



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:39 AM UTC

PDB ID : 8WRO / pdb_00008wro
EMDB ID : EMD-37784
Title : XBB.1.5.10 spike protein in complex with ACE2
Authors : Feng, L.L.; Feng, L.L.
Deposited on : 2023-10-15
Resolution : 3.90 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

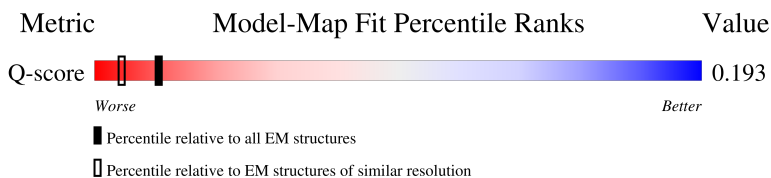
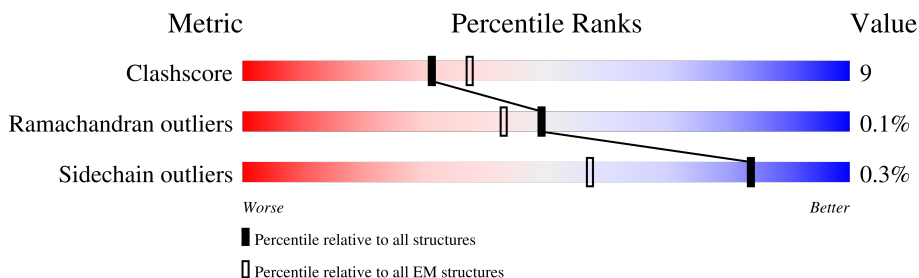
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	8855 (3.40 - 4.40)

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	1318	9% 63% 18% 19%
1	B	1318	• 64% 16% 20%
1	C	1318	5% 62% 19% 20%
2	D	594	36% 78% 22%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29807 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 Spike glycoprotein,Spike glycoprotein,Spike glycoprotein,Fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1067	Total	C	N	O	S	0	0
			8364	5347	1397	1581	39		
1	B	1059	Total	C	N	O	S	0	0
			8295	5304	1384	1568	39		
1	C	1060	Total	C	N	O	S	0	0
			8303	5310	1385	1569	39		

There are 159 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	24	SER	ALA	variant	UNP P0DTC2
A	80	ALA	VAL	variant	UNP P0DTC2
A	139	ASP	GLY	variant	UNP P0DTC2
A	143	GLN	HIS	variant	UNP P0DTC2
A	180	GLU	GLN	variant	UNP P0DTC2
A	210	GLU	VAL	variant	UNP P0DTC2
A	249	VAL	GLY	variant	UNP P0DTC2
A	336	HIS	GLY	variant	UNP P0DTC2
A	343	THR	ARG	variant	UNP P0DTC2
A	365	ILE	LEU	variant	UNP P0DTC2
A	368	PHE	SER	variant	UNP P0DTC2
A	370	PRO	SER	variant	UNP P0DTC2
A	372	PHE	SER	variant	UNP P0DTC2
A	373	ALA	THR	variant	UNP P0DTC2
A	402	ASN	ASP	variant	UNP P0DTC2
A	405	SER	ARG	variant	UNP P0DTC2
A	414	ASN	LYS	variant	UNP P0DTC2
A	437	LYS	ASN	variant	UNP P0DTC2
A	442	PRO	VAL	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	443	SER	GLY	variant	UNP P0DTC2
A	453	LEU	PHE	variant	UNP P0DTC2
A	457	LYS	ASN	variant	UNP P0DTC2
A	474	ASN	SER	variant	UNP P0DTC2
A	475	LYS	THR	variant	UNP P0DTC2
A	481	ALA	GLU	variant	UNP P0DTC2
A	483	PRO	PHE	conflict	UNP P0DTC2
A	487	SER	PHE	variant	UNP P0DTC2
A	495	ARG	GLN	variant	UNP P0DTC2
A	498	TYR	ASN	variant	UNP P0DTC2
A	502	HIS	TYR	variant	UNP P0DTC2
A	611	GLY	ASP	variant	UNP P0DTC2
A	652	TYR	HIS	variant	UNP P0DTC2
A	676	LYS	ASN	variant	UNP P0DTC2
A	678	HIS	PRO	variant	UNP P0DTC2
A	679	GLY	ARG	conflict	UNP P0DTC2
A	680	SER	ARG	conflict	UNP P0DTC2
A	682	SER	ARG	conflict	UNP P0DTC2
A	761	LYS	ASN	variant	UNP P0DTC2
A	793	TYR	ASP	variant	UNP P0DTC2
A	814	PRO	PHE	conflict	UNP P0DTC2
A	826	THR	ALA	conflict	UNP P0DTC2
A	833	LYS	GLN	conflict	UNP P0DTC2
A	889	PRO	ALA	conflict	UNP P0DTC2
A	896	PRO	ALA	conflict	UNP P0DTC2
A	939	PRO	ALA	conflict	UNP P0DTC2
A	951	HIS	GLN	variant	UNP P0DTC2
A	966	LYS	ASN	variant	UNP P0DTC2
A	983	PRO	LYS	variant	UNP P0DTC2
A	984	PRO	VAL	variant	UNP P0DTC2
B	19	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	24	SER	ALA	variant	UNP P0DTC2
B	80	ALA	VAL	variant	UNP P0DTC2
B	139	ASP	GLY	variant	UNP P0DTC2
B	143	GLN	HIS	variant	UNP P0DTC2
B	180	GLU	GLN	variant	UNP P0DTC2
B	210	GLU	VAL	variant	UNP P0DTC2
B	249	VAL	GLY	variant	UNP P0DTC2
B	336	HIS	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	343	THR	ARG	variant	UNP P0DTC2
B	365	ILE	LEU	variant	UNP P0DTC2
B	368	PHE	SER	variant	UNP P0DTC2
B	370	PRO	SER	variant	UNP P0DTC2
B	372	PHE	SER	variant	UNP P0DTC2
B	373	ALA	THR	variant	UNP P0DTC2
B	402	ASN	ASP	variant	UNP P0DTC2
B	405	SER	ARG	variant	UNP P0DTC2
B	414	ASN	LYS	variant	UNP P0DTC2
B	437	LYS	ASN	variant	UNP P0DTC2
B	442	PRO	VAL	variant	UNP P0DTC2
B	443	SER	GLY	variant	UNP P0DTC2
B	453	LEU	PHE	variant	UNP P0DTC2
B	457	LYS	ASN	variant	UNP P0DTC2
B	474	ASN	SER	variant	UNP P0DTC2
B	475	LYS	THR	variant	UNP P0DTC2
B	481	ALA	GLU	variant	UNP P0DTC2
B	483	PRO	PHE	conflict	UNP P0DTC2
B	487	SER	PHE	variant	UNP P0DTC2
B	495	ARG	GLN	variant	UNP P0DTC2
B	498	TYR	ASN	variant	UNP P0DTC2
B	502	HIS	TYR	variant	UNP P0DTC2
B	611	GLY	ASP	variant	UNP P0DTC2
B	652	TYR	HIS	variant	UNP P0DTC2
B	676	LYS	ASN	variant	UNP P0DTC2
B	678	HIS	PRO	variant	UNP P0DTC2
B	679	GLY	ARG	conflict	UNP P0DTC2
B	680	SER	ARG	conflict	UNP P0DTC2
B	682	SER	ARG	conflict	UNP P0DTC2
B	761	LYS	ASN	variant	UNP P0DTC2
B	793	TYR	ASP	variant	UNP P0DTC2
B	814	PRO	PHE	conflict	UNP P0DTC2
B	826	THR	ALA	conflict	UNP P0DTC2
B	833	LYS	GLN	conflict	UNP P0DTC2
B	889	PRO	ALA	conflict	UNP P0DTC2
B	896	PRO	ALA	conflict	UNP P0DTC2
B	939	PRO	ALA	conflict	UNP P0DTC2
B	951	HIS	GLN	variant	UNP P0DTC2
B	966	LYS	ASN	variant	UNP P0DTC2
B	983	PRO	LYS	variant	UNP P0DTC2
B	984	PRO	VAL	variant	UNP P0DTC2
C	19	ILE	THR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	24	SER	ALA	variant	UNP P0DTC2
C	80	ALA	VAL	variant	UNP P0DTC2
C	139	ASP	GLY	variant	UNP P0DTC2
C	143	GLN	HIS	variant	UNP P0DTC2
C	180	GLU	GLN	variant	UNP P0DTC2
C	210	GLU	VAL	variant	UNP P0DTC2
C	249	VAL	GLY	variant	UNP P0DTC2
C	336	HIS	GLY	variant	UNP P0DTC2
C	343	THR	ARG	variant	UNP P0DTC2
C	365	ILE	LEU	variant	UNP P0DTC2
C	368	PHE	SER	variant	UNP P0DTC2
C	370	PRO	SER	variant	UNP P0DTC2
C	372	PHE	SER	variant	UNP P0DTC2
C	373	ALA	THR	variant	UNP P0DTC2
C	402	ASN	ASP	variant	UNP P0DTC2
C	405	SER	ARG	variant	UNP P0DTC2
C	414	ASN	LYS	variant	UNP P0DTC2
C	437	LYS	ASN	variant	UNP P0DTC2
C	442	PRO	VAL	variant	UNP P0DTC2
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C	453	LEU	PHE	variant	UNP P0DTC2
C	457	LYS	ASN	variant	UNP P0DTC2
C	474	ASN	SER	variant	UNP P0DTC2
C	475	LYS	THR	variant	UNP P0DTC2
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C	498	TYR	ASN	variant	UNP P0DTC2
C	502	HIS	TYR	variant	UNP P0DTC2
C	611	GLY	ASP	variant	UNP P0DTC2
C	652	TYR	HIS	variant	UNP P0DTC2
C	676	LYS	ASN	variant	UNP P0DTC2
C	678	HIS	PRO	variant	UNP P0DTC2
C	679	GLY	ARG	conflict	UNP P0DTC2
C	680	SER	ARG	conflict	UNP P0DTC2
C	682	SER	ARG	conflict	UNP P0DTC2
C	761	LYS	ASN	variant	UNP P0DTC2
C	793	TYR	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	814	PRO	PHE	conflict	UNP P0DTC2
C	826	THR	ALA	conflict	UNP P0DTC2
C	833	LYS	GLN	conflict	UNP P0DTC2
C	889	PRO	ALA	conflict	UNP P0DTC2
C	896	PRO	ALA	conflict	UNP P0DTC2
C	939	PRO	ALA	conflict	UNP P0DTC2
C	951	HIS	GLN	variant	UNP P0DTC2
C	966	LYS	ASN	variant	UNP P0DTC2
C	983	PRO	LYS	variant	UNP P0DTC2
C	984	PRO	VAL	variant	UNP P0DTC2

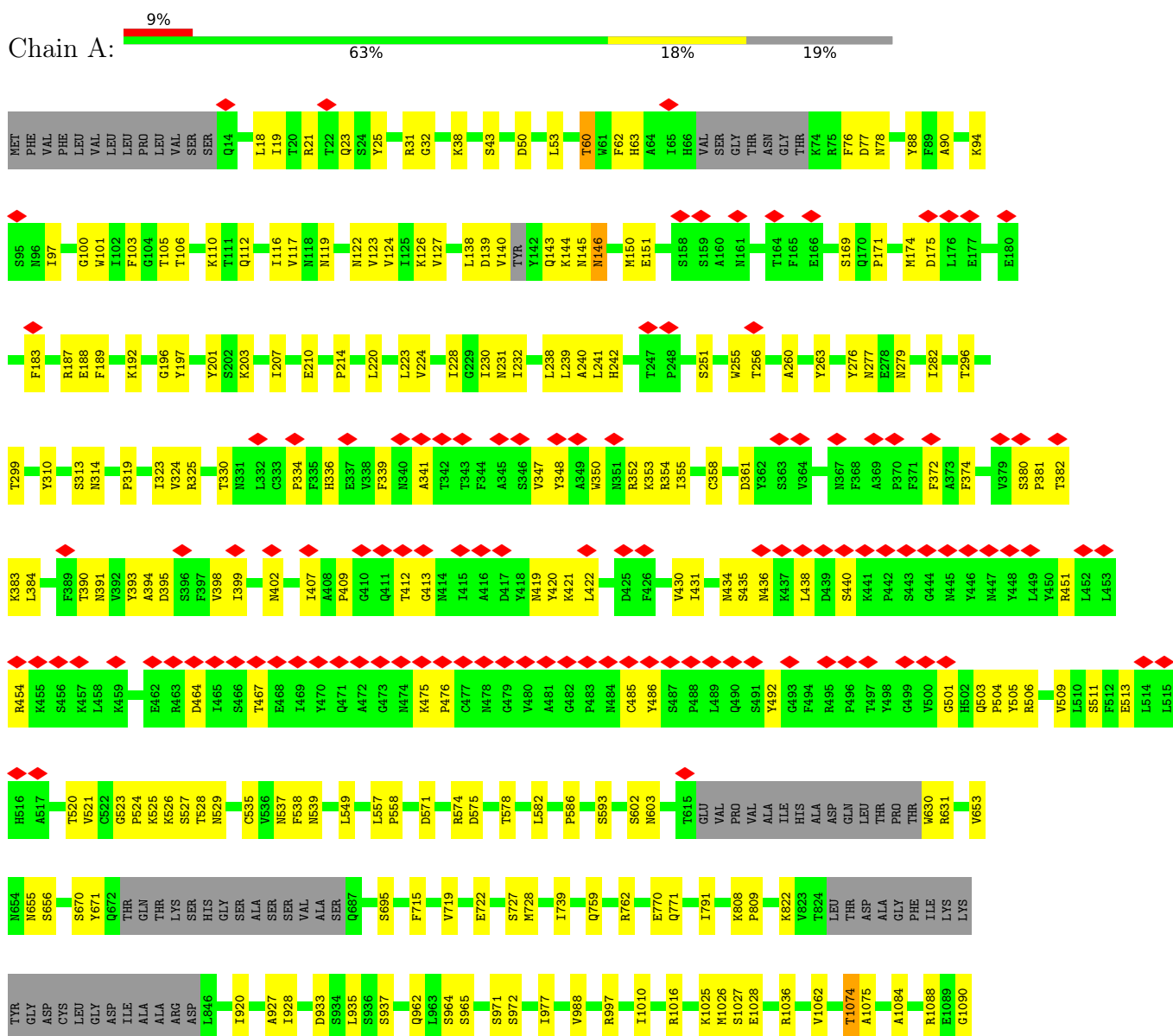
- Molecule 2 is a protein called Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	594	Total	C	N	O	S	0	0
			4845	3099	803	914	29		

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: Spike glycoprotein,Spike glycoprotein,Spike glycoprotein,Fusion protein



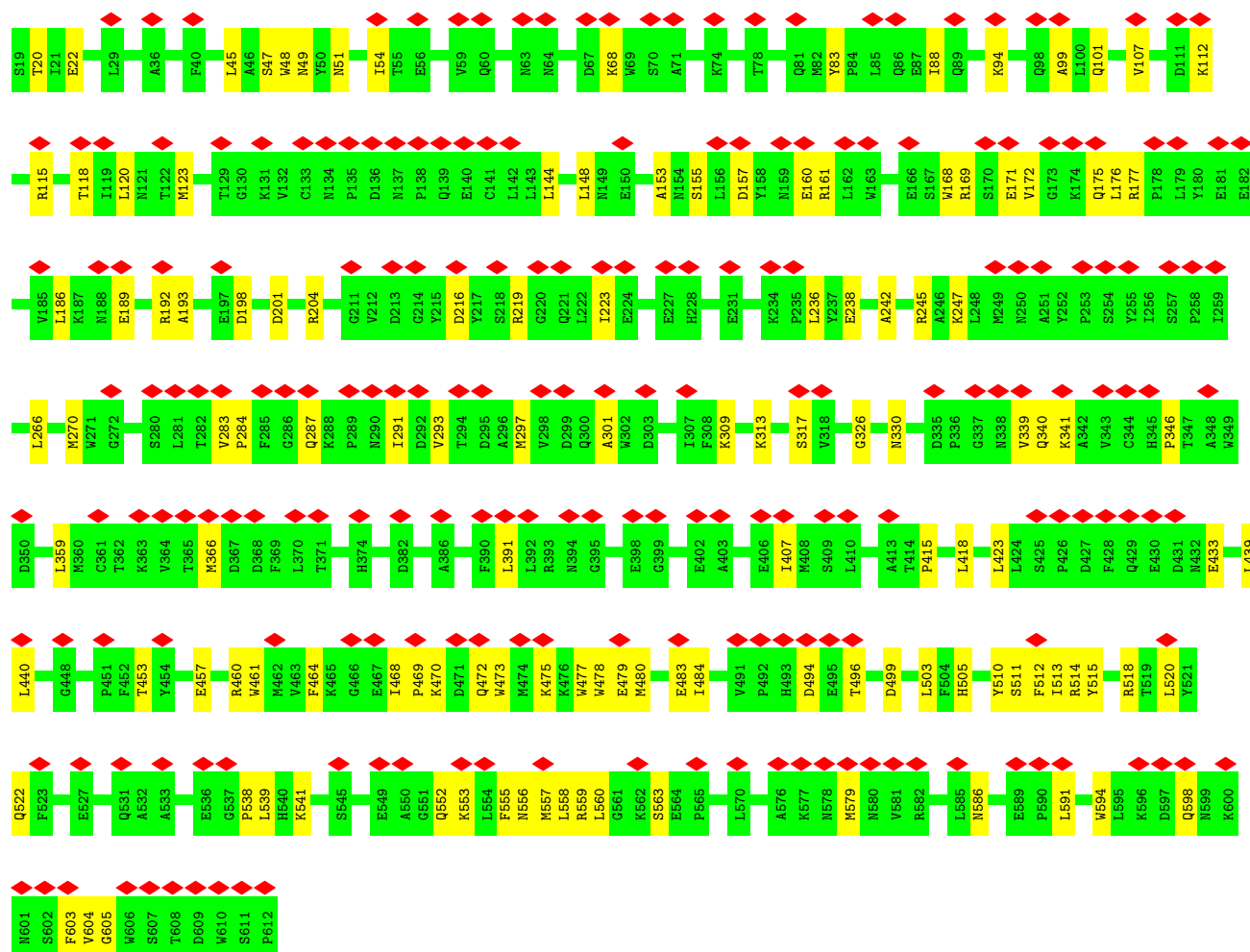




GLY
GLY
SER
SER
ALA
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS
HIS
HIS
HIS
HIS
HIS
HIS
HIS

● Molecule 2: Processed angiotensin-converting enzyme 2

Chain D: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76881	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.686	Depositor
Minimum map value	-0.786	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.19	0/8565	0.44	0/11656
1	B	0.19	0/8495	0.43	1/11563 (0.0%)
1	C	0.21	0/8503	0.47	0/11574
2	D	0.16	0/4981	0.42	2/6767 (0.0%)
All	All	0.19	0/30544	0.44	3/41560 (0.0%)

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	ILE	CG1-CB-CG2	-5.21	95.07	110.70
2	D	479	GLU	CA-C-N	-5.16	112.47	122.06
2	D	479	GLU	C-N-CA	-5.16	112.47	122.06

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	980	ARG	Sidechain

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	8364	0	8184	150	0
1	B	8295	0	8111	137	0
1	C	8303	0	8124	158	0
2	D	4845	0	4625	83	0
All	All	29807	0	29044	517	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 9.

All (517) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:VAL:O	1:A:123:VAL:HA	1.74	0.86
1:C:1025:LYS:O	1:C:1029:CYS:HB2	1.83	0.78
1:B:90:ALA:HB3	1:B:263:TYR:HB2	1.71	0.72
1:A:1084:ALA:HB3	1:A:1120:SER:O	1.89	0.72
2:D:480:MET:O	2:D:484:ILE:HB	1.90	0.72
2:D:594:TRP:O	2:D:598:GLN:HB2	1.90	0.72
1:C:902:ARG:NH1	1:C:1047:MET:SD	2.64	0.70
2:D:204:ARG:HE	2:D:219:ARG:HB3	1.57	0.69
1:C:882:GLY:HA2	1:C:898:GLN:HE21	1.57	0.68
1:C:22:THR:HG1	1:C:63:HIS:HD1	1.42	0.68
1:B:98:ILE:HA	1:B:239:LEU:HA	1.75	0.67
2:D:480:MET:HA	2:D:483:GLU:HG2	1.77	0.67
1:A:558:PRO:HA	1:A:574:ARG:HH12	1.58	0.67
1:C:122:ASN:HA	1:C:171:PRO:HD3	1.77	0.67
1:B:190:VAL:HG12	1:B:201:TYR:HB2	1.77	0.66
1:C:520:THR:HG23	1:C:521:VAL:HG12	1.76	0.65
1:A:31:ARG:HD2	1:A:214:PRO:HD2	1.79	0.65
1:C:355:ILE:HD13	1:C:392:VAL:HG13	1.79	0.65
1:A:63:HIS:NE2	1:A:260:ALA:O	2.30	0.65
1:C:1047:MET:HE3	1:C:1048:SER:H	1.62	0.64
1:A:380:SER:HG	1:A:382:THR:HG1	1.42	0.64
1:A:728:MET:SD	1:A:771:GLN:NE2	2.71	0.64
1:B:183:PHE:H	1:B:210:GLU:HG3	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:270:MET:SD	2:D:270:MET:N	2.70	0.64
2:D:120:LEU:HA	2:D:123:MET:HE2	1.81	0.63
1:C:425:ASP:OD1	1:C:426:PHE:N	2.30	0.63
1:C:90:ALA:O	1:C:262:TYR:HA	1.99	0.63
1:B:93:GLU:OE2	1:B:187:ARG:NH2	2.32	0.63
2:D:503:LEU:HD23	2:D:505:HIS:H	1.64	0.63
1:B:471:GLN:HB2	1:B:477:CYS:HB2	1.81	0.62
1:A:277:ASN:HD21	1:A:279:ASN:HB2	1.64	0.62
2:D:177:ARG:HH11	2:D:470:LYS:HE2	1.64	0.62
1:C:788:THR:HG21	1:C:803:LEU:HD21	1.81	0.62
1:B:155:ARG:HH22	1:B:243:ARG:HH22	1.45	0.62
1:A:435:SER:HB2	1:A:438:LEU:HB2	1.82	0.62
1:C:1090:GLY:HA3	1:C:1102:THR:O	1.99	0.62
1:C:299:THR:O	1:C:301:LYS:NZ	2.34	0.61
1:A:223:LEU:HG	1:A:224:VAL:HG23	1.81	0.61
1:B:421:LYS:HB2	1:B:458:LEU:HB3	1.83	0.61
1:A:653:VAL:HG22	1:A:655:ASN:H	1.66	0.60
1:C:981:LEU:HB3	1:C:985:GLU:HG3	1.82	0.60
1:A:100:GLY:HA3	1:A:238:LEU:HB2	1.82	0.60
1:C:104:GLY:H	1:C:232:ILE:HG23	1.66	0.60
1:B:223:LEU:HG	1:B:224:VAL:HG23	1.84	0.60
1:C:415:ILE:O	1:C:421:LYS:NZ	2.35	0.60
1:B:21:ARG:HH21	1:B:80:ALA:HB2	1.67	0.59
1:C:352:ARG:HH12	1:C:393:TYR:HB3	1.67	0.59
1:C:403:GLU:HB3	1:C:406:GLN:HG3	1.84	0.59
1:B:947:ASP:N	1:B:947:ASP:OD1	2.32	0.59
1:B:812:ARG:HD2	1:B:816:GLU:HB3	1.84	0.59
1:A:549:LEU:HD12	1:A:582:LEU:HB3	1.85	0.59
1:B:523:GLY:O	1:B:525:LYS:NZ	2.36	0.59
1:A:348:TYR:O	1:A:451:ARG:NH2	2.35	0.59
1:A:1088:ARG:NH2	1:A:1115:ASP:O	2.36	0.59
1:C:347:VAL:HB	1:C:399:ILE:HD11	1.84	0.59
1:C:417:ASP:OD1	1:C:419:ASN:ND2	2.36	0.59
1:B:106:THR:HG21	1:B:110:LYS:HB2	1.83	0.58
1:C:314:ASN:ND2	1:C:590:GLY:O	2.36	0.58
1:A:183:PHE:HB3	1:A:210:GLU:HG3	1.84	0.58
1:B:816:GLU:OE2	1:B:1051:GLN:NE2	2.35	0.58
1:A:43:SER:HA	1:A:276:TYR:O	2.03	0.58
1:B:429:CYS:SG	1:B:430:VAL:N	2.76	0.58
1:B:381:PRO:HA	1:B:384:LEU:HG	1.85	0.58
1:C:140:VAL:O	1:C:243:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:TYR:O	2:D:101:GLN:NE2	2.36	0.58
1:A:174:MET:SD	1:A:175:ASP:N	2.76	0.58
1:C:308:GLY:HA2	1:C:661:ILE:HG23	1.85	0.58
1:C:971:SER:HB3	1:C:977:ILE:HD11	1.86	0.58
1:A:63:HIS:HE2	1:A:260:ALA:H	1.51	0.58
1:B:34:TYR:HB3	1:B:220:LEU:HD23	1.86	0.58
1:C:347:VAL:HG13	1:C:451:ARG:HH21	1.68	0.58
2:D:155:SER:H	2:D:161:ARG:HH21	1.50	0.58
1:A:106:THR:HG21	1:A:110:LYS:HB2	1.86	0.57
1:C:325:ARG:HD2	1:C:576:PRO:HD2	1.85	0.57
1:C:312:THR:HG22	1:C:313:SER:H	1.70	0.57
1:A:119:ASN:ND2	1:A:122:ASN:O	2.38	0.57
1:A:189:PHE:HA	1:A:201:TYR:O	2.05	0.57
1:B:602:SER:OG	1:B:603:ASN:N	2.35	0.57
2:D:460:ARG:NH1	2:D:510:TYR:O	2.36	0.57
1:A:355:ILE:O	1:A:391:ASN:HA	2.05	0.57
1:B:402:ASN:ND2	1:B:501:GLY:O	2.37	0.57
1:C:412:THR:HB	1:C:416:ALA:HB2	1.85	0.57
1:A:353:LYS:HB3	1:A:394:ALA:HB3	1.86	0.56
1:B:353:LYS:O	1:B:393:TYR:HA	2.06	0.56
1:C:26:THR:HG22	1:C:61:TRP:HB2	1.85	0.56
1:A:139:ASP:OD1	1:A:139:ASP:N	2.37	0.56
1:C:435:SER:HB2	1:C:506:ARG:HG3	1.87	0.56
1:A:197:TYR:OH	1:C:391:ASN:ND2	2.38	0.56
2:D:539:LEU:HG	2:D:586:ASN:HB3	1.86	0.56
2:D:510:TYR:HB3	2:D:514:ARG:HH12	1.71	0.56
1:A:313:SER:OG	1:A:314:ASN:N	2.39	0.56
1:A:409:PRO:HG3	1:A:422:LEU:HD11	1.88	0.56
1:B:660:ASP:OD1	1:B:660:ASP:N	2.37	0.56
1:C:325:ARG:HB3	1:C:576:PRO:HG2	1.88	0.55
1:B:14:GLN:HB3	1:B:155:ARG:HD2	1.89	0.55
1:B:20:THR:OG1	1:B:21:ARG:NH1	2.38	0.55
1:C:361:ASP:OD1	1:C:361:ASP:N	2.39	0.55
1:A:391:ASN:ND2	1:A:513:GLU:OE2	2.37	0.55
1:A:485:CYS:SG	1:A:486:TYR:N	2.80	0.55
1:A:1090:GLY:HA3	1:A:1102:THR:O	2.07	0.55
1:C:982:ASP:HB2	1:C:983:PRO:HD2	1.88	0.55
2:D:326:GLY:O	2:D:330:ASN:ND2	2.39	0.55
1:B:115:LEU:HD13	1:B:126:LYS:HE3	1.87	0.55
1:C:103:PHE:HB2	1:C:114:LEU:HB2	1.89	0.55
1:B:103:PHE:HD2	1:B:114:LEU:HB2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:PHE:H	1:B:590:GLY:HA3	1.72	0.55
1:B:571:ASP:OD1	1:B:571:ASP:N	2.37	0.55
1:C:987:GLU:N	1:C:987:GLU:OE1	2.40	0.55
1:B:902:ARG:NH1	1:B:1046:LEU:O	2.40	0.54
1:B:278:GLU:OE2	1:B:279:ASN:ND2	2.41	0.54
1:B:672:GLN:OE1	1:B:687:GLN:N	2.40	0.54
1:A:436:ASN:O	1:A:440:SER:OG	2.26	0.54
1:A:145:ASN:ND2	1:A:151:GLU:O	2.40	0.54
1:A:101:TRP:HB2	1:A:116:ILE:HB	1.89	0.54
1:A:475:LYS:NZ	1:A:476:PRO:O	2.40	0.54
1:C:376:CYS:HB2	1:C:381:PRO:HD3	1.89	0.54
2:D:155:SER:HB3	2:D:161:ARG:HE	1.73	0.54
2:D:511:SER:O	2:D:514:ARG:NH1	2.41	0.53
1:C:730:LYS:NZ	1:C:772:ASP:OD2	2.39	0.53
1:C:983:PRO:O	1:C:984:PRO:C	2.49	0.53
1:A:122:ASN:ND2	1:A:169:SER:O	2.42	0.53
1:A:203:LYS:HB2	1:A:220:LEU:HD13	1.90	0.53
1:C:439:ASP:HB3	1:C:504:PRO:HG2	1.90	0.53
2:D:238:GLU:HG2	2:D:605:GLY:HA2	1.90	0.53
1:A:76:PHE:N	1:A:256:THR:O	2.41	0.53
1:A:334:PRO:HD2	1:A:355:ILE:HG23	1.90	0.53
1:C:100:GLY:HA3	1:C:238:LEU:HB2	1.91	0.53
1:C:325:ARG:NH1	1:C:528:THR:O	2.41	0.53
2:D:477:TRP:HA	2:D:480:MET:SD	2.48	0.53
1:A:150:MET:SD	1:A:151:GLU:N	2.82	0.53
1:C:554:LYS:NZ	1:C:571:ASP:OD2	2.41	0.53
1:C:375:LYS:HB3	1:C:430:VAL:HB	1.91	0.53
1:A:770:GLU:OE2	1:A:1016:ARG:NH1	2.42	0.53
1:C:54:PRO:HB2	1:C:57:SER:HB2	1.91	0.53
1:B:441:LYS:NZ	1:B:445:ASN:OD1	2.37	0.53
2:D:171:GLU:O	2:D:175:GLN:NE2	2.41	0.53
1:B:325:ARG:HH21	1:B:530:LEU:HD22	1.74	0.52
1:B:730:LYS:NZ	1:B:772:ASP:OD2	2.42	0.52
1:C:103:PHE:HD1	1:C:235:PHE:HB2	1.74	0.52
1:C:270:ARG:NH2	1:C:287:ASP:OD2	2.41	0.52
2:D:201:ASP:OD1	2:D:219:ARG:NE	2.41	0.52
1:A:90:ALA:HB3	1:A:263:TYR:HB2	1.91	0.52
1:A:138:LEU:HD12	1:A:240:ALA:HB2	1.91	0.52
1:B:407:ILE:HA	1:B:422:LEU:HD11	1.92	0.52
1:C:22:THR:OG1	1:C:63:HIS:ND1	2.31	0.52
1:C:555:LYS:NZ	1:C:556:PHE:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:866:MET:SD	1:C:866:MET:N	2.73	0.52
1:A:571:ASP:OD1	1:A:571:ASP:N	2.41	0.52
1:B:203:LYS:HG3	1:B:205:THR:HG23	1.90	0.52
1:C:324:VAL:HB	1:C:527:SER:HA	1.92	0.52
1:A:971:SER:OG	1:A:972:SER:N	2.39	0.52
1:B:415:ILE:HA	1:B:419:ASN:HB2	1.91	0.52
1:B:445:ASN:N	1:B:493:GLY:O	2.43	0.52
1:A:358:CYS:H	1:A:521:VAL:HG22	1.74	0.52
1:C:302:SER:OG	1:C:303:PHE:N	2.41	0.52
2:D:107:VAL:HB	2:D:193:ALA:HB1	1.92	0.52
1:B:1089:GLU:OE2	1:B:1104:ARG:NH2	2.42	0.52
1:C:138:LEU:HD12	1:C:240:ALA:HB2	1.91	0.52
1:C:351:ASN:ND2	1:C:394:ALA:O	2.43	0.52
2:D:407:ILE:HG23	2:D:522:GLN:HB2	1.91	0.52
1:A:143:GLN:HB3	1:A:242:HIS:HB3	1.92	0.52
1:C:313:SER:OG	1:C:314:ASN:N	2.43	0.52
1:A:354:ARG:HG3	1:A:391:ASN:HB3	1.92	0.52
1:B:653:VAL:HG23	1:B:655:ASN:H	1.75	0.52
1:C:775:THR:HA	1:C:778:VAL:HG12	1.92	0.52
2:D:45:LEU:O	2:D:49:ASN:ND2	2.43	0.52
2:D:284:PRO:HG3	2:D:440:LEU:HD13	1.91	0.52
1:A:196:GLY:O	1:C:354:ARG:NH2	2.43	0.51
1:A:440:SER:HB3	1:A:504:PRO:HG3	1.92	0.51
1:C:187:ARG:HD2	1:C:204:HIS:HD2	1.74	0.51
1:C:983:PRO:HB2	1:C:984:PRO:HD3	1.91	0.51
1:B:355:ILE:HB	1:B:392:VAL:HB	1.92	0.51
2:D:475:LYS:HA	2:D:478:TRP:HD1	1.74	0.51
1:A:341:ALA:O	1:A:506:ARG:NH1	2.39	0.51
1:C:31:ARG:NH2	1:C:214:PRO:O	2.43	0.51
1:B:427:THR:OG1	1:B:512:PHE:O	2.29	0.51
1:A:94:LYS:HA	1:A:187:ARG:HH22	1.76	0.51
1:C:340:ASN:HB3	1:C:368:PHE:HZ	1.73	0.51
1:C:84:ASN:N	1:C:84:ASN:OD1	2.43	0.51
1:B:498:TYR:O	1:B:503:GLN:NE2	2.43	0.51
2:D:157:ASP:HB2	2:D:160:GLU:HB3	1.93	0.51
1:A:122:ASN:HA	1:A:171:PRO:HD3	1.92	0.51
1:B:54:PRO:HB3	1:B:270:ARG:HH12	1.76	0.51
1:C:602:SER:OG	1:C:603:ASN:N	2.44	0.51
1:A:523:GLY:O	1:A:525:LYS:NZ	2.44	0.51
1:A:971:SER:HB3	1:A:977:ILE:HD11	1.92	0.51
1:B:967:PHE:HB2	1:B:993:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:287:GLN:NE2	2:D:433:GLU:OE1	2.42	0.51
1:A:602:SER:OG	1:A:603:ASN:N	2.43	0.50
1:A:1124:ASP:OD1	1:A:1124:ASP:N	2.44	0.50
1:C:402:ASN:ND2	1:C:501:GLY:O	2.38	0.50
1:C:638:ASN:HD22	1:C:651:GLU:HA	1.76	0.50
1:A:808:LYS:HZ3	1:A:809:PRO:HD2	1.77	0.50
2:D:177:ARG:HH22	2:D:473:TRP:HE3	1.59	0.50
2:D:515:TYR:HB3	2:D:518:ARG:HH21	1.77	0.50
1:B:115:LEU:HD13	1:B:126:LYS:HG2	1.94	0.50
1:B:234:ARG:HB3	1:B:236:GLN:HE22	1.77	0.50
1:C:400:ARG:HA	1:C:504:PRO:HA	1.93	0.50
1:C:430:VAL:HA	1:C:509:VAL:HG12	1.94	0.50
1:C:452:LEU:HB2	1:C:488:PRO:HA	1.94	0.50
1:C:66:HIS:O	1:C:74:LYS:N	2.45	0.50
1:B:102:ILE:HB	1:B:236:GLN:HB2	1.94	0.50
1:B:380:SER:HG	1:B:382:THR:HG1	1.60	0.50
1:B:475:LYS:NZ	1:B:476:PRO:O	2.42	0.50
1:B:428:GLY:HA3	1:B:510:LEU:O	2.12	0.50
2:D:153:ALA:O	2:D:161:ARG:NH2	2.45	0.50
1:A:527:SER:OG	1:A:528:THR:N	2.44	0.50
1:A:1027:SER:OG	1:C:1038:ASP:OD2	2.28	0.49
1:A:1028:GLU:OE2	1:C:1036:ARG:NE	2.45	0.49
1:B:313:SER:OG	1:B:314:ASN:N	2.45	0.49
1:C:986:ALA:O	1:C:987:GLU:C	2.55	0.49
1:B:630:TRP:HE1	1:B:631:ARG:HH21	1.60	0.49
1:A:670:SER:OG	1:A:671:TYR:N	2.43	0.49
1:B:131:GLN:H	1:B:160:ALA:HB3	1.78	0.49
1:B:486:TYR:OH	2:D:83:TYR:OH	2.29	0.49
1:A:759:GLN:OE1	1:A:762:ARG:NH2	2.41	0.49
1:B:449:LEU:HD12	1:B:489:LEU:HB3	1.95	0.49
1:C:911:ASN:N	1:C:911:ASN:OD1	2.46	0.49
2:D:468:ILE:HD12	2:D:473:TRP:HE1	1.77	0.49
1:B:61:TRP:HE1	1:B:261:ALA:HA	1.76	0.49
1:B:400:ARG:HE	1:B:402:ASN:HD21	1.60	0.49
1:C:980:ARG:O	1:C:981:LEU:C	2.54	0.49
1:A:722:GLU:OE2	1:A:1025:LYS:NZ	2.45	0.49
1:B:325:ARG:HB2	1:B:540:PHE:HA	1.95	0.49
1:B:359:VAL:HB	1:B:524:PRO:HD3	1.95	0.49
1:A:94:LYS:HD3	1:A:187:ARG:HH12	1.78	0.49
1:A:430:VAL:HG22	1:A:509:VAL:HG13	1.94	0.49
1:A:434:ASN:ND2	1:A:503:GLN:OE1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:THR:OG1	1:A:1075:ALA:N	2.46	0.49
1:C:601:THR:OG1	1:C:602:SER:N	2.46	0.49
1:A:528:THR:OG1	1:A:529:ASN:N	2.45	0.48
1:C:965:SER:OG	1:C:966:LYS:N	2.46	0.48
1:C:1007:GLN:HE22	1:C:1011:ARG:HE	1.61	0.48
1:C:1080:HIS:O	1:C:1083:LYS:HB2	2.12	0.48
2:D:339:VAL:HG23	2:D:340:GLN:HG2	1.95	0.48
1:A:144:LYS:NZ	1:A:146:ASN:O	2.38	0.48
1:A:381:PRO:HA	1:A:384:LEU:HB2	1.95	0.48
1:C:398:VAL:HG13	1:C:506:ARG:HG2	1.94	0.48
1:C:635:THR:OG1	1:C:636:GLY:N	2.46	0.48
2:D:216:ASP:OD1	2:D:216:ASP:N	2.43	0.48
1:A:112:GLN:HB3	1:A:230:ILE:HG23	1.94	0.48
1:A:430:VAL:HG13	1:A:509:VAL:HG22	1.95	0.48
1:C:114:LEU:HD12	1:C:116:ILE:HD11	1.96	0.48
1:B:149:TRP:O	1:B:151:GLU:N	2.47	0.48
1:C:125:ILE:HB	1:C:167:TYR:HB3	1.93	0.48
2:D:48:TRP:HZ3	2:D:359:LEU:HB2	1.78	0.48
2:D:198:ASP:H	2:D:201:ASP:HB3	1.78	0.48
1:B:173:LEU:HD13	1:B:176:LEU:HD12	1.95	0.48
1:C:346:SER:OG	1:C:347:VAL:N	2.45	0.48
1:C:1124:ASP:OD1	1:C:1124:ASP:N	2.45	0.48
2:D:47:SER:O	2:D:51:ASN:ND2	2.46	0.48
1:B:595:ILE:HD13	1:B:663:ILE:HD11	1.96	0.48
1:A:933:ASP:O	1:A:937:SER:OG	2.24	0.48
1:A:962:GLN:O	1:A:965:SER:OG	2.31	0.48
1:C:877:GLY:O	1:C:881:SER:OG	2.32	0.48
2:D:291:ILE:HD13	2:D:415:PRO:HG3	1.96	0.48
1:C:388:CYS:HA	1:C:522:CYS:HB3	1.96	0.48
1:A:105:THR:OG1	1:A:231:ASN:O	2.32	0.48
1:A:529:ASN:N	1:A:529:ASN:OD1	2.47	0.48
1:A:964:SER:O	1:A:964:SER:OG	2.27	0.48
1:B:30:THR:O	1:B:31:ARG:NH1	2.39	0.48
1:C:596:THR:HB	1:C:605:VAL:HG12	1.94	0.48
2:D:54:ILE:HB	2:D:341:LYS:HB2	1.96	0.48
1:A:140:VAL:HG22	1:A:251:SER:HB3	1.96	0.47
1:A:399:ILE:HD13	1:A:407:ILE:HD11	1.95	0.47
1:B:112:GLN:NE2	1:B:129:GLU:OE2	2.47	0.47
1:C:117:VAL:HG12	1:C:119:ASN:HD22	1.79	0.47
1:C:785:ILE:HG13	1:C:873:ALA:HB2	1.96	0.47
1:A:336:HIS:HA	1:A:339:PHE:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:297:MET:O	2:D:301:ALA:N	2.46	0.47
1:B:980:ARG:HG3	1:B:981:LEU:HG	1.96	0.47
1:C:960:VAL:O	1:C:963:LEU:HB2	2.14	0.47
2:D:460:ARG:HE	2:D:464:PHE:HE2	1.61	0.47
1:A:372:PHE:HZ	1:A:434:ASN:HB2	1.79	0.47
1:A:719:VAL:HG12	1:A:1062:VAL:HG22	1.96	0.47
1:B:801:GLN:NE2	1:B:932:GLN:OE1	2.39	0.47
1:B:200:ILE:HB	1:B:224:VAL:HB	1.96	0.47
2:D:99:ALA:HB3	2:D:391:LEU:HD21	1.97	0.47
2:D:313:LYS:O	2:D:317:SER:OG	2.30	0.47
1:A:739:ILE:O	1:A:997:ARG:NH1	2.48	0.47
1:B:459:LYS:HB2	1:B:462:GLU:HB2	1.97	0.47
2:D:555:PHE:HA	2:D:558:LEU:HB2	1.97	0.47
1:B:27:ASN:OD1	1:B:58:ASN:ND2	2.46	0.47
1:B:66:HIS:HB3	1:B:260:ALA:HA	1.96	0.47
2:D:494:ASP:OD1	2:D:496:THR:OG1	2.29	0.47
1:A:380:SER:H	1:A:383:LYS:HE3	1.80	0.47
1:C:333:CYS:HA	1:C:358:CYS:HB2	1.96	0.47
1:C:414:ASN:O	1:C:419:ASN:ND2	2.44	0.47
1:B:131:GLN:OE1	1:B:159:SER:OG	2.34	0.46
1:B:1122:ASN:OD1	1:B:1122:ASN:N	2.48	0.46
1:C:24:SER:OG	1:C:25:TYR:N	2.48	0.46
1:C:51:LEU:HG	1:C:267:LEU:HB3	1.97	0.46
1:A:715:PHE:HE2	1:A:920:ILE:HD11	1.79	0.46
1:C:121:THR:OG1	1:C:122:ASN:N	2.49	0.46
1:C:409:PRO:HD3	1:C:422:LEU:HD11	1.97	0.46
2:D:553:LYS:HA	2:D:556:ASN:HD22	1.79	0.46
1:A:127:VAL:HG11	1:A:228:ILE:HG21	1.97	0.46
1:A:325:ARG:NH2	1:A:528:THR:O	2.49	0.46
1:B:173:LEU:HD23	1:B:173:LEU:HA	1.80	0.46
2:D:247:LYS:NZ	2:D:283:VAL:O	2.43	0.46
2:D:560:LEU:O	2:D:563:SER:OG	2.33	0.46
1:A:324:VAL:HG23	1:A:539:ASN:HB3	1.95	0.46
1:A:656:SER:HB3	1:A:695:SER:HB3	1.97	0.46
1:B:736:THR:HA	1:B:739:ILE:HG22	1.97	0.46
1:B:790:PRO:HG2	1:B:791:ILE:HD12	1.96	0.46
1:A:347:VAL:HG22	1:A:419:ASN:HB3	1.98	0.46
1:C:123:VAL:HB	1:C:171:PRO:HA	1.98	0.46
1:A:21:ARG:HG3	1:A:77:ASP:HA	1.98	0.46
1:A:575:ASP:OD2	1:A:578:THR:N	2.43	0.46
1:B:1087:PRO:HA	1:B:1117:THR:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:VAL:HG22	1:C:201:TYR:HB2	1.98	0.46
1:C:342:THR:OG1	1:C:343:THR:N	2.48	0.46
1:C:534:LYS:HD2	1:C:534:LYS:HA	1.81	0.46
1:B:135:ASP:N	1:B:135:ASP:OD1	2.49	0.46
1:C:963:LEU:O	1:C:997:ARG:NH2	2.46	0.46
1:C:1029:CYS:O	1:C:1048:SER:OG	2.34	0.46
2:D:309:LYS:HA	2:D:309:LYS:HD3	1.78	0.46
1:B:203:LYS:HD2	1:B:203:LYS:HA	1.67	0.46
1:A:330:THR:O	1:A:330:THR:OG1	2.34	0.45
1:B:243:ARG:HE	1:B:255:TRP:HZ2	1.64	0.45
1:B:287:ASP:OD1	1:B:288:CYS:N	2.49	0.45
1:B:481:ALA:HB3	1:B:485:CYS:HB2	1.97	0.45
1:C:183:PHE:HB2	1:C:210:GLU:HG3	1.96	0.45
2:D:20:THR:HG23	2:D:22:GLU:H	1.80	0.45
1:A:282:ILE:HD13	1:A:282:ILE:HA	1.84	0.45
1:A:361:ASP:H	1:A:524:PRO:HD3	1.81	0.45
1:C:597:PRO:HG3	1:C:671:TYR:HD2	1.81	0.45
1:A:1111:ILE:HD12	1:A:1111:ILE:HA	1.82	0.45
1:C:105:THR:OG1	1:C:231:ASN:O	2.34	0.45
1:A:19:ILE:O	1:A:78:ASN:ND2	2.34	0.45
1:A:241:LEU:HD22	1:A:255:TRP:HH2	1.82	0.45
1:A:451:ARG:HH12	1:A:464:ASP:HB3	1.80	0.45
1:C:431:ILE:HB	1:C:508:VAL:HG23	1.98	0.45
1:A:390:THR:O	1:A:520:THR:OG1	2.31	0.45
1:A:467:THR:O	1:A:467:THR:OG1	2.35	0.45
1:A:822:LYS:NZ	1:A:935:LEU:O	2.50	0.45
1:C:125:ILE:HD13	1:C:167:TYR:HD2	1.81	0.45
1:C:450:TYR:HD2	1:C:492:TYR:HE1	1.64	0.45
1:A:63:HIS:ND1	1:A:77:ASP:OD1	2.50	0.45
1:B:19:ILE:HG22	1:B:20:THR:H	1.81	0.45
2:D:168:TRP:HD1	2:D:169:ARG:HH11	1.64	0.45
2:D:346:PRO:HA	2:D:359:LEU:O	2.16	0.45
1:A:18:LEU:HG	1:A:78:ASN:HD21	1.82	0.45
1:A:728:MET:N	1:A:771:GLN:OE1	2.46	0.45
1:B:406:GLN:HB3	1:B:416:ALA:HB2	1.99	0.45
1:A:207:ILE:HD12	1:A:214:PRO:HG3	1.99	0.44
1:A:419:ASN:HA	1:A:454:ARG:HH21	1.82	0.44
1:A:1036:ARG:NE	1:B:1028:GLU:OE2	2.49	0.44
1:B:980:ARG:HE	1:B:981:LEU:H	1.65	0.44
1:C:440:SER:HA	1:C:494:PHE:HE2	1.82	0.44
1:C:1097:THR:OG1	1:C:1098:HIS:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:245:ARG:HH22	2:D:603:PHE:HB3	1.81	0.44
1:A:962:GLN:OE1	1:B:755:SER:OG	2.35	0.44
1:B:436:ASN:HA	1:B:504:PRO:HG2	1.99	0.44
2:D:293:VAL:HG21	2:D:423:LEU:HD13	1.99	0.44
1:A:402:ASN:N	1:A:501:GLY:O	2.50	0.44
1:B:1104:ARG:HD3	1:C:901:TYR:CZ	2.52	0.44
1:C:97:ILE:HG22	1:C:239:LEU:HD12	2.00	0.44
1:C:961:LYS:HB2	1:C:961:LYS:HE2	1.74	0.44
2:D:68:LYS:HA	2:D:68:LYS:HD3	1.70	0.44
1:A:526:LYS:HD2	1:A:526:LYS:HA	1.73	0.44
1:C:726:VAL:HG11	1:C:778:VAL:HG11	1.98	0.44
1:A:528:THR:OG1	1:A:529:ASN:OD1	2.36	0.44
1:A:586:PRO:HD2	1:B:852:PHE:HD2	1.82	0.44
1:B:451:ARG:HH21	1:B:454:ARG:HA	1.81	0.44
1:B:1040:CYS:HB2	1:B:1045:HIS:CD2	2.53	0.44
1:C:614:CYS:O	1:C:630:TRP:N	2.50	0.44
2:D:223:ILE:HG12	2:D:461:TRP:CZ3	2.52	0.44
2:D:520:LEU:HD13	2:D:579:MET:HG2	2.00	0.44
1:C:525:LYS:HA	1:C:525:LYS:HD3	1.68	0.44
1:C:920:ILE:HD13	1:C:920:ILE:HA	1.91	0.44
2:D:293:VAL:O	2:D:297:MET:N	2.46	0.44
2:D:538:PRO:HG2	2:D:541:LYS:HB3	1.99	0.44
1:B:783:LYS:HD2	1:B:783:LYS:HA	1.77	0.44
1:A:38:LYS:HE2	1:A:38:LYS:HB2	1.71	0.44
2:D:287:GLN:H	2:D:287:GLN:HG3	1.64	0.44
1:A:23:GLN:HB3	1:A:62:PHE:HA	1.99	0.43
1:A:97:ILE:HG22	1:A:239:LEU:HD11	2.00	0.43
1:B:97:ILE:O	1:B:240:ALA:N	2.51	0.43
1:B:114:LEU:HD21	1:B:230:ILE:HG21	2.00	0.43
1:B:934:SER:O	1:B:937:SER:OG	2.35	0.43
2:D:457:GLU:OE1	2:D:513:ILE:N	2.51	0.43
1:A:310:TYR:O	1:A:593:SER:OG	2.32	0.43
1:A:1104:ARG:HD3	1:B:901:TYR:CZ	2.53	0.43
1:B:334:PRO:HB2	1:B:337:GLU:HB2	1.99	0.43
1:B:563:GLY:HA3	1:B:572:ALA:HB3	2.00	0.43
1:B:614:CYS:HA	1:B:630:TRP:HB3	1.99	0.43
1:C:517:ALA:HB2	1:C:562:PHE:HD2	1.83	0.43
1:C:981:LEU:HB3	1:C:985:GLU:CG	2.47	0.43
1:A:103:PHE:HB3	1:A:232:ILE:HG21	2.01	0.43
1:A:928:ILE:HD13	1:A:928:ILE:HA	1.89	0.43
1:B:163:CYS:SG	1:B:164:THR:N	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:ARG:HH22	1:C:530:LEU:H	1.65	0.43
1:C:719:VAL:HG22	1:C:927:ALA:HB1	1.99	0.43
2:D:291:ILE:HG21	2:D:415:PRO:HG3	2.01	0.43
1:A:50:ASP:OD1	1:A:192:LYS:NZ	2.51	0.43
1:B:140:VAL:HG23	1:B:245:TYR:HA	2.01	0.43
1:A:537:ASN:OD1	1:A:537:ASN:N	2.51	0.43
1:C:127:VAL:HG11	1:C:228:ILE:HD12	2.01	0.43
1:C:739:ILE:HG23	1:C:994:ILE:HD12	2.00	0.43
1:A:88:TYR:OH	1:A:188:GLU:OE1	2.32	0.43
1:B:201:TYR:CZ	1:B:222:PRO:HB3	2.54	0.43
1:B:719:VAL:HG12	1:B:1062:VAL:HG22	2.00	0.43
1:B:86:GLY:CA	1:B:191:PHE:O	2.67	0.43
1:B:722:GLU:OE2	1:B:1061:HIS:NE2	2.51	0.43
1:C:207:ILE:HG21	1:C:214:PRO:HG3	2.00	0.43
1:C:418:TYR:HB2	1:C:454:ARG:HB3	2.00	0.43
1:A:117:VAL:HG12	1:A:119:ASN:HD22	1.84	0.43
1:A:296:THR:HA	1:A:299:THR:HG22	2.01	0.43
1:A:374:PHE:HD1	1:A:431:ILE:HG12	1.84	0.43
1:B:419:ASN:HA	1:B:454:ARG:HH21	1.84	0.43
1:C:365:ILE:HD12	1:C:365:ILE:HA	1.85	0.43
1:C:935:LEU:HD23	1:C:935:LEU:HA	1.86	0.43
1:A:393:TYR:HB2	1:A:511:SER:HB2	2.01	0.42
1:B:597:PRO:HD3	1:B:689:ILE:HD11	2.00	0.42
1:B:1083:LYS:HA	1:B:1083:LYS:HD2	1.82	0.42
2:D:88:ILE:HB	2:D:94:LYS:HG3	2.01	0.42
2:D:418:LEU:O	2:D:423:LEU:N	2.52	0.42
2:D:469:PRO:HD2	2:D:472:GLN:HG2	2.01	0.42
2:D:556:ASN:OD1	2:D:559:ARG:NH2	2.52	0.42
1:A:43:SER:CA	1:A:276:TYR:O	2.66	0.42
1:B:173:LEU:HD21	1:B:187:ARG:HD3	2.01	0.42
1:B:427:THR:OG1	1:B:427:THR:O	2.33	0.42
1:C:83:PHE:N	1:C:233:THR:O	2.51	0.42
1:C:964:SER:O	1:C:964:SER:OG	2.30	0.42
2:D:484:ILE:HD13	2:D:484:ILE:HA	1.89	0.42
1:A:727:SER:OG	1:A:728:MET:N	2.53	0.42
1:C:700:ASN:OD1	1:C:701:SER:N	2.52	0.42
1:B:213:LEU:HD12	1:B:214:PRO:HD2	2.01	0.42
1:C:959:LEU:HD12	1:C:959:LEU:HA	1.86	0.42
2:D:169:ARG:HE	2:D:499:ASP:HB3	1.84	0.42
1:A:124:VAL:HG12	1:A:126:LYS:HG2	2.02	0.42
1:B:117:VAL:HG12	1:B:119:ASN:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LYS:HE2	1:B:199:LYS:HB2	2.02	0.42
1:C:211:ARG:HD2	1:C:211:ARG:HA	1.95	0.42
1:A:239:LEU:HD12	1:A:240:ALA:H	1.85	0.42
1:A:398:VAL:HA	1:A:505:TYR:O	2.19	0.42
1:C:443:SER:O	1:C:443:SER:OG	2.38	0.42
2:D:189:GLU:HG2	2:D:192:ARG:HH22	1.84	0.42
1:A:421:LYS:HA	1:A:421:LYS:HD3	1.77	0.42
1:C:434:ASN:OD1	1:C:434:ASN:N	2.52	0.42
1:C:706:ASN:OD1	1:C:706:ASN:N	2.43	0.42
1:C:739:ILE:HG21	1:C:750:LEU:HD13	2.02	0.42
2:D:115:ARG:NH1	2:D:118:THR:OG1	2.52	0.42
1:C:712:PRO:HA	1:C:1069:GLU:HA	2.00	0.42
2:D:515:TYR:HA	2:D:518:ARG:HE	1.85	0.42
1:B:1074:THR:OG1	1:B:1075:ALA:N	2.53	0.42
1:C:1046:LEU:HD23	1:C:1046:LEU:HA	1.89	0.42
1:A:1026:MET:HE2	1:A:1026:MET:HB2	1.97	0.41
1:B:176:LEU:HD23	1:B:176:LEU:HA	1.94	0.41
1:B:416:ALA:O	1:B:421:LYS:NZ	2.46	0.41
1:C:291:ASP:O	1:C:294:SER:OG	2.29	0.41
1:C:1122:ASN:OD1	1:C:1122:ASN:N	2.51	0.41
1:C:273:LEU:HD13	1:C:273:LEU:HA	1.95	0.41
2:D:171:GLU:H	2:D:171:GLU:HG3	1.66	0.41
1:A:350:TRP:HZ3	1:A:352:ARG:HD3	1.85	0.41
1:A:25:TYR:HA	1:A:60:THR:HA	2.02	0.41
1:A:719:VAL:HG22	1:A:927:ALA:HB1	2.01	0.41
2:D:144:LEU:HA	2:D:148:LEU:HD12	2.02	0.41
2:D:293:VAL:HB	2:D:423:LEU:HD22	2.02	0.41
2:D:439:LEU:HB3	2:D:591:LEU:HB2	2.01	0.41
1:A:21:ARG:NH1	1:A:76:PHE:O	2.47	0.41
1:A:1132:ASN:OD1	1:A:1133:THR:N	2.53	0.41
1:B:393:TYR:HE2	1:B:513:GLU:HG2	1.86	0.41
1:B:465:ILE:HD12	1:B:465:ILE:HA	1.93	0.41
1:C:443:SER:H	1:C:495:ARG:HG3	1.85	0.41
1:A:32:GLY:HA3	1:A:53:LEU:HD23	2.03	0.41
1:A:395:ASP:OD2	1:A:420:TYR:OH	2.31	0.41
1:B:446:TYR:OH	1:B:495:ARG:NH2	2.53	0.41
1:C:14:GLN:N	1:C:158:SER:HG	2.19	0.41
2:D:242:ALA:HB2	2:D:604:VAL:HA	2.02	0.41
1:A:319:PRO:HA	1:A:535:CYS:HB3	2.03	0.41
1:A:412:THR:OG1	1:A:413:GLY:N	2.54	0.41
1:A:791:ILE:H	1:A:791:ILE:HG13	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:ASP:OD2	1:C:578:THR:N	2.46	0.41
1:C:608:LEU:HD12	1:C:647:LEU:HD12	2.01	0.41
2:D:557:MET:HA	2:D:560:LEU:HG	2.02	0.41
1:B:183:PHE:HB2	1:B:210:GLU:HA	2.02	0.41
1:B:451:ARG:HE	1:B:454:ARG:HG2	1.86	0.41
1:B:943:GLY:HA2	1:B:946:GLN:HB2	2.03	0.41
1:C:150:MET:HE2	1:C:150:MET:N	2.36	0.41
1:C:803:LEU:HD12	1:C:803:LEU:HA	1.90	0.41
1:A:630:TRP:CD1	1:A:631:ARG:HG2	2.56	0.41
1:B:119:ASN:ND2	1:B:122:ASN:O	2.53	0.41
1:B:325:ARG:HA	1:B:325:ARG:HD3	1.80	0.41
1:B:387:LEU:HA	1:B:387:LEU:HD23	1.86	0.41
1:B:574:ARG:HH11	1:B:579:LEU:HD12	1.86	0.41
1:C:805:ASP:HA	1:C:806:PRO:HD3	1.96	0.41
1:C:931:ILE:HD12	1:C:931:ILE:HA	1.83	0.41
2:D:172:VAL:O	2:D:176:LEU:HB2	2.21	0.41
2:D:236:LEU:HD12	2:D:236:LEU:H	1.85	0.41
2:D:366:MET:O	2:D:366:MET:HE3	2.21	0.41
1:C:390:THR:OG1	1:C:513:GLU:OE2	2.35	0.41
1:A:557:LEU:HD12	1:A:558:PRO:HD2	2.03	0.40
1:B:928:ILE:HD12	1:B:928:ILE:HA	1.94	0.40
1:C:422:LEU:HD12	1:C:426:PHE:CG	2.56	0.40
1:C:653:VAL:HG22	1:C:655:ASN:H	1.86	0.40
2:D:112:LYS:HE3	2:D:186:LEU:HD22	2.02	0.40
1:A:43:SER:N	1:A:277:ASN:O	2.53	0.40
1:A:323:ILE:O	1:A:538:PHE:HA	2.21	0.40
1:A:1010:ILE:HD13	1:A:1010:ILE:HA	1.91	0.40
1:B:116:ILE:HA	1:B:124:VAL:O	2.21	0.40
1:B:945:LEU:O	1:B:948:VAL:HB	2.20	0.40
1:C:862:LEU:HD12	1:C:862:LEU:HA	1.86	0.40
1:B:539:ASN:ND2	1:B:541:ASN:O	2.54	0.40
1:B:977:ILE:HD12	1:B:980:ARG:HB3	2.03	0.40
2:D:453:THR:HG23	2:D:512:PHE:HD1	1.85	0.40
2:D:552:GLN:O	2:D:556:ASN:ND2	2.55	0.40
1:B:300:LEU:HD12	1:B:300:LEU:HA	1.94	0.40
1:B:702:VAL:HG11	1:C:880:THR:HG21	2.02	0.40
1:B:760:LEU:HD13	1:B:1005:VAL:HG21	2.03	0.40
1:C:185:ASN:OD1	1:C:185:ASN:N	2.54	0.40
1:C:557:LEU:HD12	1:C:557:LEU:HA	1.99	0.40
1:C:560:GLN:O	1:C:574:ARG:NH2	2.53	0.40
1:B:18:LEU:O	1:B:134:ASN:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:959:LEU:HD12	1:B:959:LEU:HA	1.80	0.40
1:C:749:LEU:HD13	1:C:990:ILE:HG21	2.04	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	1055/1318 (80%)	956 (91%)	98 (9%)	1 (0%)	48	80
1	B	1047/1318 (79%)	959 (92%)	88 (8%)	0	100	100
1	C	1048/1318 (80%)	942 (90%)	103 (10%)	3 (0%)	36	69
2	D	592/594 (100%)	565 (95%)	27 (5%)	0	100	100
All	All	3742/4548 (82%)	3422 (91%)	316 (8%)	4 (0%)	49	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	C	980	ARG
1	C	151	GLU
1	C	251	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	935/1140 (82%)	931 (100%)	4 (0%)	84	83
1	B	927/1140 (81%)	924 (100%)	3 (0%)	86	85
1	C	928/1140 (81%)	925 (100%)	3 (0%)	86	85
2	D	525/525 (100%)	524 (100%)	1 (0%)	87	87
All	All	3315/3945 (84%)	3304 (100%)	11 (0%)	84	85

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	THR
1	A	492	TYR
1	A	988	VAL
1	A	1074	THR
1	B	543	LEU
1	B	756	PHE
1	B	1134	VAL
1	C	335	PHE
1	C	604	GLN
1	C	648	ILE
2	D	266	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	119	ASN
1	A	122	ASN
1	A	402	ASN
1	A	411	GLN
1	A	561	GLN
1	A	910	GLN
1	A	946	GLN
1	A	957	ASN
1	A	1033	GLN
1	A	1051	GLN
1	B	122	ASN
1	B	182	ASN
1	B	193	ASN
1	B	268	GLN
1	B	560	GLN

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Mol	Chain	Res	Type
1	B	603	ASN
1	B	748	ASN
1	B	952	ASN
1	B	957	ASN
1	B	989	GLN
1	B	999	GLN
1	B	1002	GLN
1	C	112	GLN
1	C	268	GLN
1	C	277	ASN
1	C	367	ASN
1	C	419	ASN
1	C	445	ASN
1	C	471	GLN
1	C	478	ASN
1	C	484	ASN
1	C	490	GLN
1	C	600	ASN
1	C	638	ASN
1	C	752	GLN
1	C	853	ASN
1	C	898	GLN
1	C	989	GLN
1	C	999	GLN
1	C	1055	HIS
2	D	60	GLN
2	D	397	ASN
2	D	472	GLN
2	D	508	ASN
2	D	524	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

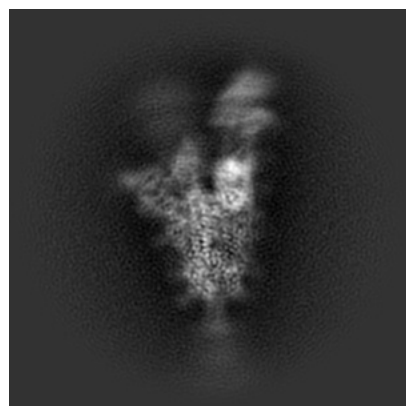
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37784. These allow visual inspection of the internal detail of the map and identification of artifacts.

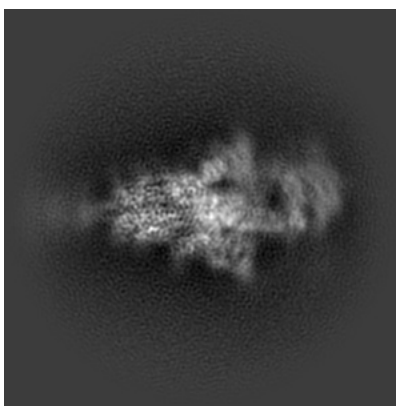
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

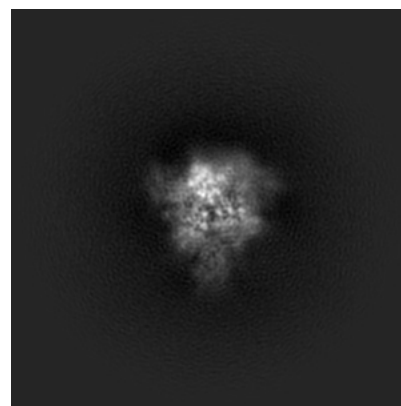
6.1.1 Primary map



X

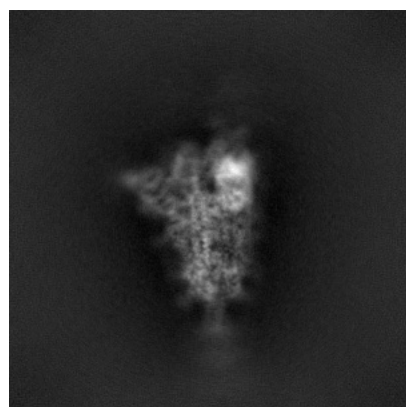


Y

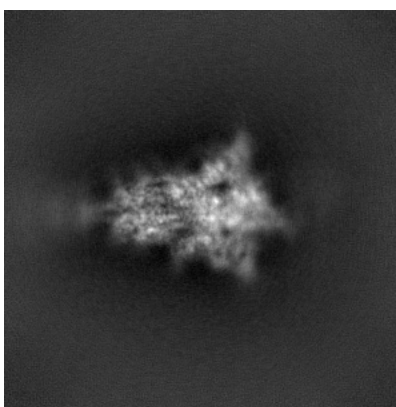


Z

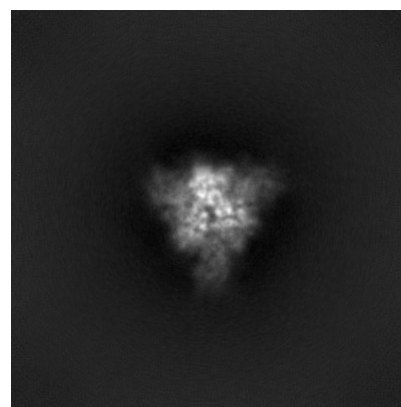
6.1.2 Raw map



X



Y



Z

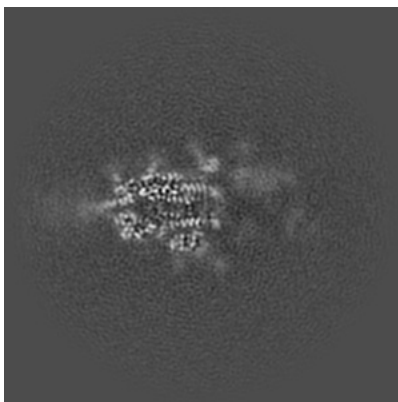
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

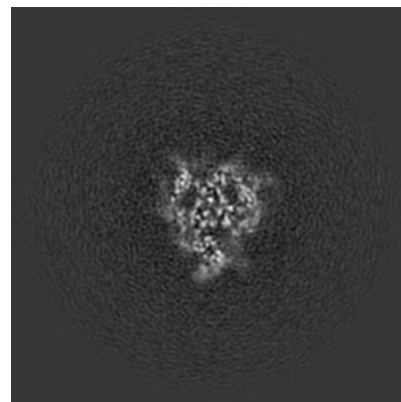
6.2.1 Primary map



X Index: 180

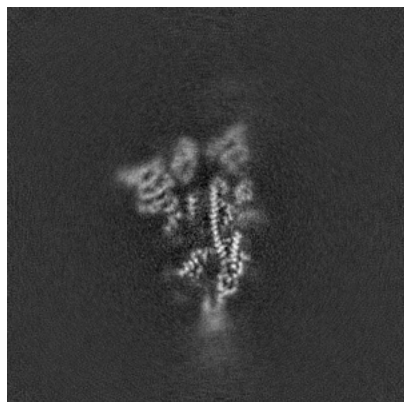


Y Index: 180

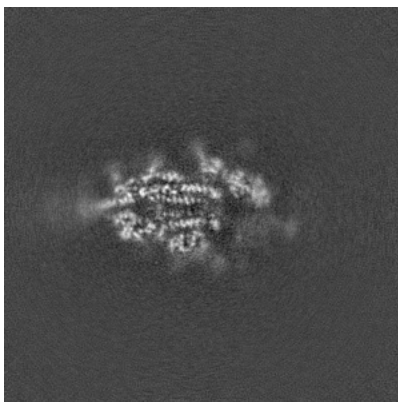


Z Index: 180

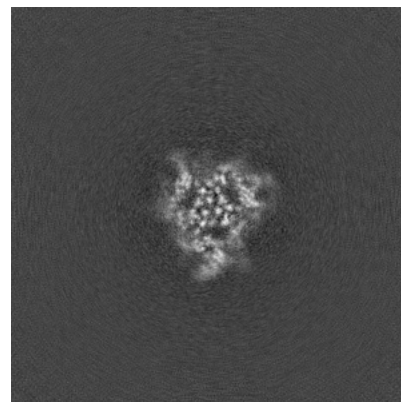
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

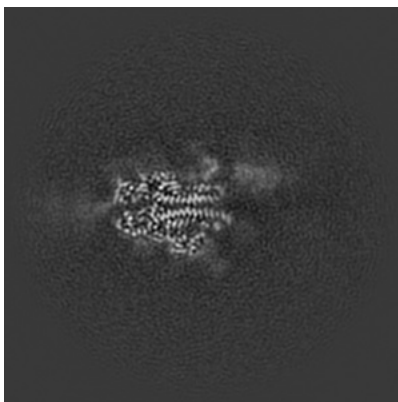
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

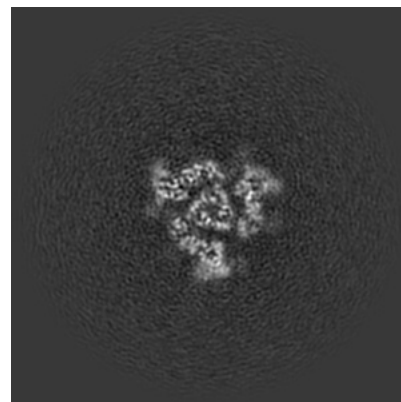
6.3.1 Primary map



X Index: 173

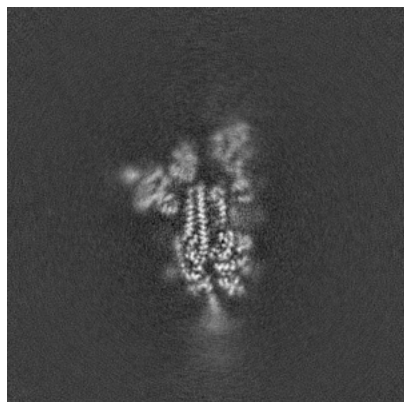


Y Index: 176

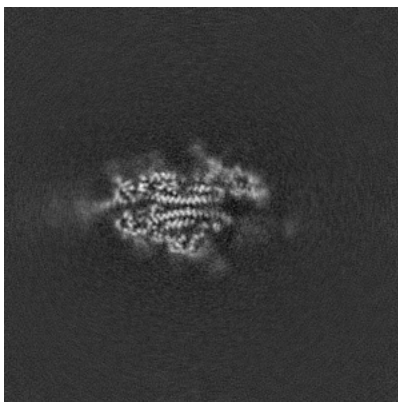


Z Index: 189

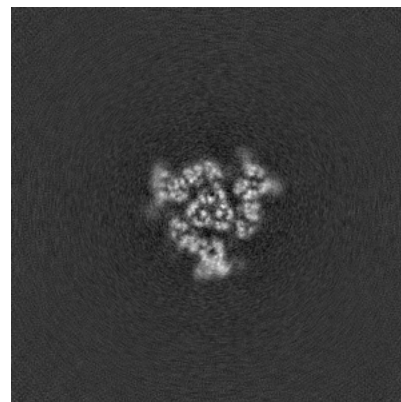
6.3.2 Raw map



X Index: 173



Y Index: 177

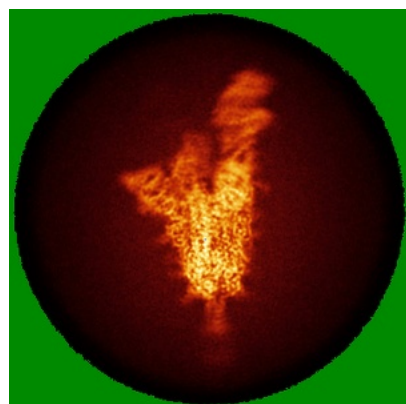


Z Index: 190

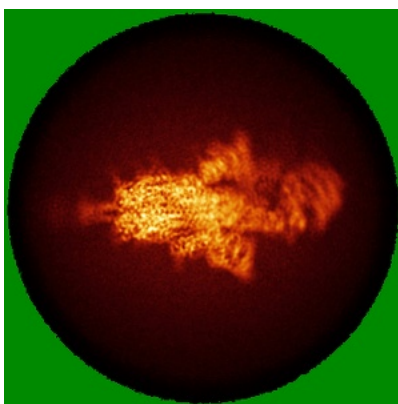
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

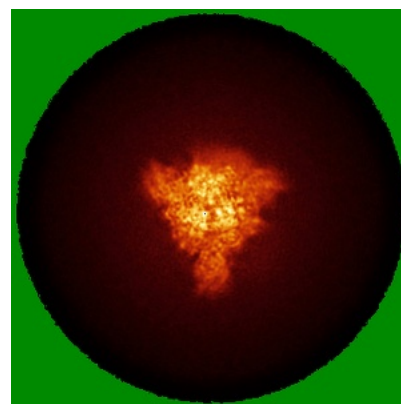
6.4.1 Primary map



X

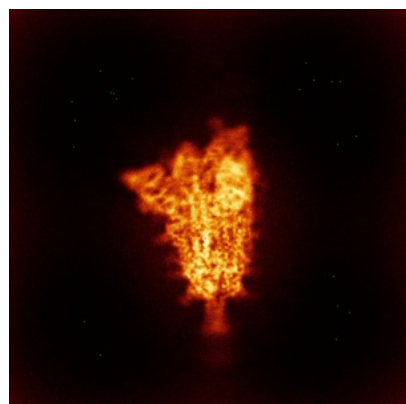


Y

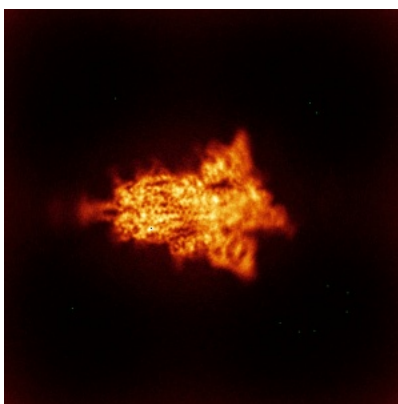


Z

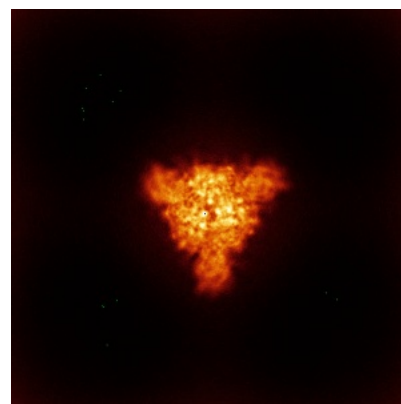
6.4.2 Raw map



X



Y

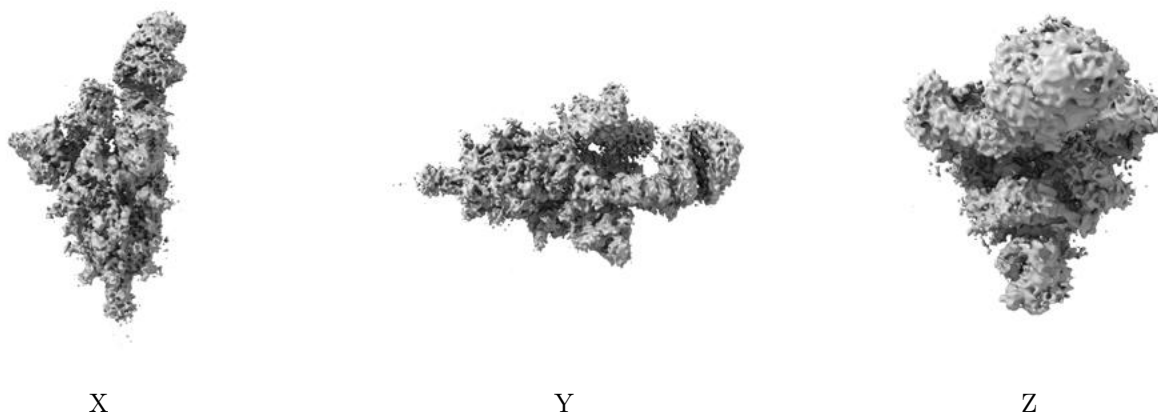


Z

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.

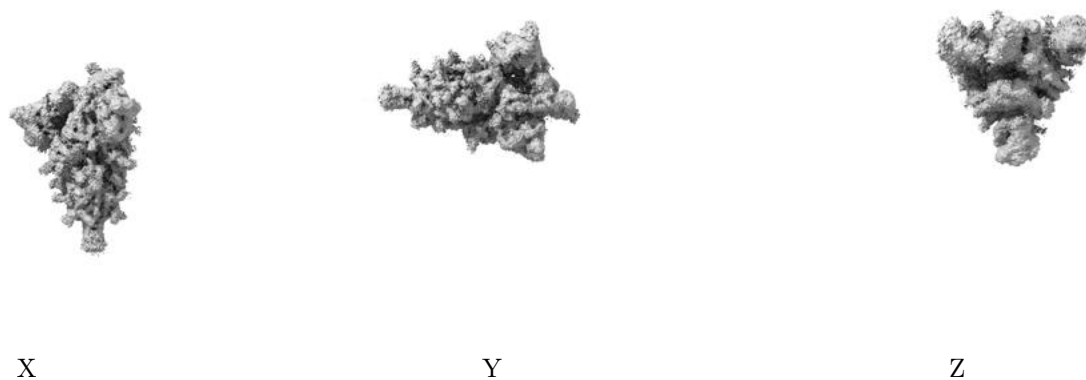
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

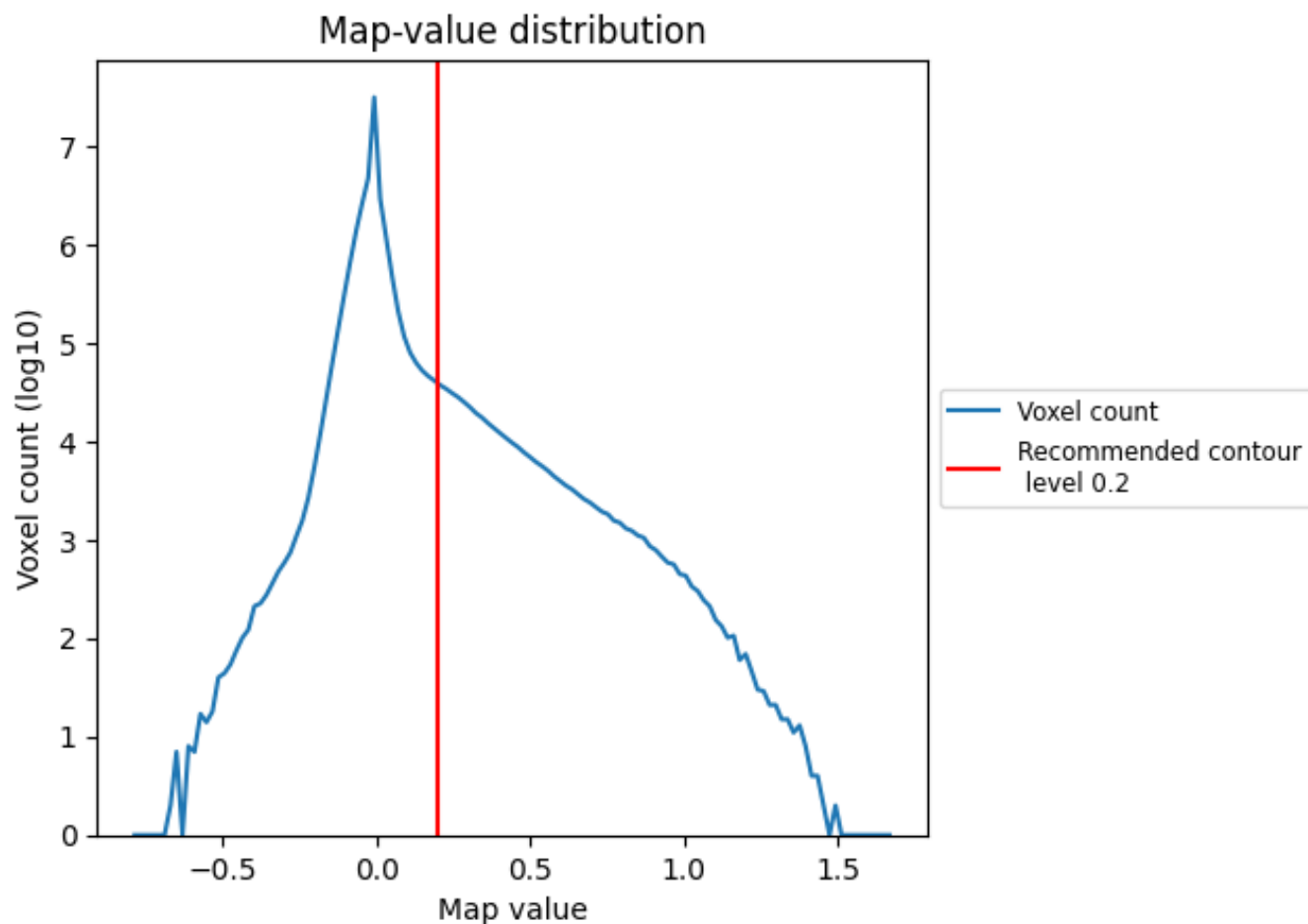
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

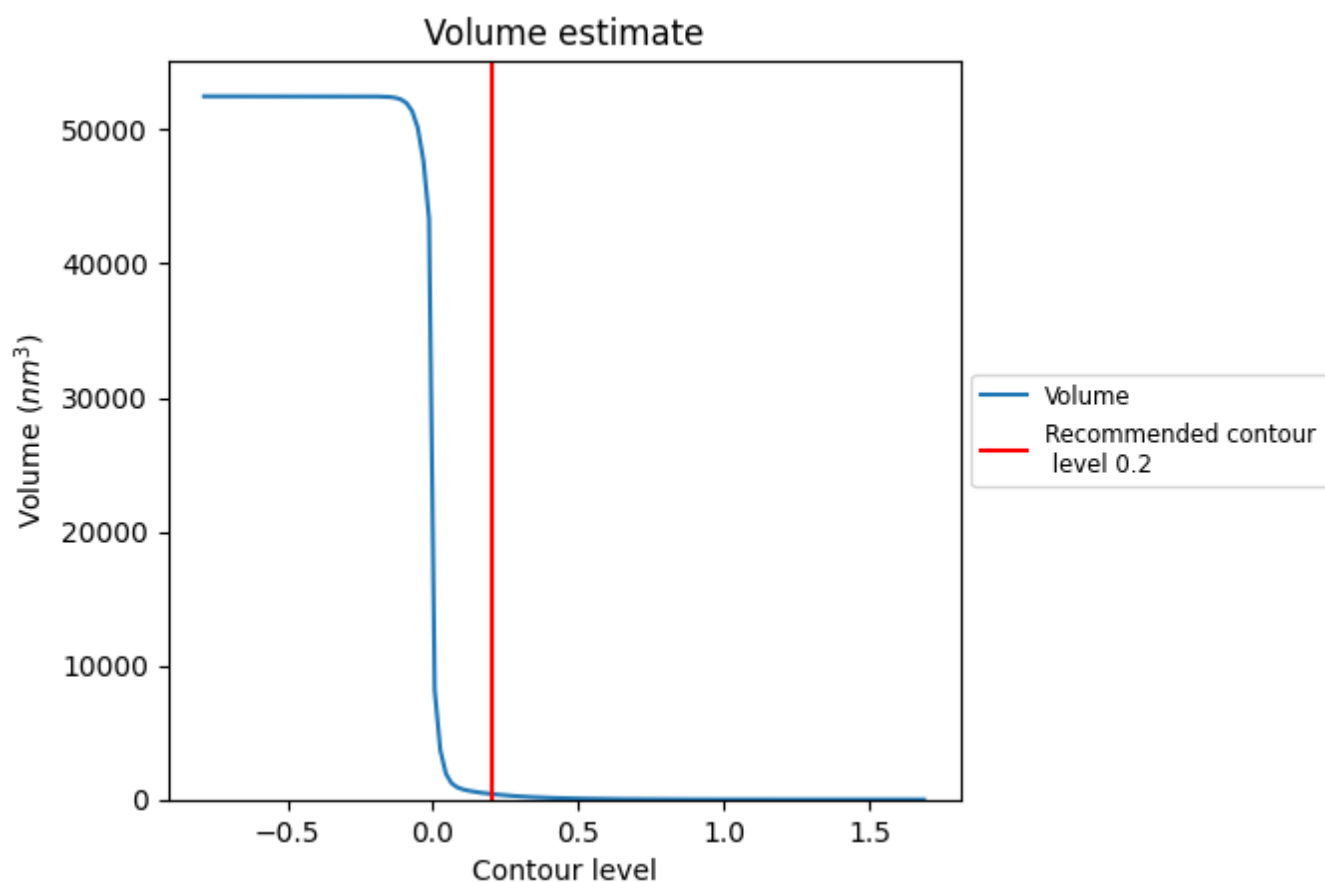
This section contains the results of statistical analysis of the map.

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.

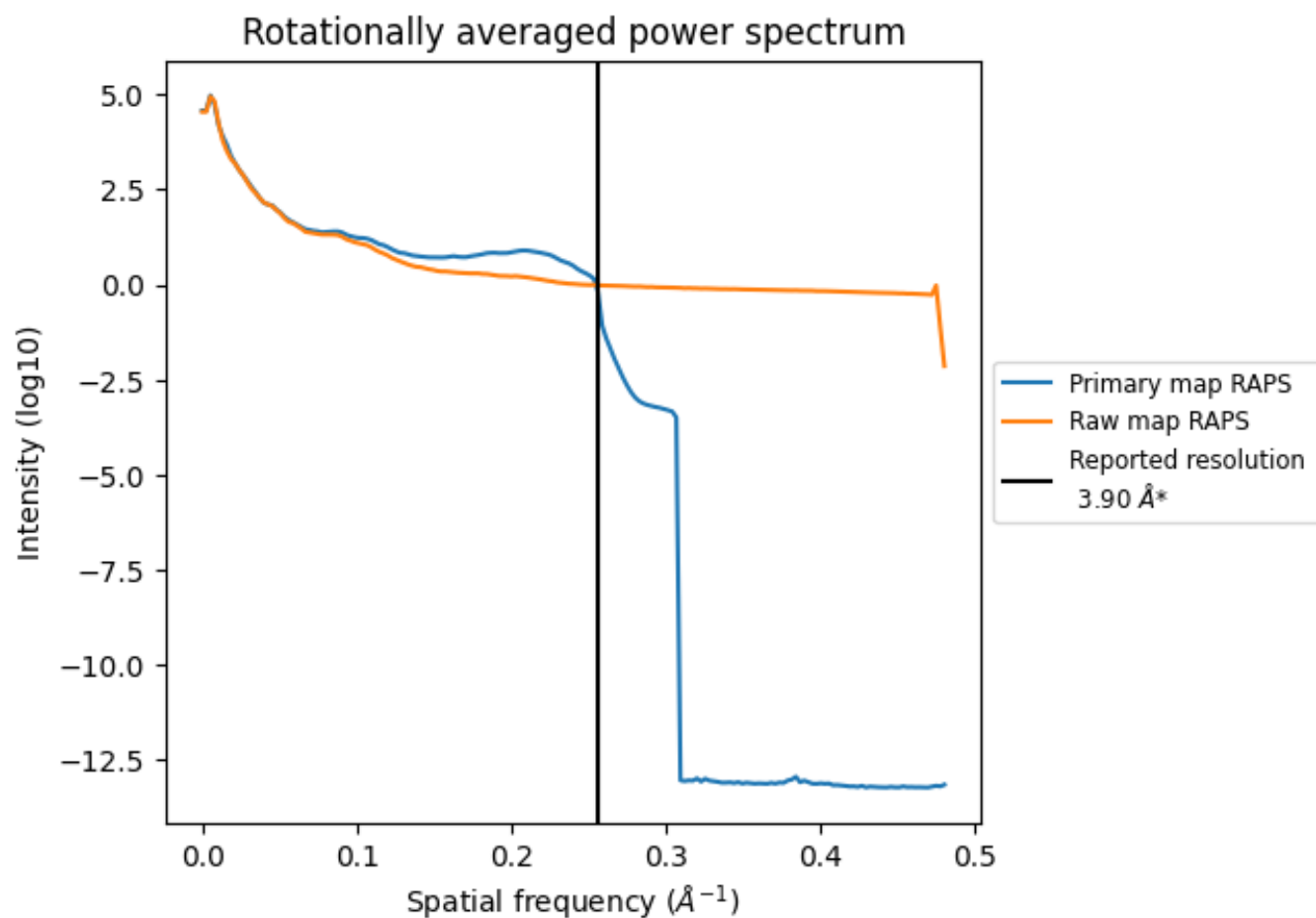
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 419 nm^3 ; this corresponds to an approximate mass of 378 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 ⓘ

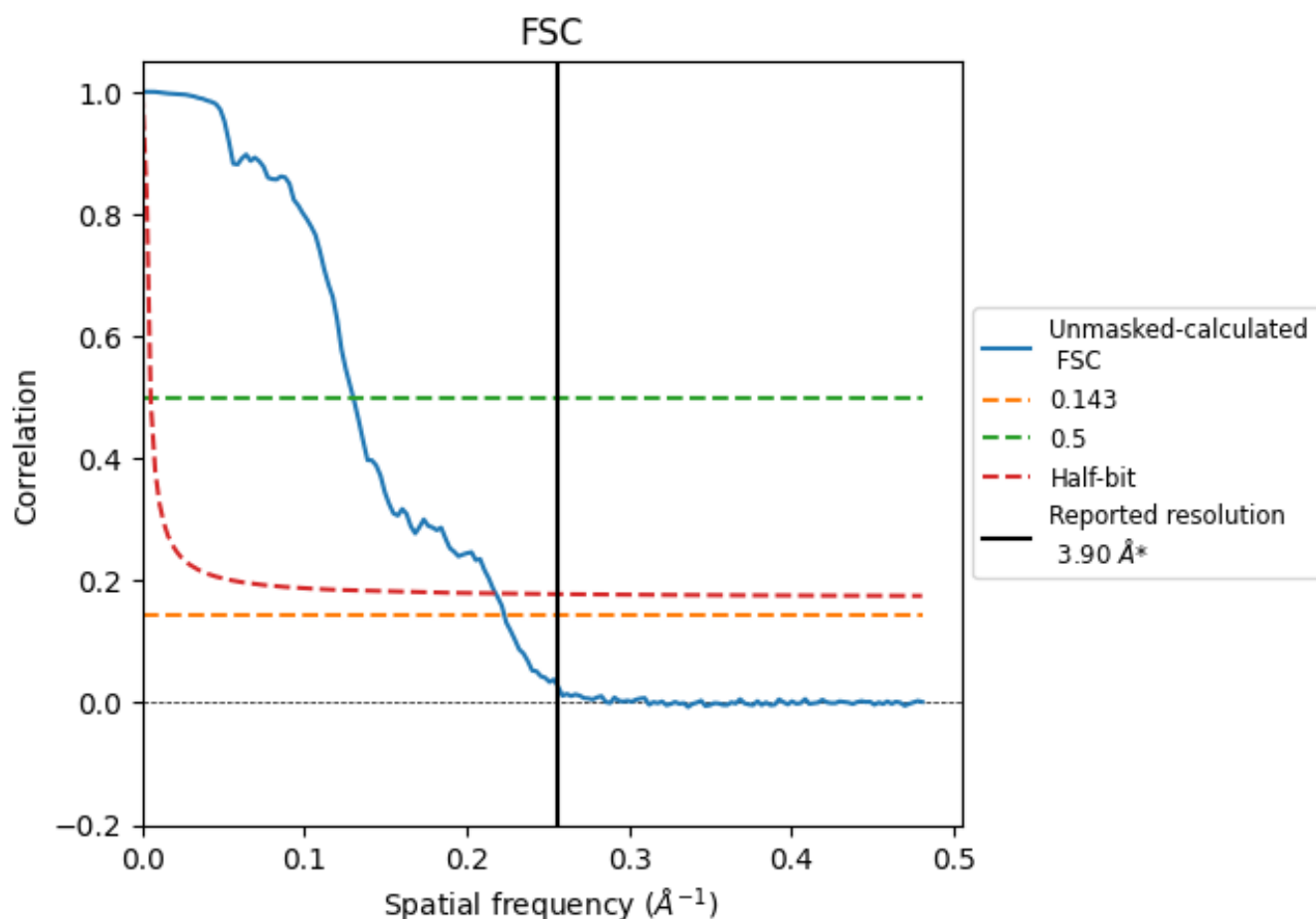


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

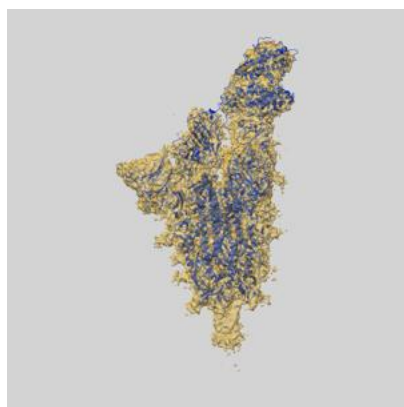
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.48	7.69	4.59

*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 4.48 differs from the reported value 3.9 by more than 10 %

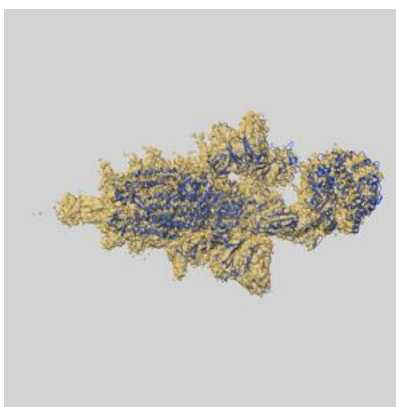
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37784 and PDB model 8WRO. Per-residue inclusion information can be found in section [3](#) on page [8](#).

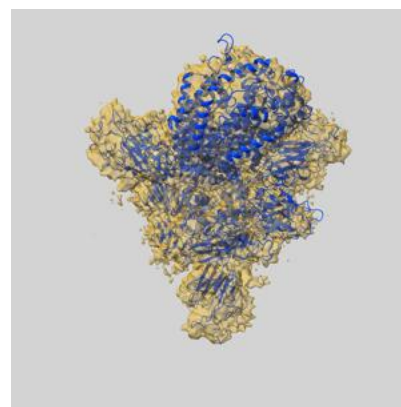
9.1 Map-model overlay [i](#)



X



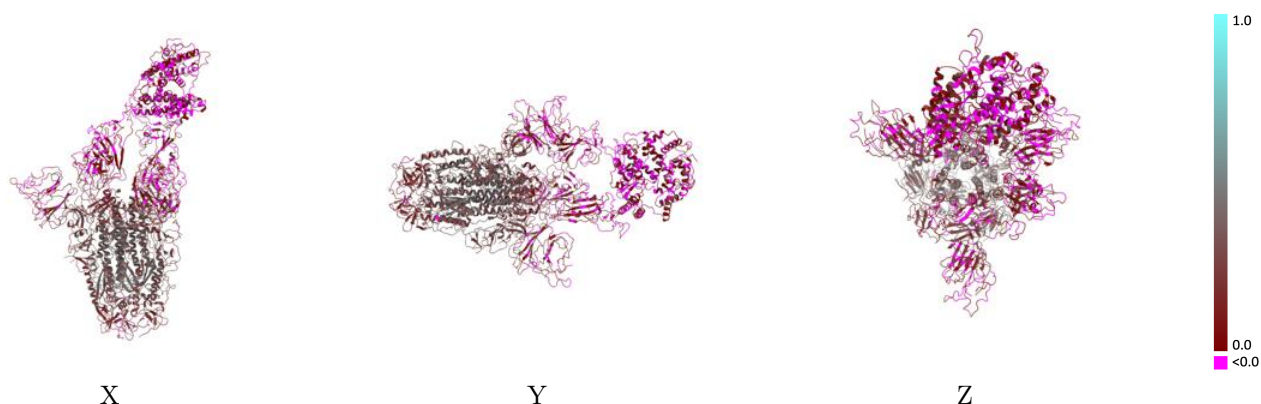
Y



Z

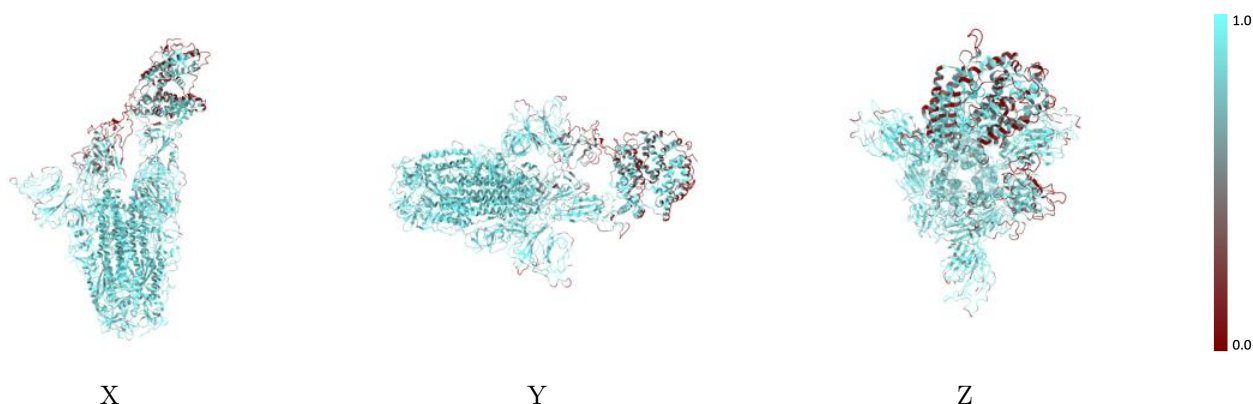
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



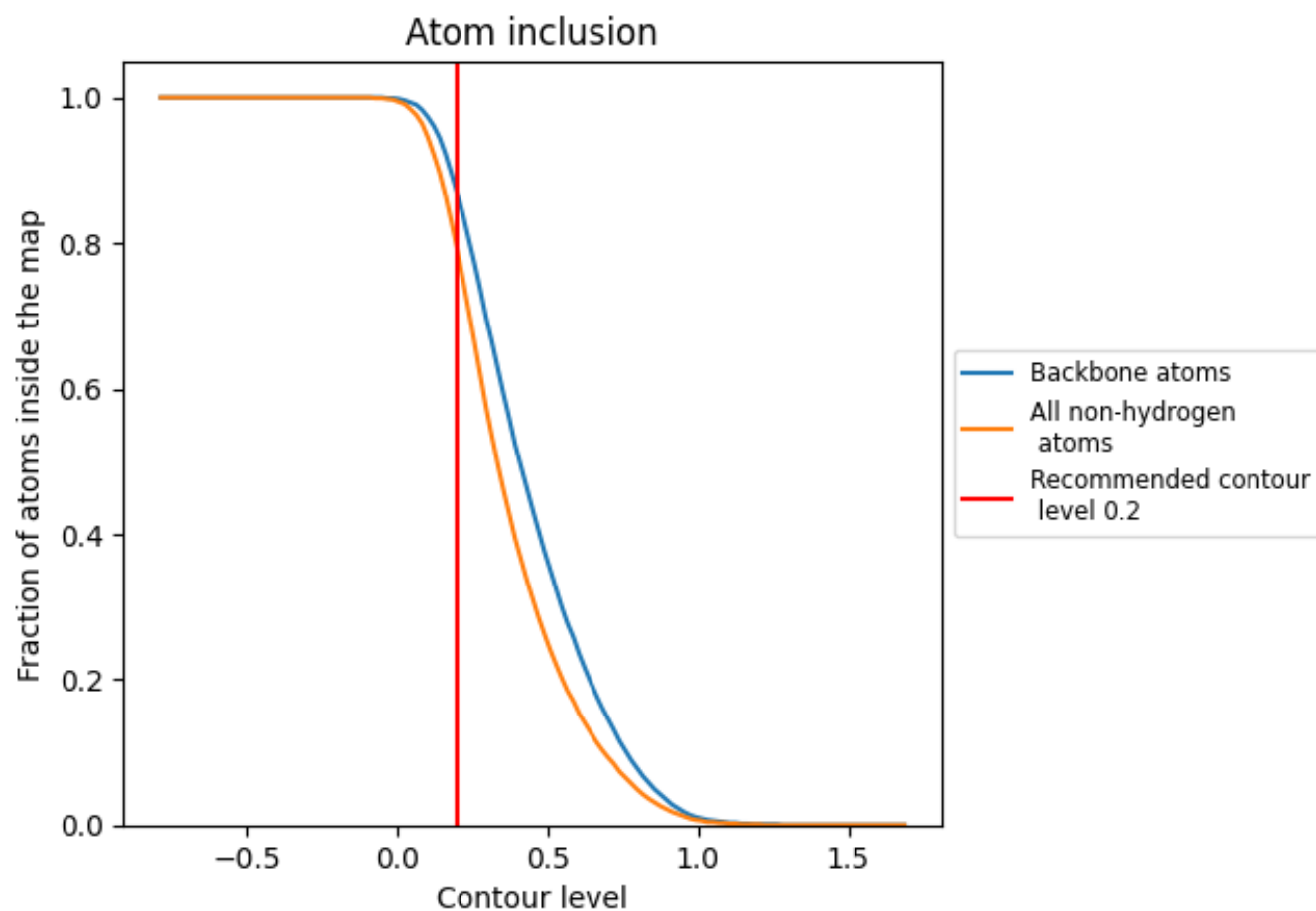
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 79% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7900	0.1930
A	0.7920	0.2200
B	0.8520	0.2200
C	0.8380	0.2330
D	0.5940	0.0300

