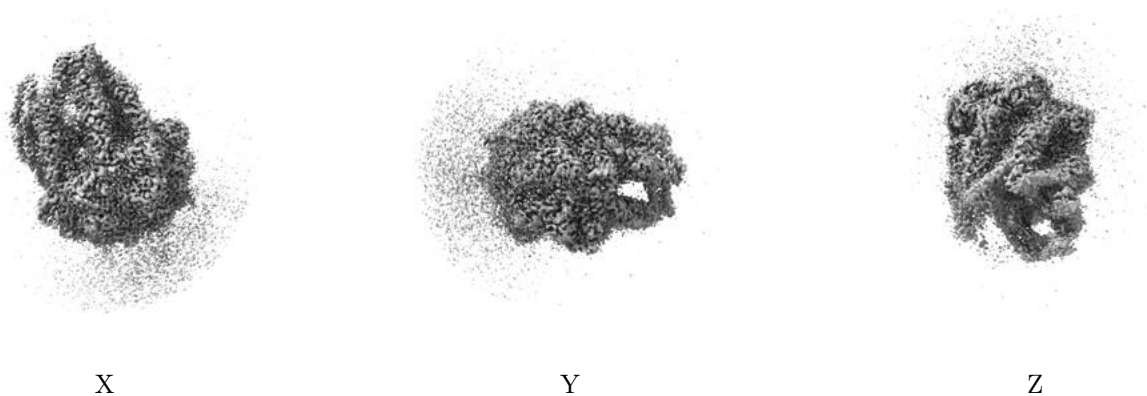


Z

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.

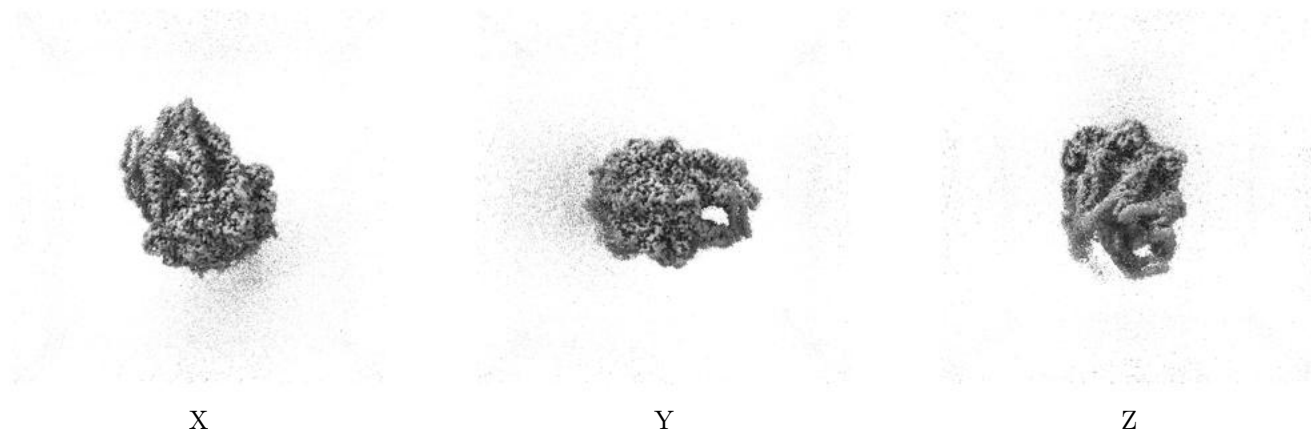
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

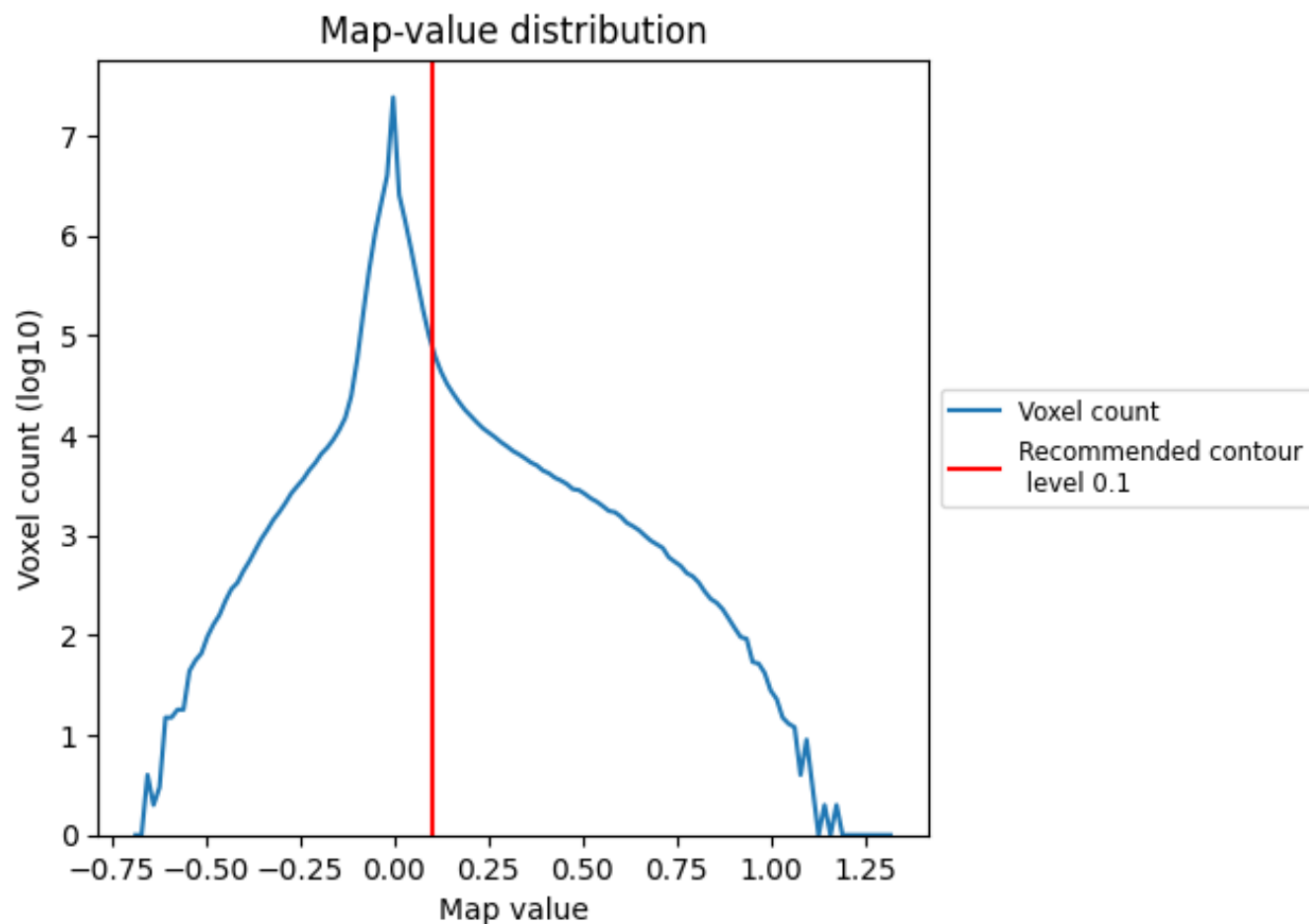
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

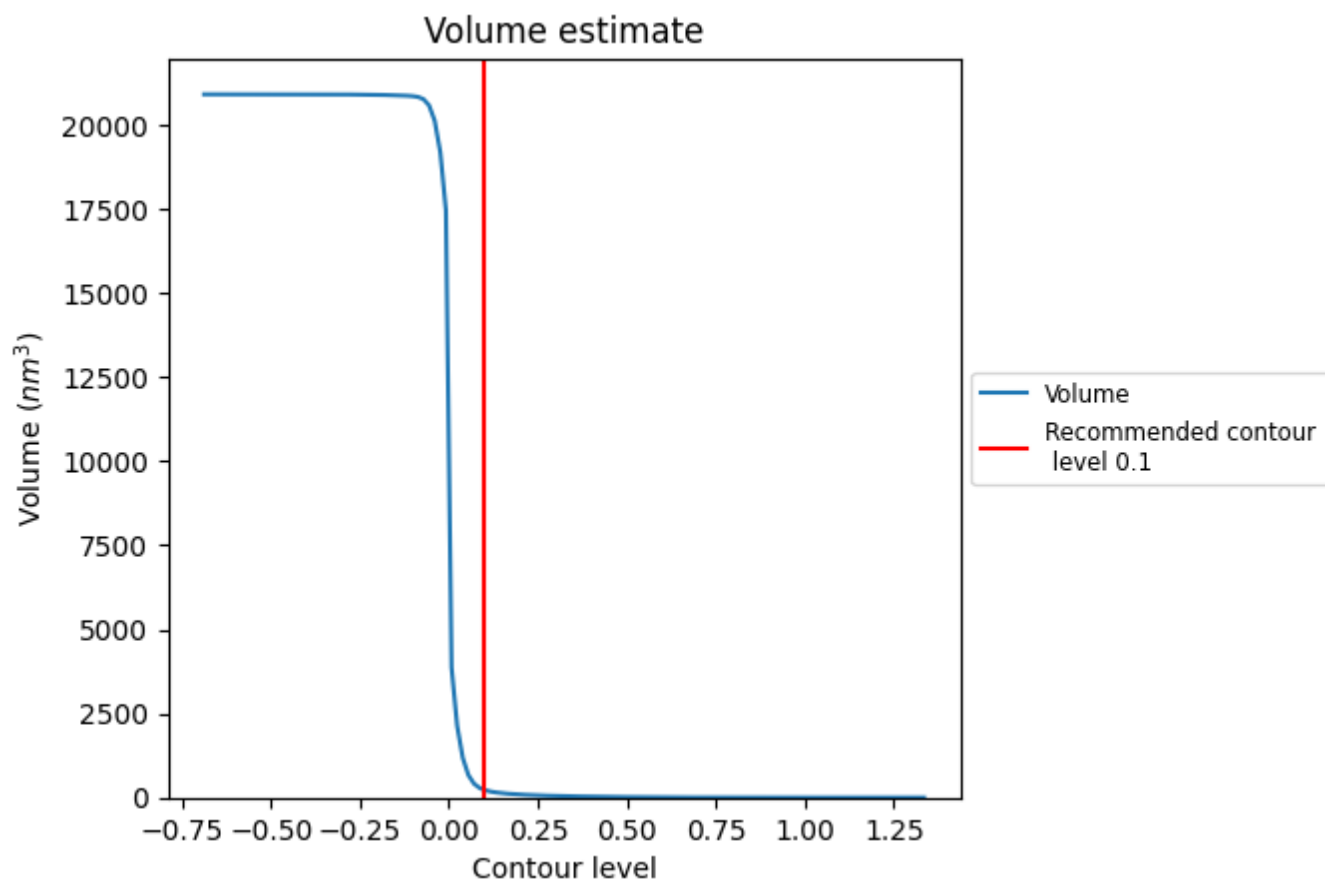
This section contains the results of statistical analysis of the map.

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.

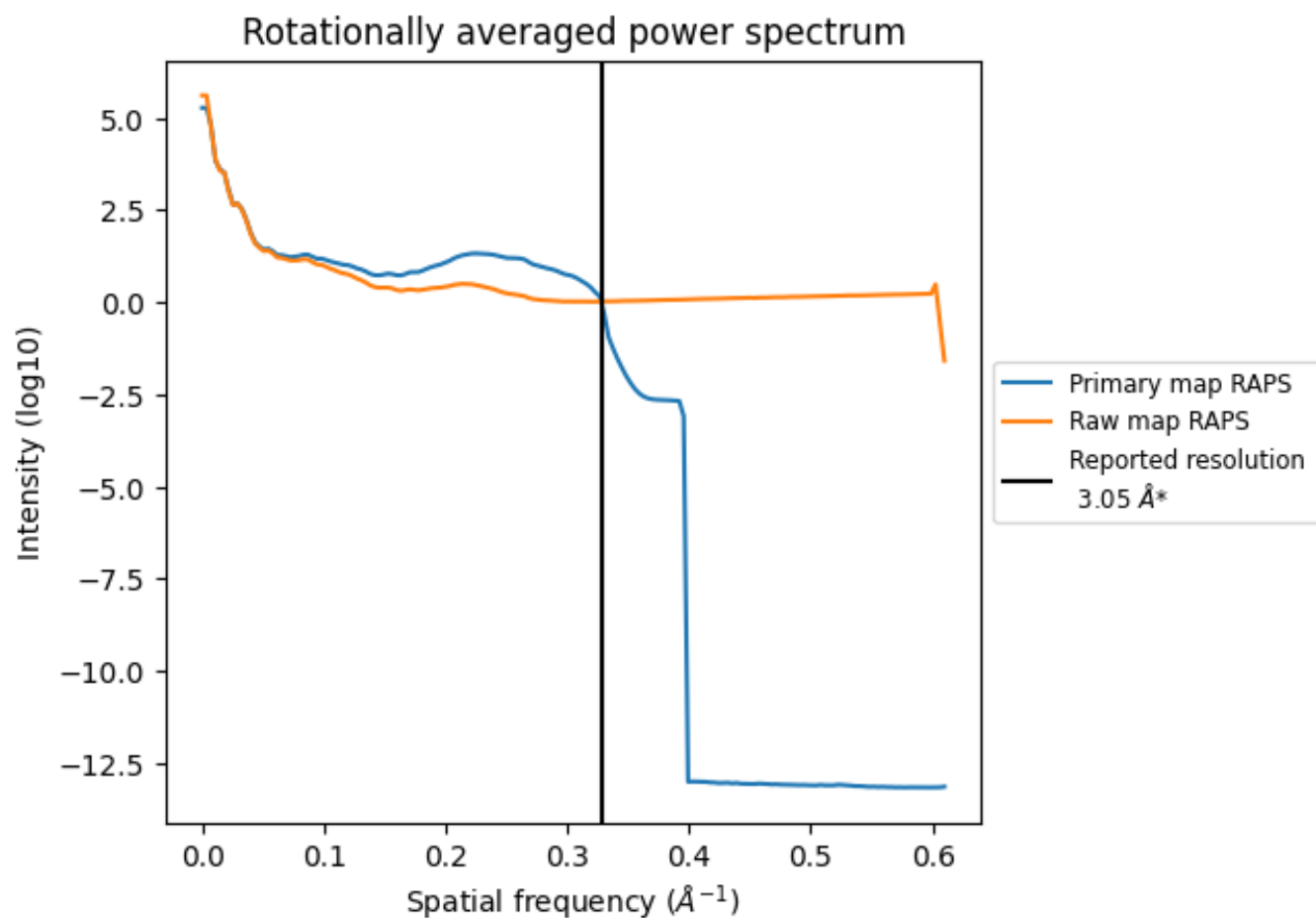
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 227 nm^3 ; this corresponds to an approximate mass of 205 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 ⓘ

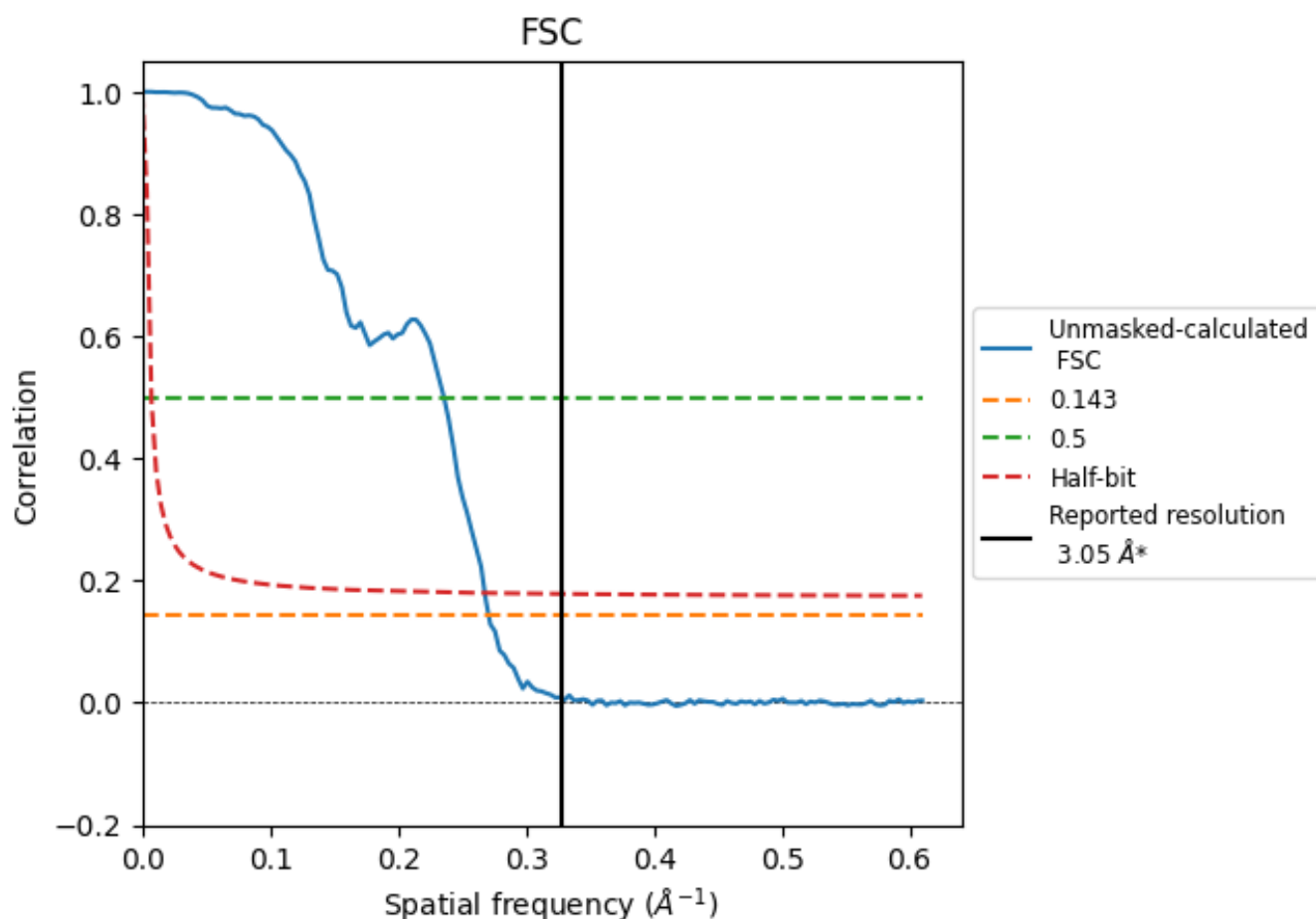


*Reported resolution corresponds to spatial frequency of 0.328 Å⁻¹

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 $0.328 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.05	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.69	4.24	3.73

*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 3.69 differs from the reported value 3.05 by more than 10 %

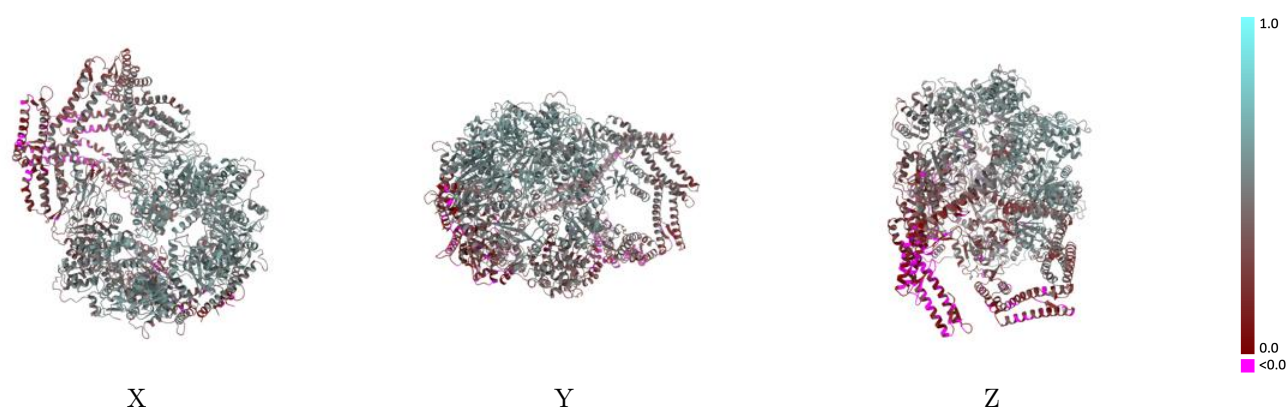
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-36975 and PDB model 8K95. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

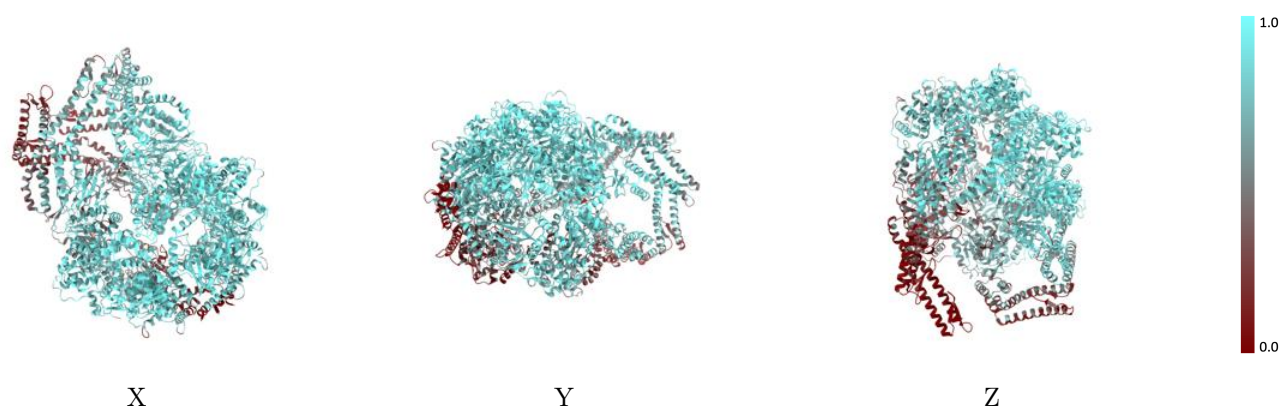
This section was not generated.

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



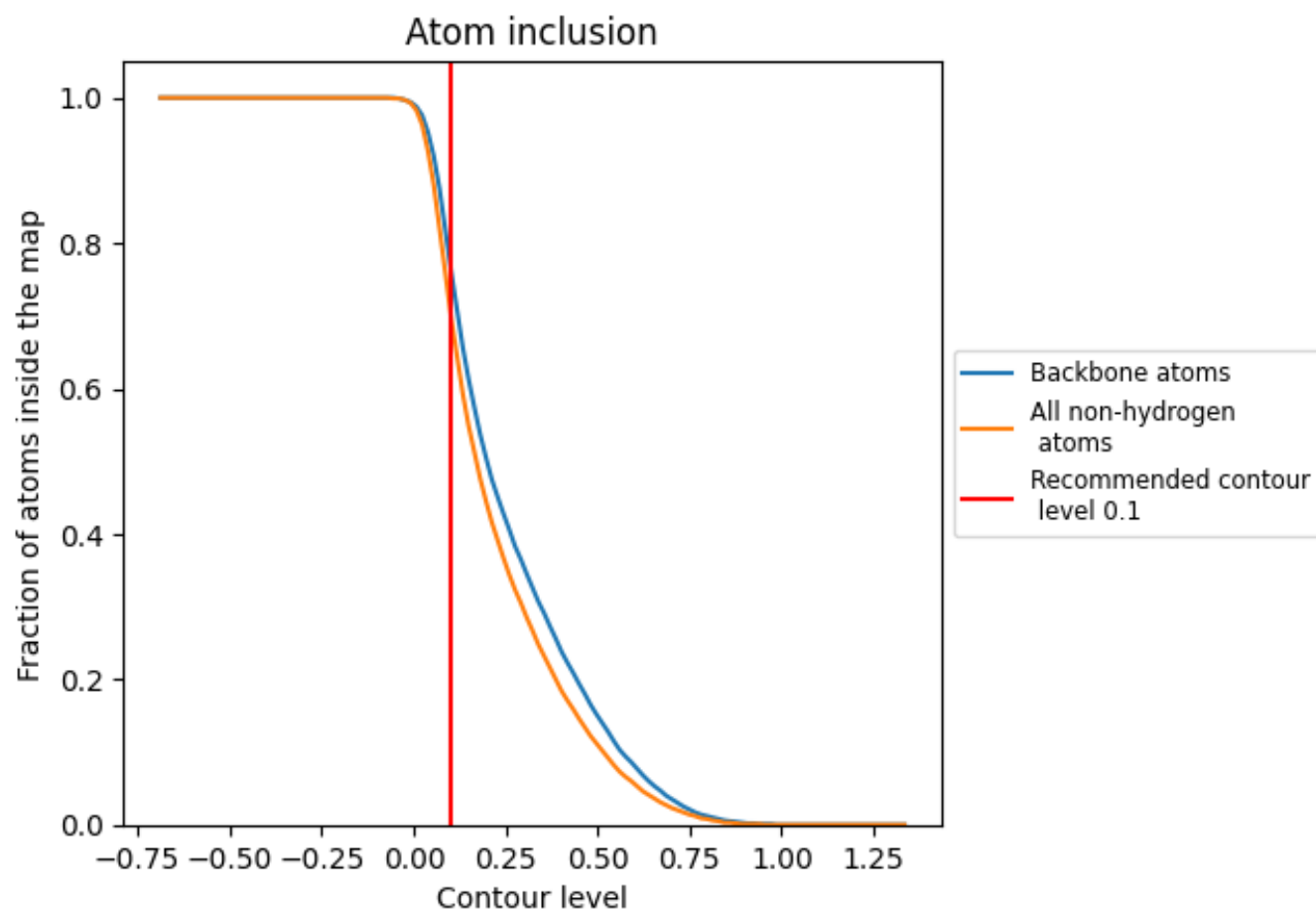
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 71% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7060	0.4040
A	0.5330	0.3050
B	0.7810	0.4380
C	0.8560	0.4930
D	0.8610	0.5020
E	0.8100	0.4510
F	0.3970	0.2350

