



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 01:48 AM UTC

PDB ID : 8XAV / pdb_00008xav
EMDB ID : EMD-38204
Title : Cryo-EM structure of an anti-phage defense complex
Authors : Wang, Y.; Deng, Z.
Deposited on : 2023-12-05
Resolution : 2.87 Å(reported)

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

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

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
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

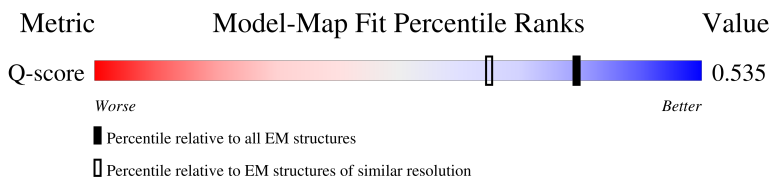
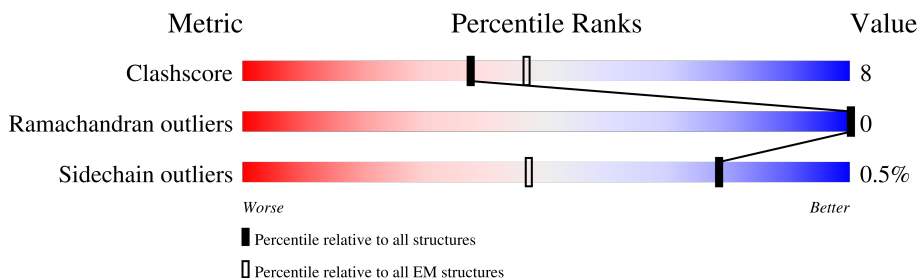
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

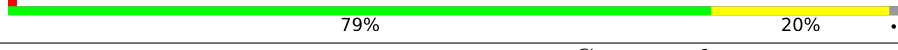
The reported resolution of this entry is 2.87 Å.

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	12062 (2.37 - 3.37)

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	571	
1	B	571	
1	C	571	
1	D	571	

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Mol	Chain	Length	Quality of chain
1	E	571	 77% 22% .
1	F	571	 79% 20% .
2	G	394	 52% 10% 38%
2	H	394	 51% 11% 38%
2	I	394	 53% 9% 38%
2	J	394	 54% 8% 38%
2	K	394	 50% 12% 38%
2	L	394	 51% 11% 38%
2	M	394	 36% 7% 57%
2	N	394	 36% 7% 57%
2	O	394	 34% 9% 57%
2	P	394	 35% 8% 57%
2	Q	394	 33% 10% 57%
2	R	394	 36% 7% 57%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 48264 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 ATP-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	567	Total	C	N	O	S	0	0
			4539	2882	762	889	6		
1	B	567	Total	C	N	O	S	0	0
			4539	2882	762	889	6		
1	C	567	Total	C	N	O	S	0	0
			4539	2882	762	889	6		
1	D	567	Total	C	N	O	S	0	0
			4539	2882	762	889	6		
1	E	564	Total	C	N	O	S	0	0
			4518	2870	758	884	6		
1	F	564	Total	C	N	O	S	0	0
			4518	2870	758	884	6		

- Molecule 2 is a protein called DUF4297.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	244	Total	C	N	O	S	0	0
			2076	1339	343	389	5		
2	H	244	Total	C	N	O	S	0	0
			2076	1339	343	389	5		
2	I	244	Total	C	N	O	S	0	0
			2076	1339	343	389	5		
2	J	244	Total	C	N	O	S	0	0
			2076	1339	343	389	5		
2	K	244	Total	C	N	O	S	0	0
			2076	1339	343	389	5		
2	L	244	Total	C	N	O	S	0	0
			2076	1339	343	389	5		
2	M	171	Total	C	N	O	S	0	0
			1436	928	236	269	3		
2	N	171	Total	C	N	O	S	0	0
			1436	928	236	269	3		
2	O	171	Total	C	N	O	S	0	0
			1436	928	236	269	3		

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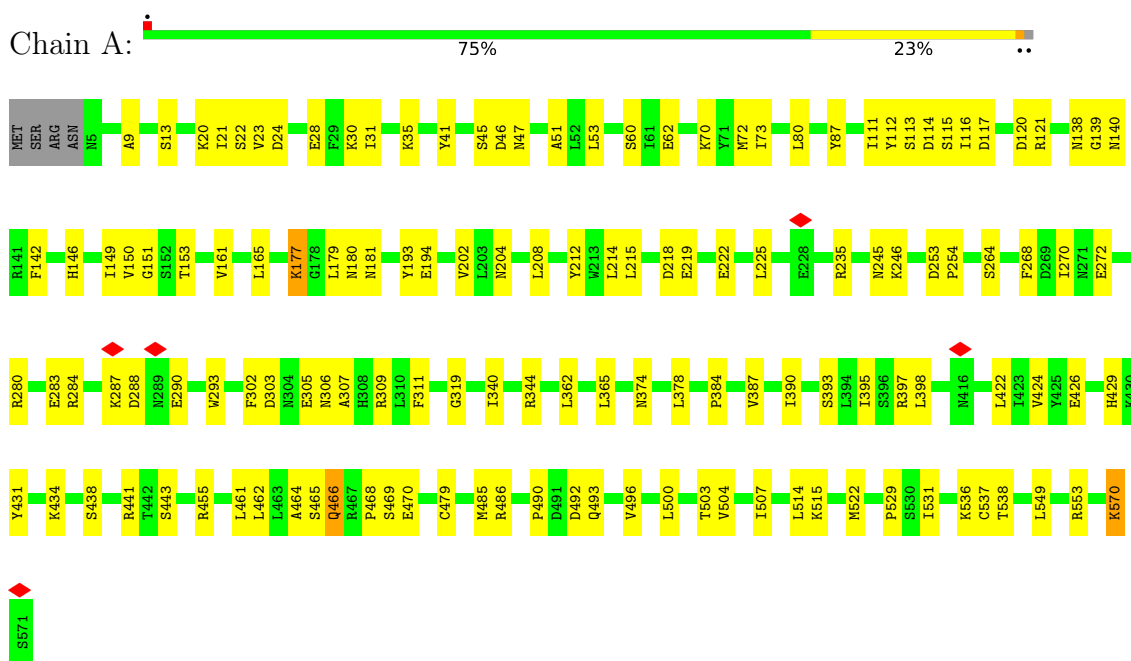
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	171	Total 1436	C 928	N 236	O 269	S 3	0	0
2	Q	171	Total 1436	C 928	N 236	O 269	S 3	0	0
2	R	171	Total 1436	C 928	N 236	O 269	S 3	0	0

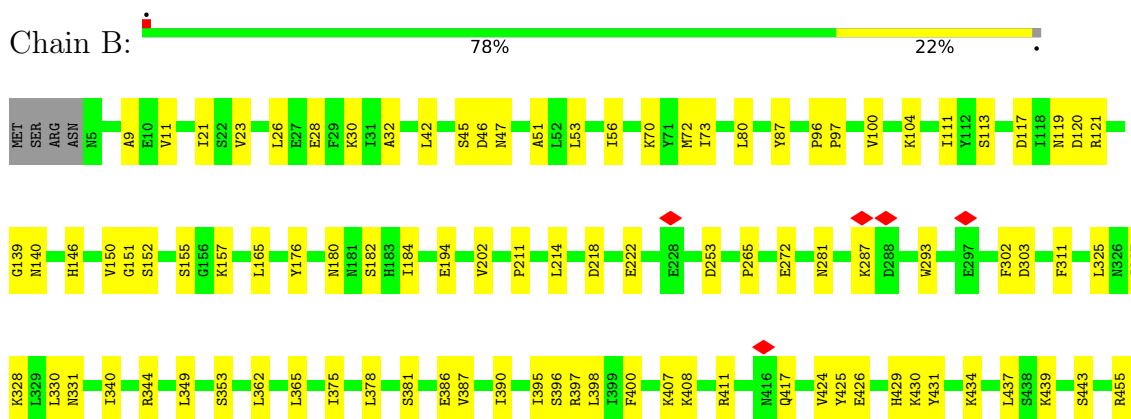
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ATP-binding protein

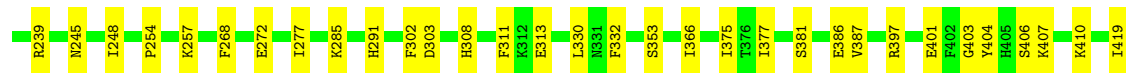
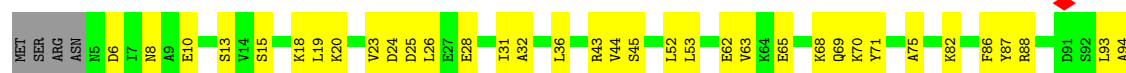


- Molecule 1: ATP-binding protein

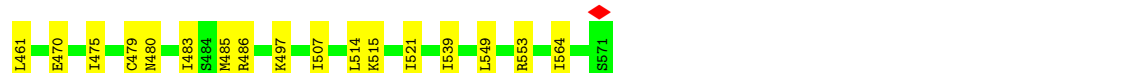




- Molecule 1: ATP-binding protein

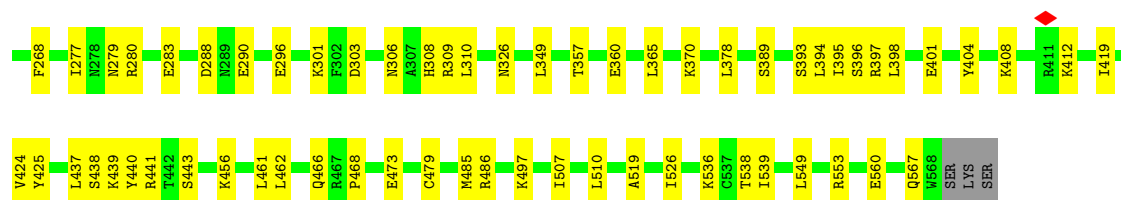


- Molecule 1: ATP-binding protein



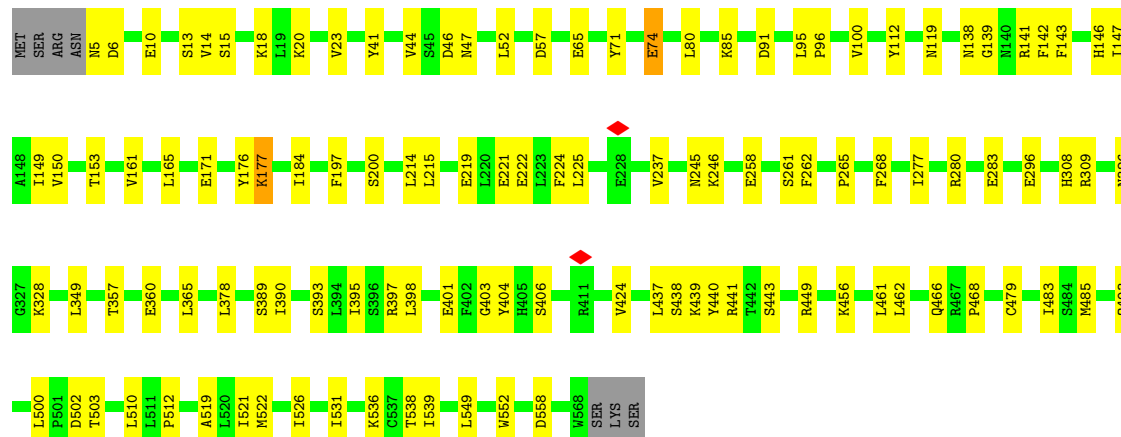
- Molecule 1: ATP-binding protein





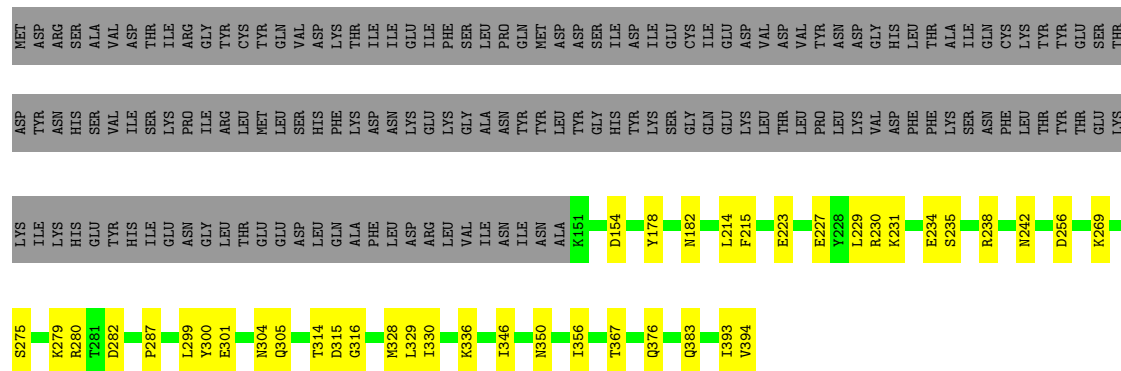
• Molecule 1: ATP-binding protein

Chain F: 79% 20%



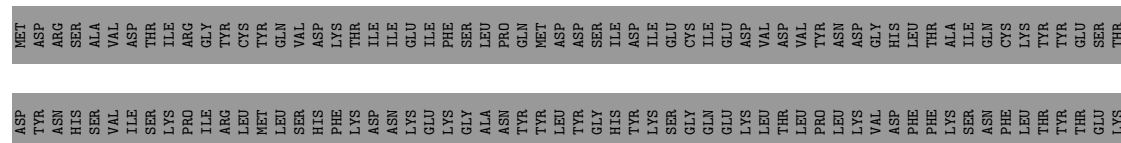
• Molecule 2: DUF4297

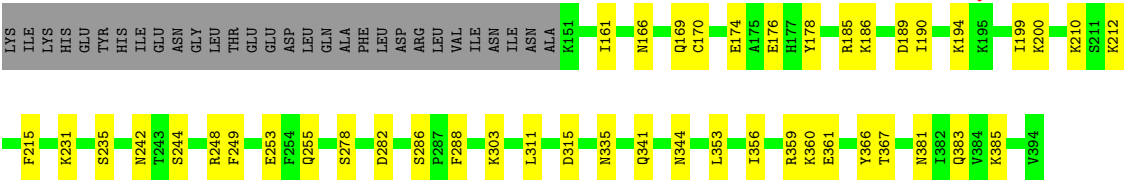
Chain G: 52% 10% 38%



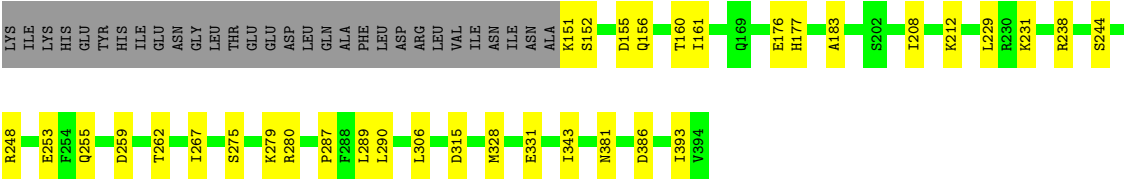
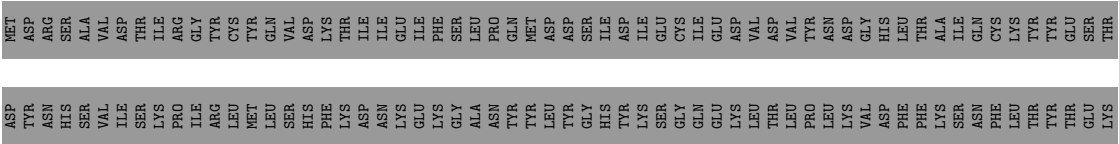
• Molecule 2: DUF4297

Chain H: 51% 11% 38%

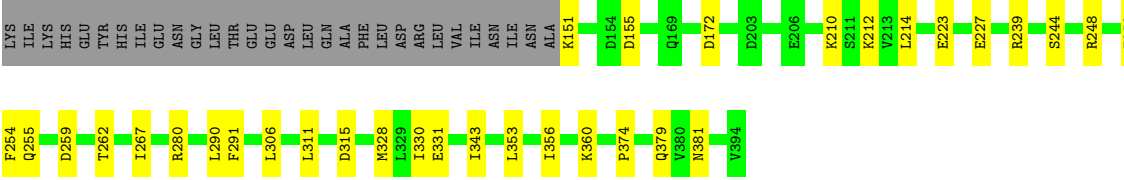
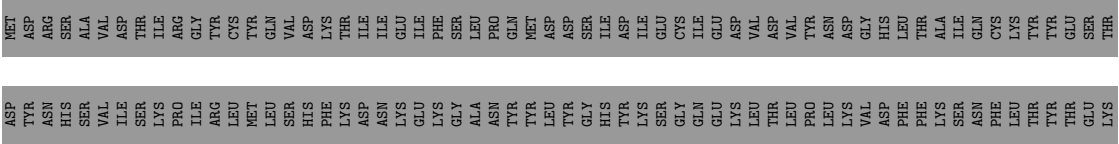




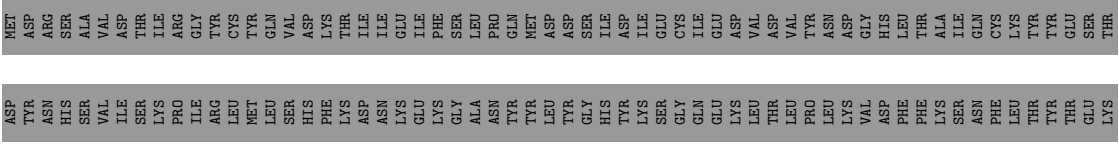
• Molecule 2: DUF4297



• Molecule 2: DUF4297



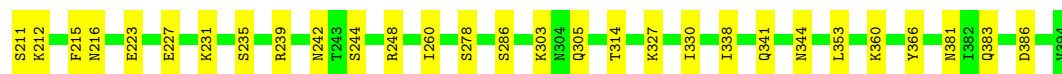
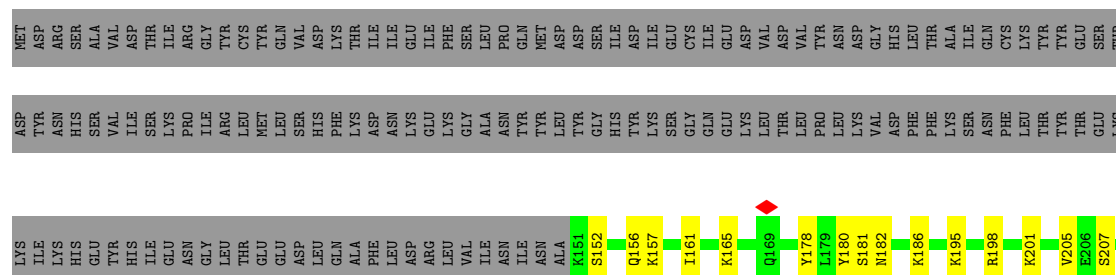
• Molecule 2: DUF4297





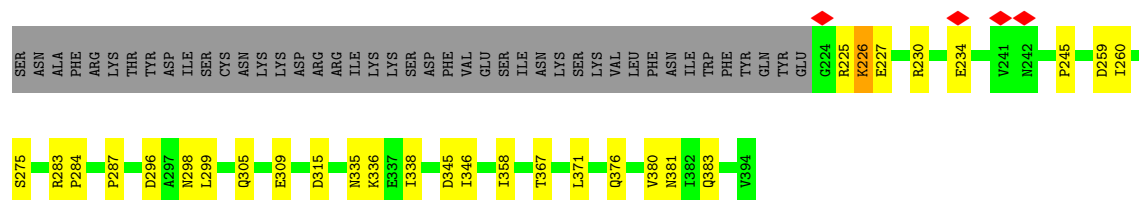
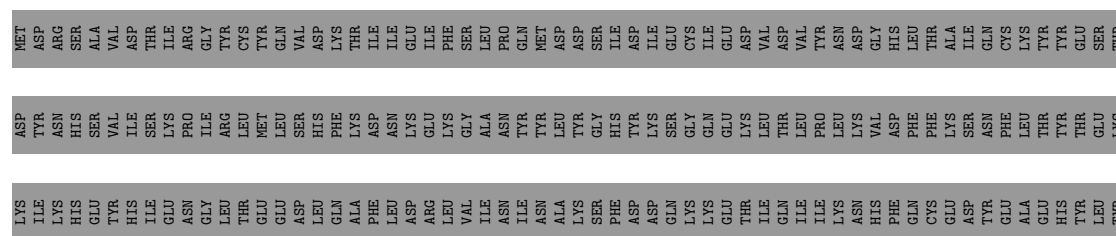
• Molecule 2: DUF4297

Chain L: 51% 11% 38%



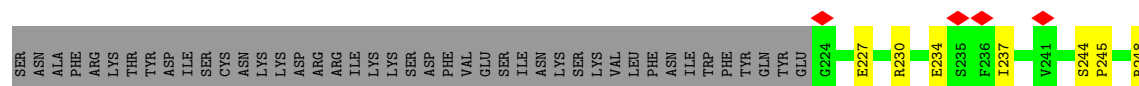
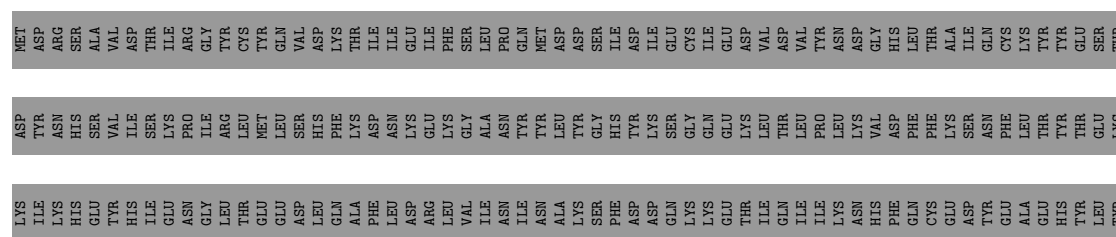
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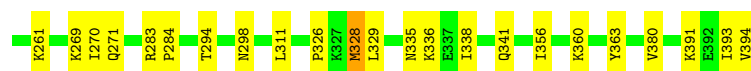
Chain M: 36% 7% 57%



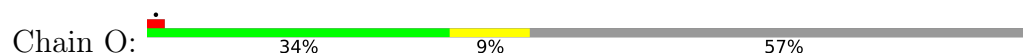
• Molecule 2: DUF4297

Chain N: 36% 7% 57%

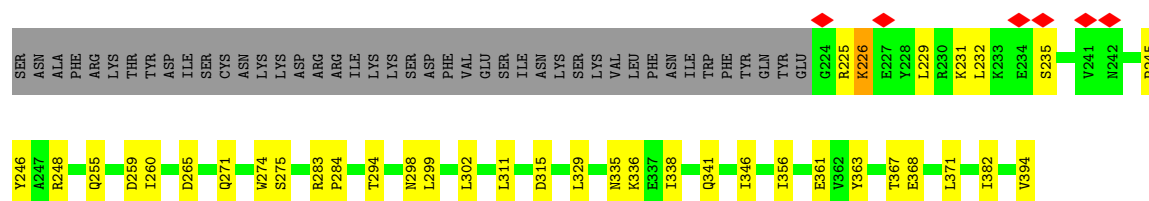




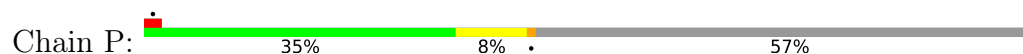
• Molecule 2: DUF4297



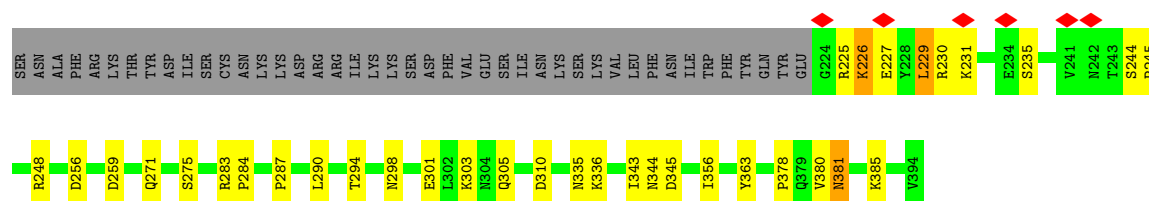
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LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	R283
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	P294
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	T294
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	N298
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LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	K326
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LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	L329
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	K335
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	K336
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	E337
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	I338
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	Q341
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	I356
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LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	Y363
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LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	K391
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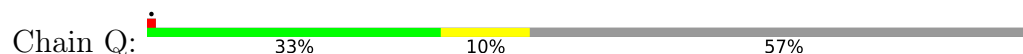
• Molecule 2: DUF4297



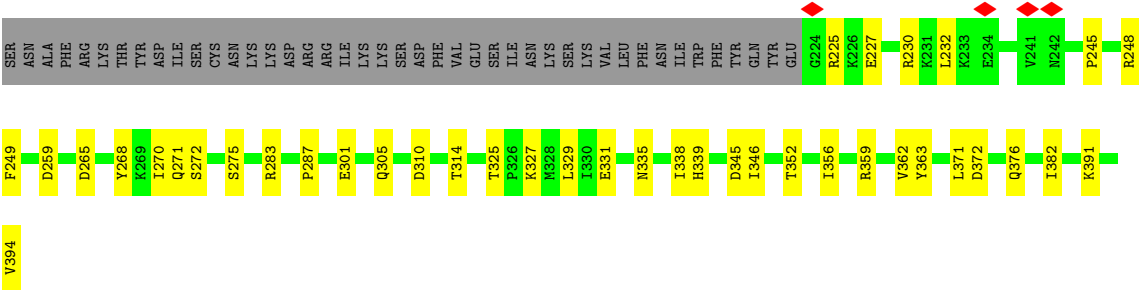
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LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	E337
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	I338
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	Q341
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LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	E234
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	S235
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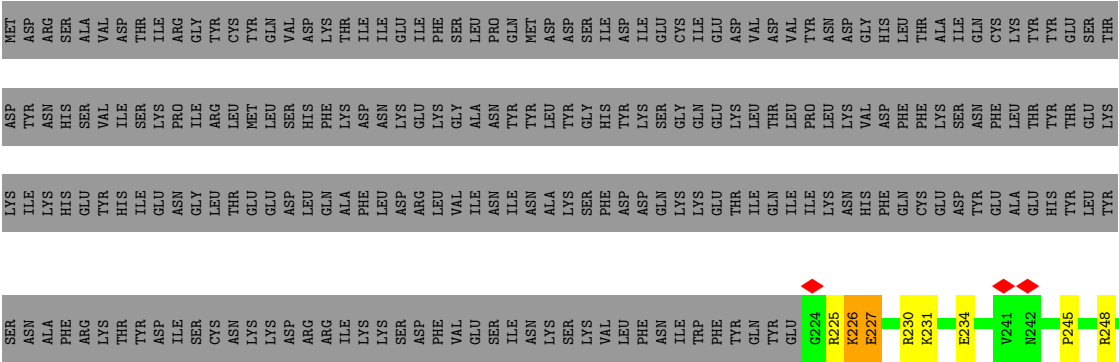
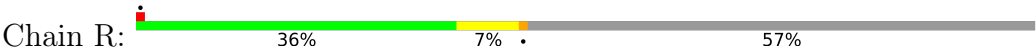
• Molecule 2: DUF4297



MET	ASP	THR	ILE	THR	ASP	VAL	ALA	SER	ARG	ASP	K261
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LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	S275
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	R283
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	P284
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	P287
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LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	T294
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	N298
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	E301
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LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	K303
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	M304
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	Q305
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	D310
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	N335
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	K336
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	I343
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	N344
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	D345
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	I356
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	Y363
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	P378
LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	Q379
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LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	M381
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LYS	ILE	LYS	HIS	GLU	THR	ASP	THR	ASP	THR	ASP	V394



• Molecule 2: DUF4297



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	290611	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.971	Depositor
Minimum map value	-1.203	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.108	Depositor
Map size ($\text{\AA}$)	304.0, 304.0, 304.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.95, 0.95, 0.95	Depositor

5 Model quality

5.1 Standard geometry

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	0.20	0/4625	0.50	2/6248 (0.0%)
1	B	0.17	0/4625	0.42	2/6248 (0.0%)
1	C	0.18	0/4625	0.45	1/6248 (0.0%)
1	D	0.17	0/4625	0.42	1/6248 (0.0%)
1	E	0.18	0/4604	0.45	2/6221 (0.0%)
1	F	0.18	0/4604	0.45	2/6221 (0.0%)
2	G	0.17	0/2126	0.42	0/2861
2	H	0.15	0/2126	0.40	0/2861
2	I	0.14	0/2126	0.35	0/2861
2	J	0.16	0/2126	0.41	0/2861
2	K	0.15	0/2126	0.38	0/2861
2	L	0.14	0/2126	0.36	0/2861
2	M	0.21	0/1470	0.54	2/1983 (0.1%)
2	N	0.22	0/1470	0.57	1/1983 (0.1%)
2	O	0.18	0/1470	0.51	1/1983 (0.1%)
2	P	0.20	0/1470	0.55	1/1983 (0.1%)
2	Q	0.20	0/1470	0.49	1/1983 (0.1%)
2	R	0.20	0/1470	0.50	1/1983 (0.1%)
All	All	0.18	0/49284	0.45	17/66498 (0.0%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	265	PRO	CA-N-CD	-8.74	99.76	112.00
1	F	265	PRO	CA-N-CD	-7.24	101.86	112.00
2	R	226	LYS	CA-CB-CG	6.93	127.97	114.10
2	M	226	LYS	CA-CB-CG	6.70	127.50	114.10
1	B	265	PRO	CA-N-CD	-5.97	103.65	112.00
2	M	225	ARG	CA-CB-CG	5.62	125.34	114.10
1	A	570	LYS	CB-CG-CD	5.54	124.05	111.30
1	B	570	LYS	CB-CG-CD	5.51	123.97	111.30
1	D	177	LYS	CB-CG-CD	5.45	123.83	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	177	LYS	CB-CG-CD	5.42	123.77	111.30
2	N	328	MET	CB-CG-SD	5.42	128.97	112.70
2	P	226	LYS	CA-CB-CG	5.38	124.85	114.10
1	F	177	LYS	CB-CG-CD	5.36	123.64	111.30
1	C	177	LYS	CB-CG-CD	5.33	123.56	111.30
2	Q	225	ARG	CA-CB-CG	5.32	124.74	114.10
2	O	226	LYS	CA-CB-CG	5.28	124.67	114.10
1	A	177	LYS	CB-CG-CD	5.21	123.28	111.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4539	0	4525	90	0
1	B	4539	0	4525	82	0
1	C	4539	0	4525	80	0
1	D	4539	0	4525	76	0
1	E	4518	0	4502	84	0
1	F	4518	0	4502	82	0
2	G	2076	0	2029	28	0
2	H	2076	0	2029	30	0
2	I	2076	0	2029	26	0
2	J	2076	0	2029	19	0
2	K	2076	0	2029	33	0
2	L	2076	0	2029	27	0
2	M	1436	0	1412	18	0
2	N	1436	0	1412	20	0
2	O	1436	0	1412	24	0
2	P	1436	0	1412	21	0
2	Q	1436	0	1412	24	0
2	R	1436	0	1412	19	0
All	All	48264	0	47750	723	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 (723) 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)
2:P:227:GLU:HG3	2:P:230:ARG:HH22	1.42	0.83
1:F:153:THR:HA	1:F:466:GLN:HE22	1.47	0.76
2:I:152:SER:H	2:I:155:ASP:HB2	1.51	0.73
1:C:151:GLY:HA3	1:C:485:MET:HB2	1.70	0.72
1:C:549:LEU:HA	1:C:552:TRP:HB2	1.73	0.70
1:B:522:MET:HE2	1:B:529:PRO:HB3	1.74	0.69
1:A:522:MET:HE2	1:A:529:PRO:HB3	1.74	0.68
1:B:139:GLY:HA3	1:E:549:LEU:HD22	1.76	0.68
1:A:28:GLU:HG2	1:A:30:LYS:H	1.60	0.67
1:C:62:GLU:HB2	1:C:70:LYS:HB3	1.77	0.66
2:J:267:ILE:HD13	2:J:306:LEU:HD11	1.77	0.66
1:A:218:ASP:HB2	1:A:441:ARG:HH22	1.61	0.65
2:I:275:SER:HB3	2:I:287:PRO:HD3	1.77	0.65
2:H:212:LYS:HA	2:H:381:ASN:HB2	1.79	0.65
1:E:62:GLU:HB2	1:E:70:LYS:HB3	1.79	0.65
1:B:151:GLY:HA3	1:B:485:MET:HB2	1.80	0.64
1:C:401:GLU:HA	1:C:404:TYR:HB3	1.79	0.64
2:H:190:ILE:HG21	2:H:199:ILE:HD13	1.80	0.64
2:O:260:ILE:HD12	2:O:302:LEU:HB2	1.80	0.64
1:C:138:ASN:HB3	1:C:141:ARG:HB2	1.79	0.64
2:G:223:GLU:HB3	2:G:227:GLU:HB3	1.80	0.64
1:B:340:ILE:HG22	1:B:349:LEU:HD22	1.79	0.63
1:A:31:ILE:HG23	1:A:35:LYS:HB2	1.79	0.63
1:C:245:ASN:HB3	1:C:268:PHE:HB2	1.80	0.63
1:A:549:LEU:HD22	1:C:139:GLY:HA3	1.81	0.63
1:F:258:GLU:N	1:F:258:GLU:OE1	2.31	0.63
2:I:267:ILE:HD13	2:I:306:LEU:HD11	1.81	0.63
1:D:407:LYS:HA	1:D:410:LYS:HG3	1.81	0.62
2:P:301:GLU:OE2	2:P:305:GLN:NE2	2.32	0.62
2:P:380:VAL:C	2:P:381:ASN:HD22	2.08	0.62
1:B:455:ARG:NH1	1:E:153:THR:OG1	2.33	0.62
2:O:245:PRO:HG3	2:O:283:ARG:HB3	1.80	0.62
1:B:293:TRP:HE1	1:B:302:PHE:HB2	1.65	0.62
2:P:385:LYS:HE2	2:P:385:LYS:H	1.64	0.62
1:A:139:GLY:HA3	1:F:549:LEU:HD22	1.81	0.62
1:D:483:ILE:HG12	1:D:521:ILE:HG23	1.81	0.62
1:A:151:GLY:HA3	1:A:485:MET:HB2	1.83	0.61
1:B:549:LEU:HD22	1:D:139:GLY:HA3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:GLU:OE1	1:F:397:ARG:NH2	2.34	0.61
1:F:401:GLU:HA	1:F:404:TYR:HB3	1.81	0.61
2:G:367:THR:O	2:G:383:GLN:NE2	2.34	0.61
1:B:119:ASN:O	1:E:553:ARG:NH1	2.34	0.61
1:D:401:GLU:HA	1:D:404:TYR:HB3	1.83	0.61
1:D:138:ASN:HB3	1:D:141:ARG:HB2	1.82	0.60
1:D:549:LEU:HD11	1:F:171:GLU:HG2	1.83	0.60
1:E:99:LYS:NZ	1:E:101:GLU:OE1	2.34	0.60
2:K:223:GLU:HB3	2:K:227:GLU:HB3	1.84	0.60
2:J:328:MET:HA	2:J:331:GLU:HG2	1.83	0.60
2:K:176:GLU:HA	2:K:180:TYR:HB3	1.82	0.60
2:I:151:LYS:HZ2	2:I:156:GLN:HG3	1.67	0.60
1:D:245:ASN:HB3	1:D:268:PHE:HB2	1.84	0.59
1:A:306:ASN:OD1	1:A:309:ARG:NH1	2.35	0.59
1:C:24:ASP:O	1:C:68:LYS:NZ	2.35	0.59
2:H:166:ASN:O	2:H:169:GLN:NE2	2.36	0.59
1:A:22:SER:OG	2:I:280:ARG:NH2	2.35	0.59
1:E:219:GLU:OE1	1:E:397:ARG:NH2	2.36	0.59
2:I:328:MET:HA	2:I:331:GLU:HG2	1.84	0.59
2:Q:301:GLU:OE1	2:Q:305:GLN:NE2	2.36	0.59
1:C:221:GLU:OE2	1:C:239:ARG:NH1	2.35	0.59
2:P:245:PRO:HG3	2:P:283:ARG:HB3	1.84	0.59
1:D:24:ASP:O	1:D:68:LYS:NZ	2.36	0.59
1:A:146:HIS:HB2	1:A:479:CYS:HA	1.85	0.59
2:R:301:GLU:OE2	2:R:305:GLN:NE2	2.34	0.59
2:N:227:GLU:OE1	2:N:230:ARG:NE	2.36	0.58
2:O:346:ILE:HD13	2:O:371:LEU:HD13	1.85	0.58
1:A:222:GLU:HB3	1:A:390:ILE:HD11	1.84	0.58
1:B:437:LEU:HD23	1:B:439:LYS:HE3	1.86	0.58
1:D:549:LEU:HD22	1:F:139:GLY:HA3	1.84	0.58
2:K:275:SER:HB3	2:K:287:PRO:HD3	1.85	0.58
1:D:219:GLU:OE1	1:D:397:ARG:NH2	2.36	0.58
1:F:13:SER:HB2	1:F:20:LYS:HB2	1.85	0.58
1:E:22:SER:OG	2:K:280:ARG:NH2	2.36	0.58
2:O:231:LYS:O	2:O:235:SER:OG	2.20	0.58
2:M:380:VAL:C	2:M:381:ASN:HD22	2.11	0.58
1:B:331:ASN:OD1	1:D:239:ARG:NH1	2.36	0.58
1:B:381:SER:HB2	1:D:456:LYS:HD2	1.85	0.58
2:N:245:PRO:HG3	2:N:283:ARG:HB3	1.85	0.58
2:G:275:SER:HB3	2:G:287:PRO:HD3	1.85	0.58
1:B:146:HIS:HB2	1:B:479:CYS:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:VAL:HB	1:D:71:TYR:HB3	1.86	0.58
2:P:231:LYS:O	2:P:235:SER:OG	2.21	0.58
1:A:165:LEU:HD11	1:A:424:VAL:HG21	1.86	0.57
1:A:246:LYS:NZ	1:A:264:SER:O	2.31	0.57
2:M:227:GLU:OE2	2:M:230:ARG:NH2	2.36	0.57
1:B:378:LEU:HD13	1:B:395:ILE:HD13	1.86	0.57
2:Q:271:GLN:O	2:Q:275:SER:OG	2.23	0.57
1:E:401:GLU:HA	1:E:404:TYR:HB3	1.85	0.57
1:E:485:MET:HE3	1:E:519:ALA:HB2	1.86	0.57
1:C:6:ASP:OD2	1:C:6:ASP:N	2.36	0.57
1:A:429:HIS:HD1	1:A:465:SER:HG	1.48	0.57
1:D:185:ILE:HD11	1:D:366:ILE:HG22	1.86	0.57
1:C:219:GLU:OE1	1:C:397:ARG:NH2	2.38	0.57
1:E:153:THR:HA	1:E:466:GLN:HE22	1.70	0.57
2:G:282:ASP:OD1	2:G:282:ASP:N	2.37	0.57
1:D:6:ASP:N	1:D:6:ASP:OD2	2.36	0.57
2:P:271:GLN:O	2:P:275:SER:OG	2.23	0.56
1:D:44:VAL:HB	1:D:52:LEU:HB3	1.86	0.56
1:F:521:ILE:HG22	1:F:526:ILE:HG21	1.86	0.56
1:B:281:ASN:HD21	1:B:330:LEU:HB2	1.70	0.56
1:C:146:HIS:HB2	1:C:479:CYS:HA	1.87	0.56
1:C:185:ILE:HD11	1:C:366:ILE:HG22	1.86	0.56
2:O:284:PRO:HG3	2:O:336:LYS:HE3	1.88	0.56
2:G:279:LYS:HA	2:G:336:LYS:HD2	1.88	0.56
2:K:279:LYS:HA	2:K:336:LYS:HD2	1.88	0.56
1:B:253:ASP:OD1	1:B:253:ASP:N	2.39	0.56
1:C:407:LYS:HD2	1:C:457:TYR:HA	1.88	0.56
1:E:6:ASP:N	1:E:6:ASP:OD1	2.36	0.56
1:E:44:VAL:HB	1:E:52:LEU:HB2	1.87	0.56
2:M:376:GLN:OE1	2:M:376:GLN:N	2.38	0.56
2:N:294:THR:OG1	2:N:298:ASN:ND2	2.38	0.56
1:D:184:ILE:HB	1:D:375:ILE:HG12	1.88	0.56
1:C:93:LEU:O	2:L:242:ASN:ND2	2.38	0.55
2:I:212:LYS:HA	2:I:381:ASN:HB2	1.89	0.55
1:A:215:LEU:HD22	1:A:219:GLU:HB3	1.88	0.55
1:C:549:LEU:HD12	1:E:171:GLU:HG2	1.87	0.55
1:D:145:LYS:HB3	1:D:480:ASN:HB2	1.89	0.55
2:O:271:GLN:O	2:O:275:SER:OG	2.19	0.55
2:R:227:GLU:OE2	2:R:230:ARG:NH2	2.39	0.55
1:A:153:THR:OG1	1:A:466:GLN:NE2	2.38	0.55
1:A:344:ARG:NH2	1:C:453:GLU:OE1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:ASP:OD1	1:C:303:ASP:N	2.39	0.55
1:F:20:LYS:HE2	1:F:74:GLU:HG3	1.89	0.55
2:J:253:GLU:OE2	2:J:255:GLN:NE2	2.39	0.55
2:Q:232:LEU:HD23	2:Q:382:ILE:HG23	1.88	0.55
1:E:26:LEU:HD21	1:E:32:ALA:HB2	1.89	0.55
1:B:470:GLU:N	1:B:470:GLU:OE1	2.38	0.55
2:K:171:GLU:N	2:K:171:GLU:OE1	2.39	0.55
1:C:44:VAL:HB	1:C:52:LEU:HB3	1.87	0.55
1:A:378:LEU:HD13	1:A:395:ILE:HD13	1.89	0.55
1:B:549:LEU:HD11	1:D:171:GLU:HG2	1.89	0.55
1:C:184:ILE:HB	1:C:375:ILE:HG12	1.89	0.55
1:C:445:GLU:OE2	1:C:445:GLU:N	2.38	0.55
1:E:137:VAL:HG12	1:E:526:ILE:HB	1.89	0.55
1:E:288:ASP:HB3	1:E:290:GLU:HG2	1.88	0.55
2:G:300:TYR:O	2:G:304:ASN:ND2	2.39	0.55
2:L:386:ASP:N	2:L:386:ASP:OD1	2.39	0.55
2:Q:271:GLN:HE21	2:Q:339:HIS:HB3	1.72	0.55
1:B:434:LYS:N	1:B:470:GLU:O	2.40	0.55
1:C:553:ARG:O	1:E:176:TYR:OH	2.20	0.55
1:F:536:LYS:HE2	1:F:536:LYS:H	1.72	0.55
2:R:245:PRO:HG3	2:R:283:ARG:HB3	1.89	0.55
1:E:245:ASN:HB3	1:E:268:PHE:HB2	1.87	0.55
1:F:10:GLU:OE2	2:G:280:ARG:NH1	2.37	0.55
2:G:269:LYS:NZ	2:G:394:VAL:O	2.40	0.55
2:K:279:LYS:O	2:K:336:LYS:NZ	2.40	0.55
1:E:536:LYS:H	1:E:536:LYS:HE2	1.72	0.55
1:B:184:ILE:HB	1:B:375:ILE:HG12	1.89	0.54
2:G:315:ASP:OD1	2:G:315:ASP:N	2.39	0.54
1:D:515:LYS:NZ	1:F:91:ASP:OD2	2.40	0.54
1:E:24:ASP:OD1	2:K:280:ARG:NH2	2.40	0.54
1:F:221:GLU:HG2	1:F:225:LEU:HD12	1.89	0.54
1:A:24:ASP:OD1	2:I:280:ARG:NH2	2.41	0.54
1:B:180:ASN:ND2	1:B:182:SER:OG	2.40	0.54
1:F:485:MET:HE3	1:F:519:ALA:HB2	1.90	0.54
2:L:353:LEU:HD12	2:L:360:LYS:HD3	1.89	0.54
2:O:329:LEU:HD23	2:O:341:GLN:HB3	1.89	0.54
2:O:255:GLN:N	2:O:255:GLN:OE1	2.40	0.54
1:C:43:ARG:NH2	1:C:45:SER:OG	2.40	0.54
1:C:493:GLN:HB3	1:C:497:LYS:HZ3	1.71	0.54
1:E:438:SER:HA	1:E:441:ARG:HB2	1.89	0.54
1:F:389:SER:HB3	1:F:440:TYR:HD1	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:LYS:NZ	1:E:567:GLN:OE1	2.41	0.54
1:C:536:LYS:HE2	1:C:536:LYS:H	1.72	0.54
2:O:367:THR:OG1	2:O:368:GLU:OE2	2.26	0.54
1:A:193:TYR:HE2	1:A:426:GLU:HG3	1.72	0.54
1:C:211:PRO:HA	1:C:353:SER:HB3	1.90	0.54
2:M:245:PRO:HG3	2:M:283:ARG:HB3	1.89	0.54
2:R:315:ASP:OD1	2:R:315:ASP:N	2.39	0.54
1:A:120:ASP:OD2	1:A:140:ASN:ND2	2.41	0.54
1:C:434:LYS:N	1:C:470:GLU:O	2.40	0.53
1:D:43:ARG:NH2	1:D:47:ASN:O	2.41	0.53
1:D:553:ARG:O	1:F:176:TYR:OH	2.24	0.53
2:K:269:LYS:HD2	2:K:391:LYS:HG3	1.89	0.53
1:A:253:ASP:N	1:A:253:ASP:OD1	2.41	0.53
1:D:211:PRO:HA	1:D:353:SER:HB3	1.89	0.53
1:F:6:ASP:OD1	1:F:6:ASP:N	2.35	0.53
1:B:70:LYS:HD2	1:B:72:MET:HG2	1.90	0.53
1:E:378:LEU:HD13	1:E:395:ILE:HD13	1.89	0.53
1:D:445:GLU:OE2	1:D:445:GLU:N	2.38	0.53
1:F:18:LYS:NZ	1:F:57:ASP:OD1	2.41	0.53
1:F:146:HIS:HB2	1:F:479:CYS:HA	1.90	0.53
1:D:407:LYS:HD2	1:D:457:TYR:HA	1.89	0.53
1:F:438:SER:HA	1:F:441:ARG:HB2	1.89	0.53
1:A:280:ARG:NE	1:A:283:GLU:OE2	2.41	0.53
1:B:53:LEU:HD23	1:B:111:ILE:HD11	1.90	0.53
1:E:146:HIS:HB2	1:E:479:CYS:HA	1.90	0.53
1:C:254:PRO:HA	1:C:257:LYS:HB2	1.91	0.53
1:A:53:LEU:HD23	1:A:111:ILE:HD11	1.91	0.53
1:D:215:LEU:HA	1:D:397:ARG:HH22	1.74	0.53
2:H:215:PHE:HB2	2:H:383:GLN:HG2	1.91	0.53
1:D:230:ASN:HD22	1:D:235:ARG:HE	1.56	0.53
1:E:389:SER:HB3	1:E:440:TYR:HD1	1.74	0.53
2:N:234:GLU:OE2	2:N:234:GLU:N	2.36	0.53
1:A:214:LEU:HD13	1:A:398:LEU:HD11	1.90	0.52
1:B:117:ASP:OD1	1:B:117:ASP:N	2.42	0.52
1:F:15:SER:HB2	1:F:18:LYS:HB3	1.91	0.52
2:K:184:PHE:HE2	2:K:218:TRP:HD1	1.57	0.52
2:N:326:PRO:HA	2:N:329:LEU:HD12	1.89	0.52
1:C:130:ASN:OD1	1:C:132:LYS:NZ	2.42	0.52
1:D:180:ASN:ND2	1:D:182:SER:OG	2.42	0.52
1:E:221:GLU:OE1	1:E:235:ARG:NH2	2.42	0.52
1:F:245:ASN:HB3	1:F:268:PHE:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:172:ASP:OD2	2:J:172:ASP:N	2.37	0.52
1:B:21:ILE:O	1:B:73:ILE:N	2.43	0.52
1:D:434:LYS:N	1:D:470:GLU:O	2.41	0.52
1:A:180:ASN:O	1:A:374:ASN:ND2	2.43	0.52
1:E:15:SER:HB2	1:E:18:LYS:HB3	1.90	0.52
1:C:180:ASN:ND2	1:C:182:SER:OG	2.43	0.52
1:E:18:LYS:NZ	1:E:57:ASP:OD2	2.43	0.52
2:M:234:GLU:OE2	2:M:234:GLU:N	2.38	0.52
1:D:93:LEU:O	2:H:242:ASN:ND2	2.43	0.52
1:D:130:ASN:OD1	1:D:132:LYS:NZ	2.42	0.52
2:G:154:ASP:OD1	2:G:154:ASP:N	2.38	0.52
2:G:256:ASP:OD1	2:G:256:ASP:N	2.40	0.52
2:K:300:TYR:O	2:K:304:ASN:ND2	2.43	0.52
1:D:386:GLU:OE2	1:F:449:ARG:NH1	2.41	0.52
1:F:280:ARG:NE	1:F:283:GLU:OE2	2.42	0.52
2:O:246:TYR:H	2:O:248:ARG:HH12	1.58	0.52
1:B:424:VAL:HG13	1:B:462:LEU:HD22	1.90	0.52
1:D:146:HIS:HB2	1:D:479:CYS:HA	1.92	0.52
1:B:120:ASP:OD2	1:B:140:ASN:ND2	2.42	0.51
1:A:429:HIS:HB2	1:A:470:GLU:HB2	1.91	0.51
2:J:306:LEU:HD22	2:J:311:LEU:HD23	1.92	0.51
2:M:259:ASP:OD1	2:M:260:ILE:N	2.43	0.51
2:R:248:ARG:HG2	2:R:363:TYR:HE2	1.75	0.51
2:H:282:ASP:OD1	2:H:282:ASP:N	2.37	0.51
2:Q:372:ASP:OD1	2:Q:372:ASP:N	2.43	0.51
1:E:14:VAL:HG23	1:E:96:PRO:HG3	1.93	0.51
2:H:286:SER:OG	2:H:341:GLN:OE1	2.29	0.51
2:I:290:LEU:HD13	2:I:343:ILE:HG22	1.92	0.51
2:J:315:ASP:OD1	2:J:315:ASP:N	2.44	0.51
1:F:149:ILE:HD12	1:F:161:VAL:HG22	1.93	0.51
1:F:365:LEU:HD13	1:F:395:ILE:HG23	1.93	0.51
2:I:315:ASP:OD1	2:I:315:ASP:N	2.43	0.51
2:J:353:LEU:HD12	2:J:360:LYS:HD3	1.92	0.51
1:B:113:SER:O	1:B:121:ARG:NH2	2.43	0.51
1:C:165:LEU:HD22	1:C:184:ILE:HD13	1.92	0.51
1:E:23:VAL:HB	1:E:71:TYR:HB3	1.93	0.51
2:Q:335:ASN:HD22	2:Q:338:ILE:HD12	1.75	0.51
1:E:165:LEU:HD13	1:E:184:ILE:HG21	1.93	0.51
2:J:151:LYS:N	2:J:155:ASP:OD2	2.43	0.51
2:L:244:SER:O	2:L:248:ARG:NH1	2.36	0.51
1:E:94:ALA:HA	2:K:242:ASN:HD21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:374:PRO:O	2:J:379:GLN:NE2	2.44	0.51
2:Q:345:ASP:OD1	2:Q:345:ASP:N	2.42	0.51
1:D:47:ASN:C	1:D:47:ASN:HD22	2.17	0.51
2:H:253:GLU:OE1	2:H:367:THR:OG1	2.27	0.51
2:K:178:TYR:O	2:K:182:ASN:ND2	2.44	0.51
2:O:226:LYS:HD2	2:O:226:LYS:O	2.11	0.51
1:B:21:ILE:HG12	1:B:100:VAL:HG21	1.94	0.50
1:B:194:GLU:HG3	1:B:202:VAL:HG11	1.93	0.50
1:E:13:SER:HB3	1:E:20:LYS:HB2	1.93	0.50
1:F:502:ASP:OD1	1:F:503:THR:N	2.41	0.50
2:N:271:GLN:HG2	2:N:311:LEU:HD11	1.93	0.50
2:Q:346:ILE:HD11	2:Q:371:LEU:HD11	1.93	0.50
1:A:194:GLU:HG3	1:A:202:VAL:HG21	1.94	0.50
1:A:270:ILE:HG12	1:A:340:ILE:HD11	1.92	0.50
1:B:11:VAL:HG12	1:B:96:PRO:HB3	1.93	0.50
1:D:165:LEU:HD22	1:D:184:ILE:HD13	1.92	0.50
2:N:244:SER:O	2:N:248:ARG:NH1	2.39	0.50
1:B:165:LEU:HD22	1:B:184:ILE:HG12	1.93	0.50
1:C:193:TYR:HE2	1:C:426:GLU:HG3	1.76	0.50
2:P:259:ASP:OD1	2:P:259:ASP:N	2.39	0.50
2:Q:248:ARG:HG2	2:Q:363:TYR:HE2	1.75	0.50
2:R:226:LYS:HE3	2:R:230:ARG:HH12	1.76	0.50
1:A:507:ILE:HD11	1:A:531:ILE:HG12	1.92	0.50
1:D:43:ARG:NH2	1:D:45:SER:OG	2.45	0.50
1:D:149:ILE:HD12	1:D:161:VAL:HG22	1.92	0.50
1:F:437:LEU:HD12	1:F:439:LYS:HE3	1.94	0.50
2:N:237:ILE:HG21	2:N:393:ILE:HG22	1.94	0.50
1:A:181:ASN:HB3	1:F:552:TRP:HA	1.93	0.50
2:H:186:LYS:HA	2:H:189:ASP:HB2	1.94	0.50
2:M:335:ASN:HD22	2:M:338:ILE:HD12	1.77	0.50
2:J:244:SER:O	2:J:248:ARG:NH1	2.36	0.50
1:F:23:VAL:HB	1:F:71:TYR:HB3	1.94	0.50
1:F:138:ASN:HB3	1:F:141:ARG:HB2	1.92	0.50
2:K:162:GLN:HA	2:K:165:LYS:HB2	1.94	0.50
1:A:431:TYR:O	1:A:443:SER:OG	2.23	0.50
1:E:303:ASP:HB3	1:E:306:ASN:HB3	1.94	0.50
1:E:437:LEU:HD12	1:E:439:LYS:HE3	1.93	0.49
2:O:274:TRP:HE1	2:O:394:VAL:HG23	1.76	0.49
2:P:345:ASP:N	2:P:345:ASP:OD1	2.44	0.49
1:C:149:ILE:HD12	1:C:161:VAL:HG22	1.94	0.49
1:C:23:VAL:HB	1:C:71:TYR:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:230:ARG:NH1	2:G:234:GLU:OE1	2.45	0.49
2:M:226:LYS:HD2	2:M:226:LYS:O	2.12	0.49
2:O:265:ASP:OD1	2:Q:359:ARG:NH2	2.40	0.49
2:L:286:SER:OG	2:L:341:GLN:OE1	2.30	0.49
2:M:315:ASP:OD1	2:M:315:ASP:N	2.44	0.49
1:E:538:THR:HG23	1:E:539:ILE:HG13	1.94	0.49
2:O:294:THR:OG1	2:O:298:ASN:ND2	2.43	0.49
1:A:434:LYS:N	1:A:470:GLU:O	2.42	0.49
2:J:330:ILE:HD12	2:J:356:ILE:HG12	1.94	0.49
1:A:46:ASP:OD1	1:A:47:ASN:ND2	2.45	0.49
1:A:113:SER:O	1:A:121:ARG:NH2	2.45	0.49
1:E:279:ASN:ND2	1:E:310:LEU:O	2.46	0.49
2:H:303:LYS:NZ	2:H:344:ASN:OD1	2.46	0.49
2:L:157:LYS:NZ	2:L:180:TYR:OH	2.45	0.49
1:B:426:GLU:HA	1:B:464:ALA:HB3	1.94	0.49
1:C:8:ASN:ND2	1:C:25:ASP:OD1	2.36	0.49
1:E:280:ARG:NE	1:E:283:GLU:OE2	2.43	0.49
2:H:359:ARG:NH1	2:H:361:GLU:OE2	2.46	0.49
1:A:70:LYS:HD2	1:A:72:MET:HG2	1.94	0.49
1:C:215:LEU:HA	1:C:397:ARG:HH22	1.77	0.49
2:H:161:ILE:HG21	2:H:176:GLU:HG2	1.94	0.49
1:E:150:VAL:HG11	1:E:468:PRO:HB3	1.95	0.49
1:E:254:PRO:HA	1:E:257:LYS:HB2	1.94	0.49
2:H:244:SER:O	2:H:248:ARG:NH1	2.35	0.49
1:D:286:ASN:HD21	1:D:290:GLU:HG2	1.78	0.48
1:F:296:GLU:OE2	1:F:296:GLU:N	2.46	0.48
2:P:248:ARG:HG2	2:P:363:TYR:HE2	1.78	0.48
2:P:256:ASP:OD1	2:P:298:ASN:ND2	2.46	0.48
1:C:291:HIS:HB2	1:C:302:PHE:HB3	1.94	0.48
1:C:548:TYR:O	1:C:552:TRP:N	2.44	0.48
1:E:296:GLU:OE2	1:E:296:GLU:N	2.43	0.48
1:E:497:LYS:HD3	1:E:507:ILE:HG23	1.95	0.48
2:J:212:LYS:HA	2:J:381:ASN:HB2	1.95	0.48
1:A:305:GLU:HG3	1:A:306:ASN:ND2	2.28	0.48
1:A:553:ARG:O	1:C:176:TYR:OH	2.27	0.48
1:C:28:GLU:HG2	1:C:31:ILE:HG13	1.94	0.48
1:D:193:TYR:HE2	1:D:426:GLU:HG3	1.77	0.48
1:F:14:VAL:HG23	1:F:96:PRO:HG3	1.93	0.48
1:A:365:LEU:HD13	1:A:395:ILE:HG23	1.94	0.48
1:C:65:GLU:HB3	2:K:279:LYS:NZ	2.29	0.48
1:C:272:GLU:HB3	1:C:311:PHE:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:VAL:HG12	1:E:277:ILE:HG12	1.96	0.48
2:R:345:ASP:N	2:R:345:ASP:OD1	2.45	0.48
1:F:95:LEU:N	2:G:242:ASN:OD1	2.40	0.48
1:F:150:VAL:HG11	1:F:468:PRO:HB3	1.94	0.48
1:B:327:GLY:O	1:D:236:ASN:ND2	2.39	0.48
2:G:178:TYR:O	2:G:182:ASN:ND2	2.47	0.48
2:H:353:LEU:HD12	2:H:360:LYS:HD2	1.95	0.48
2:G:279:LYS:O	2:G:336:LYS:NZ	2.47	0.48
2:N:270:ILE:HG12	2:N:394:VAL:HG21	1.96	0.48
1:B:303:ASP:OD1	1:B:303:ASP:N	2.44	0.48
2:K:198:ARG:NH1	2:K:199:ILE:O	2.46	0.48
1:A:553:ARG:NH1	1:C:119:ASN:O	2.45	0.47
1:F:378:LEU:HD13	1:F:395:ILE:HD13	1.95	0.47
2:O:315:ASP:OD1	2:O:315:ASP:N	2.46	0.47
1:A:177:LYS:HE2	1:A:177:LYS:HA	1.96	0.47
2:L:212:LYS:HA	2:L:381:ASN:HB2	1.97	0.47
1:F:197:PHE:O	1:F:200:SER:OG	2.29	0.47
2:R:226:LYS:HD2	2:R:226:LYS:O	2.14	0.47
1:B:553:ARG:O	1:D:176:TYR:OH	2.27	0.47
1:C:155:SER:HB3	1:C:486:ARG:HB3	1.95	0.47
1:A:116:ILE:HG23	1:A:138:ASN:HD22	1.80	0.47
1:A:490:PRO:HA	1:A:493:GLN:HB2	1.97	0.47
1:E:65:GLU:HA	2:J:280:ARG:HA	1.97	0.47
2:L:152:SER:O	2:L:156:GLN:N	2.46	0.47
1:E:224:PHE:HZ	1:E:349:LEU:HD21	1.80	0.47
2:L:215:PHE:HB2	2:L:383:GLN:HG2	1.97	0.47
2:P:226:LYS:HD2	2:P:226:LYS:O	2.15	0.47
1:A:21:ILE:O	1:A:73:ILE:N	2.48	0.47
1:A:503:THR:OG1	1:A:504:VAL:N	2.48	0.47
1:C:23:VAL:HG11	1:C:26:LEU:HG	1.95	0.47
1:C:549:LEU:O	1:C:553:ARG:HG3	2.14	0.47
1:E:396:SER:OG	1:E:425:TYR:OH	2.27	0.47
1:F:65:GLU:HG3	2:I:279:LYS:HD2	1.97	0.47
2:G:229:LEU:HD22	2:G:393:ILE:HD11	1.97	0.47
2:H:315:ASP:OD1	2:H:315:ASP:N	2.47	0.47
2:L:231:LYS:O	2:L:235:SER:OG	2.29	0.47
1:F:165:LEU:HD22	1:F:184:ILE:HD13	1.96	0.47
1:F:502:ASP:HB3	1:F:522:MET:HE3	1.97	0.47
2:G:215:PHE:HB2	2:G:383:GLN:HG2	1.96	0.47
2:G:234:GLU:O	2:G:238:ARG:NH1	2.48	0.47
2:H:200:LYS:HD2	2:H:200:LYS:HA	1.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:ARG:HG2	1:B:470:GLU:OE1	2.15	0.47
2:M:367:THR:O	2:M:383:GLN:NE2	2.48	0.47
2:O:259:ASP:OD1	2:O:259:ASP:N	2.47	0.47
2:Q:245:PRO:HG3	2:Q:283:ARG:HB3	1.97	0.47
1:D:15:SER:HB2	1:D:18:LYS:HB3	1.97	0.46
1:E:283:GLU:O	1:E:326:ASN:ND2	2.44	0.46
1:F:224:PHE:HZ	1:F:349:LEU:HD21	1.80	0.46
2:G:314:THR:HG23	2:G:329:LEU:HD23	1.95	0.46
2:Q:275:SER:HB3	2:Q:287:PRO:HD3	1.95	0.46
1:E:370:LYS:HE2	1:E:370:LYS:HA	1.96	0.46
1:F:558:ASP:OD1	1:F:558:ASP:N	2.43	0.46
2:M:345:ASP:N	2:M:345:ASP:OD1	2.48	0.46
2:Q:268:TYR:O	2:Q:272:SER:OG	2.30	0.46
1:D:155:SER:HB3	1:D:486:ARG:HB3	1.96	0.46
2:G:231:LYS:O	2:G:235:SER:OG	2.27	0.46
2:P:303:LYS:NZ	2:P:344:ASN:OD1	2.49	0.46
1:A:549:LEU:HD11	1:C:171:GLU:HG2	1.98	0.46
1:B:80:LEU:N	1:B:87:TYR:O	2.46	0.46
1:B:344:ARG:NH2	1:D:453:GLU:OE1	2.46	0.46
1:C:32:ALA:HA	1:C:36:LEU:HB2	1.98	0.46
1:C:386:GLU:HG2	1:C:387:VAL:HG13	1.97	0.46
1:E:215:LEU:HA	1:E:397:ARG:HH22	1.81	0.46
1:F:403:GLY:HA2	1:F:406:SER:HB3	1.98	0.46
2:J:223:GLU:HB2	2:J:227:GLU:HG2	1.97	0.46
2:P:310:ASP:HB2	2:R:358:ILE:HG22	1.97	0.46
2:Q:259:ASP:OD1	2:Q:259:ASP:N	2.44	0.46
1:A:62:GLU:HG2	1:A:70:LYS:HZ2	1.80	0.46
1:B:222:GLU:HB3	1:B:390:ILE:HD11	1.97	0.46
1:C:146:HIS:HB3	1:C:461:LEU:HD12	1.96	0.46
1:C:497:LYS:HD3	1:C:507:ILE:HG23	1.97	0.46
1:E:204:ASN:OD1	1:E:204:ASN:N	2.41	0.46
2:G:330:ILE:HD12	2:G:356:ILE:HG13	1.98	0.46
2:K:154:ASP:N	2:K:154:ASP:OD1	2.45	0.46
1:A:284:ARG:HB3	1:A:319:GLY:HA3	1.97	0.46
1:F:424:VAL:HG13	1:F:462:LEU:HD22	1.98	0.46
2:L:161:ILE:O	2:L:165:LYS:N	2.44	0.46
2:L:223:GLU:HB3	2:L:227:GLU:HB3	1.97	0.46
2:N:269:LYS:HB2	2:N:269:LYS:HE3	1.73	0.46
2:Q:270:ILE:HG12	2:Q:394:VAL:HG21	1.97	0.46
2:R:225:ARG:NH2	2:R:226:LYS:HB2	2.31	0.46
1:B:407:LYS:O	1:B:411:ARG:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:486:ARG:NE	1:D:514:LEU:O	2.49	0.46
2:K:374:PRO:O	2:K:379:GLN:NE2	2.49	0.46
1:D:381:SER:HB2	1:F:456:LYS:HD2	1.97	0.46
1:E:257:LYS:HA	1:E:260:ILE:HD12	1.96	0.46
1:E:507:ILE:HA	1:E:510:LEU:HG	1.97	0.46
2:H:366:TYR:CZ	2:H:383:GLN:HB2	2.51	0.46
2:K:165:LYS:NZ	2:K:170:CYS:O	2.44	0.46
1:C:407:LYS:HB3	1:C:410:LYS:HE2	1.98	0.46
1:C:547:LYS:HD2	1:E:140:ASN:HB3	1.99	0.46
1:E:365:LEU:HD13	1:E:395:ILE:HG23	1.97	0.46
2:Q:227:GLU:HG3	2:Q:230:ARG:HH21	1.79	0.46
1:B:176:TYR:OH	1:E:553:ARG:O	2.28	0.45
1:D:13:SER:HB3	1:D:20:LYS:HB2	1.96	0.45
1:E:536:LYS:HE2	1:E:536:LYS:N	2.30	0.45
1:F:177:LYS:HE3	1:F:177:LYS:HA	1.97	0.45
2:H:185:ARG:O	2:H:189:ASP:N	2.49	0.45
2:R:252:LEU:HD23	2:R:365:PHE:HB2	1.97	0.45
2:R:259:ASP:OD1	2:R:260:ILE:N	2.48	0.45
1:B:211:PRO:HA	1:B:353:SER:HB3	1.98	0.45
1:C:10:GLU:OE2	2:L:278:SER:OG	2.28	0.45
1:E:64:LYS:HB2	1:E:64:LYS:HE2	1.72	0.45
2:H:178:TYR:OH	2:H:210:LYS:O	2.25	0.45
2:L:303:LYS:NZ	2:L:344:ASN:OD1	2.46	0.45
2:M:346:ILE:HD11	2:M:371:LEU:HD13	1.98	0.45
2:N:356:ILE:HB	2:N:360:LYS:HD3	1.97	0.45
1:A:117:ASP:OD1	1:A:117:ASP:N	2.43	0.45
1:D:65:GLU:HB3	2:G:279:LYS:NZ	2.32	0.45
1:F:165:LEU:HD11	1:F:424:VAL:HG21	1.97	0.45
1:F:237:VAL:HG12	1:F:277:ILE:HG12	1.97	0.45
2:R:234:GLU:OE2	2:R:234:GLU:N	2.44	0.45
1:E:165:LEU:HD11	1:E:424:VAL:HG21	1.99	0.45
2:G:214:LEU:HA	2:G:383:GLN:HB3	1.97	0.45
2:I:259:ASP:HB3	2:I:262:THR:HG23	1.99	0.45
1:A:288:ASP:OD2	1:A:290:GLU:HG2	2.16	0.45
1:B:507:ILE:HD11	1:B:531:ILE:HG12	1.97	0.45
1:C:15:SER:HB2	1:C:18:LYS:HB3	1.97	0.45
1:D:202:VAL:HA	1:D:377:ILE:HB	1.99	0.45
1:F:510:LEU:HD21	1:F:531:ILE:HD11	1.98	0.45
2:P:275:SER:HB3	2:P:287:PRO:HD3	1.98	0.45
1:A:426:GLU:HA	1:A:464:ALA:HB3	1.99	0.45
1:D:146:HIS:HB3	1:D:461:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:346:ILE:H	2:K:346:ILE:HD12	1.82	0.45
1:A:193:TYR:CE2	1:A:426:GLU:HG3	2.52	0.45
1:C:277:ILE:HG21	1:C:332:PHE:HD2	1.82	0.45
1:E:357:THR:HG23	1:E:360:GLU:H	1.80	0.45
2:O:335:ASN:HD22	2:O:338:ILE:HD12	1.81	0.45
2:R:294:THR:OG1	2:R:298:ASN:OD1	2.32	0.45
1:A:303:ASP:O	1:A:307:ALA:N	2.50	0.45
1:D:28:GLU:HG2	1:D:31:ILE:HG13	1.98	0.45
1:D:485:MET:HE3	1:D:485:MET:HB3	1.78	0.45
1:F:138:ASN:O	1:F:142:PHE:N	2.50	0.45
2:J:290:LEU:HD13	2:J:343:ILE:HG22	1.97	0.45
2:L:327:LYS:HA	2:L:330:ILE:HD13	1.99	0.45
1:A:219:GLU:OE2	1:A:393:SER:OG	2.32	0.45
1:C:19:LEU:N	1:C:75:ALA:O	2.41	0.45
1:F:46:ASP:OD1	1:F:47:ASN:ND2	2.49	0.45
1:F:538:THR:HG23	1:F:539:ILE:HG13	1.98	0.45
2:I:177:HIS:ND1	2:I:231:LYS:HD2	2.32	0.45
2:K:329:LEU:HD22	2:K:341:GLN:HB3	1.99	0.45
1:B:365:LEU:HD13	1:B:395:ILE:HG23	1.98	0.45
1:C:13:SER:HB3	1:C:20:LYS:HB2	1.98	0.45
1:C:486:ARG:NE	1:C:514:LEU:O	2.50	0.45
1:D:32:ALA:HA	1:D:36:LEU:HB2	1.99	0.45
1:E:393:SER:HB2	1:E:443:SER:HA	1.99	0.45
1:F:222:GLU:HB2	1:F:390:ILE:HD11	1.98	0.45
2:O:368:GLU:OE2	2:O:368:GLU:N	2.50	0.45
2:Q:314:THR:HG23	2:Q:329:LEU:HD23	1.99	0.45
2:R:284:PRO:HG3	2:R:336:LYS:HE3	1.98	0.45
1:A:28:GLU:HG3	1:A:31:ILE:HG12	2.00	0.44
1:A:422:LEU:HD11	1:A:462:LEU:HB2	1.99	0.44
1:B:281:ASN:ND2	1:B:330:LEU:HB2	2.31	0.44
1:E:85:LYS:HA	1:E:85:LYS:HD3	1.79	0.44
2:H:215:PHE:CE2	2:H:385:LYS:HG3	2.52	0.44
1:B:218:ASP:OD1	1:B:218:ASP:N	2.49	0.44
1:C:221:GLU:HA	1:C:225:LEU:HG	1.99	0.44
1:F:500:LEU:HD12	1:F:500:LEU:HA	1.88	0.44
2:Q:325:THR:HG22	2:Q:327:LYS:HG2	1.99	0.44
2:Q:376:GLN:OE1	2:Q:376:GLN:N	2.47	0.44
1:D:291:HIS:HB2	1:D:302:PHE:HB3	1.98	0.44
1:E:149:ILE:HD12	1:E:161:VAL:HG22	1.99	0.44
1:F:146:HIS:HB3	1:F:461:LEU:HD12	1.99	0.44
2:G:316:GLY:HA2	2:G:328:MET:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:GLY:HA2	1:C:406:SER:HB3	2.00	0.44
1:E:214:LEU:HD13	1:E:398:LEU:HD21	1.99	0.44
1:F:52:LEU:HD12	1:F:80:LEU:HD12	1.99	0.44
2:K:356:ILE:HG22	2:K:360:LYS:HE3	1.99	0.44
2:M:284:PRO:HG3	2:M:336:LYS:HE3	1.99	0.44
2:O:356:ILE:HD12	2:O:356:ILE:H	1.82	0.44
1:A:455:ARG:NH1	1:F:153:THR:OG1	2.50	0.44
1:B:553:ARG:NH1	1:D:119:ASN:O	2.50	0.44
1:C:330:LEU:HD12	1:C:330:LEU:HA	1.86	0.44
2:G:301:GLU:OE2	2:G:305:GLN:NE2	2.50	0.44
2:G:376:GLN:OE1	2:G:376:GLN:N	2.41	0.44
2:Q:327:LYS:NZ	2:Q:331:GLU:OE1	2.50	0.44
1:A:13:SER:HB3	1:A:20:LYS:HB2	2.00	0.44
1:A:149:ILE:HD12	1:A:161:VAL:HG22	1.99	0.44
1:B:9:ALA:HB2	1:B:23:VAL:HG22	2.00	0.44
1:B:503:THR:OG1	1:B:504:VAL:N	2.49	0.44
1:C:248:ILE:HG13	1:C:308:HIS:HB2	2.00	0.44
1:D:86:PHE:HE2	1:D:88:ARG:HG2	1.82	0.44
2:N:335:ASN:HD22	2:N:338:ILE:HD12	1.83	0.44
2:P:381:ASN:HD22	2:P:381:ASN:N	2.13	0.44
1:A:204:ASN:OD1	1:A:204:ASN:N	2.49	0.44
1:B:272:GLU:HB3	1:B:311:PHE:HB3	1.99	0.44
1:D:63:VAL:HG21	1:F:96:PRO:HB2	1.99	0.44
2:K:226:LYS:HE2	2:K:226:LYS:HB2	1.74	0.44
2:K:231:LYS:O	2:K:235:SER:OG	2.28	0.44
2:Q:265:ASP:HB3	2:Q:391:LYS:HE3	1.99	0.44
1:C:431:TYR:O	1:C:443:SER:OG	2.32	0.44
1:F:328:LYS:HB3	1:F:328:LYS:HE3	1.70	0.44
1:F:536:LYS:HE2	1:F:536:LYS:N	2.31	0.44
2:J:239:ARG:HD2	2:J:239:ARG:HA	1.71	0.44
1:A:245:ASN:HB3	1:A:268:PHE:HB2	2.00	0.43
1:B:214:LEU:HD13	1:B:398:LEU:HD11	1.99	0.43
1:B:429:HIS:ND1	1:B:465:SER:OG	2.45	0.43
2:K:151:LYS:HB3	2:K:152:SER:H	1.68	0.43
2:K:282:ASP:OD1	2:K:282:ASP:N	2.38	0.43
1:A:486:ARG:HB2	1:A:514:LEU:HB2	2.01	0.43
1:B:45:SER:HB2	1:B:51:ALA:HA	2.00	0.43
1:E:146:HIS:HB3	1:E:461:LEU:HD12	2.00	0.43
1:B:157:LYS:HA	1:B:485:MET:HG3	2.00	0.43
2:K:229:LEU:HD22	2:K:393:ILE:HD11	2.00	0.43
1:A:179:LEU:HD23	1:A:179:LEU:HA	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:LYS:NZ	1:A:537:CYS:O	2.51	0.43
1:E:183:HIS:CD2	1:E:419:ILE:HG23	2.53	0.43
1:F:65:GLU:HA	2:I:280:ARG:HA	2.01	0.43
2:H:253:GLU:OE2	2:H:255:GLN:NE2	2.51	0.43
2:I:253:GLU:OE2	2:I:255:GLN:NE2	2.51	0.43
2:M:275:SER:HB3	2:M:287:PRO:HD3	2.00	0.43
2:N:328:MET:HE3	2:N:328:MET:HA	1.99	0.43
2:Q:249:PHE:HB2	2:Q:362:VAL:HA	1.99	0.43
1:A:80:LEU:N	1:A:87:TYR:O	2.49	0.43
1:C:86:PHE:HE2	1:C:88:ARG:HG2	1.83	0.43
1:D:10:GLU:OE2	2:H:278:SER:OG	2.29	0.43
1:D:403:GLY:HA2	1:D:406:SER:HB3	2.00	0.43
1:F:393:SER:HB2	1:F:443:SER:HA	2.00	0.43
2:G:346:ILE:O	2:G:350:ASN:ND2	2.51	0.43
2:L:211:SER:O	2:L:211:SER:OG	2.34	0.43
2:L:314:THR:HG22	2:L:338:ILE:HG21	2.01	0.43
2:R:227:GLU:O	2:R:231:LYS:HG3	2.18	0.43
1:F:219:GLU:OE2	1:F:393:SER:OG	2.31	0.43
1:A:272:GLU:HB3	1:A:311:PHE:HB3	1.99	0.43
1:A:570:LYS:HE3	1:A:570:LYS:HA	1.99	0.43
1:B:407:LYS:HD3	1:B:407:LYS:HA	1.68	0.43
1:B:536:LYS:NZ	1:B:537:CYS:O	2.51	0.43
1:C:123:THR:HG21	1:C:134:SER:HB2	2.01	0.43
2:I:289:LEU:O	2:I:343:ILE:N	2.47	0.43
2:K:172:ASP:OD1	2:K:173:TYR:N	2.52	0.43
1:C:202:VAL:HA	1:C:377:ILE:HB	2.00	0.43
2:L:198:ARG:HA	2:L:198:ARG:HD2	1.76	0.43
1:B:546:ILE:O	1:D:144:ASN:ND2	2.48	0.43
1:C:82:LYS:HB2	1:C:87:TYR:HE2	1.84	0.43
1:D:564:ILE:HD13	1:F:406:SER:HB2	2.00	0.43
1:E:197:PHE:O	1:E:200:SER:OG	2.31	0.43
2:H:311:LEU:HD12	2:H:311:LEU:HA	1.93	0.43
1:A:293:TRP:HE1	1:A:302:PHE:HB2	1.82	0.43
1:A:515:LYS:HB3	1:A:515:LYS:HE3	1.83	0.43
1:B:396:SER:OG	1:B:425:TYR:OH	2.32	0.43
1:B:547:LYS:HB2	1:B:550:ASP:HB2	2.00	0.43
1:C:63:VAL:HG22	1:C:69:GLN:HG3	2.01	0.43
2:H:231:LYS:O	2:H:235:SER:OG	2.34	0.43
2:J:259:ASP:HB3	2:J:262:THR:HG23	2.01	0.43
2:K:181:SER:O	2:K:216:ASN:ND2	2.52	0.43
1:D:19:LEU:N	1:D:75:ALA:O	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:ILE:H	1:D:248:ILE:HG13	1.66	0.42
2:I:386:ASP:OD1	2:I:386:ASP:N	2.49	0.42
2:L:195:LYS:HB3	2:L:195:LYS:HE2	1.74	0.42
2:N:230:ARG:NH1	2:N:234:GLU:OE1	2.52	0.42
2:P:284:PRO:HG3	2:P:336:LYS:HE3	2.00	0.42
1:A:469:SER:OG	1:A:492:ASP:OD1	2.31	0.42
1:E:219:GLU:OE2	1:E:393:SER:OG	2.31	0.42
1:F:283:GLU:O	1:F:326:ASN:ND2	2.46	0.42
1:A:146:HIS:HB3	1:A:461:LEU:HD12	2.00	0.42
1:B:152:SER:O	1:B:155:SER:OG	2.27	0.42
1:E:82:LYS:HB2	1:E:87:TYR:HE1	1.84	0.42
1:F:44:VAL:HG22	1:F:100:VAL:HG22	2.00	0.42
2:N:284:PRO:HG3	2:N:336:LYS:HE3	2.01	0.42
1:B:386:GLU:HG2	1:B:387:VAL:HG13	2.00	0.42
1:B:522:MET:HE2	1:B:522:MET:HB3	1.83	0.42
1:E:308:HIS:CE1	1:E:309:ARG:HG3	2.55	0.42
2:K:248:ARG:HG2	2:K:361:GLU:HB2	2.02	0.42
1:A:9:ALA:HB2	1:A:23:VAL:HG22	2.02	0.42
1:A:208:LEU:HD11	1:A:378:LEU:HD22	2.00	0.42
1:B:97:PRO:HD3	1:E:63:VAL:HG21	2.02	0.42
1:B:150:VAL:HB	1:B:468:PRO:HG3	2.02	0.42
1:B:400:PHE:HA	1:B:459:VAL:HG21	2.01	0.42
1:D:553:ARG:NH1	1:F:119:ASN:O	2.38	0.42
2:H:170:CYS:HB2	2:H:174:GLU:HB3	2.01	0.42
2:L:201:LYS:O	2:L:205:VAL:HG23	2.20	0.42
2:R:275:SER:HB3	2:R:287:PRO:HD3	2.01	0.42
1:A:384:PRO:HB2	1:A:387:VAL:HG22	2.01	0.42
1:D:272:GLU:HB3	1:D:311:PHE:HB3	2.01	0.42
1:D:303:ASP:OD1	1:D:303:ASP:N	2.52	0.42
1:F:308:HIS:CE1	1:F:309:ARG:HG3	2.55	0.42
2:H:166:ASN:OD1	2:H:166:ASN:N	2.49	0.42
2:P:225:ARG:HH12	2:P:229:LEU:HD22	1.85	0.42
1:C:94:ALA:HB1	1:C:98:LYS:HD2	2.02	0.42
1:C:313:GLU:H	1:C:313:GLU:CD	2.27	0.42
2:H:249:PHE:HA	2:H:288:PHE:HB2	2.02	0.42
2:N:248:ARG:HG2	2:N:363:TYR:HE1	1.85	0.42
2:P:294:THR:OG1	2:P:298:ASN:ND2	2.47	0.42
1:B:325:LEU:HD23	1:B:328:LYS:HD3	2.02	0.42
1:B:431:TYR:O	1:B:443:SER:OG	2.24	0.42
1:C:53:LEU:HD23	1:C:53:LEU:HA	1.93	0.42
1:D:8:ASN:ND2	1:D:25:ASP:OD2	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:GLN:H	1:E:67:GLN:HG2	1.56	0.42
1:F:389:SER:HB3	1:F:440:TYR:CD1	2.54	0.42
2:O:225:ARG:HH12	2:O:229:LEU:HD23	1.85	0.42
1:A:28:GLU:OE2	1:A:28:GLU:N	2.44	0.42
1:C:183:HIS:CD2	1:C:419:ILE:HG23	2.54	0.42
1:D:183:HIS:CD2	1:D:419:ILE:HG23	2.54	0.42
1:E:181:ASN:OD1	1:E:183:HIS:NE2	2.52	0.42
1:E:301:LYS:HZ1	1:E:303:ASP:HB2	1.85	0.42
1:F:215:LEU:HA	1:F:397:ARG:HH22	1.84	0.42
1:F:493:GLN:NE2	1:F:512:PRO:HG3	2.35	0.42
2:I:244:SER:O	2:I:248:ARG:NH1	2.40	0.42
2:P:290:LEU:HB2	2:P:343:ILE:HB	2.02	0.42
1:A:114:ASP:OD2	1:A:115:SER:N	2.53	0.41
1:C:461:LEU:HD13	1:C:463:LEU:HD13	2.02	0.41
1:E:117:ASP:HB2	1:E:120:ASP:HB2	2.01	0.41
2:I:151:LYS:NZ	2:I:156:GLN:HG3	2.34	0.41
1:A:41:TYR:HH	1:A:112:TYR:HH	1.63	0.41
1:A:212:TYR:OH	1:A:268:PHE:O	2.34	0.41
1:B:570:LYS:HA	1:B:570:LYS:HE3	2.01	0.41
1:E:389:SER:HB3	1:E:440:TYR:CD1	2.54	0.41
1:F:214:LEU:HD13	1:F:398:LEU:HD21	2.02	0.41
2:G:299:LEU:HD23	2:G:299:LEU:HA	1.89	0.41
2:H:253:GLU:HB2	2:H:366:TYR:HA	2.02	0.41
2:L:239:ARG:HA	2:L:239:ARG:HD2	1.68	0.41
2:Q:352:THR:HG22	2:Q:356:ILE:HD11	2.02	0.41
2:R:374:PRO:O	2:R:379:GLN:NE2	2.53	0.41
1:A:522:MET:HE2	1:A:522:MET:HB3	1.89	0.41
1:B:26:LEU:HD21	1:B:32:ALA:HB2	2.02	0.41
1:B:486:ARG:HB2	1:B:514:LEU:HB2	2.02	0.41
1:B:520:LEU:HD13	1:B:531:ILE:HD13	2.01	0.41
1:D:432:ALA:HB1	1:D:475:ILE:HD13	2.03	0.41
2:I:156:GLN:O	2:I:160:THR:OG1	2.30	0.41
2:I:328:MET:HE3	2:I:328:MET:HB3	1.84	0.41
2:L:181:SER:OG	2:L:216:ASN:OD1	2.25	0.41
1:A:150:VAL:HB	1:A:468:PRO:HG3	2.01	0.41
1:C:65:GLU:HB3	2:K:279:LYS:HZ2	1.85	0.41
1:E:408:LYS:O	1:E:412:LYS:NZ	2.46	0.41
1:D:144:ASN:HA	1:D:460:THR:HG21	2.02	0.41
1:D:431:TYR:O	1:D:443:SER:OG	2.31	0.41
1:E:301:LYS:NZ	1:E:303:ASP:HB2	2.35	0.41
1:F:261:SER:OG	1:F:262:PHE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:356:ILE:HB	2:H:360:LYS:HD3	2.01	0.41
2:I:183:ALA:HB2	2:I:208:ILE:HD13	2.02	0.41
2:K:315:ASP:OD1	2:K:315:ASP:N	2.53	0.41
2:N:261:LYS:HD3	2:P:378:PRO:HA	2.01	0.41
2:O:248:ARG:HG2	2:O:363:TYR:HE2	1.84	0.41
1:A:225:LEU:HD21	1:A:235:ARG:HG3	2.02	0.41
1:B:362:LEU:HD23	1:B:362:LEU:HA	1.86	0.41
1:E:231:ASP:HB3	1:E:234:GLN:HB2	2.03	0.41
1:F:143:PHE:HA	1:F:147:ILE:HD11	2.01	0.41
2:I:229:LEU:HD22	2:I:393:ILE:HD11	2.02	0.41
1:A:138:ASN:O	1:A:142:PHE:N	2.51	0.41
1:A:362:LEU:HD23	1:A:362:LEU:HA	1.81	0.41
1:B:430:LYS:NZ	1:D:452:LYS:HD2	2.35	0.41
1:D:230:ASN:OD1	1:D:234:GLN:NE2	2.48	0.41
1:E:215:LEU:HD23	1:E:394:LEU:HD13	2.02	0.41
1:E:235:ARG:HH21	1:E:239:ARG:HH21	1.68	0.41
1:F:41:TYR:OH	1:F:112:TYR:OH	2.34	0.41
1:F:357:THR:HG23	1:F:360:GLU:H	1.86	0.41
2:L:223:GLU:N	2:L:223:GLU:OE1	2.54	0.41
2:N:363:TYR:HA	2:N:380:VAL:HG22	2.02	0.41
1:A:253:ASP:HA	1:A:254:PRO:HD3	1.97	0.41
1:B:28:GLU:HG3	1:B:30:LYS:H	1.86	0.41
1:B:214:LEU:O	1:B:397:ARG:NH2	2.36	0.41
1:C:381:SER:HB2	1:E:456:LYS:HD2	2.01	0.41
1:F:85:LYS:HA	1:F:85:LYS:HD3	1.79	0.41
2:J:210:LYS:HD3	2:J:214:LEU:HD11	2.03	0.41
2:K:311:LEU:HD23	2:K:311:LEU:HA	1.92	0.41
2:M:296:ASP:HA	2:M:299:LEU:HB3	2.03	0.41
2:R:386:ASP:OD1	2:R:386:ASP:N	2.54	0.41
1:A:45:SER:HB2	1:A:51:ALA:HA	2.02	0.41
1:A:60:SER:O	1:A:60:SER:OG	2.37	0.41
1:A:287:LYS:NZ	1:B:287:LYS:HE3	2.36	0.41
1:B:429:HIS:HB2	1:B:470:GLU:HB2	2.02	0.41
1:C:192:GLU:HG2	1:C:543:SER:HB3	2.03	0.41
1:C:407:LYS:HA	1:C:410:LYS:HG3	2.03	0.41
1:E:424:VAL:HG13	1:E:462:LEU:HD22	2.02	0.41
2:I:161:ILE:HG13	2:I:176:GLU:HG2	2.03	0.41
2:I:238:ARG:H	2:I:238:ARG:HG2	1.68	0.41
2:L:178:TYR:O	2:L:182:ASN:ND2	2.54	0.41
2:L:260:ILE:HG21	2:L:305:GLN:HE22	1.86	0.41
2:M:358:ILE:HG22	2:Q:310:ASP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:232:LEU:HD22	2:O:382:ILE:HD13	2.03	0.41
2:O:271:GLN:HG2	2:O:311:LEU:HD11	2.02	0.41
1:B:46:ASP:OD1	1:B:47:ASN:ND2	2.52	0.41
1:B:417:GLN:HB3	1:E:560:GLU:HG3	2.03	0.41
1:F:483:ILE:HG12	1:F:521:ILE:HD12	2.01	0.41
1:F:246:LYS:HG3	1:F:268:PHE:HB3	2.01	0.40
2:H:194:LYS:HE3	2:H:194:LYS:HA	2.02	0.40
1:A:214:LEU:O	1:A:397:ARG:NH2	2.38	0.40
1:A:393:SER:HB2	1:A:443:SER:HA	2.03	0.40
1:C:500:LEU:HD23	1:C:500:LEU:HA	1.90	0.40
2:J:254:PHE:HB2	2:J:291:PHE:HD1	1.86	0.40
2:O:361:GLU:OE1	2:O:363:TYR:OH	2.31	0.40
1:B:42:LEU:HD21	1:B:56:ILE:HD11	2.03	0.40
1:B:456:LYS:HE2	1:B:456:LYS:HB3	1.88	0.40
1:F:5:ASN:HB3	1:F:6:ASP:H	1.77	0.40
2:I:381:ASN:OD1	2:I:381:ASN:N	2.54	0.40
2:L:366:TYR:CZ	2:L:383:GLN:HB2	2.57	0.40
1:A:438:SER:HA	1:A:441:ARG:HB2	2.04	0.40
1:C:432:ALA:HB1	1:C:475:ILE:HD13	2.02	0.40
1:D:165:LEU:HD11	1:D:424:VAL:HG21	2.03	0.40
1:E:152:SER:N	1:E:486:ARG:O	2.54	0.40
1:F:441:ARG:HB3	1:F:441:ARG:NH1	2.37	0.40
2:M:260:ILE:HD11	2:M:298:ASN:HB2	2.03	0.40
2:M:305:GLN:O	2:M:309:GLU:HG3	2.21	0.40
2:N:341:GLN:HE21	2:N:341:GLN:HB2	1.76	0.40
2:N:391:LYS:HE2	2:N:391:LYS:HB3	1.82	0.40
1:D:49:ASP:N	1:D:49:ASP:OD1	2.53	0.40
1:D:497:LYS:HG2	1:D:507:ILE:HD13	2.04	0.40
2:L:186:LYS:NZ	2:L:207:SER:O	2.53	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	565/571 (99%)	543 (96%)	22 (4%)	0	100	100
1	B	565/571 (99%)	545 (96%)	20 (4%)	0	100	100
1	C	565/571 (99%)	544 (96%)	21 (4%)	0	100	100
1	D	565/571 (99%)	548 (97%)	17 (3%)	0	100	100
1	E	562/571 (98%)	548 (98%)	14 (2%)	0	100	100
1	F	562/571 (98%)	549 (98%)	13 (2%)	0	100	100
2	G	242/394 (61%)	236 (98%)	6 (2%)	0	100	100
2	H	242/394 (61%)	236 (98%)	6 (2%)	0	100	100
2	I	242/394 (61%)	234 (97%)	8 (3%)	0	100	100
2	J	242/394 (61%)	233 (96%)	9 (4%)	0	100	100
2	K	242/394 (61%)	238 (98%)	4 (2%)	0	100	100
2	L	242/394 (61%)	232 (96%)	10 (4%)	0	100	100
2	M	169/394 (43%)	165 (98%)	4 (2%)	0	100	100
2	N	169/394 (43%)	166 (98%)	3 (2%)	0	100	100
2	O	169/394 (43%)	164 (97%)	5 (3%)	0	100	100
2	P	169/394 (43%)	164 (97%)	5 (3%)	0	100	100
2	Q	169/394 (43%)	164 (97%)	5 (3%)	0	100	100
2	R	169/394 (43%)	162 (96%)	7 (4%)	0	100	100
All	All	5850/8154 (72%)	5671 (97%)	179 (3%)	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	516/520 (99%)	512 (99%)	4 (1%)	73	89
1	B	516/520 (99%)	513 (99%)	3 (1%)	78	92
1	C	516/520 (99%)	511 (99%)	5 (1%)	68	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	516/520 (99%)	511 (99%)	5 (1%)	68	87
1	E	513/520 (99%)	510 (99%)	3 (1%)	78	92
1	F	513/520 (99%)	512 (100%)	1 (0%)	87	96
2	G	234/373 (63%)	234 (100%)	0	100	100
2	H	234/373 (63%)	233 (100%)	1 (0%)	84	94
2	I	234/373 (63%)	234 (100%)	0	100	100
2	J	234/373 (63%)	234 (100%)	0	100	100
2	K	234/373 (63%)	234 (100%)	0	100	100
2	L	234/373 (63%)	234 (100%)	0	100	100
2	M	163/373 (44%)	163 (100%)	0	100	100
2	N	163/373 (44%)	163 (100%)	0	100	100
2	O	163/373 (44%)	162 (99%)	1 (1%)	78	92
2	P	163/373 (44%)	158 (97%)	5 (3%)	35	66
2	Q	163/373 (44%)	163 (100%)	0	100	100
2	R	163/373 (44%)	161 (99%)	2 (1%)	63	84
All	All	5472/7596 (72%)	5442 (100%)	30 (0%)	78	93

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	466	GLN
1	A	496	VAL
1	A	500	LEU
1	A	538	THR
1	B	104	LYS
1	B	500	LEU
1	B	539	ILE
1	C	234	GLN
1	C	285	LYS
1	C	463	LEU
1	C	522	MET
1	C	549	LEU
1	D	26	LEU
1	D	33	GLU
1	D	47	ASN
1	D	53	LEU
1	D	539	ILE

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Mol	Chain	Res	Type
1	E	27	GLU
1	E	61	ILE
1	E	473	GLU
1	F	74	GLU
2	H	335	ASN
2	O	299	LEU
2	P	229	LEU
2	P	244	SER
2	P	335	ASN
2	P	356	ILE
2	P	381	ASN
2	R	227	GLU
2	R	364	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	HIS
1	A	236	ASN
1	A	251	GLN
1	A	466	GLN
1	A	478	GLN
1	B	236	ASN
1	B	478	GLN
1	B	480	ASN
1	C	5	ASN
1	C	48	GLN
1	C	138	ASN
1	C	140	ASN
1	C	190	HIS
1	C	281	ASN
1	C	326	ASN
1	C	337	GLN
1	C	493	GLN
1	D	47	ASN
1	D	69	GLN
1	D	83	ASN
1	D	138	ASN
1	D	190	HIS
1	D	245	ASN
1	D	278	ASN
1	D	308	HIS

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Mol	Chain	Res	Type
1	D	326	ASN
1	D	480	ASN
1	D	493	GLN
1	E	17	ASN
1	E	69	GLN
1	E	83	ASN
1	E	138	ASN
1	E	159	HIS
1	E	245	ASN
1	E	337	GLN
1	F	17	ASN
1	F	67	GLN
1	F	69	GLN
1	F	138	ASN
1	F	337	GLN
1	F	417	GLN
1	F	466	GLN
1	F	509	ASN
2	G	169	GLN
2	G	182	ASN
2	G	276	ASN
2	G	304	ASN
2	G	305	GLN
2	G	369	ASN
2	H	350	ASN
2	H	379	GLN
2	I	162	GLN
2	I	166	ASN
2	I	276	ASN
2	I	369	ASN
2	I	379	GLN
2	I	383	GLN
2	J	166	ASN
2	J	193	ASN
2	J	276	ASN
2	J	350	ASN
2	J	369	ASN
2	K	166	ASN
2	K	276	ASN
2	K	369	ASN
2	K	381	ASN
2	L	162	GLN

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Mol	Chain	Res	Type
2	L	166	ASN
2	L	305	GLN
2	L	350	ASN
2	L	364	GLN
2	M	305	GLN
2	M	335	ASN
2	M	379	GLN
2	M	381	ASN
2	N	304	ASN
2	N	335	ASN
2	N	350	ASN
2	N	369	ASN
2	N	379	GLN
2	O	304	ASN
2	O	335	ASN
2	O	354	ASN
2	O	357	ASN
2	O	379	GLN
2	P	381	ASN
2	Q	379	GLN
2	R	273	ASN
2	R	381	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

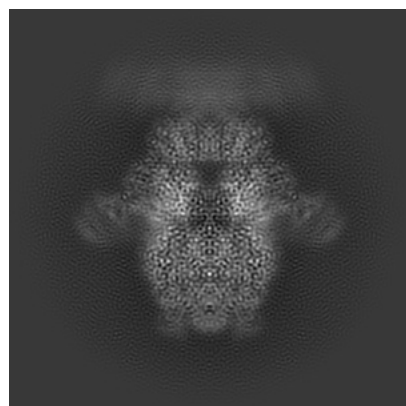
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38204. These allow visual inspection of the internal detail of the map and identification of artifacts.

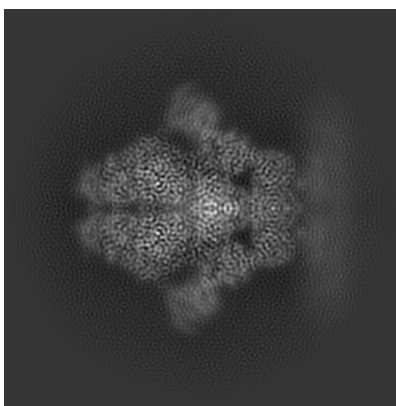
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

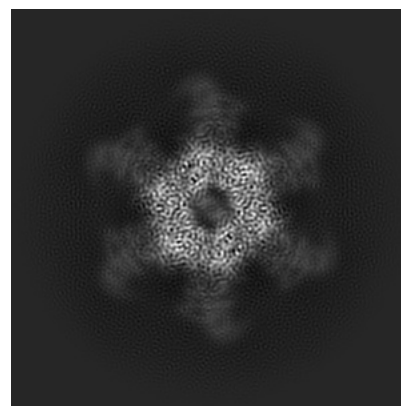
6.1.1 Primary map



X

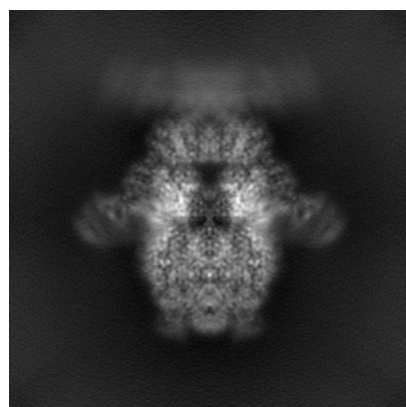


Y

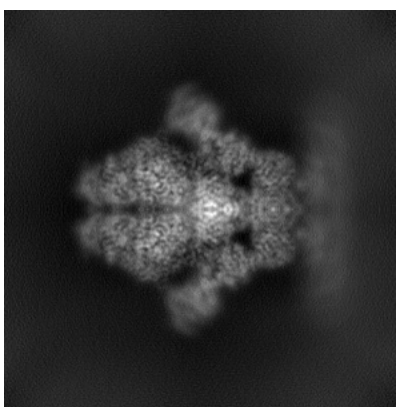


Z

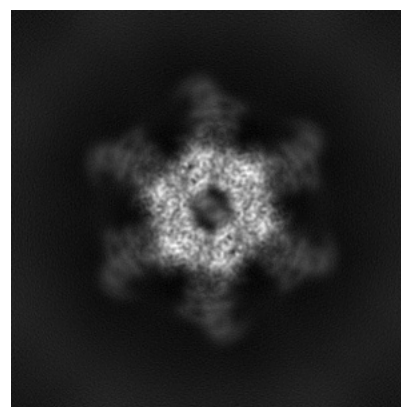
6.1.2 Raw map



X



Y

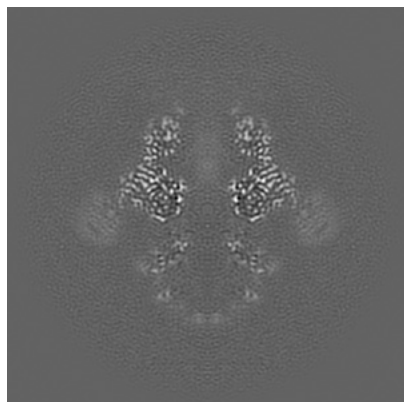


Z

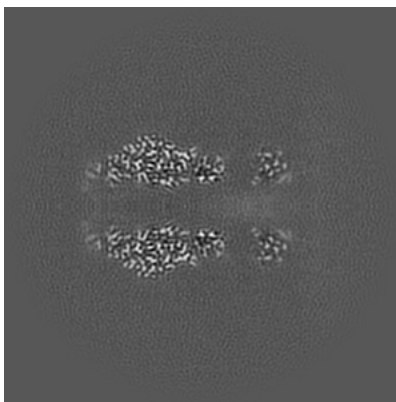
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

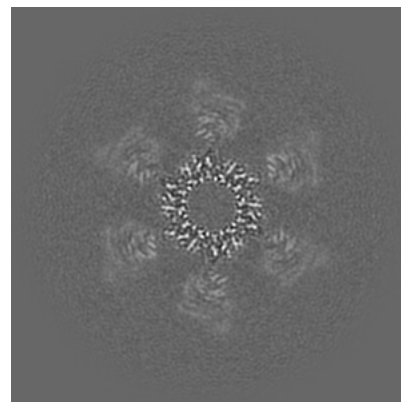
6.2.1 Primary map



X Index: 160

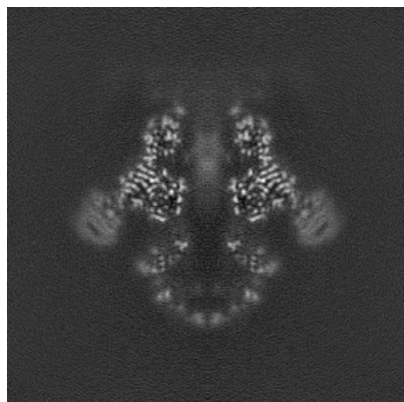


Y Index: 160

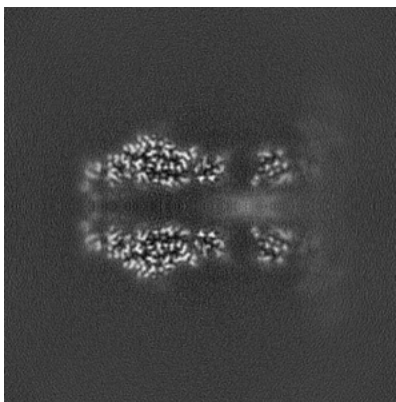


Z Index: 160

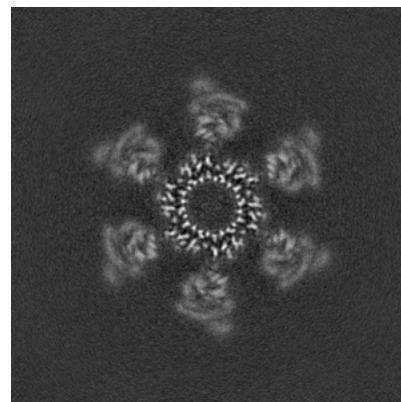
6.2.2 Raw map



X Index: 160



Y Index: 160

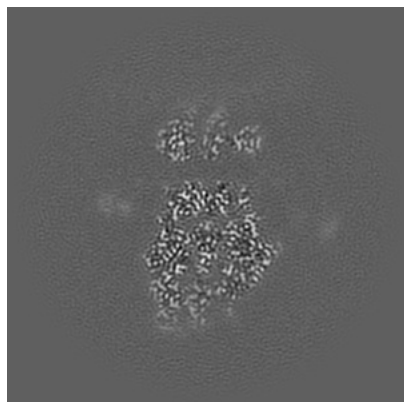


Z Index: 160

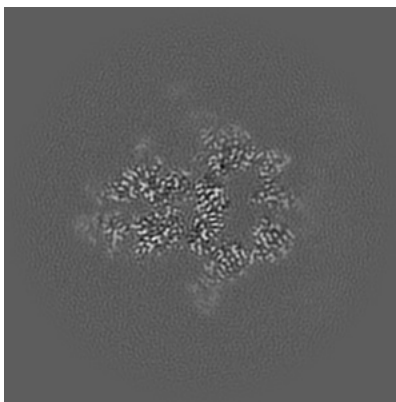
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

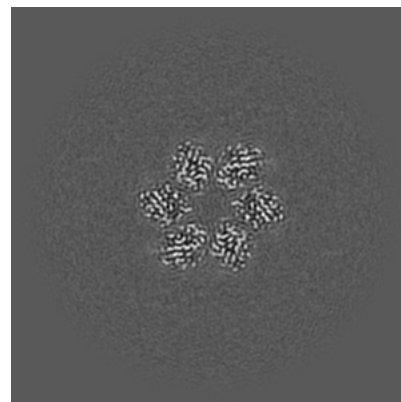
6.3.1 Primary map



X Index: 139

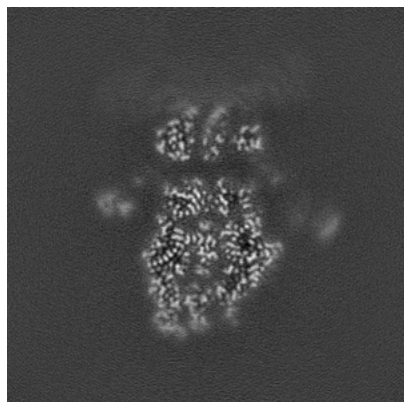


Y Index: 136

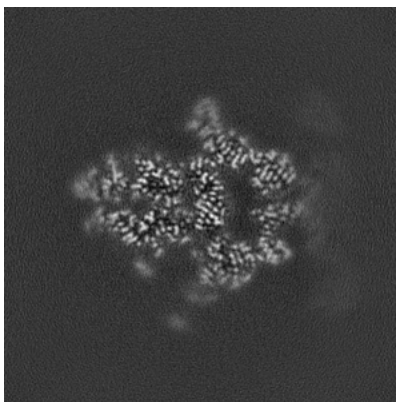


Z Index: 118

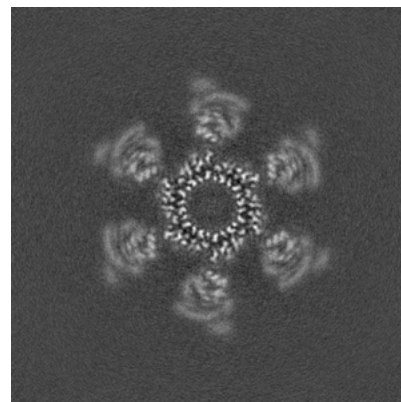
6.3.2 Raw map



X Index: 140



Y Index: 184

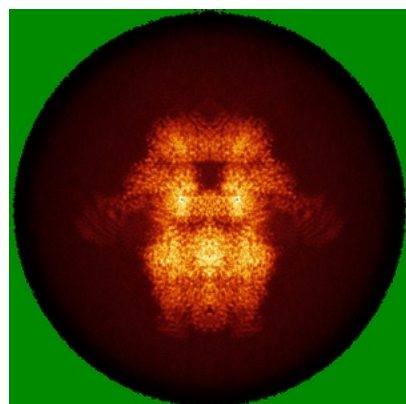


Z Index: 161

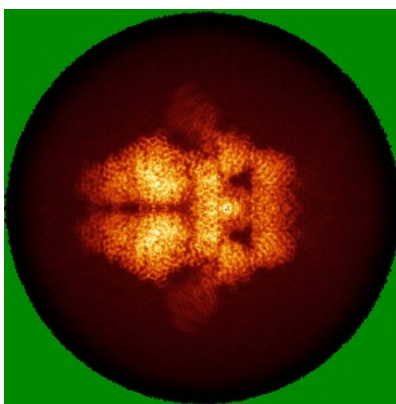
The images above show the largest variance slices of the map in three orthogonal directions.

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

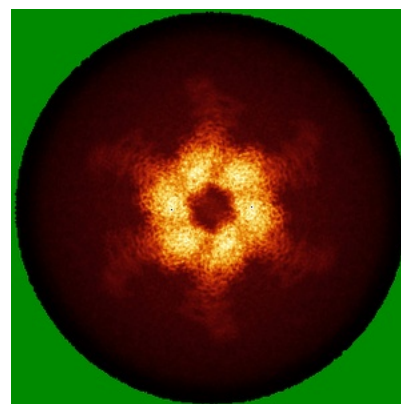
6.4.1 Primary map



X

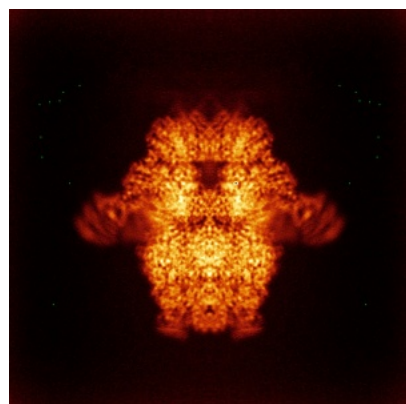


Y

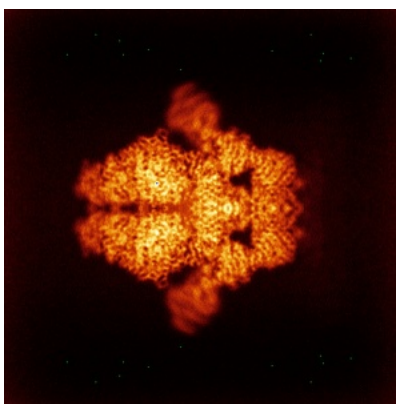


Z

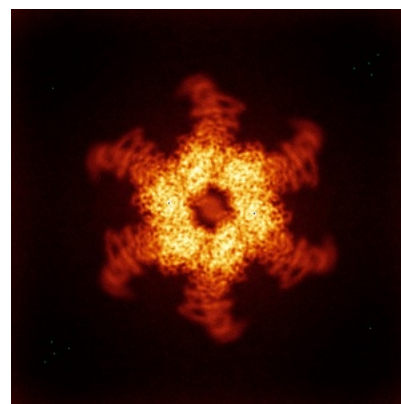
6.4.2 Raw map



X



Y

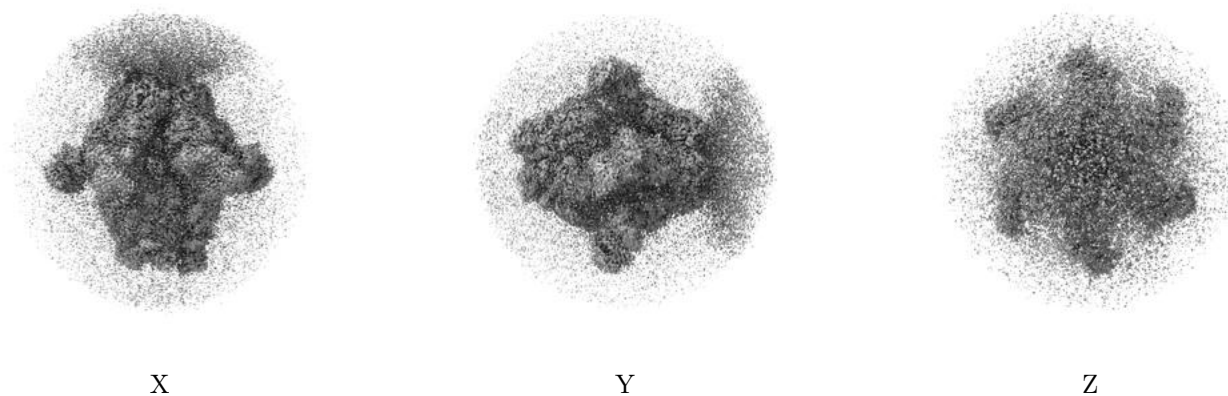


Z

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.

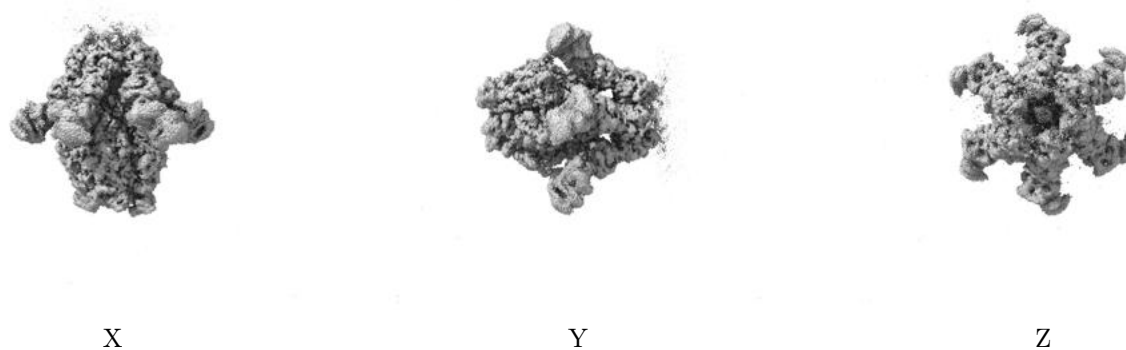
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.108. 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.

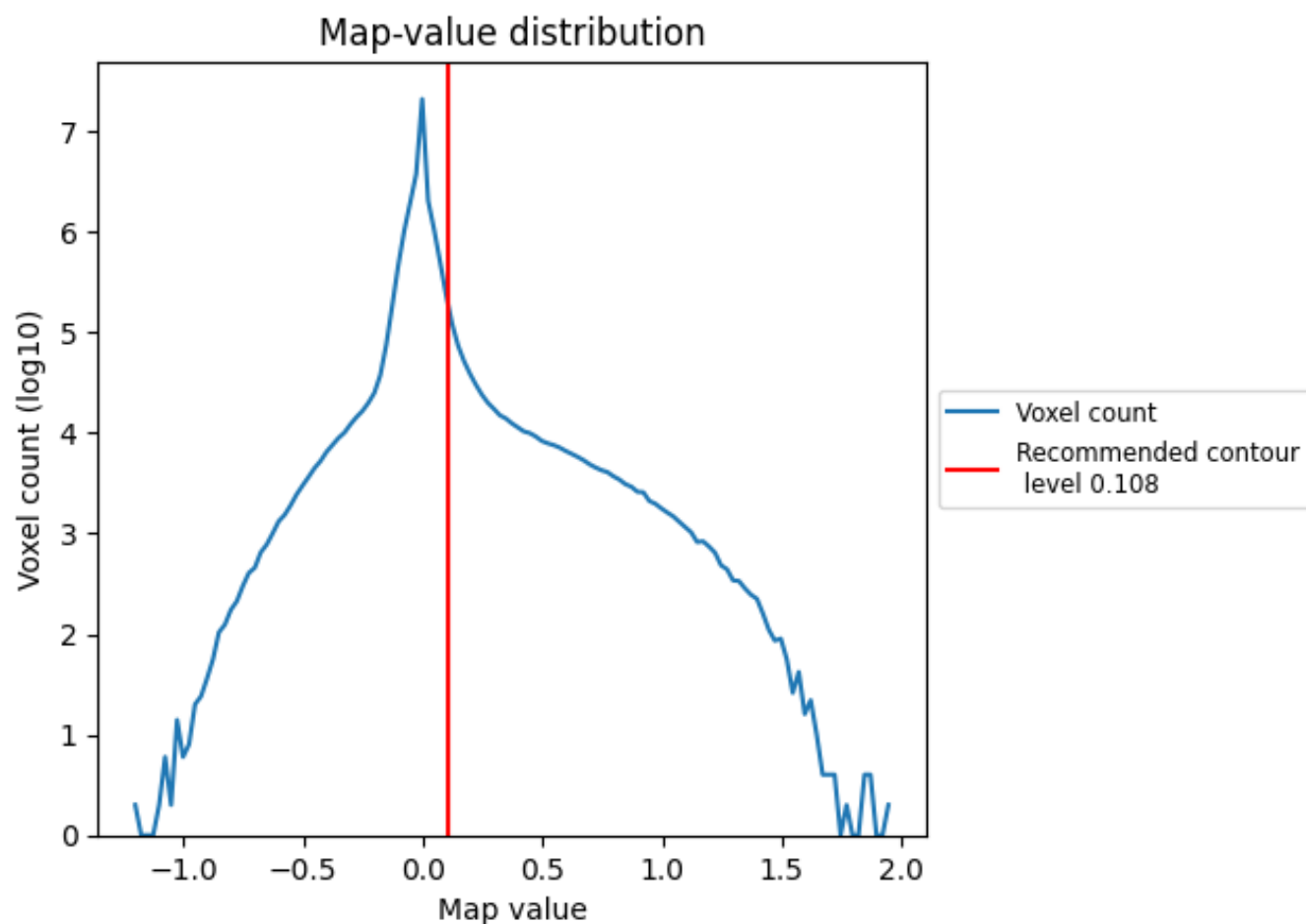
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

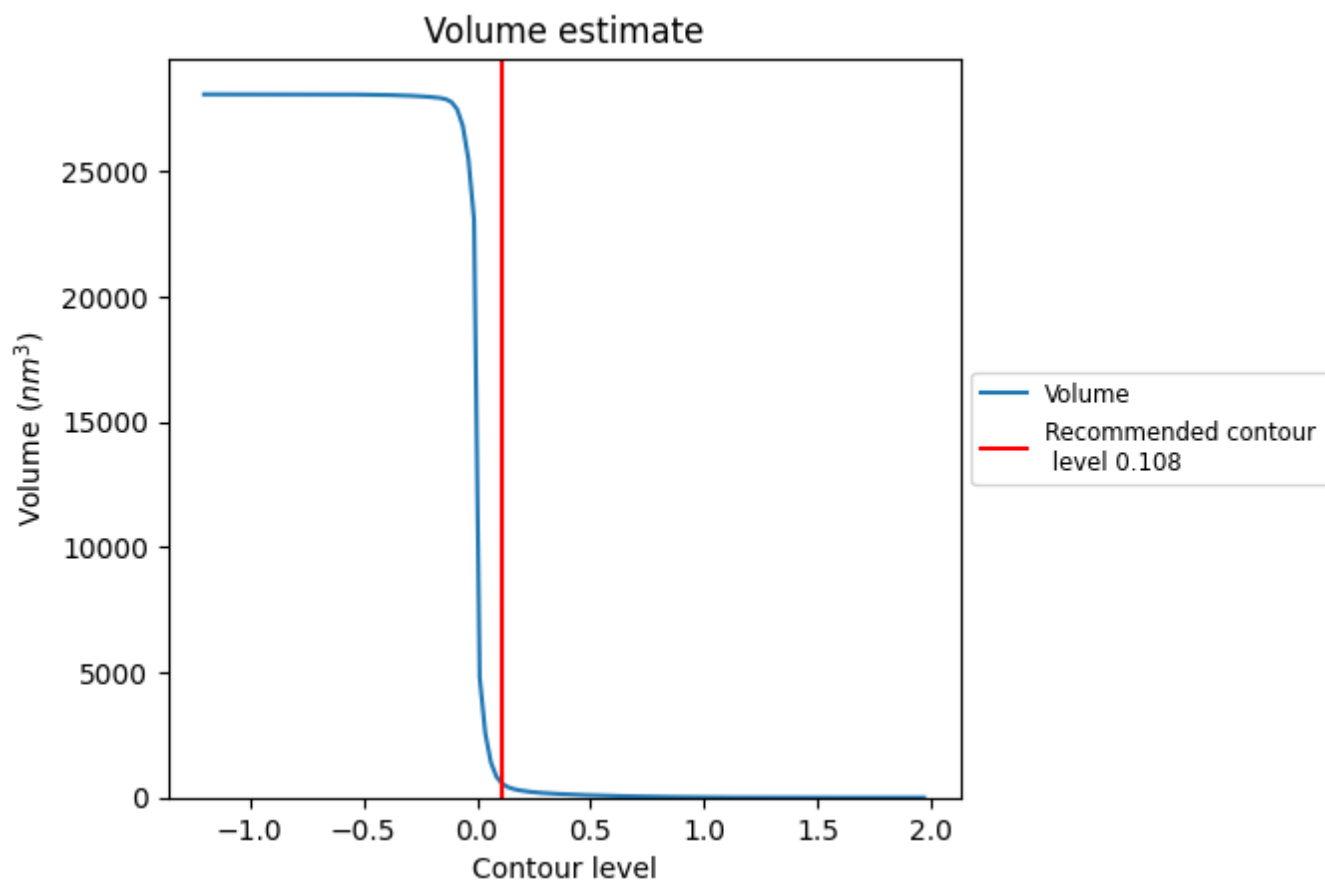
This section contains the results of statistical analysis of the map.

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.

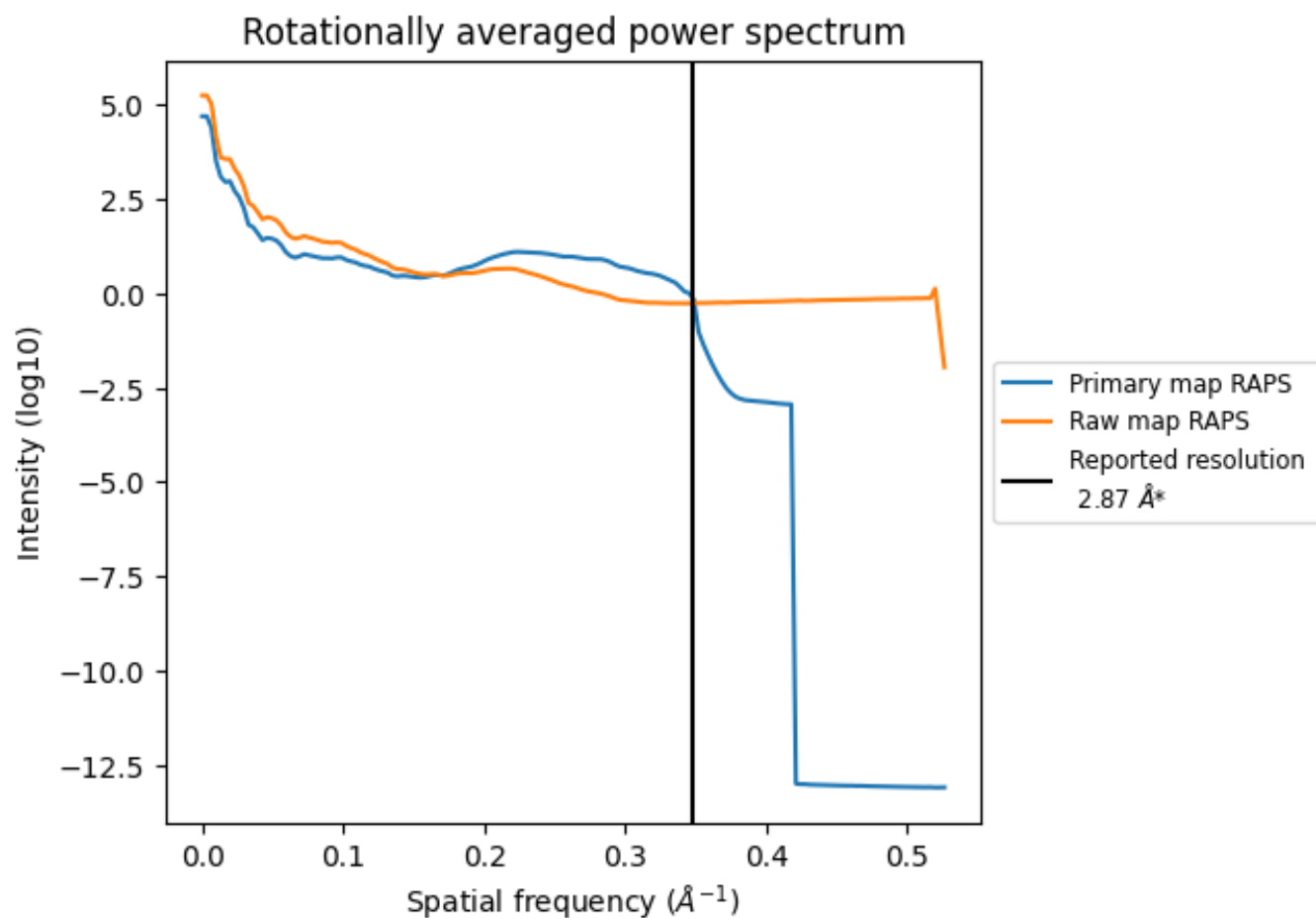
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 589 nm^3 ; this corresponds to an approximate mass of 532 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 ⓘ

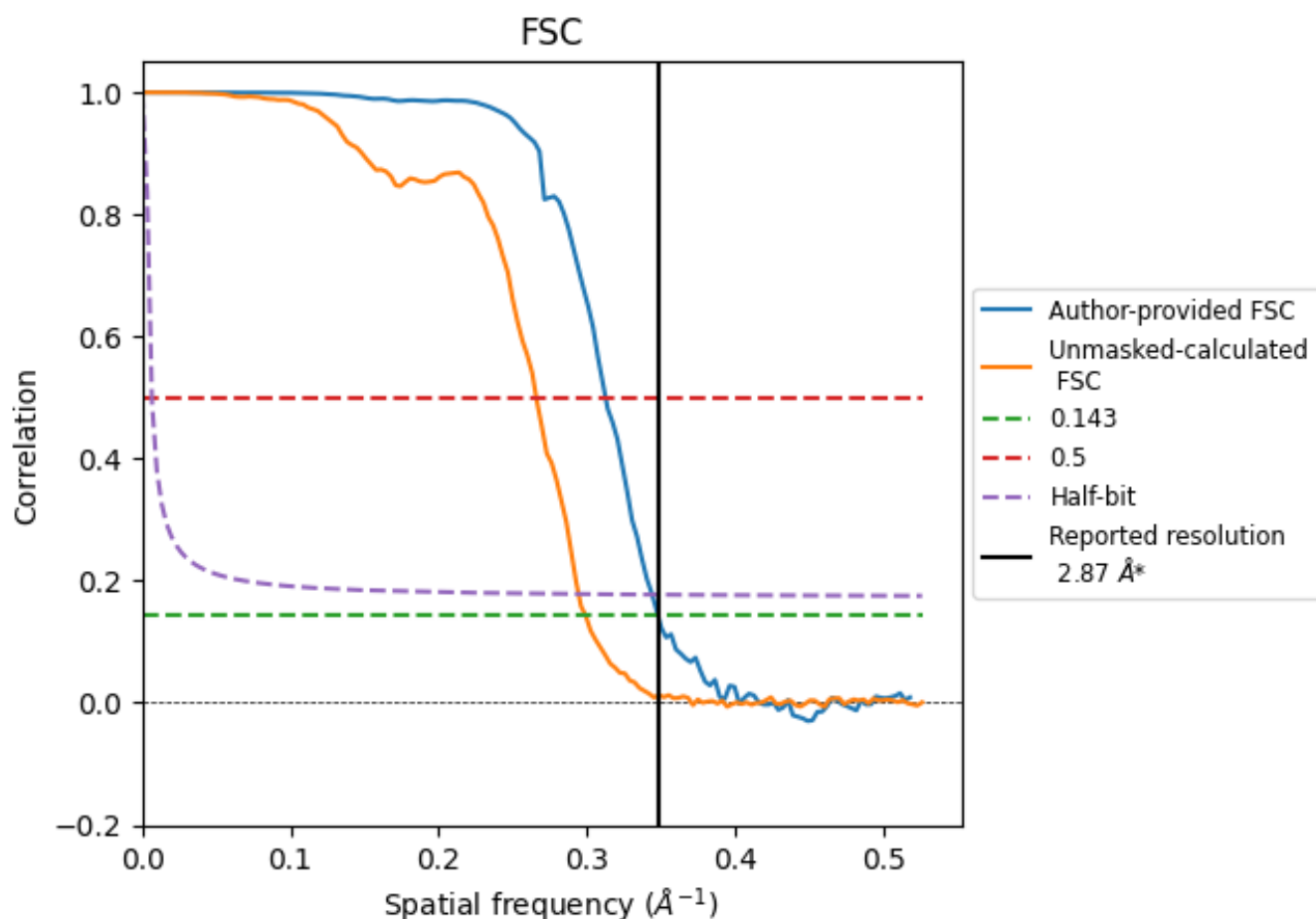


*Reported resolution corresponds to spatial frequency of 0.348 Å⁻¹

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 0.348 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

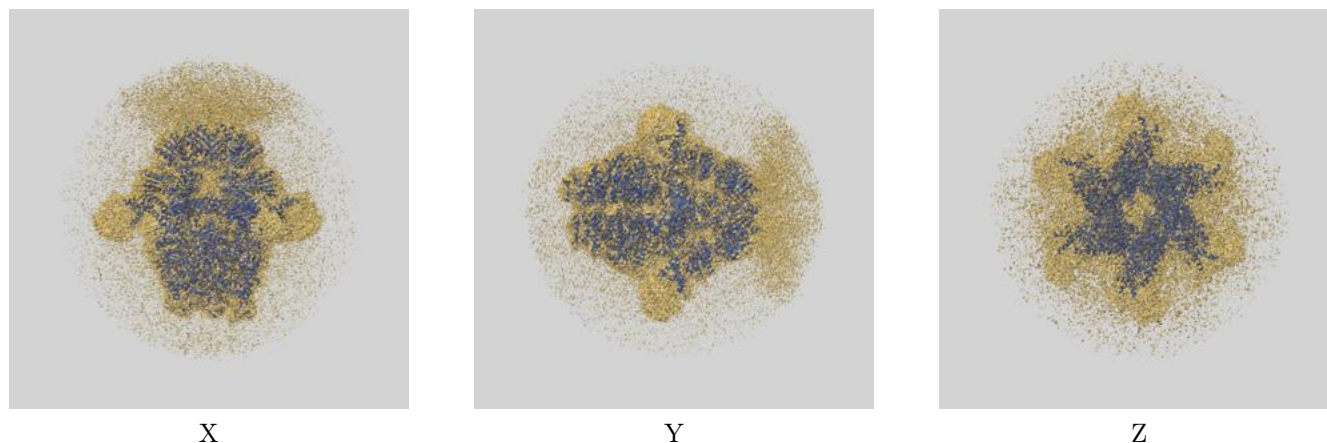
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	2.87	3.20	2.91
Unmasked-calculated*	3.34	3.76	3.40

*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 3.34 differs from the reported value 2.87 by more than 10 %

9 Map-model fit [i](#)

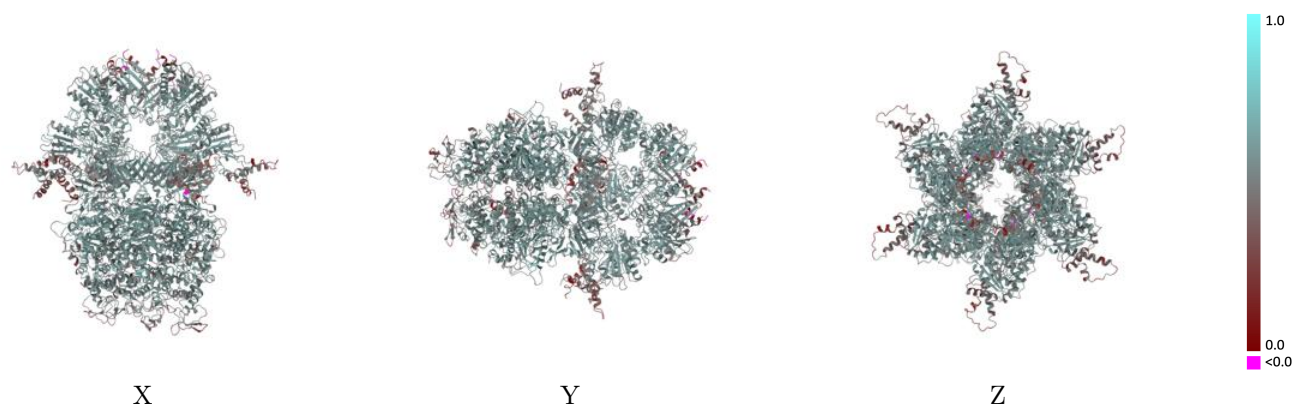
This section contains information regarding the fit between EMDB map EMD-38204 and PDB model 8XAV. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



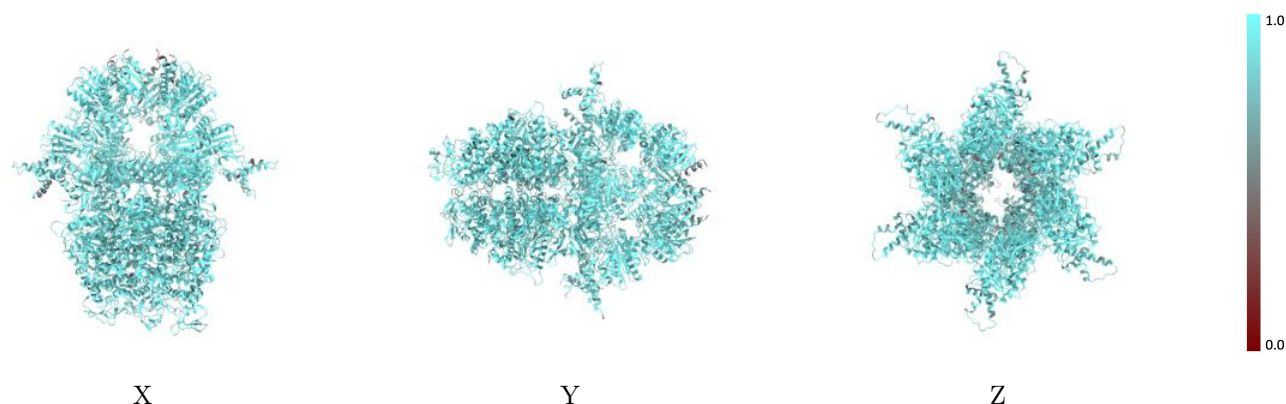
The images above show the 3D surface view of the map at the recommended contour level 0.108 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



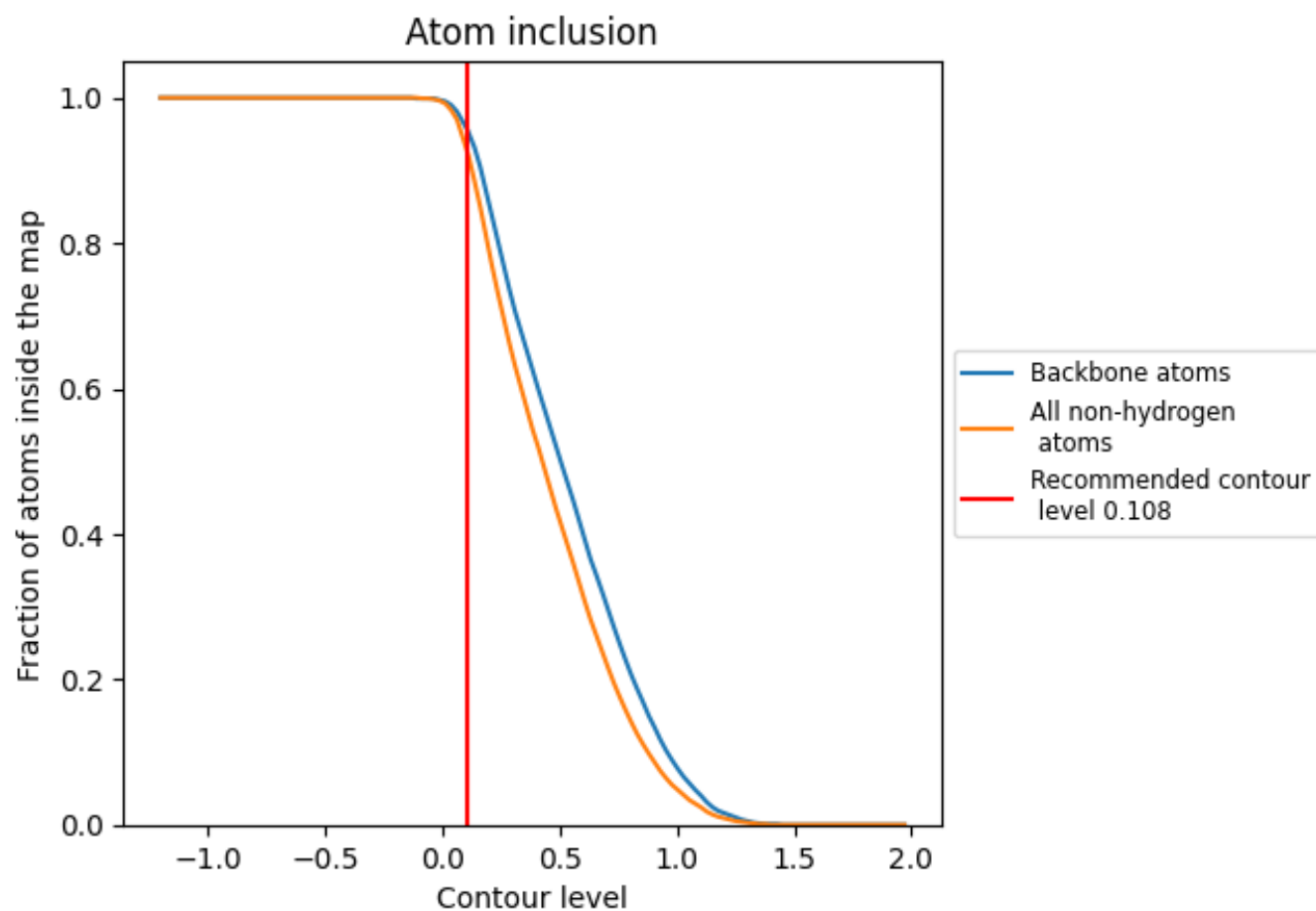
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.108).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 92% 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 (0.108) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9240	0.5350
A	0.9420	0.5590
B	0.9340	0.5490
C	0.9370	0.5570
D	0.9420	0.5600
E	0.9380	0.5520
F	0.9370	0.5520
G	0.9150	0.5000
H	0.9070	0.5000
I	0.9080	0.5060
J	0.9090	0.5010
K	0.9200	0.5060
L	0.9090	0.5030
M	0.8870	0.5190
N	0.9010	0.5220
O	0.8990	0.5150
P	0.8970	0.5200
Q	0.9030	0.5250
R	0.8960	0.5180

1.0

0.0

<0.0