



## Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 12:01 AM UTC

PDB ID : 9BJ9 / pdb\_00009bj9  
EMDB ID : EMD-44631  
Title : Human CRL-2 ZYG11B binding to human NLRP1 Gly/N degnon  
Authors : Liu, X.; Gross, J.D.  
Deposited on : 2024-04-25  
Resolution : 4.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

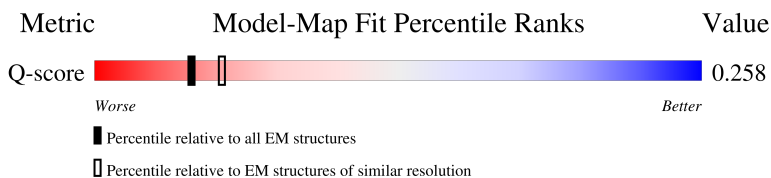
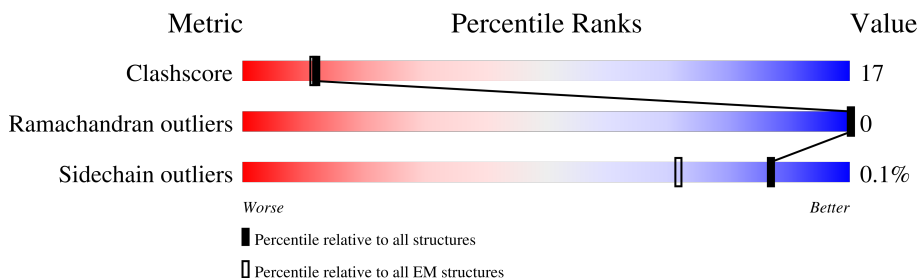
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 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.



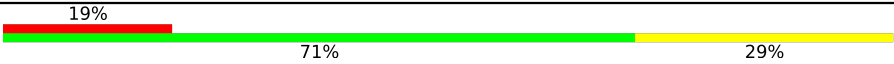

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 ( 3.70 - 4.70 )

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

Mol	Chain	Length	Quality of chain
1	A	748	 60% 36% .
2	B	118	 52% 31% 17%
3	C	96	 59% 39% .
4	D	779	 59% 36% .

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Mol	Chain	Length	Quality of chain
5	P	21	
6	R	108	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14204 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 Protein zyg-11 homolog B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	721	Total	C	N	O	S	0	0
			5714	3627	1000	1051	36		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	SER	-	expression tag	UNP Q9C0D3
A	-2	HIS	-	expression tag	UNP Q9C0D3
A	-1	MET	-	expression tag	UNP Q9C0D3
A	0	VAL	-	expression tag	UNP Q9C0D3
A	1	ASP	-	expression tag	UNP Q9C0D3

- Molecule 2 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	98	Total	C	N	O	S	0	0
			775	489	131	151	4		

- Molecule 3 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	96	Total	C	N	O	S	0	0
			760	487	122	145	6		

- Molecule 4 is a protein called Cullin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	744	Total	C	N	O	S	0	0
			6092	3870	1032	1145	45		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	746	LEU	-	expression tag	UNP Q13617
D	747	GLU	-	expression tag	UNP Q13617
D	748	GLY	-	expression tag	UNP Q13617
D	749	GLY	-	expression tag	UNP Q13617
D	750	GLY	-	expression tag	UNP Q13617
D	751	GLY	-	expression tag	UNP Q13617
D	752	TRP	-	expression tag	UNP Q13617
D	753	SER	-	expression tag	UNP Q13617
D	754	HIS	-	expression tag	UNP Q13617
D	755	PRO	-	expression tag	UNP Q13617
D	756	GLN	-	expression tag	UNP Q13617
D	757	PHE	-	expression tag	UNP Q13617
D	758	GLU	-	expression tag	UNP Q13617
D	759	LYS	-	expression tag	UNP Q13617
D	760	GLY	-	expression tag	UNP Q13617
D	761	GLY	-	expression tag	UNP Q13617
D	762	GLY	-	expression tag	UNP Q13617
D	763	SER	-	expression tag	UNP Q13617
D	764	GLY	-	expression tag	UNP Q13617
D	765	GLY	-	expression tag	UNP Q13617
D	766	GLY	-	expression tag	UNP Q13617
D	767	SER	-	expression tag	UNP Q13617
D	768	GLY	-	expression tag	UNP Q13617
D	769	GLY	-	expression tag	UNP Q13617
D	770	GLY	-	expression tag	UNP Q13617
D	771	SER	-	expression tag	UNP Q13617
D	772	TRP	-	expression tag	UNP Q13617
D	773	SER	-	expression tag	UNP Q13617
D	774	HIS	-	expression tag	UNP Q13617
D	775	PRO	-	expression tag	UNP Q13617
D	776	GLN	-	expression tag	UNP Q13617
D	777	PHE	-	expression tag	UNP Q13617
D	778	GLU	-	expression tag	UNP Q13617
D	779	LYS	-	expression tag	UNP Q13617

- Molecule 5 is a protein called Peptide from NACHT, LRR and PYD domains-containing protein 1, N-terminus.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	P	21	Total	C	N	O	0	0
			136	80	31	25		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	10	UNK	-	cloning artifact	UNP Q9C000
P	11	UNK	-	cloning artifact	UNP Q9C000
P	12	UNK	-	cloning artifact	UNP Q9C000
P	13	UNK	-	cloning artifact	UNP Q9C000
P	14	UNK	-	cloning artifact	UNP Q9C000
P	15	UNK	-	cloning artifact	UNP Q9C000
P	16	UNK	-	cloning artifact	UNP Q9C000
P	17	UNK	-	cloning artifact	UNP Q9C000
P	18	UNK	-	cloning artifact	UNP Q9C000
P	19	UNK	-	cloning artifact	UNP Q9C000
P	20	UNK	-	cloning artifact	UNP Q9C000
P	21	UNK	-	cloning artifact	UNP Q9C000

- Molecule 6 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	87	Total	C	N	O	S	0	0
			724	460	134	121	9		

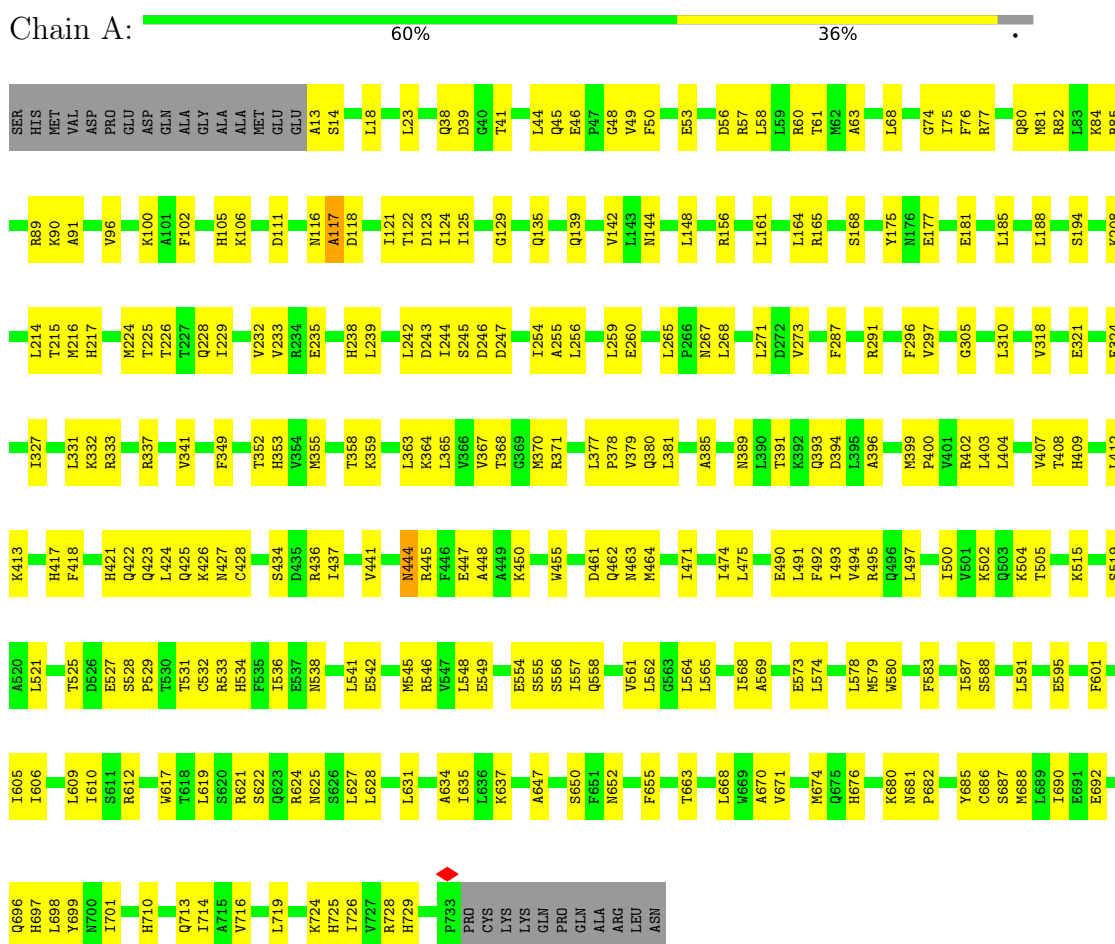
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	R	3	Total	Zn	0
			3	3	

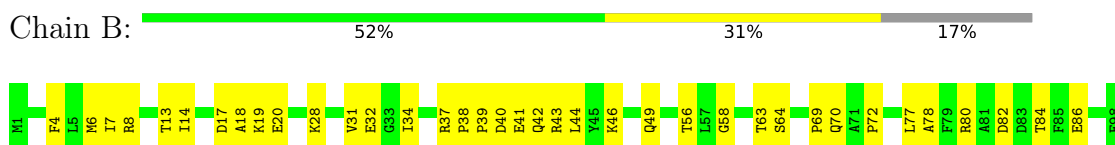
### 3 Residue-property plots

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: Protein zyg-11 homolog B



#### • Molecule 2: Elongin-B



LEU PRO ASP VAL MET LYS PRO GLN ASP SER GLY SER SER ALA ASN GLN VAL GLN

• Molecule 3: Elongin-C

Chain C:  59% 39%

M17 I22 S23 S24 E28 F29 I30 V31 K32 R33 E34 H35 A36 L37 T41 I42 K43 A44 M45 L46 S47 G48 P49 G50 Q51 F52 A53 E54 N55 E56 T57 V60 V69 Y76 K80 V81 E82 Y83 T84 N85 S86 S87 P91 L101 E102 L103 L104 M105 C112

• Molecule 4: Cullin-2

Chain D:  59% 36%

MET S2 L3 K4 P5 R6 D9 F10 D11 E12 T13 W14 L17 L18 T19 T20 T21 K22 V25 M26 R32 A33 T34 N36 D37 R38 Y42 Y43 V47 A48 Y49 E55 T59 K62 E80 Q82 V83 L84 R89 E92 C103 R106 Y107 L108

M109 T110 K114 K115 L118 T119 Q124 Y125 G126 Y127 G128 V130 D131 M132 N133 L136 M137 E138 I139 G140 E141 L142 N143 A144 W147 R148 K149 M151 V152 L155 Q156 I160 L164 K168 N169 D170 R171 G172 G173 Q178 I181 V184 I185 N186 S187 F188

V189 H190 V191 F198 K201 F202 Y203 I206 S209 P210 F211 T215 A223 L226 L227 S230 M236 V239 G241 R242 L243 K252 Y253 L254 H255 P256 K261 H264 E265 C266 Q267 R269 L278 H283 R284 L285 R287 D293 M294 N297

V298 V299 L300 V301 R302 S305 L308 P309 H310 K311 E314 L315 Q316 T319 T327 L330 T331 E332 E333 N334 M335 L338 F339 V340 E341 L344 Q342 K343 F344 F350 V351 Q352 L353 L354 V357 L358 D361 Q362 H363 F364 M365 K370 A371 L372 T373 S374 V375 V376 N377

K382 S383 V384 K385 K386 L390 L391 A392 K393 Y394 C395 D396 L399 K400 K401 M409 E410 L415 F418 T419 N334 W421 F422 K423 Y424 L425 F431 Q432 K433 F434 R437 M438 L439 A440 K441 L443 L444 H445 Q446 M451 D452 S453 A456 M457 T458 M459 K460 L461

T470 S471 K472 L473 V384 H474 R475 H476 M480 A484 D485 L486 M487 F490 D502 S506 F507 Q508 T509 Y510 V511 L512 M517 P518 L519 E534 V537 Q538 M539 F540 F543 Y544 B551 V552 L553 L556 L559 C560 T561 Q562 V563 V564 K565 M566 H567 V568 P572

A575 M576 V577 T578 M582 L585 M589 V594 S595 Y596 K597 E598 L599 M600 M601 S602 M605 K608 E609 L610 T611 T612 T613 L614 K615 S616 L617 K621 P622 T623 M624 K629 E630 D631 T632 D633 A634 S637 F638 S639 L640 K647 R648 T649 K652 I653 S656

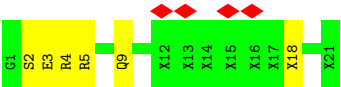
M657 Q658 R659 D660 T661 P662 Q663 E664 M665 E666 S670 A671 V672 D673 E674 D675 M678 V679 L680 Q681 R686 T687 R691 L694 R695 H696 M697 A698 L699 I700 Q701 E702 V703 I704 S705 Q706 S707 R708 F711 N712 P713 S714 T715 S716 R717 T718 L725 T726 D727 K728 Q735

A736 S737 A738 A745 LEU GLU GLY GLY GLY GLY TRP SER HIS PRO GLN PHE E674 GLU LYS GLY GLY GLY SER GLY GLY GLY GLY TRP SER HIS PRO GLN PHE GLU LYS

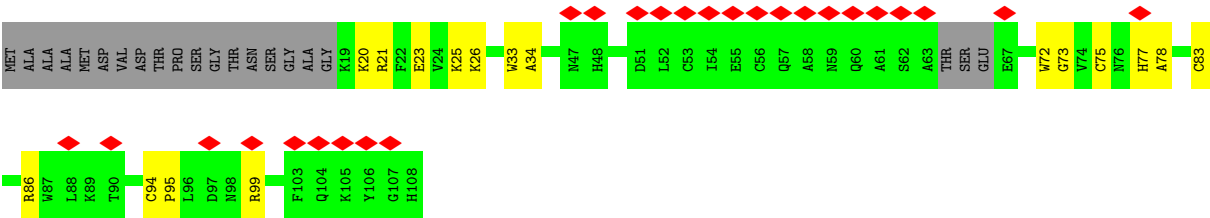
• Molecule 5: Peptide from NACHT, LRR and PYD domains-containing protein 1, N-terminus

Chain P:  19% 71% 29%





• Molecule 6: E3 ubiquitin-protein ligase RBX1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80380	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)	5000	Depositor
Maximum defocus (nm)	20000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	39.928	Depositor
Minimum map value	-20.928	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3	Depositor
Map size ( $\text{\AA}$ )	300.6, 300.6, 300.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.83500004, 0.83500004, 0.83500004	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.16	0/5824	0.47	2/7891 (0.0%)
2	B	0.14	0/790	0.44	0/1067
3	C	0.18	0/777	0.61	1/1050 (0.1%)
4	D	0.16	0/6211	0.46	2/8368 (0.0%)
5	P	0.17	0/75	0.50	0/97
6	R	0.12	0/745	0.35	0/1007
All	All	0.16	0/14422	0.47	5/19480 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	105	MET	CA-CB-CG	8.61	131.33	114.10
1	A	117	ALA	CA-C-N	6.95	137.19	124.82
1	A	117	ALA	C-N-CA	6.95	137.19	124.82
4	D	150	LEU	CA-C-N	-5.12	113.12	122.38
4	D	150	LEU	C-N-CA	-5.12	113.12	122.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	32	LYS	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5714	0	5783	216	0
2	B	775	0	771	30	0
3	C	760	0	749	38	0
4	D	6092	0	6079	216	0
5	P	136	0	95	6	0
6	R	724	0	680	15	0
7	R	3	0	0	0	0
All	All	14204	0	14157	487	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 17.

All (487) 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)
4:D:3:LEU:HD13	4:D:43:TYR:HE2	1.26	0.98
4:D:589:ASN:HD21	6:R:21:ARG:HB3	1.31	0.96
4:D:534:GLU:HA	4:D:537:VAL:HG22	1.58	0.84
1:A:655:PHE:HB3	1:A:697:HIS:HE1	1.46	0.81
1:A:536:ILE:HG21	1:A:574:LEU:HD11	1.64	0.80
1:A:634:ALA:HA	1:A:637:LYS:HE3	1.63	0.78
4:D:3:LEU:HD13	4:D:43:TYR:CE2	2.17	0.77
2:B:7:ILE:HD11	2:B:77:LEU:HB2	1.69	0.75
4:D:551:ARG:HG2	6:R:34:ALA:HB3	1.70	0.74
4:D:663:GLN:O	4:D:667:GLN:NE2	2.21	0.73
2:B:19:LYS:HD3	2:B:20:GLU:H	1.53	0.73
1:A:519:SER:OG	5:P:5:ARG:NH2	2.22	0.72
4:D:594:VAL:HG11	4:D:638:PHE:HB2	1.71	0.72
1:A:461:ASP:HB3	1:A:464:MET:SD	2.29	0.71
1:A:619:LEU:O	1:A:621:ARG:NH2	2.23	0.71
1:A:578:LEU:HD23	1:A:609:LEU:HD11	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:75:CYS:HB2	6:R:77:HIS:ND1	2.05	0.70
4:D:144:LEU:HD12	4:D:191:VAL:HA	1.73	0.70
4:D:487:ASN:ND2	4:D:509:ILE:O	2.24	0.70
1:A:353:HIS:HA	1:A:389:ASN:HD21	1.57	0.70
4:D:470:THR:O	4:D:474:HIS:ND1	2.24	0.70
1:A:655:PHE:HB3	1:A:697:HIS:CE1	2.28	0.69
1:A:352:THR:HA	1:A:355:MET:HG2	1.75	0.69
4:D:534:GLU:O	4:D:538:GLN:HG2	1.93	0.69
3:C:22:ILE:HG22	3:C:28:GLU:HG3	1.74	0.69
4:D:127:TYR:O	4:D:133:ASN:ND2	2.26	0.68
4:D:599:LEU:O	4:D:602:SER:OG	2.11	0.68
3:C:101:LEU:O	3:C:105:MET:HB2	1.93	0.68
1:A:76:PHE:HD1	1:A:81:MET:HG3	1.59	0.67
4:D:330:LEU:HD11	4:D:338:LEU:HB3	1.77	0.67
4:D:357:VAL:HG13	4:D:358:LEU:HD12	1.77	0.66
4:D:316:GLN:HG3	4:D:371:ALA:HB2	1.76	0.66
4:D:420:THR:HA	4:D:423:LYS:HZ2	1.60	0.66
1:A:76:PHE:CD1	1:A:81:MET:HG3	2.31	0.66
3:C:43:LYS:O	3:C:47:SER:OG	2.14	0.66
3:C:17:MET:N	3:C:56:GLU:OE1	2.28	0.66
1:A:68:LEU:HD11	1:A:91:ALA:HA	1.77	0.66
1:A:161:LEU:HB3	1:A:164:LEU:HD22	1.78	0.66
2:B:4:PHE:HE2	2:B:69:PRO:HG3	1.61	0.65
1:A:696:GLN:HA	1:A:699:TYR:CD1	2.31	0.65
4:D:362:GLN:N	4:D:362:GLN:OE1	2.30	0.65
3:C:48:GLY:H	4:D:32:ARG:HH12	1.44	0.65
1:A:425:GLN:HE21	1:A:455:TRP:NE1	1.95	0.65
4:D:354:ILE:HD11	4:D:364:PHE:HB3	1.79	0.65
4:D:4:LYS:O	4:D:6:ARG:NH1	2.30	0.64
4:D:471:SER:HA	4:D:474:HIS:CE1	2.31	0.64
4:D:308:LEU:HA	4:D:311:MET:HE2	1.79	0.64
4:D:441:LYS:O	4:D:445:HIS:ND1	2.31	0.64
1:A:671:VAL:HG22	1:A:714:ILE:HG22	1.78	0.64
2:B:4:PHE:CE2	2:B:69:PRO:HG3	2.33	0.63
1:A:331:LEU:HD22	1:A:365:LEU:HB3	1.80	0.63
1:A:381:LEU:HD23	1:A:424:LEU:HB2	1.80	0.63
1:A:635:ILE:HG21	1:A:668:LEU:HG	1.80	0.63
4:D:399:LEU:HB3	4:D:442:ARG:HH22	1.62	0.63
4:D:451:MET:HE3	4:D:480:MET:HE1	1.81	0.63
1:A:287:PHE:HD1	1:A:291:ARG:HH12	1.44	0.63
1:A:305:GLY:HA2	1:A:310:LEU:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:GLU:OE2	1:A:650:SER:OG	2.17	0.62
1:A:444:ASN:O	1:A:444:ASN:ND2	2.32	0.62
1:A:652:ASN:HA	1:A:655:PHE:CE1	2.35	0.62
3:C:17:MET:HA	3:C:33:ARG:HH21	1.65	0.62
3:C:32:LYS:HG3	3:C:35:HIS:ND1	2.15	0.62
1:A:724:LYS:HE3	1:A:724:LYS:HA	1.81	0.61
6:R:72:TRP:CZ3	6:R:78:ALA:HB2	2.35	0.61
1:A:412:LEU:HD11	1:A:448:ALA:HA	1.82	0.61
4:D:400:LYS:HE3	4:D:400:LYS:HA	1.80	0.61
4:D:623:ILE:HG22	4:D:640:LEU:HA	1.83	0.61
1:A:409:HIS:O	1:A:413:LYS:HG2	2.01	0.61
1:A:573:GLU:OE1	1:A:573:GLU:N	2.32	0.61
1:A:606:ILE:HD11	1:A:627:LEU:HD13	1.83	0.61
1:A:74:GLY:HA2	1:A:77:ARG:HD2	1.82	0.60
4:D:401:LYS:HD2	4:D:401:LYS:O	2.01	0.60
1:A:165:ARG:HH12	4:D:127:TYR:HB2	1.67	0.60
1:A:238:HIS:HD2	1:A:267:ASN:HB2	1.66	0.60
4:D:178:GLN:NE2	4:D:252:LYS:O	2.35	0.60
3:C:32:LYS:HE2	3:C:35:HIS:CE1	2.37	0.60
1:A:647:ALA:HB3	5:P:2:SER:HB3	1.84	0.59
1:A:425:GLN:HA	1:A:428:CYS:SG	2.42	0.59
1:A:194:SER:HB3	1:A:217:HIS:HB3	1.83	0.59
1:A:393:GLN:HG3	1:A:394:ASP:H	1.67	0.59
1:A:385:ALA:HA	1:A:427:ASN:HD21	1.68	0.59
2:B:31:VAL:HA	2:B:34:ILE:HG22	1.85	0.59
2:B:86:GLU:N	2:B:86:GLU:OE1	2.35	0.59
1:A:525:THR:HG21	1:A:564:LEU:HD12	1.83	0.59
4:D:38:ARG:O	4:D:42:ILE:HG12	2.02	0.59
1:A:123:ASP:OD1	1:A:124:ILE:N	2.36	0.58
2:B:32:GLU:OE2	2:B:42:GLN:NE2	2.35	0.58
1:A:359:LYS:HE3	1:A:359:LYS:HA	1.83	0.58
1:A:606:ILE:O	1:A:610:ILE:HG12	2.04	0.58
1:A:533:ARG:HA	1:A:536:ILE:HG12	1.85	0.58
1:A:569:ALA:O	1:A:612:ARG:NH2	2.34	0.58
1:A:377:LEU:HG	1:A:378:PRO:HD3	1.85	0.58
1:A:370:MET:HE1	1:A:379:VAL:HG22	1.85	0.58
4:D:399:LEU:O	4:D:442:ARG:NH2	2.37	0.58
1:A:23:LEU:HD12	1:A:57:ARG:HG2	1.85	0.58
1:A:57:ARG:HG3	1:A:60:ARG:HH22	1.67	0.58
1:A:102:PHE:HA	1:A:105:HIS:HD2	1.69	0.58
1:A:418:PHE:HE2	1:A:421:HIS:HB2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:308:LEU:HD23	4:D:309:PRO:HD3	1.86	0.57
4:D:566:MET:HE1	4:D:568:TYR:HB2	1.86	0.57
4:D:372:LEU:HD22	4:D:424:TYR:HD2	1.68	0.57
3:C:37:LEU:HD13	3:C:43:LYS:HB3	1.86	0.57
4:D:510:TYR:HE1	4:D:512:LEU:HD23	1.69	0.57
4:D:148:ARG:O	4:D:152:VAL:HG23	2.04	0.57
4:D:419:ILE:HA	4:D:422:PHE:HB3	1.86	0.57
3:C:53:ALA:HB2	4:D:32:ARG:HH21	1.70	0.57
1:A:121:ILE:HD12	1:A:148:LEU:HB3	1.86	0.57
4:D:511:VAL:HB	6:R:33:TRP:HE3	1.70	0.57
1:A:215:THR:HG23	1:A:243:ASP:HB2	1.86	0.57
1:A:631:LEU:O	1:A:635:ILE:HG13	2.04	0.57
4:D:611:THR:HB	4:D:615:LYS:HZ1	1.69	0.57
2:B:63:THR:HG22	2:B:64:SER:H	1.70	0.56
1:A:57:ARG:HG3	1:A:60:ARG:NH2	2.20	0.56
1:A:63:ALA:HA	1:A:68:LEU:HD23	1.86	0.56
4:D:440:ALA:O	4:D:444:ILE:HG12	2.06	0.56
4:D:611:THR:HB	4:D:615:LYS:NZ	2.20	0.56
1:A:565:LEU:HA	1:A:568:ILE:HG22	1.88	0.56
1:A:245:SER:OG	1:A:337:ARG:NH1	2.39	0.56
4:D:399:LEU:HB3	4:D:442:ARG:NH2	2.20	0.56
1:A:436:ARG:NH2	3:C:87:SER:OG	2.39	0.56
4:D:575:ALA:C	4:D:576:MET:HE2	2.30	0.56
4:D:624:ASN:OD1	4:D:639:SER:OG	2.21	0.56
1:A:455:TRP:CH2	1:A:464:MET:HE3	2.41	0.56
4:D:283:HIS:O	4:D:287:ARG:HG2	2.07	0.55
4:D:703:VAL:HA	4:D:706:GLN:HE21	1.71	0.55
4:D:148:ARG:HA	4:D:151:MET:SD	2.47	0.55
4:D:597:LYS:HB2	4:D:600:GLN:HE21	1.71	0.55
1:A:370:MET:HE2	1:A:370:MET:HA	1.88	0.55
4:D:422:PHE:O	4:D:425:ILE:HG22	2.07	0.55
1:A:239:LEU:HD23	1:A:265:LEU:HD11	1.89	0.55
1:A:358:THR:HG23	1:A:399:MET:HE1	1.88	0.55
1:A:463:ASN:OD1	1:A:464:MET:N	2.38	0.55
1:A:545:MET:HA	1:A:548:LEU:HG	1.88	0.55
4:D:55:GLU:N	4:D:55:GLU:OE1	2.38	0.55
4:D:377:ASN:HD21	4:D:712:ASN:HD22	1.53	0.55
2:B:6:MET:HE1	2:B:72:PRO:HB2	1.89	0.55
6:R:94:CYS:SG	6:R:95:PRO:HD2	2.47	0.55
1:A:400:PRO:HD2	1:A:403:LEU:HD12	1.88	0.54
1:A:129:GLY:O	1:A:135:GLN:NE2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:472:LYS:O	4:D:476:MET:HG2	2.08	0.54
3:C:49:PRO:O	4:D:32:ARG:NH2	2.41	0.54
4:D:255:HIS:CG	4:D:256:PRO:HD2	2.43	0.54
4:D:517:TRP:HB3	4:D:519:LEU:HD13	1.90	0.54
1:A:352:THR:HG23	1:A:389:ASN:ND2	2.23	0.54
2:B:40:ASP:OD1	2:B:41:GLU:N	2.40	0.54
4:D:418:PHE:HZ	4:D:431:PHE:HZ	1.56	0.54
4:D:486:LEU:HA	4:D:489:LYS:HE2	1.89	0.54
4:D:59:THR:HA	4:D:62:LYS:HE3	1.89	0.54
1:A:647:ALA:HB2	5:P:4:ARG:HH22	1.73	0.53
3:C:32:LYS:HG3	3:C:35:HIS:CE1	2.43	0.53
1:A:404:LEU:O	1:A:408:THR:HG23	2.08	0.53
1:A:621:ARG:O	1:A:625:ASN:ND2	2.41	0.53
1:A:545:MET:O	1:A:549:GLU:HG3	2.07	0.53
4:D:107:TYR:O	4:D:110:THR:OG1	2.25	0.53
4:D:255:HIS:CD2	4:D:256:PRO:HD2	2.44	0.53
4:D:354:ILE:HG13	4:D:358:LEU:HD22	1.91	0.53
4:D:561:THR:HA	4:D:578:THR:HA	1.89	0.53
1:A:698:LEU:HD21	1:A:719:LEU:HG	1.89	0.53
1:A:497:LEU:O	1:A:500:ILE:HG22	2.07	0.53
4:D:34:THR:O	4:D:38:ARG:HG2	2.09	0.53
4:D:136:LEU:HD22	4:D:142:LEU:HA	1.90	0.53
4:D:392:ALA:O	4:D:438:MET:HE1	2.09	0.53
6:R:20:LYS:NZ	6:R:23:GLU:OE1	2.35	0.53
1:A:89:ARG:O	1:A:90:LYS:HG2	2.09	0.53
1:A:493:ILE:HG13	1:A:494:VAL:N	2.24	0.53
3:C:46:LEU:H	3:C:46:LEU:HD23	1.75	0.52
4:D:9:ASP:N	4:D:9:ASP:OD1	2.42	0.52
4:D:694:LEU:HG	4:D:699:LEU:HB2	1.90	0.52
4:D:265:GLU:OE2	4:D:269:ARG:NH1	2.42	0.52
4:D:691:ARG:HE	4:D:694:LEU:HD13	1.74	0.52
2:B:17:ASP:OD1	2:B:18:ALA:N	2.42	0.52
4:D:702:GLU:O	4:D:706:GLN:HG3	2.09	0.52
1:A:413:LYS:O	1:A:417:HIS:ND1	2.42	0.52
1:A:46:GLU:O	1:A:80:GLN:NE2	2.42	0.52
1:A:337:ARG:O	1:A:341:VAL:HG23	2.10	0.52
1:A:534:HIS:O	1:A:538:ASN:HB2	2.10	0.52
1:A:696:GLN:HA	1:A:699:TYR:HD1	1.73	0.52
4:D:286:ILE:HG21	4:D:314:GLU:HG3	1.91	0.52
5:P:3:GLU:OE1	5:P:3:GLU:N	2.36	0.52
2:B:43:ARG:HG3	2:B:80:ARG:HE	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:490:PHE:HB3	4:D:507:PHE:HE1	1.74	0.52
1:A:515:LYS:HE3	1:A:556:SER:OG	2.10	0.52
1:A:687:SER:OG	1:A:725:HIS:NE2	2.41	0.52
4:D:211:PHE:O	4:D:215:THR:HG23	2.10	0.51
1:A:53:GLU:OE2	4:D:114:LYS:NZ	2.43	0.51
1:A:156:ARG:NH2	1:A:181:GLU:OE2	2.44	0.51
4:D:226:LEU:O	4:D:230:SER:OG	2.27	0.51
4:D:456:ALA:HA	4:D:459:ASN:HD21	1.76	0.51
4:D:415:LEU:HB3	4:D:460:LYS:HZ1	1.75	0.51
1:A:497:LEU:HB3	1:A:521:LEU:HD21	1.93	0.51
4:D:131:ASP:OD1	4:D:132:MET:N	2.44	0.51
1:A:224:MET:HE2	1:A:229:ILE:HG13	1.91	0.51
1:A:502:LYS:HA	1:A:505:THR:HG22	1.93	0.51
1:A:445:ARG:HG2	1:A:475:LEU:HD11	1.93	0.51
2:B:56:THR:HG22	2:B:58:GLY:H	1.76	0.51
3:C:55:ASN:OD1	3:C:57:THR:OG1	2.27	0.51
3:C:102:GLU:O	3:C:105:MET:HB3	2.11	0.51
4:D:17:LEU:HA	4:D:20:THR:HG22	1.92	0.51
4:D:181:ILE:O	4:D:185:ILE:HG12	2.11	0.51
1:A:690:ILE:HD13	1:A:726:ILE:HD13	1.92	0.51
3:C:45:MET:HG2	3:C:60:VAL:HG13	1.93	0.51
4:D:327:THR:O	4:D:331:THR:HG23	2.11	0.51
4:D:490:PHE:HB3	4:D:507:PHE:CE1	2.46	0.51
1:A:528:SER:O	1:A:531:THR:OG1	2.24	0.50
1:A:208:LYS:HD2	1:A:235:GLU:HG3	1.94	0.50
1:A:554:GLU:HB3	1:A:557:ILE:HD13	1.92	0.50
1:A:685:TYR:HA	1:A:688:MET:HG3	1.93	0.50
1:A:156:ARG:HA	1:A:156:ARG:NE	2.26	0.50
4:D:589:ASN:ND2	6:R:21:ARG:HB3	2.14	0.50
4:D:301:LEU:HD23	4:D:311:MET:SD	2.51	0.50
4:D:370:LYS:HA	4:D:373:THR:HG22	1.93	0.50
1:A:216:MET:HB2	1:A:244:ILE:HG13	1.92	0.50
1:A:332:LYS:HD2	1:A:333:ARG:HH12	1.76	0.50
1:A:492:PHE:HB2	1:A:495:ARG:HH12	1.77	0.50
4:D:647:LYS:HA	4:D:647:LYS:HE2	1.93	0.50
1:A:226:THR:HG23	1:A:254:ILE:HD13	1.94	0.49
1:A:391:THR:HG23	1:A:396:ALA:HB2	1.94	0.49
4:D:294:MET:HG3	4:D:358:LEU:HD11	1.93	0.49
4:D:371:ALA:O	4:D:375:VAL:HG23	2.12	0.49
4:D:675:ASP:HA	4:D:678:MET:HG3	1.93	0.49
1:A:57:ARG:NH1	1:A:57:ARG:HB2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:NH1	4:D:49:TYR:O	2.46	0.49
4:D:138:GLU:HB2	4:D:141:GLU:HB2	1.94	0.49
1:A:50:PHE:CD2	1:A:81:MET:HE1	2.48	0.49
1:A:117:ALA:O	1:A:118:ASP:OD1	2.31	0.49
1:A:580:TRP:HB2	1:A:583:PHE:HD2	1.78	0.49
4:D:605:MET:HE3	4:D:605:MET:HA	1.94	0.49
4:D:663:GLN:NE2	4:D:664:GLU:HG3	2.28	0.49
4:D:22:LYS:HD2	4:D:22:LYS:O	2.13	0.49
4:D:119:THR:HA	4:D:124:GLN:HB2	1.95	0.49
4:D:264:HIS:O	4:D:267:GLN:HG2	2.12	0.49
1:A:404:LEU:HD12	1:A:437:ILE:HD12	1.94	0.49
4:D:456:ALA:HA	4:D:459:ASN:ND2	2.28	0.49
4:D:572:PRO:O	4:D:649:THR:OG1	2.29	0.49
1:A:14:SER:HB3	3:C:80:LYS:NZ	2.28	0.49
1:A:273:VAL:HG12	1:A:273:VAL:O	2.12	0.49
4:D:294:MET:HE2	4:D:294:MET:HA	1.95	0.49
4:D:442:ARG:O	4:D:446:GLY:N	2.46	0.49
1:A:13:ALA:HB3	3:C:85:ASN:HA	1.95	0.49
1:A:332:LYS:HG2	1:A:333:ARG:HH22	1.77	0.49
1:A:490:GLU:O	1:A:493:ILE:HG12	2.13	0.48
4:D:409:ASN:OD1	4:D:410:GLU:N	2.45	0.48
4:D:485:ASP:O	4:D:489:LYS:HG2	2.13	0.48
1:A:580:TRP:HB2	1:A:583:PHE:CD2	2.48	0.48
2:B:63:THR:HG22	2:B:64:SER:N	2.27	0.48
4:D:681:GLN:HA	4:D:725:LEU:HD11	1.95	0.48
1:A:268:LEU:HD21	1:A:271:LEU:HB2	1.95	0.48
4:D:419:ILE:HD13	4:D:460:LYS:HG2	1.96	0.48
1:A:41:THR:HB	1:A:74:GLY:HA3	1.96	0.48
1:A:710:HIS:O	1:A:713:GLN:HG2	2.14	0.48
3:C:45:MET:HE3	4:D:36:ASN:HA	1.94	0.48
4:D:713:PRO:HG2	4:D:718:ILE:HD11	1.94	0.48
1:A:698:LEU:HA	1:A:701:ILE:HG22	1.96	0.48
4:D:261:LYS:HE2	4:D:261:LYS:HA	1.96	0.48
4:D:544:TYR:HE2	4:D:553:LEU:HD13	1.78	0.48
1:A:165:ARG:NH1	4:D:127:TYR:HB2	2.28	0.48
4:D:434:PHE:HD2	4:D:437:ARG:HH21	1.60	0.48
4:D:564:VAL:HG11	4:D:585:LEU:HD21	1.96	0.48
1:A:333:ARG:NE	1:A:333:ARG:HA	2.29	0.48
4:D:472:LYS:HA	4:D:475:ARG:HG2	1.95	0.48
1:A:77:ARG:NH2	1:A:100:LYS:HE3	2.29	0.48
1:A:122:THR:HA	1:A:125:ILE:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:382:LYS:O	4:D:384:VAL:HG13	2.14	0.47
4:D:178:GLN:HG2	4:D:253:TYR:CE1	2.49	0.47
1:A:18:LEU:HD12	3:C:76:TYR:CD2	2.49	0.47
4:D:633:ASP:OD1	4:D:634:ALA:N	2.39	0.47
1:A:367:VAL:HG12	1:A:371:ARG:HH12	1.79	0.47
1:A:647:ALA:N	5:P:2:SER:O	2.47	0.47
2:B:19:LYS:HD3	2:B:20:GLU:N	2.23	0.47
4:D:278:LEU:HD22	4:D:297:MET:HE1	1.97	0.47
1:A:48:GLY:O	1:A:80:GLN:NE2	2.48	0.47
1:A:628:LEU:HD22	1:A:663:THR:HG21	1.96	0.47
3:C:52:PHE:CD2	4:D:32:ARG:HG3	2.49	0.47
4:D:575:ALA:HB1	4:D:577:VAL:HG13	1.96	0.47
1:A:491:LEU:O	1:A:494:VAL:HG22	2.14	0.47
4:D:299:VAL:HG13	4:D:300:LEU:HD22	1.97	0.47
4:D:695:ARG:CZ	4:D:696:HIS:H	2.27	0.47
1:A:246:ASP:OD1	1:A:247:ASP:N	2.44	0.47
4:D:170:ASP:OD1	4:D:171:ARG:NE	2.34	0.47
4:D:347:HIS:O	4:D:351:VAL:HG23	2.15	0.47
1:A:403:LEU:O	1:A:407:VAL:HG23	2.15	0.47
1:A:605:ILE:O	1:A:609:LEU:HD23	2.15	0.47
4:D:354:ILE:O	4:D:358:LEU:HB2	2.15	0.47
1:A:297:VAL:HB	1:A:318:VAL:HG13	1.96	0.46
1:A:450:LYS:HD2	1:A:450:LYS:O	2.14	0.46
2:B:82:ASP:O	2:B:84:THR:HG23	2.15	0.46
1:A:349:PHE:CE1	1:A:385:ALA:HB1	2.50	0.46
4:D:130:VAL:HG12	4:D:130:VAL:O	2.15	0.46
1:A:377:LEU:O	1:A:380:GLN:HG2	2.15	0.46
4:D:437:ARG:HG2	4:D:517:TRP:HZ3	1.81	0.46
4:D:711:PHE:HD2	4:D:713:PRO:HD3	1.80	0.46
1:A:461:ASP:OD1	1:A:462:GLN:N	2.48	0.46
3:C:36:ALA:HB1	3:C:42:ILE:HG21	1.97	0.46
4:D:80:GLU:O	4:D:81:GLU:HG3	2.15	0.46
1:A:175:TYR:HB3	1:A:177:GLU:OE1	2.16	0.46
2:B:44:LEU:HD13	2:B:77:LEU:HD12	1.98	0.46
3:C:69:VAL:HG23	3:C:103:LEU:HD22	1.98	0.46
4:D:89:ARG:O	4:D:92:GLU:HG3	2.16	0.46
4:D:115:LYS:O	4:D:119:THR:HG23	2.16	0.46
4:D:283:HIS:O	4:D:286:ILE:HG22	2.16	0.46
4:D:353:LEU:O	4:D:357:VAL:HG12	2.16	0.46
1:A:408:THR:O	1:A:412:LEU:HD23	2.16	0.46
1:A:541:LEU:HD12	1:A:542:GLU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:198:PHE:HB2	4:D:201:LYS:HB2	1.98	0.45
1:A:529:PRO:HB2	1:A:533:ARG:HH12	1.81	0.45
1:A:541:LEU:HD12	1:A:545:MET:HE1	1.97	0.45
1:A:728:ARG:HG3	1:A:729:HIS:CE1	2.52	0.45
2:B:14:ILE:HG12	3:C:30:ILE:HB	1.98	0.45
2:B:34:ILE:HD11	3:C:30:ILE:HG21	1.96	0.45
4:D:396:ASP:HB2	4:D:438:MET:SD	2.56	0.45
1:A:321:GLU:N	1:A:321:GLU:OE1	2.50	0.45
4:D:609:GLU:HA	4:D:612:LYS:HZ2	1.81	0.45
1:A:45:GLN:N	1:A:45:GLN:OE1	2.49	0.45
1:A:404:LEU:HB2	1:A:441:VAL:HG11	1.97	0.45
4:D:576:MET:HE2	4:D:576:MET:N	2.31	0.45
1:A:229:ILE:O	1:A:233:VAL:HG22	2.17	0.45
1:A:541:LEU:HD13	1:A:583:PHE:HZ	1.80	0.45
3:C:47:SER:HB2	4:D:103:CYS:SG	2.57	0.45
4:D:351:VAL:HA	4:D:354:ILE:HG22	1.98	0.45
4:D:432:GLN:NE2	4:D:433:LYS:HG3	2.31	0.45
4:D:433:LYS:HD3	4:D:675:ASP:OD2	2.16	0.45
1:A:111:ASP:HA	1:A:142:VAL:HB	1.98	0.45
2:B:46:LYS:O	2:B:49:GLN:HG3	2.17	0.45
4:D:652:LYS:HG2	4:D:653:ILE:N	2.31	0.45
1:A:555:SER:HA	1:A:558:GLN:HE21	1.82	0.45
4:D:43:TYR:HD1	4:D:107:TYR:CE2	2.34	0.44
4:D:297:MET:HA	4:D:297:MET:HE2	1.99	0.44
4:D:608:LYS:HG2	4:D:612:LYS:NZ	2.32	0.44
4:D:5:PRO:HG3	4:D:47:VAL:HG22	1.99	0.44
6:R:72:TRP:HZ3	6:R:78:ALA:HB2	1.79	0.44
1:A:471:ILE:HA	1:A:474:ILE:HG22	1.99	0.44
1:A:529:PRO:HA	1:A:532:CYS:SG	2.57	0.44
4:D:377:ASN:HD21	4:D:712:ASN:ND2	2.13	0.44
4:D:433:LYS:NZ	4:D:672:VAL:HA	2.31	0.44
1:A:238:HIS:CD2	1:A:267:ASN:HB2	2.50	0.44
1:A:381:LEU:CD2	1:A:424:LEU:HB2	2.45	0.44
1:A:562:LEU:HG	1:A:601:PHE:HB3	1.99	0.44
3:C:41:THR:N	4:D:106:ARG:HH12	2.16	0.44
4:D:184:VAL:O	4:D:187:SER:OG	2.22	0.44
1:A:532:CYS:SG	1:A:568:ILE:HG13	2.58	0.44
1:A:271:LEU:HD21	1:A:273:VAL:HG23	2.00	0.44
4:D:242:ARG:NE	4:D:242:ARG:HA	2.32	0.44
4:D:662:PRO:HA	4:D:665:MET:HE2	2.00	0.44
1:A:377:LEU:HA	1:A:380:GLN:NE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:239:VAL:O	4:D:243:LEU:HD23	2.17	0.44
4:D:617:LEU:O	4:D:621:LYS:N	2.51	0.44
1:A:216:MET:N	1:A:243:ASP:O	2.40	0.44
1:A:558:GLN:NE2	1:A:595:GLU:OE2	2.51	0.44
1:A:256:LEU:O	1:A:260:GLU:HG2	2.17	0.44
1:A:349:PHE:HA	1:A:352:THR:HG22	1.99	0.44
1:A:434:SER:O	1:A:437:ILE:HG22	2.17	0.44
1:A:587:ILE:O	1:A:591:LEU:HG	2.17	0.44
1:A:606:ILE:HD12	1:A:606:ILE:HA	1.80	0.44
4:D:209:SER:HB2	4:D:210:PRO:HD3	1.98	0.44
1:A:579:MET:SD	1:A:579:MET:N	2.90	0.43
1:A:676:HIS:CE1	1:A:680:LYS:HG3	2.53	0.43
4:D:14:TRP:CZ2	4:D:18:LEU:HD12	2.52	0.43
1:A:504:LYS:HA	1:A:504:LYS:HD3	1.87	0.43
3:C:53:ALA:HB2	4:D:32:ARG:NH2	2.33	0.43
4:D:611:THR:O	4:D:615:LYS:HE2	2.19	0.43
1:A:422:GLN:C	1:A:426:LYS:HZ3	2.26	0.43
1:A:688:MET:O	1:A:692:GLU:HB2	2.19	0.43
4:D:361:ASP:HB3	4:D:364:PHE:CD1	2.53	0.43
1:A:624:ARG:O	1:A:628:LEU:HG	2.18	0.43
1:A:725:HIS:HA	1:A:728:ARG:NE	2.34	0.43
1:A:185:LEU:HB2	1:A:188:LEU:HD23	2.01	0.43
1:A:546:ARG:HD3	1:A:549:GLU:OE1	2.19	0.43
2:B:69:PRO:HG2	3:C:83:TYR:HE1	1.84	0.43
4:D:17:LEU:HD11	4:D:42:ILE:HD11	2.01	0.43
4:D:223:ALA:O	4:D:227:LEU:HG	2.18	0.43
4:D:236:MET:O	4:D:240:LEU:HD23	2.19	0.43
4:D:341:GLU:HA	4:D:344:LEU:HG	2.00	0.43
1:A:144:ASN:OD1	1:A:168:SER:OG	2.25	0.43
2:B:8:ARG:HG2	2:B:13:THR:HG22	2.00	0.43
4:D:25:VAL:O	4:D:26:MET:HG3	2.19	0.43
1:A:214:LEU:HB3	1:A:242:LEU:HD13	1.99	0.43
2:B:39:PRO:HA	2:B:42:GLN:NE2	2.34	0.43
1:A:425:GLN:OE1	1:A:425:GLN:N	2.48	0.43
4:D:386:LYS:O	4:D:390:LEU:HD23	2.18	0.43
1:A:14:SER:HB3	3:C:80:LYS:HZ3	1.84	0.43
1:A:363:LEU:O	1:A:367:VAL:HG23	2.19	0.43
4:D:140:GLY:O	4:D:144:LEU:HD23	2.19	0.43
4:D:147:TRP:O	4:D:150:LEU:HB3	2.19	0.43
4:D:506:SER:OG	6:R:25:LYS:O	2.26	0.43
4:D:608:LYS:HG2	4:D:612:LYS:HZ1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LYS:O	1:A:368:THR:HG23	2.18	0.43
2:B:70:GLN:HE22	3:C:91:PRO:HB2	1.83	0.43
4:D:319:ILE:HD13	4:D:350:PHE:CD2	2.54	0.43
4:D:391:LEU:HB2	4:D:431:PHE:HE2	1.83	0.43
1:A:617:TRP:O	1:A:621:ARG:NH2	2.27	0.42
4:D:461:LEU:HG	4:D:470:THR:HG21	2.01	0.42
4:D:596:TYR:HE1	4:D:637:SER:HB2	1.83	0.42
1:A:142:VAL:HG13	1:A:168:SER:HB3	2.01	0.42
1:A:558:GLN:HA	1:A:561:VAL:HG12	2.01	0.42
3:C:80:LYS:HA	3:C:80:LYS:HE2	2.00	0.42
4:D:156:GLN:O	4:D:160:ILE:HG12	2.18	0.42
4:D:156:GLN:HG3	4:D:206:ILE:HD11	2.01	0.42
4:D:185:ILE:HG23	4:D:203:TYR:OH	2.19	0.42
4:D:160:ILE:O	4:D:164:LEU:HG	2.18	0.42
1:A:139:GLN:HE22	1:A:165:ARG:NH1	2.18	0.42
1:A:622:SER:HA	1:A:625:ASN:HD21	1.85	0.42
4:D:556:LEU:HD22	4:D:559:LEU:HD21	2.02	0.42
4:D:562:GLY:HA3	4:D:582:MET:HE1	2.01	0.42
2:B:37:ARG:HD3	2:B:38:PRO:HD2	2.00	0.42
4:D:334:ASN:O	4:D:335:MET:HE2	2.20	0.42
1:A:225:THR:O	1:A:229:ILE:HD12	2.19	0.42
1:A:423:GLN:OE1	5:P:18:UNK:HA	2.20	0.42
4:D:611:THR:O	4:D:614:ILE:HG22	2.19	0.42
4:D:671:ALA:HA	4:D:674:GLU:CD	2.45	0.42
1:A:23:LEU:HD23	1:A:23:LEU:HA	1.78	0.42
1:A:96:VAL:HG22	1:A:100:LYS:HD3	2.02	0.42
3:C:23:SER:OG	3:C:24:SER:N	2.51	0.42
4:D:186:ASN:HA	4:D:189:VAL:HG12	2.01	0.42
1:A:625:ASN:HA	1:A:628:LEU:HD12	2.01	0.42
4:D:115:LYS:HA	4:D:118:LEU:HD12	2.02	0.42
6:R:25:LYS:HE2	6:R:25:LYS:HA	2.02	0.42
6:R:25:LYS:HG3	6:R:26:LYS:HG2	2.02	0.42
6:R:73:GLY:N	6:R:77:HIS:O	2.49	0.42
1:A:23:LEU:CD1	1:A:57:ARG:HG2	2.49	0.42
1:A:49:VAL:HG21	4:D:49:TYR:HE1	1.85	0.42
1:A:324:GLU:HA	1:A:327:ILE:HG22	2.02	0.42
4:D:680:LEU:HG	4:D:717:MET:HE1	2.01	0.42
1:A:58:LEU:HA	1:A:61:THR:HG22	2.02	0.42
1:A:239:LEU:H	1:A:265:LEU:HD12	1.85	0.42
3:C:105:MET:HE3	4:D:3:LEU:CD1	2.50	0.42
4:D:299:VAL:HG23	4:D:302:ARG:HH22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:MET:SD	1:A:355:MET:N	2.93	0.41
4:D:459:ASN:OD1	4:D:460:LYS:N	2.53	0.41
1:A:13:ALA:HA	1:A:402:ARG:HH12	1.84	0.41
2:B:28:LYS:HD3	2:B:42:GLN:HE21	1.85	0.41
1:A:49:VAL:HG22	1:A:80:GLN:HA	2.02	0.41
1:A:682:PRO:O	1:A:686:CYS:HB2	2.21	0.41
4:D:83:VAL:HG13	4:D:84:LEU:HD12	2.03	0.41
4:D:540:PHE:HA	4:D:543:PHE:HB3	2.02	0.41
1:A:44:LEU:HB2	1:A:75:ILE:HD11	2.02	0.41
1:A:116:ASN:CG	1:A:117:ALA:H	2.28	0.41
1:A:444:ASN:HB2	1:A:447:GLU:OE1	2.21	0.41
1:A:541:LEU:CD1	1:A:545:MET:HE1	2.50	0.41
1:A:601:PHE:O	1:A:605:ILE:HG12	2.19	0.41
3:C:52:PHE:HD2	4:D:32:ARG:HG3	1.86	0.41
4:D:340:VAL:HG21	4:D:394:TYR:CG	2.56	0.41
4:D:372:LEU:HD22	4:D:424:TYR:CD2	2.52	0.41
4:D:629:LYS:HB2	4:D:631:ASP:OD1	2.21	0.41
6:R:75:CYS:SG	6:R:99:ARG:HD3	2.61	0.41
1:A:255:ALA:O	1:A:259:LEU:HD23	2.21	0.41
4:D:471:SER:HA	4:D:474:HIS:HE1	1.83	0.41
4:D:472:LYS:HG2	4:D:475:ARG:HH21	1.85	0.41
1:A:56:ASP:OD2	1:A:85:ARG:HB2	2.20	0.41
1:A:80:GLN:C	1:A:81:MET:HE2	2.46	0.41
1:A:588:SER:HA	1:A:591:LEU:HG	2.02	0.41
3:C:81:VAL:O	3:C:84:THR:HG22	2.21	0.41
4:D:11:ASP:OD1	4:D:12:GLU:N	2.54	0.41
4:D:106:ARG:O	4:D:109:ASN:HB2	2.21	0.41
4:D:151:MET:HA	4:D:155:LEU:HD11	2.03	0.41
4:D:472:LYS:HE2	4:D:475:ARG:HH21	1.84	0.41
4:D:475:ARG:HG3	4:D:476:MET:SD	2.60	0.41
4:D:561:THR:OG1	4:D:562:GLY:N	2.54	0.41
1:A:422:GLN:OE1	1:A:422:GLN:N	2.44	0.41
1:A:681:ASN:HB3	1:A:685:TYR:HD2	1.85	0.41
2:B:46:LYS:O	2:B:49:GLN:N	2.52	0.41
4:D:333:GLU:HG3	4:D:335:MET:HG2	2.03	0.41
4:D:399:LEU:HD13	4:D:442:ARG:HH12	1.86	0.41
1:A:228:GLN:O	1:A:232:VAL:HG22	2.20	0.40
4:D:433:LYS:HZ2	4:D:672:VAL:HA	1.85	0.40
4:D:458:ILE:HD13	4:D:473:LEU:HG	2.03	0.40
4:D:508:GLN:HE21	4:D:508:GLN:HB3	1.74	0.40
1:A:84:LYS:NZ	1:A:106:LYS:HG3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:GLN:HG2	1:A:455:TRP:CH2	2.56	0.40
1:A:545:MET:HE2	1:A:545:MET:HB2	1.91	0.40
3:C:50:GLY:HA2	3:C:53:ALA:HB3	2.03	0.40
4:D:285:ILE:HG12	4:D:293:ASP:OD2	2.21	0.40
4:D:452:ASP:OD1	4:D:453:SER:N	2.54	0.40
1:A:38:GLN:HE21	1:A:39:ASP:CG	2.29	0.40
1:A:244:ILE:O	1:A:244:ILE:HG22	2.20	0.40
2:B:77:LEU:HD23	2:B:78:ALA:N	2.36	0.40
4:D:164:LEU:O	4:D:168:LYS:HG2	2.22	0.40
4:D:485:ASP:OD1	4:D:486:LEU:N	2.55	0.40
1:A:371:ARG:NH1	1:A:371:ARG:HB2	2.36	0.40
1:A:670:ALA:O	1:A:674:MET:HG2	2.22	0.40
1:A:713:GLN:HA	1:A:716:VAL:HG22	2.04	0.40
2:B:42:GLN:O	2:B:43:ARG:HD2	2.21	0.40
2:B:43:ARG:HG3	2:B:80:ARG:NE	2.35	0.40
4:D:365:MET:HA	4:D:365:MET:HE3	2.02	0.40
6:R:83:CYS:O	6:R:86:ARG:HG2	2.21	0.40
1:A:296:PHE:CE2	1:A:333:ARG:HG3	2.57	0.40
4:D:609:GLU:HA	4:D:612:LYS:NZ	2.37	0.40
4:D:670:SER:O	4:D:674:GLU:OE1	2.40	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	719/748 (96%)	679 (94%)	40 (6%)	0	100	100
2	B	96/118 (81%)	91 (95%)	5 (5%)	0	100	100
3	C	94/96 (98%)	89 (95%)	5 (5%)	0	100	100
4	D	742/779 (95%)	707 (95%)	35 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	P	8/21 (38%)	8 (100%)	0	0	100	100
6	R	83/108 (77%)	75 (90%)	8 (10%)	0	100	100
All	All	1742/1870 (93%)	1649 (95%)	93 (5%)	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	641/663 (97%)	640 (100%)	1 (0%)	87	85
2	B	86/103 (84%)	86 (100%)	0	100	100
3	C	85/85 (100%)	85 (100%)	0	100	100
4	D	680/702 (97%)	680 (100%)	0	100	100
5	P	8/8 (100%)	7 (88%)	1 (12%)	4	18
6	R	76/90 (84%)	76 (100%)	0	100	100
All	All	1576/1651 (96%)	1574 (100%)	2 (0%)	87	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	444	ASN
5	P	9	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	137	ASN
1	A	238	HIS
1	A	249	GLN
1	A	267	ASN

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Mol	Chain	Res	Type
1	A	290	GLN
1	A	389	ASN
1	A	409	HIS
1	A	558	GLN
1	A	625	ASN
1	A	667	GLN
1	A	676	HIS
1	A	697	HIS
1	A	700	ASN
2	B	42	GLN
4	D	68	HIS
4	D	334	ASN
4	D	377	ASN
4	D	497	GLN
4	D	589	ASN
4	D	667	GLN
4	D	696	HIS
5	P	9	GLN
6	R	82	HIS
6	R	98	ASN

### 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 ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

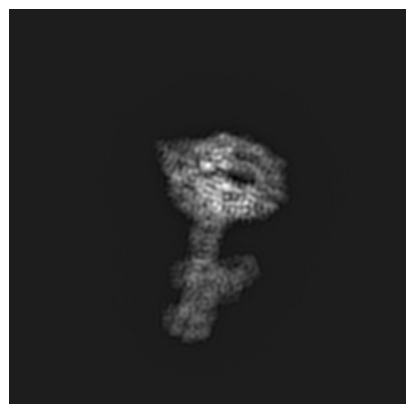
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44631. These allow visual inspection of the internal detail of the map and identification of artifacts.

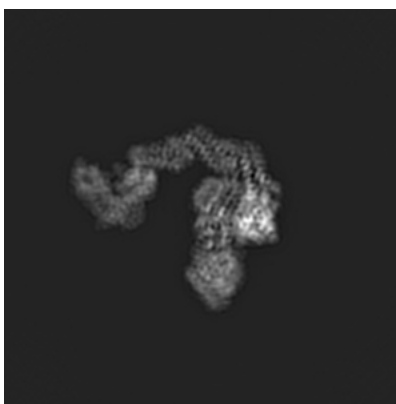
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

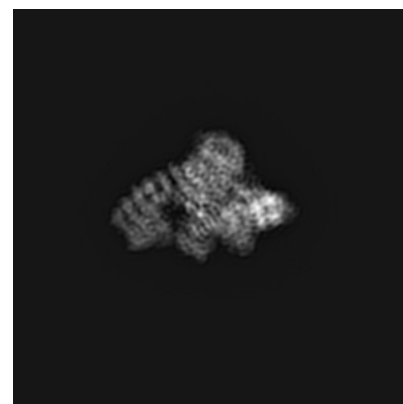
#### 6.1.1 Primary map



X

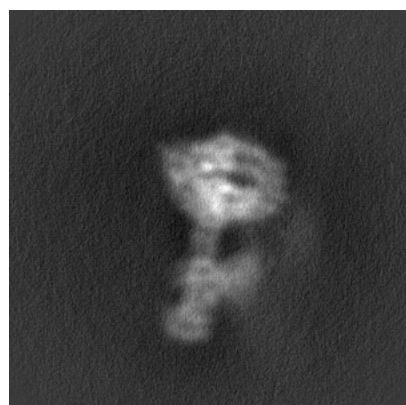


Y

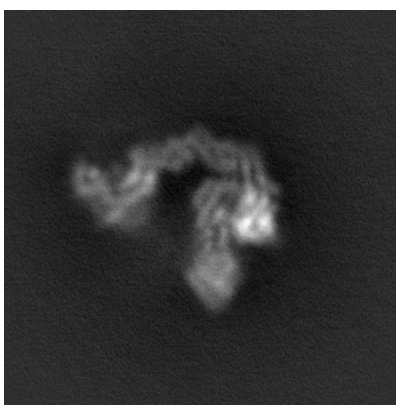


Z

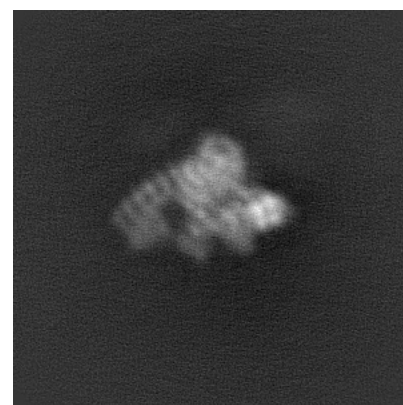
#### 6.1.2 Raw map



X



Y

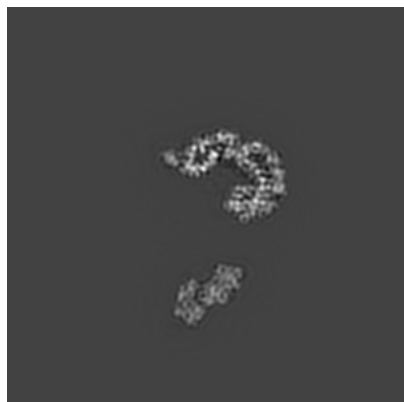


Z

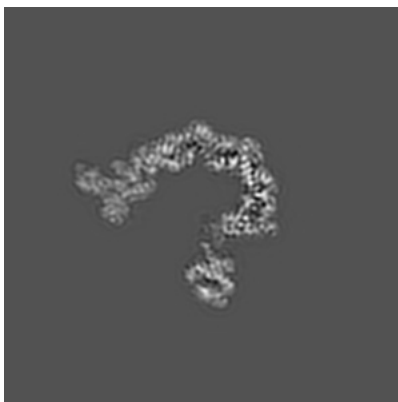
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 180



Y Index: 180

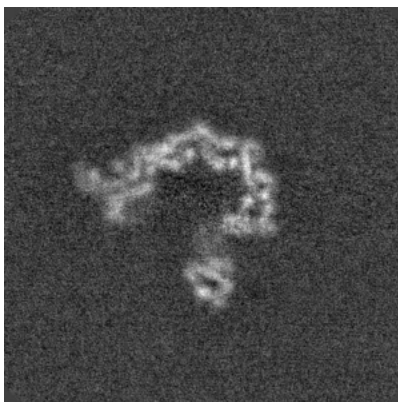


Z Index: 180

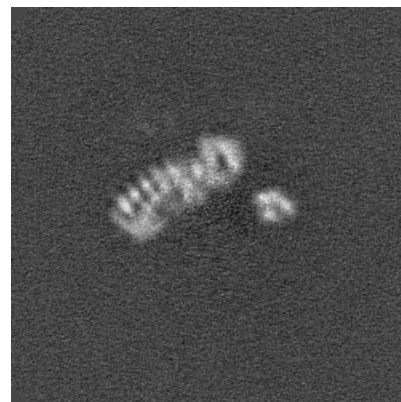
### 6.2.2 Raw map



X Index: 180



Y Index: 180

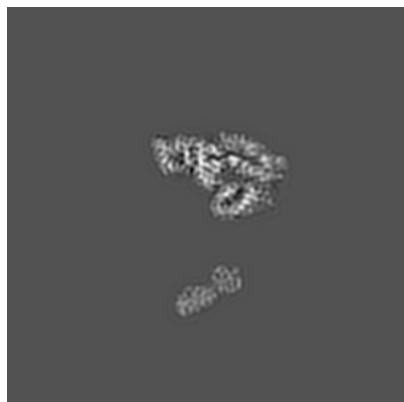


Z Index: 180

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

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

### 6.3.1 Primary map



X Index: 169



Y Index: 189

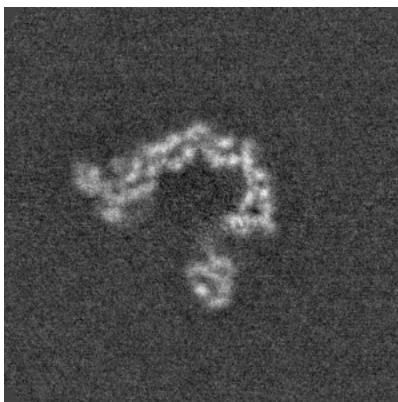


Z Index: 196

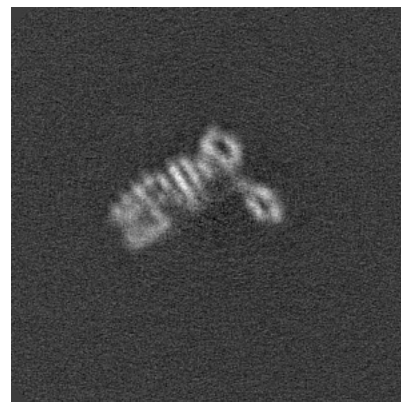
### 6.3.2 Raw map



X Index: 169



Y Index: 177

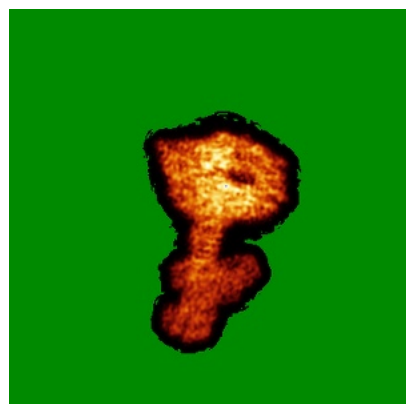


Z Index: 196

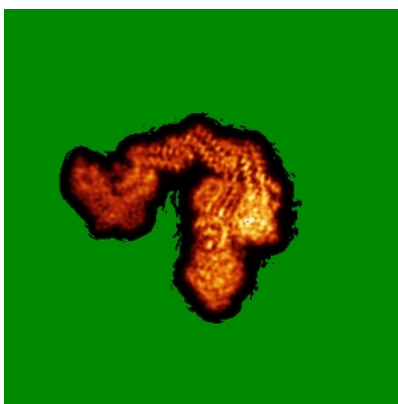
The images above show the largest variance slices of the map in three orthogonal directions.

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

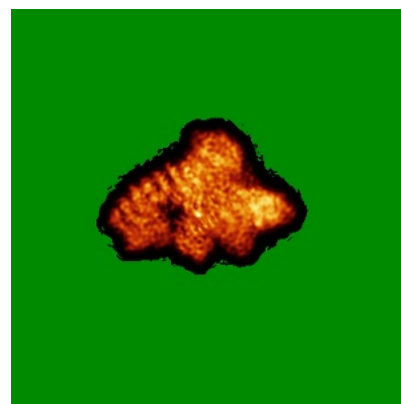
### 6.4.1 Primary map



X

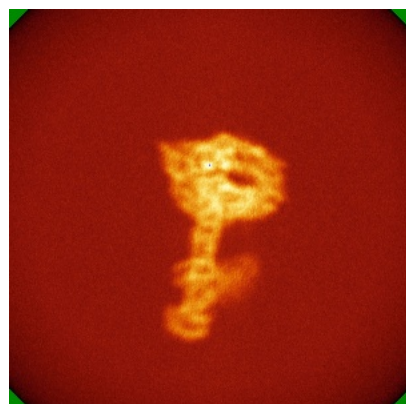


Y

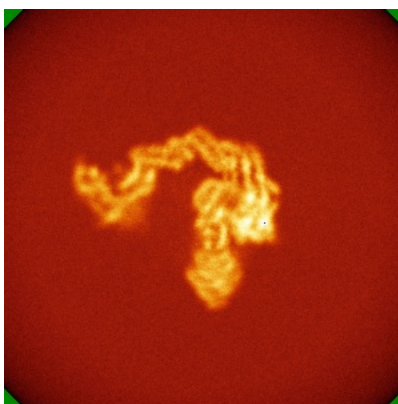


Z

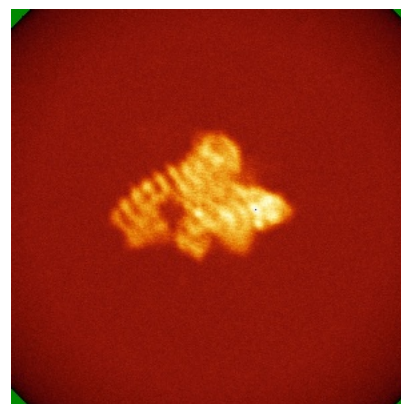
### 6.4.2 Raw map



X



Y



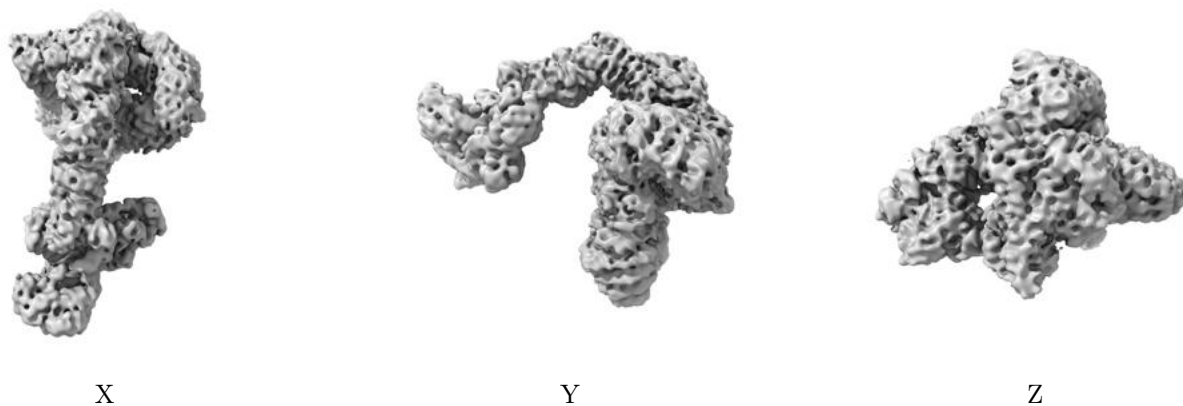
Z

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.



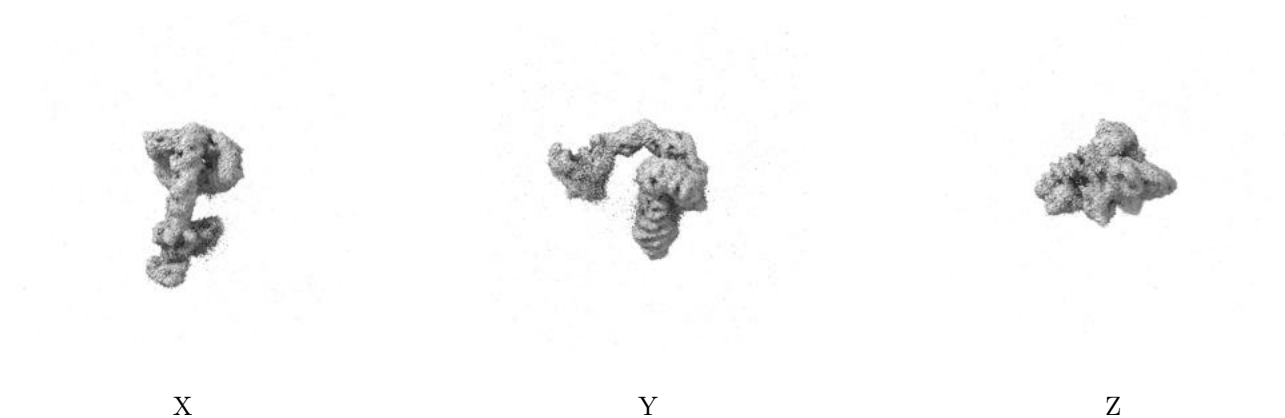
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. 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](#)

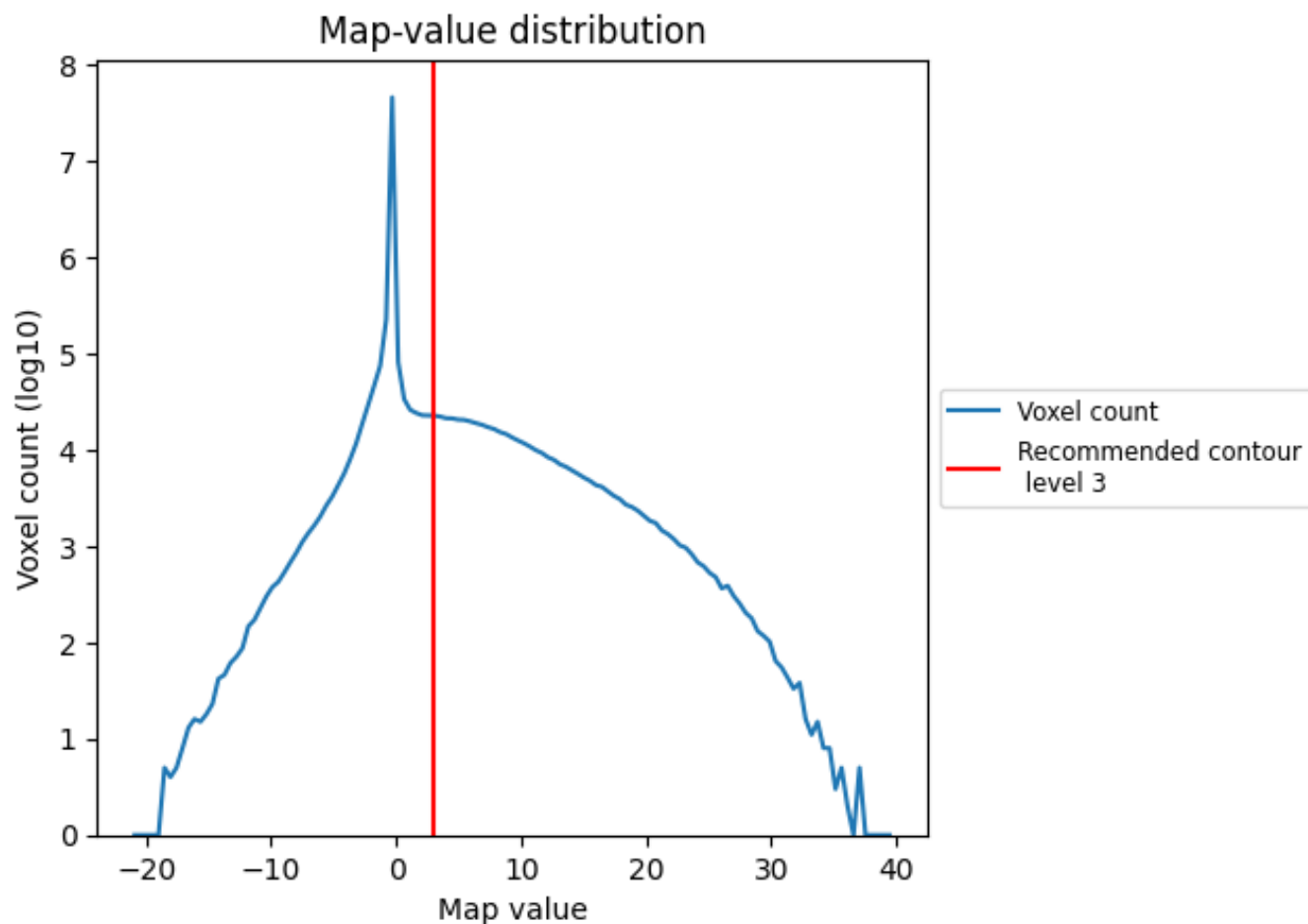
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

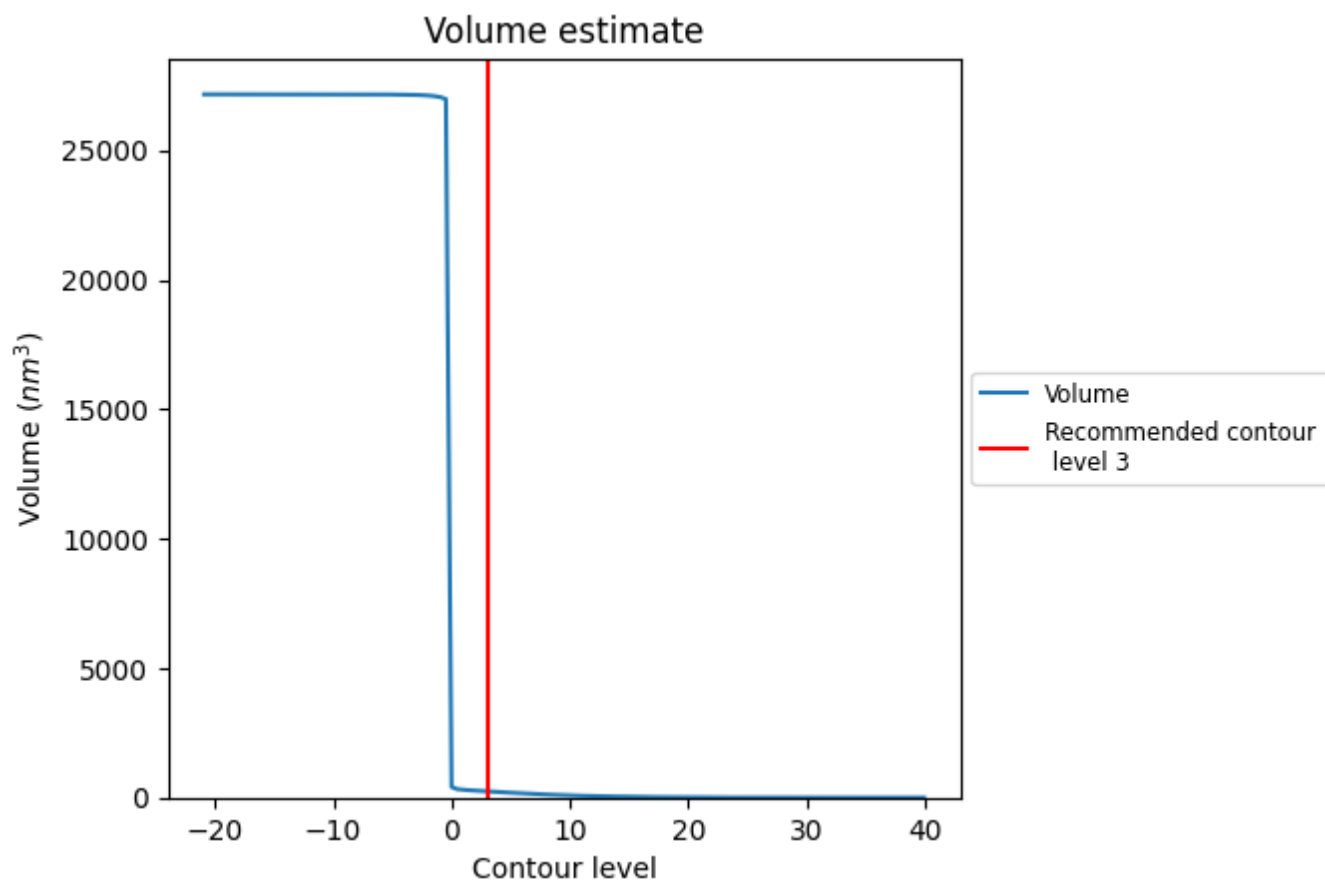
This section contains the results of statistical analysis of the map.

### 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.

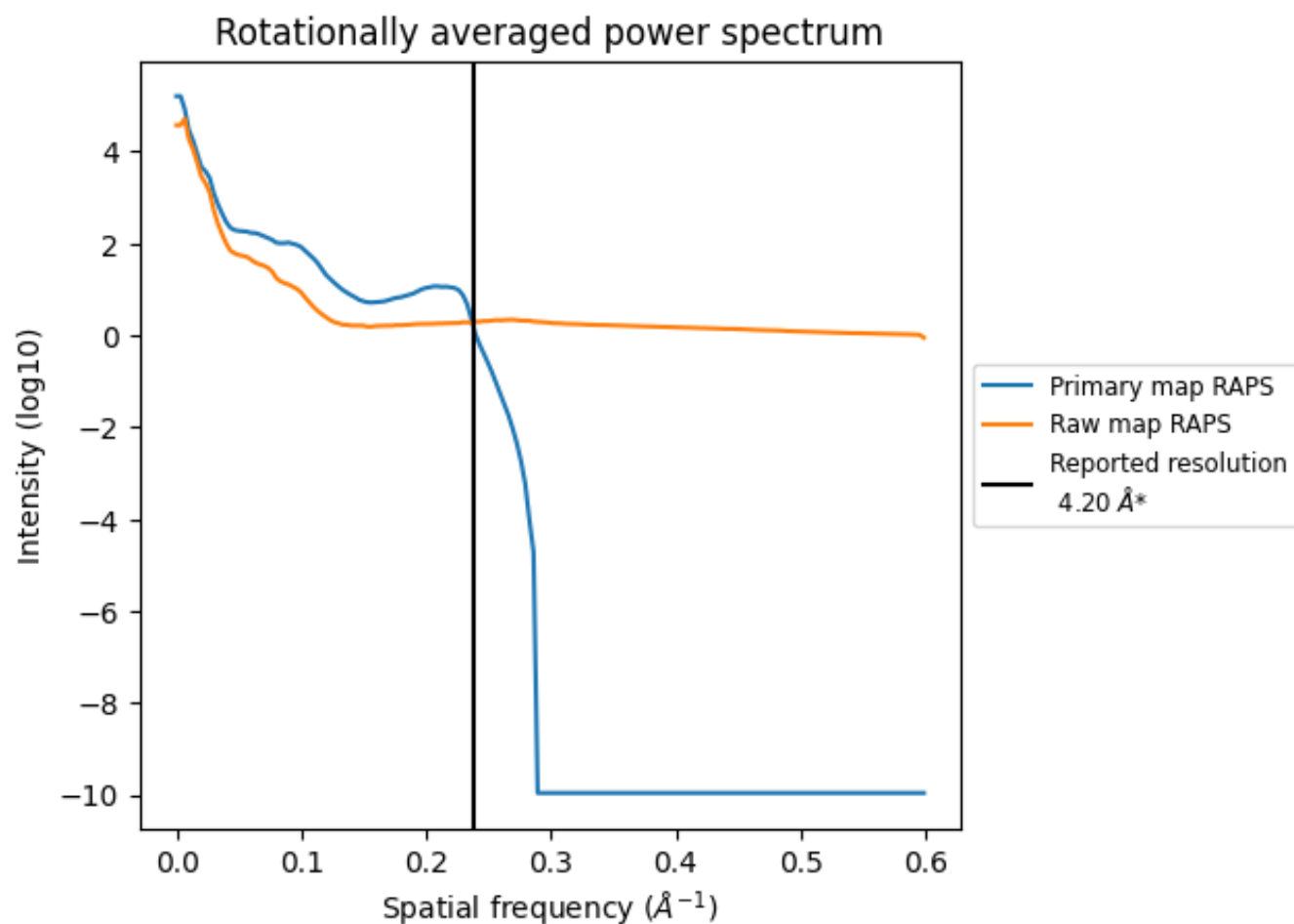
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 240  $\text{nm}^3$ ; this corresponds to an approximate mass of 217 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 ⓘ

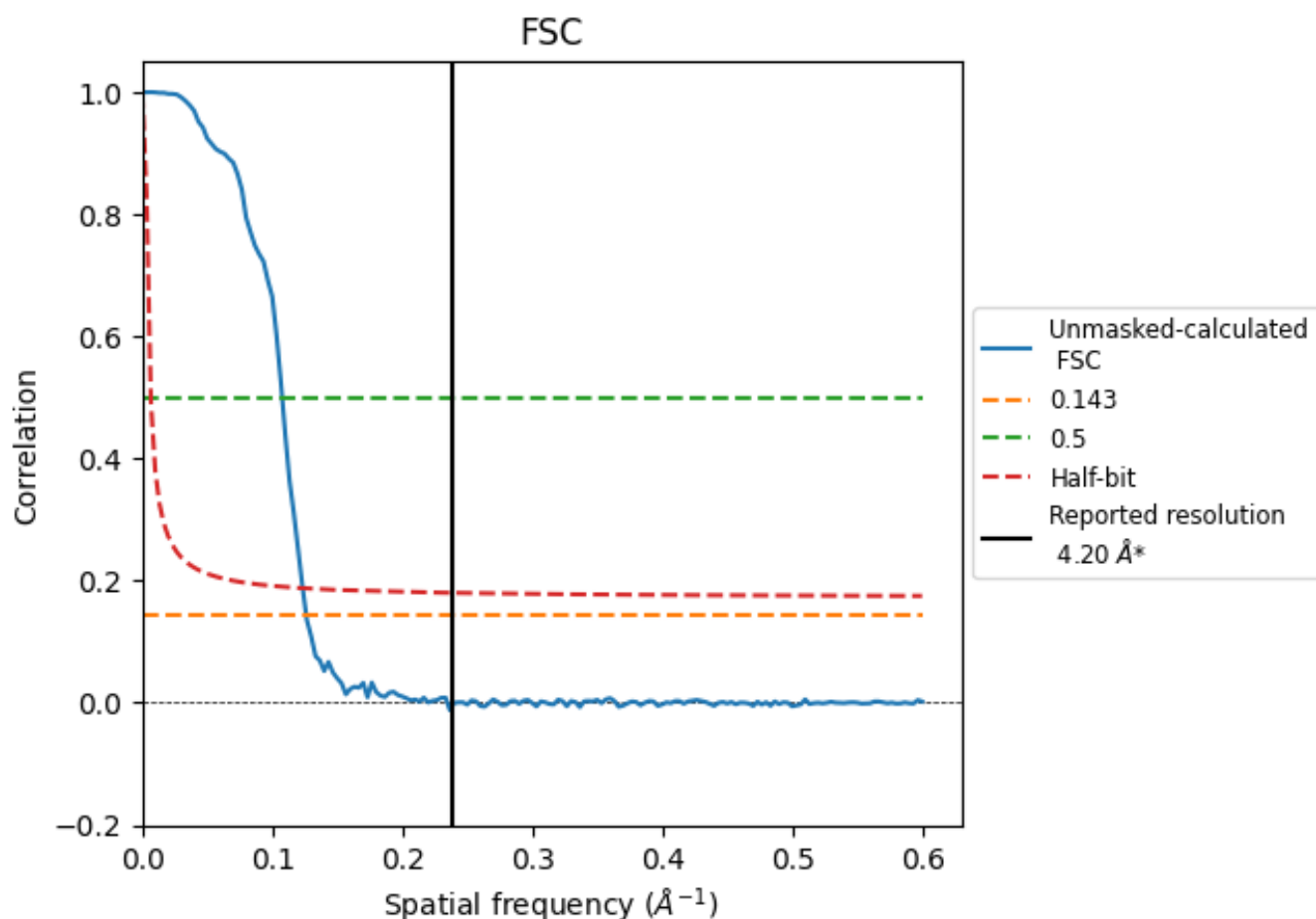


\*Reported resolution corresponds to spatial frequency of 0.238 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.238 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

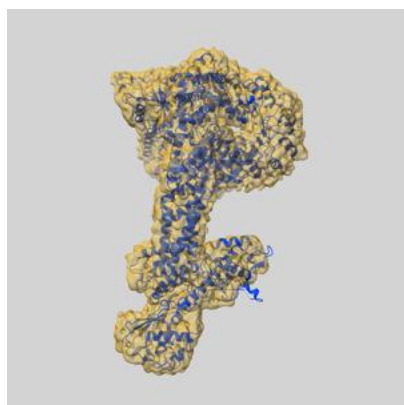
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.94	9.31	8.12

\*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 7.94 differs from the reported value 4.2 by more than 10 %

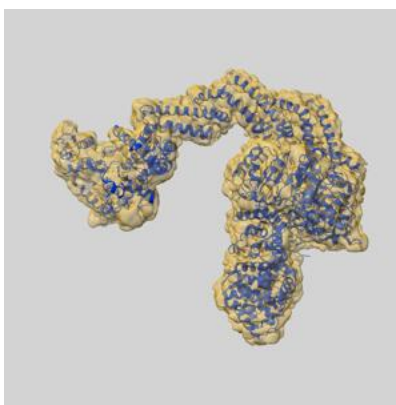
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44631 and PDB model 9BJ9. Per-residue inclusion information can be found in section [3](#) on page [7](#).

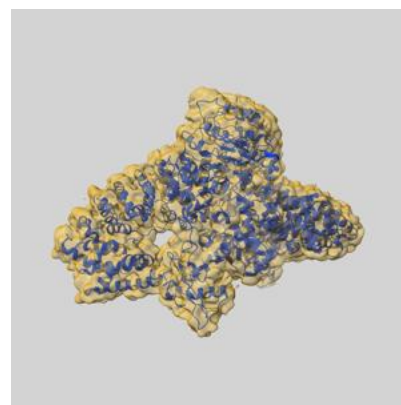
### 9.1 Map-model overlay [i](#)



X



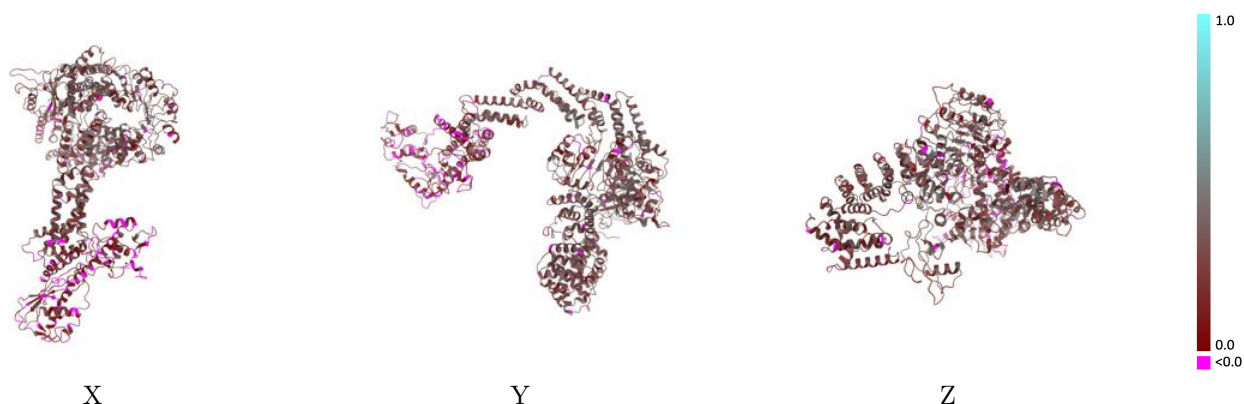
Y



Z

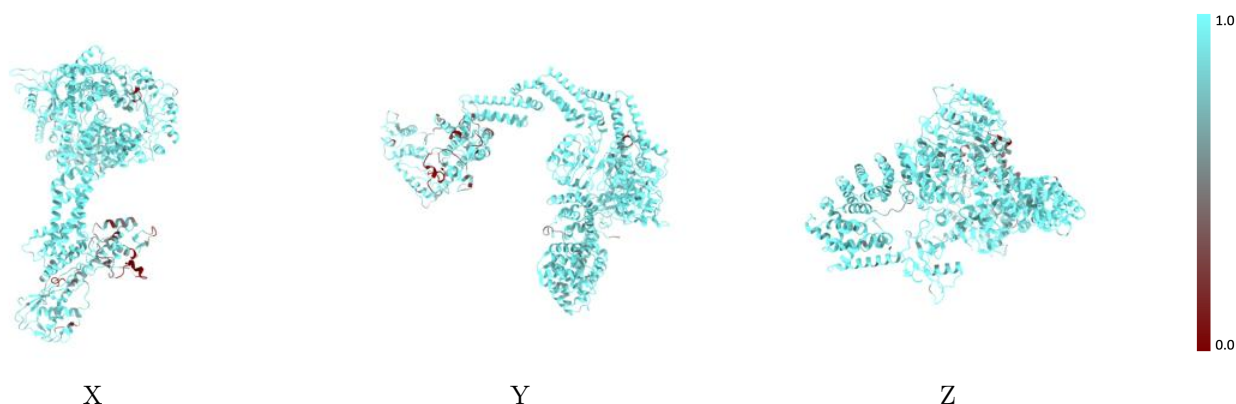
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



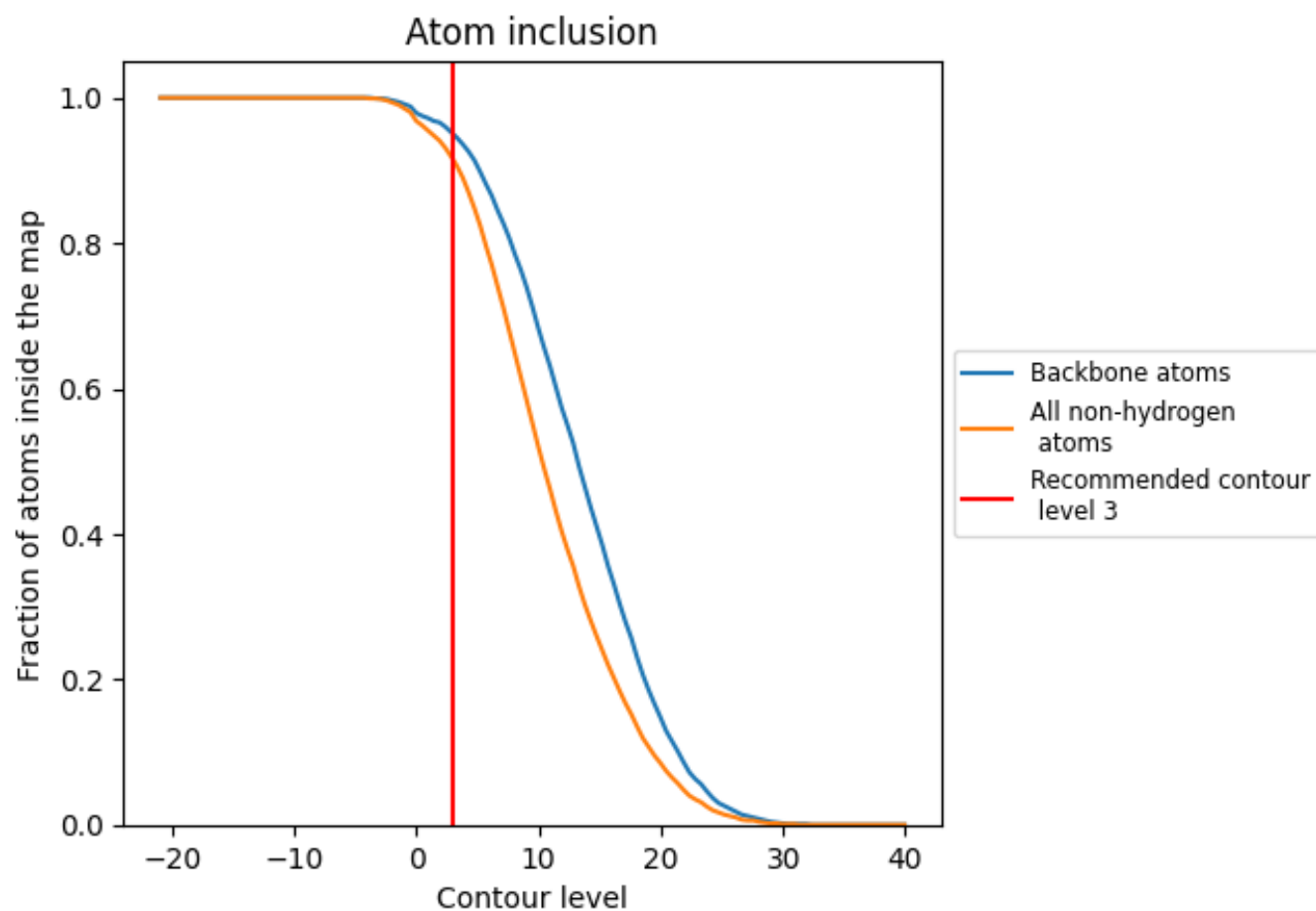
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9150</div>	<div><div></div>0.2580</div>
A	<div><div></div>0.9590</div>	<div><div></div>0.2920</div>
B	<div><div></div>0.9590</div>	<div><div></div>0.3030</div>
C	<div><div></div>0.9560</div>	<div><div></div>0.3360</div>
D	<div><div></div>0.8970</div>	<div><div></div>0.2310</div>
P	<div><div></div>0.7610</div>	<div><div></div>0.2250</div>
R	<div><div></div>0.6480</div>	<div><div></div>0.0950</div>

1.0

0.0

<0.0