



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:27 AM UTC

PDB ID : 8R2D / pdb_00008r2d
EMDB ID : EMD-18839
Title : Integrator cleavage module assembly intermediate
Authors : Sabath, K.; Qiu, C.; Jonas, S.
Deposited on : 2023-11-03
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:

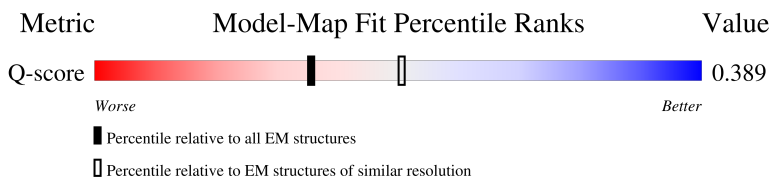
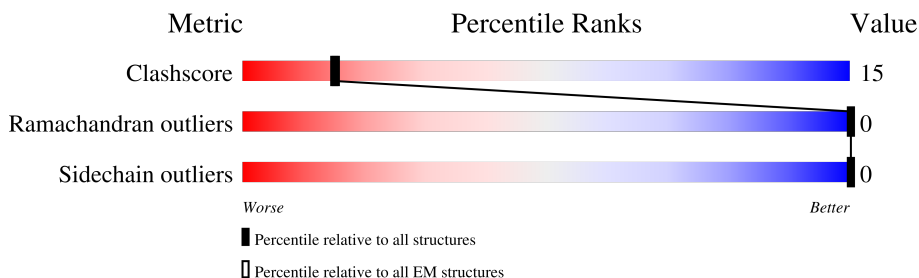
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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	827	 7% 61% 26% 13%
2	B	658	 49% 25% 27%
3	C	612	 49% 21% 30%
4	D	973	 41% 44% 29% 27%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18276 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 BRCA1-associated ATM activator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	718	Total	C	N	O	S	0	0
			5468	3482	938	1013	35		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q6PJG6
A	-4	PRO	-	expression tag	UNP Q6PJG6
A	-3	SER	-	expression tag	UNP Q6PJG6
A	-2	GLN	-	expression tag	UNP Q6PJG6
A	-1	SER	-	expression tag	UNP Q6PJG6
A	0	ASN	-	expression tag	UNP Q6PJG6

- Molecule 2 is a protein called Integrator complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	483	Total	C	N	O	S	0	0
			3786	2438	615	704	29		

- Molecule 3 is a protein called Integrator complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	429	Total	C	N	O	S	0	0
			3381	2166	576	608	31		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	GLY	-	expression tag	UNP Q5TA45
C	-10	PRO	-	expression tag	UNP Q5TA45
C	-9	SER	-	expression tag	UNP Q5TA45
C	-8	ASP	-	expression tag	UNP Q5TA45
C	-7	PRO	-	expression tag	UNP Q5TA45

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLY	-	expression tag	UNP Q5TA45
C	-5	PRO	-	expression tag	UNP Q5TA45
C	-4	LYS	-	expression tag	UNP Q5TA45
C	-3	ARG	-	expression tag	UNP Q5TA45
C	-2	ALA	-	expression tag	UNP Q5TA45
C	-1	GLU	-	expression tag	UNP Q5TA45
C	0	PHE	-	expression tag	UNP Q5TA45

- Molecule 4 is a protein called Integrator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	712	Total	C	N	O	S	0	0
			5639	3590	965	1052	32		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	GLY	-	expression tag	UNP Q96HW7
D	-8	PRO	-	expression tag	UNP Q96HW7
D	-7	SER	-	expression tag	UNP Q96HW7
D	-6	ASP	-	expression tag	UNP Q96HW7
D	-5	PRO	-	expression tag	UNP Q96HW7
D	-4	GLY	-	expression tag	UNP Q96HW7
D	-3	PRO	-	expression tag	UNP Q96HW7
D	-2	LYS	-	expression tag	UNP Q96HW7
D	-1	ARG	-	expression tag	UNP Q96HW7
D	0	ALA	-	expression tag	UNP Q96HW7

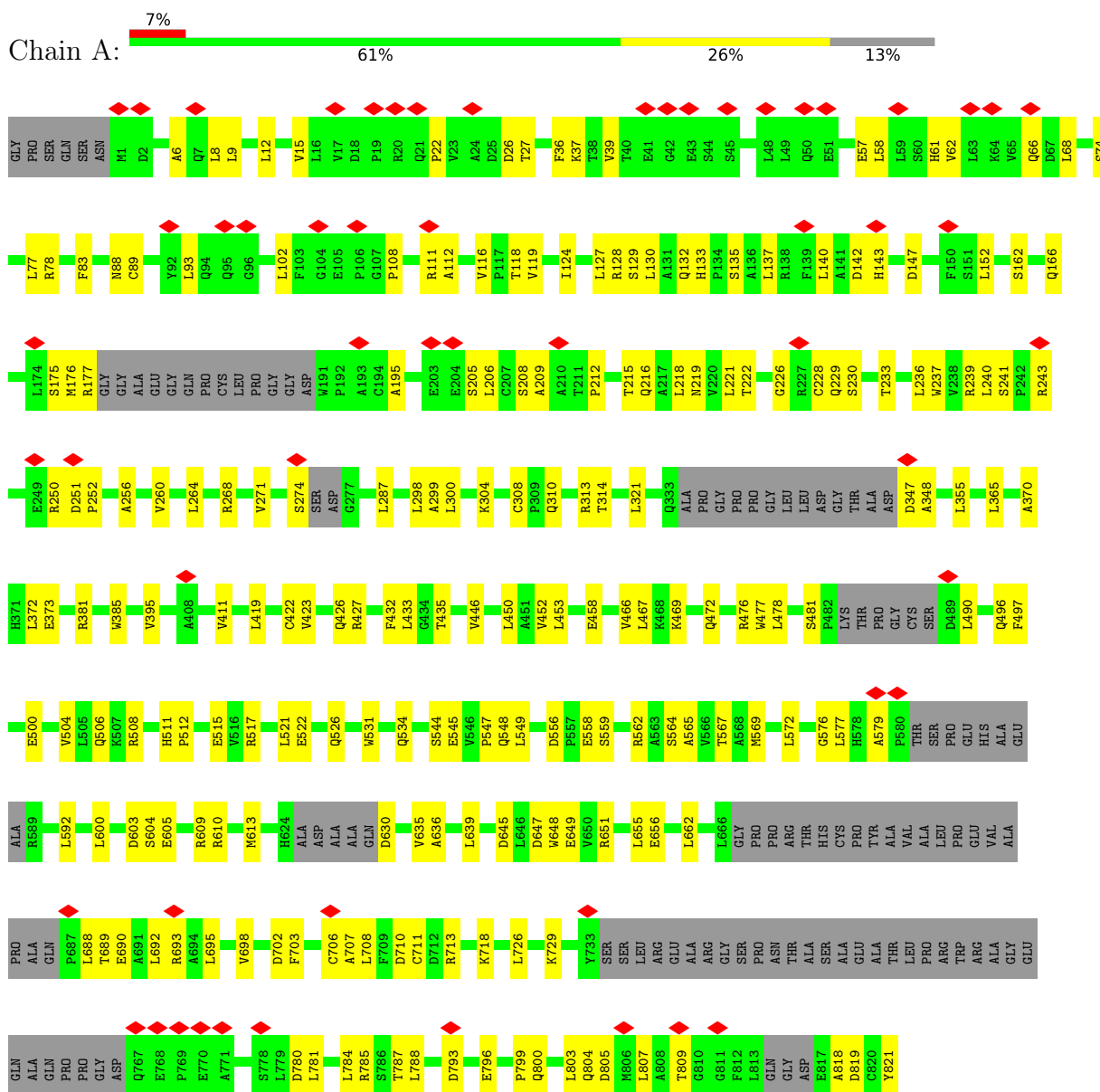
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	C	2	Total	Zn	0
			2	2	

3 Residue-property plots

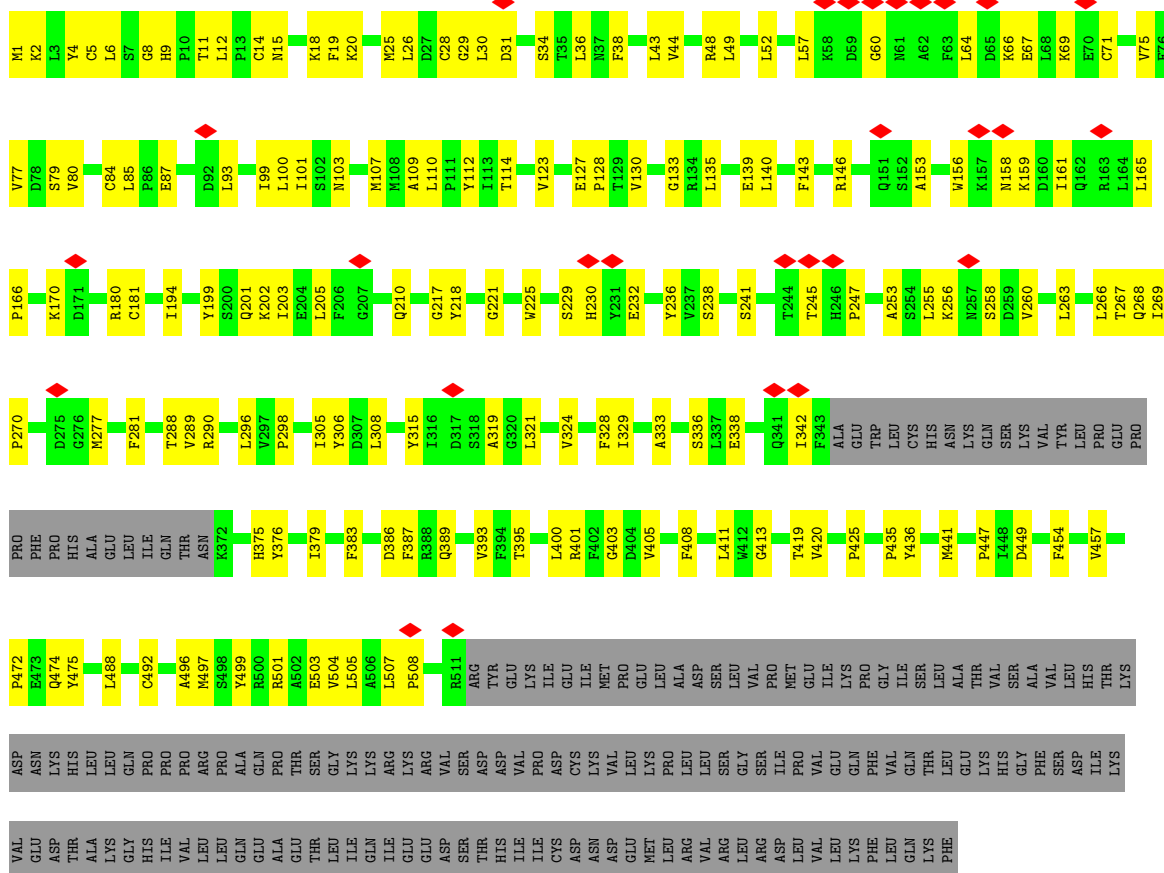
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: BRCA1-associated ATM activator 1



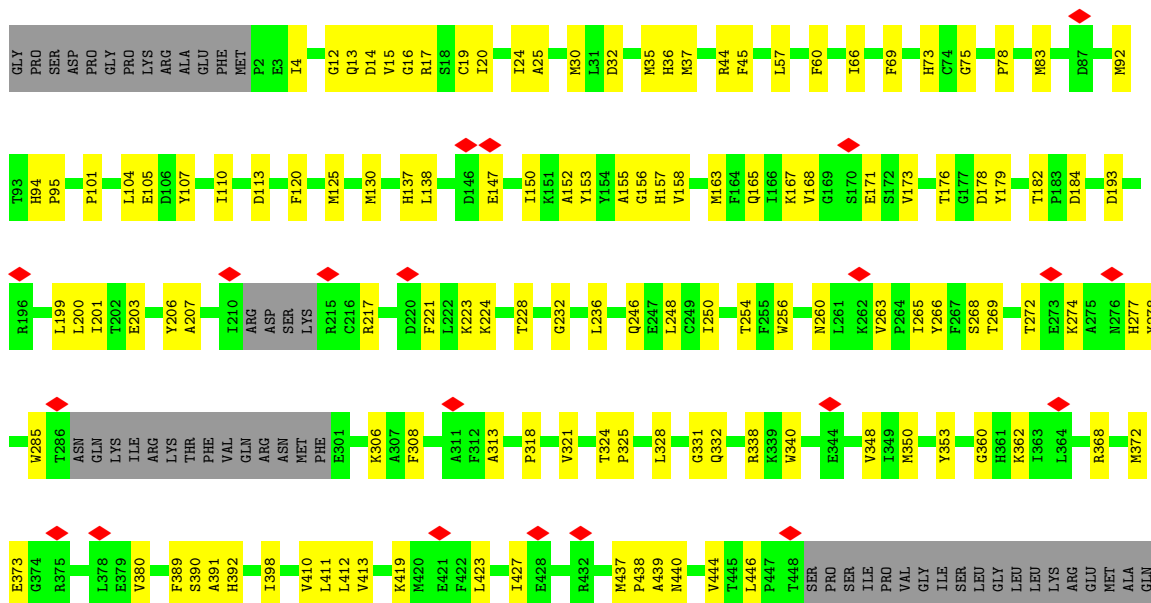
- Molecule 2: Integrator complex subunit 9

Chain B: 

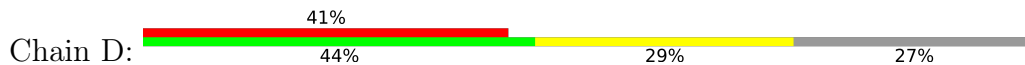


• Molecule 3: Integrator complex subunit 11

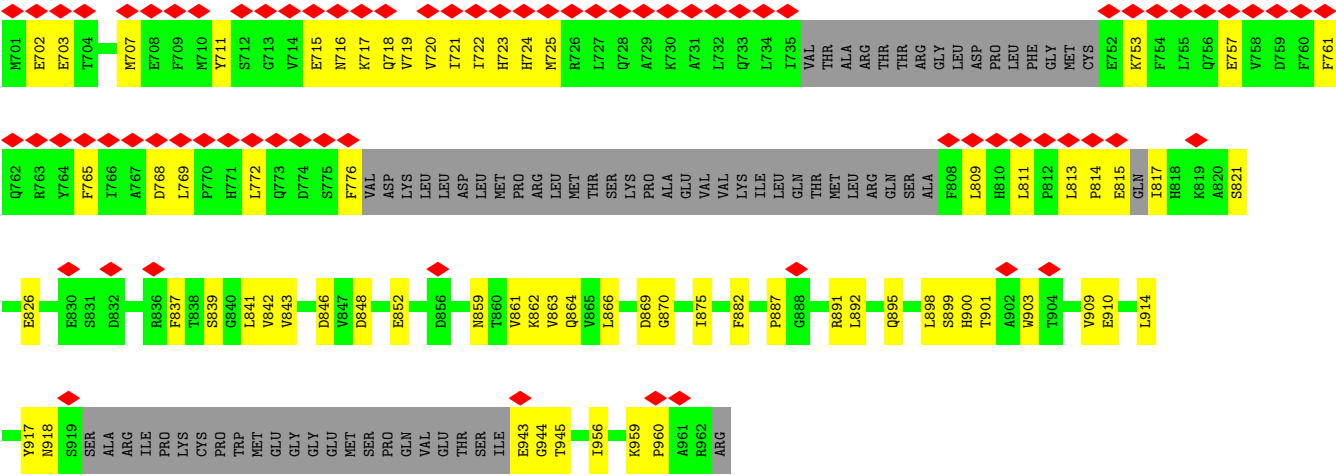
Chain C: 



- Molecule 4: Integrator complex subunit 4



R641	D642	L643	Q644	P645	L646	G647	E648	L649	Q650	S651	E652	L653	G654	A655	S656	L657	P658	D659	I660	A661	T662	Y663	L664	R665	C666	G667	L668	L669	L670	L671	K672	A673	L674	G675	L676	L677	L678	L679	L680	
S581	H582	L583	V584	P585	A586	L587	H588	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L449	D450	T451	V452	L453	A454	V455	L456	E457	D458	H459	S460	R461	D462	T463	R464	H468	F469	L470		N475	V476	S477	T478	K479	F480	A481	G482	V483	L484	L485	L486	F487	E488	L489	L490	K491	D492	L493	T494	
L521	V522	P523	E524	L525	A526	S527	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
S581	H582	L583	V584	P585	A586	L587	H588	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
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L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	V547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	V632	P633	E634	L635	A636	S637	THR	HIS	PRO	HIS	PHE	PHE	ASP																											



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97185	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.5	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.118	Depositor
Minimum map value	-1.934	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.324	Depositor
Map size (Å)	298.08, 298.08, 298.08	wwPDB
Map dimensions	230, 230, 230	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2959999, 1.2959999, 1.2959999	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.17	0/5578	0.38	0/7593
2	B	0.24	0/3884	0.47	0/5294
3	C	0.23	0/3457	0.49	0/4667
4	D	0.15	0/5739	0.38	0/7768
All	All	0.19	0/18658	0.42	0/25322

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5468	0	5506	143	0
2	B	3786	0	3787	112	0
3	C	3381	0	3371	102	0
4	D	5639	0	5693	199	0
5	C	2	0	0	0	0
All	All	18276	0	18357	541	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 15.

All (541) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:VAL:HG11	4:D:899:SER:HB2	1.55	0.88
2:B:30:LEU:HB2	2:B:109:ALA:HB2	1.62	0.81
4:D:114:ALA:HA	4:D:117:ILE:HD12	1.66	0.78
4:D:917:TYR:O	4:D:943:GLU:N	2.17	0.77
4:D:568:HIS:HA	4:D:571:ARG:HD2	1.67	0.77
4:D:385:ASP:O	4:D:391:ARG:NH1	2.19	0.76
4:D:322:ASP:HB3	4:D:325:LEU:HD23	1.68	0.74
3:C:268:SER:HB3	3:C:308:PHE:HB3	1.69	0.74
4:D:669:LEU:HD13	4:D:672:LYS:HD3	1.71	0.72
2:B:36:LEU:O	2:B:401:ARG:NH2	2.22	0.72
1:A:610:ARG:NH1	3:C:105:GLU:OE2	2.23	0.71
4:D:293:ASP:O	4:D:299:ARG:NH1	2.24	0.71
4:D:436:ARG:HG3	4:D:470:LEU:HA	1.73	0.70
4:D:178:GLY:H	4:D:225:ARG:HH12	1.39	0.70
4:D:436:ARG:HB2	4:D:470:LEU:HD12	1.73	0.70
4:D:399:CYS:SG	4:D:403:GLN:NE2	2.65	0.70
4:D:621:VAL:HG21	4:D:664:LEU:HD21	1.73	0.69
4:D:478:THR:HG23	4:D:481:GLY:H	1.58	0.68
3:C:256:TRP:HH2	3:C:263:VAL:HB	1.59	0.68
1:A:142:ASP:OD1	1:A:143:HIS:ND1	2.29	0.66
1:A:819:ASP:OD1	3:C:392:HIS:NE2	2.29	0.66
1:A:137:LEU:HA	1:A:140:LEU:HD12	1.78	0.65
3:C:157:HIS:ND1	3:C:391:ALA:O	2.24	0.65
4:D:724:HIS:HE1	4:D:776:PHE:H	1.45	0.65
1:A:57:GLU:O	1:A:61:HIS:ND1	2.30	0.64
2:B:267:THR:HG22	2:B:269:ILE:H	1.61	0.64
3:C:201:ILE:HG23	3:C:411:LEU:HB3	1.79	0.64
4:D:320:THR:HA	4:D:377:GLY:H	1.61	0.64
1:A:656:GLU:OE1	1:A:718:LYS:NZ	2.30	0.64
1:A:490:LEU:HD21	1:A:534:GLN:HB3	1.80	0.63
1:A:230:SER:O	1:A:233:THR:OG1	2.15	0.63
1:A:821:TYR:HE2	3:C:37:MET:H	1.44	0.63
2:B:112:TYR:OH	2:B:180:ARG:O	2.16	0.63
4:D:859:ASN:O	4:D:862:LYS:NZ	2.28	0.63
1:A:433:LEU:O	1:A:477:TRP:NE1	2.31	0.63
1:A:133:HIS:HD2	1:A:135:SER:HB2	1.63	0.63
4:D:196:VAL:HA	4:D:199:ILE:HD12	1.79	0.63
2:B:99:ILE:HB	2:B:123:VAL:HG12	1.80	0.62
4:D:72:VAL:HA	4:D:75:ILE:HD12	1.81	0.62
4:D:118:LEU:HD11	4:D:130:LEU:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:ASP:O	1:A:706:CYS:HB2	1.97	0.62
3:C:269:THR:HA	3:C:324:THR:HG21	1.81	0.62
4:D:617:SER:HA	4:D:620:ARG:HE	1.64	0.62
3:C:35:MET:HG2	3:C:36:HIS:H	1.65	0.62
4:D:175:GLY:O	4:D:225:ARG:NH1	2.33	0.62
4:D:391:ARG:O	4:D:395:VAL:HG23	2.00	0.62
4:D:80:TYR:OH	4:D:121:GLU:OE2	2.18	0.61
4:D:243:ASP:O	4:D:249:ARG:NH1	2.33	0.61
3:C:232:GLY:HA2	3:C:318:PRO:HG3	1.83	0.61
4:D:462:ASP:OD1	4:D:891:ARG:NH1	2.33	0.61
4:D:475:ASN:OD1	4:D:513:ARG:NH2	2.33	0.61
3:C:173:VAL:HG22	3:C:199:LEU:HB3	1.81	0.61
1:A:547:PRO:HB2	1:A:579:ALA:HB2	1.81	0.61
4:D:959:LYS:O	4:D:959:LYS:HG3	2.01	0.61
1:A:8:LEU:HD23	1:A:807:LEU:HD21	1.83	0.61
1:A:511:HIS:O	1:A:517:ARG:NH1	2.33	0.60
4:D:639:THR:O	4:D:643:LEU:HG	2.01	0.60
2:B:43:LEU:HD21	2:B:146:ARG:HH21	1.67	0.60
4:D:172:GLN:O	4:D:176:ASN:ND2	2.33	0.60
2:B:333:ALA:HB1	2:B:375:HIS:HB2	1.83	0.60
4:D:637:GLU:HB3	4:D:641:ARG:HH21	1.66	0.60
1:A:609:ARG:NE	1:A:645:ASP:OD2	2.35	0.60
1:A:208:SER:O	1:A:250:ARG:NH2	2.33	0.60
4:D:456:LEU:HD21	4:D:489:LEU:HD23	1.82	0.60
4:D:814:PRO:HG2	4:D:817:ILE:HD11	1.83	0.59
1:A:662:LEU:HD11	1:A:726:LEU:HD13	1.85	0.59
2:B:306:TYR:OH	2:B:336:SER:OG	2.19	0.59
2:B:474:GLN:OE1	2:B:474:GLN:N	2.36	0.59
3:C:368:ARG:HB3	3:C:380:VAL:HB	1.83	0.59
3:C:57:LEU:O	3:C:60:PHE:N	2.34	0.59
1:A:129:SER:O	1:A:132:GLN:NE2	2.32	0.59
1:A:422:CYS:SG	1:A:423:VAL:N	2.76	0.59
4:D:236:GLN:HA	4:D:239:LYS:HE3	1.83	0.59
4:D:493:LEU:HD21	4:D:542:PRO:HB2	1.85	0.59
4:D:221:GLN:HE21	4:D:225:ARG:HD2	1.68	0.59
1:A:22:PRO:HG2	1:A:809:THR:HG22	1.84	0.59
2:B:229:SER:OG	2:B:230:HIS:N	2.36	0.59
4:D:577:ARG:NH1	4:D:584:VAL:O	2.35	0.58
1:A:215:THR:O	1:A:219:ASN:ND2	2.36	0.58
4:D:841:LEU:O	4:D:899:SER:OG	2.14	0.58
3:C:138:LEU:HA	3:C:152:ALA:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:721:ILE:O	4:D:725:MET:HG2	2.03	0.58
1:A:219:ASN:HA	1:A:222:THR:HG22	1.83	0.58
4:D:633:GLN:HA	4:D:636:LEU:HD12	1.85	0.58
1:A:77:LEU:HD11	1:A:108:PRO:HG3	1.85	0.58
4:D:420:PHE:CD2	4:D:455:VAL:HG21	2.38	0.58
2:B:296:LEU:HD11	2:B:405:VAL:HG23	1.86	0.57
1:A:239:ARG:O	1:A:243:ARG:NH1	2.38	0.57
4:D:266:SER:O	4:D:279:LEU:N	2.35	0.57
1:A:142:ASP:OD1	1:A:143:HIS:N	2.38	0.57
1:A:260:VAL:HG13	1:A:298:LEU:HB2	1.85	0.57
3:C:256:TRP:O	3:C:260:ASN:N	2.32	0.57
4:D:476:VAL:HG13	4:D:517:LEU:HD12	1.87	0.57
4:D:718:GLN:O	4:D:722:ILE:HG12	2.05	0.57
2:B:79:SER:OG	2:B:80:VAL:N	2.38	0.57
4:D:156:CYS:HA	4:D:159:LEU:HD12	1.87	0.57
4:D:555:ALA:HB1	4:D:562:PRO:HD3	1.86	0.57
1:A:556:ASP:O	1:A:562:ARG:NH1	2.38	0.56
2:B:156:TRP:HA	2:B:161:ILE:HD13	1.85	0.56
4:D:558:CYS:HB2	4:D:561:MET:HE1	1.86	0.56
3:C:248:LEU:HD21	3:C:389:PHE:HD2	1.70	0.56
4:D:88:VAL:O	4:D:92:ILE:HG12	2.05	0.56
4:D:249:ARG:O	4:D:253:VAL:HG23	2.05	0.56
1:A:12:LEU:HD22	1:A:803:LEU:HD22	1.87	0.56
1:A:467:LEU:HD11	1:A:508:ARG:HE	1.70	0.56
2:B:14:CYS:HB2	2:B:29:GLY:H	1.70	0.56
3:C:176:THR:OG1	3:C:201:ILE:O	2.22	0.56
3:C:274:LYS:HA	3:C:277:HIS:HB3	1.87	0.56
4:D:92:ILE:O	4:D:96:LEU:HG	2.05	0.56
1:A:610:ARG:NH2	1:A:647:ASP:OD2	2.39	0.56
4:D:416:LEU:HG	4:D:435:MET:HE2	1.87	0.56
2:B:499:TYR:HB3	2:B:505:LEU:HD11	1.87	0.56
4:D:212:ARG:O	4:D:216:ILE:HG13	2.06	0.56
4:D:445:ARG:N	4:D:448:GLN:OE1	2.38	0.56
1:A:603:ASP:OD1	1:A:604:SER:N	2.39	0.56
4:D:461:ARG:HD3	4:D:891:ARG:HH21	1.71	0.55
4:D:490:LEU:O	4:D:494:THR:HG23	2.06	0.55
1:A:228:CYS:O	1:A:229:GLN:NE2	2.39	0.55
4:D:508:LYS:HA	4:D:553:ASN:ND2	2.21	0.55
4:D:903:TRP:HZ3	4:D:956:ILE:HD13	1.72	0.55
1:A:205:SER:O	1:A:208:SER:OG	2.23	0.55
4:D:129:GLN:O	4:D:133:THR:HG23	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:180:LEU:HA	4:D:227:LEU:HD12	1.88	0.55
1:A:426:GLN:HE21	1:A:466:VAL:HG11	1.71	0.55
3:C:155:ALA:HB2	3:C:163:MET:HE2	1.88	0.55
4:D:456:LEU:HD22	4:D:488:GLU:HG3	1.88	0.55
3:C:266:TYR:HB3	3:C:308:PHE:HB2	1.88	0.55
4:D:428:ARG:HE	4:D:463:ILE:HD13	1.71	0.55
2:B:260:VAL:HG21	2:B:507:LEU:HD13	1.88	0.55
2:B:376:TYR:OH	2:B:386:ASP:OD2	2.24	0.55
4:D:769:LEU:HD23	4:D:772:LEU:HD21	1.89	0.55
4:D:112:ASP:OD1	4:D:150:ARG:NH2	2.39	0.55
1:A:310:GLN:O	1:A:314:THR:HG23	2.06	0.54
4:D:180:LEU:HD23	4:D:227:LEU:HB2	1.88	0.54
2:B:158:ASN:HB3	2:B:161:ILE:HG22	1.89	0.54
2:B:158:ASN:OD1	2:B:159:LYS:N	2.40	0.54
4:D:74:ARG:NH2	4:D:113:ASP:OD2	2.38	0.54
4:D:843:VAL:HG12	4:D:898:LEU:O	2.08	0.54
1:A:300:LEU:O	1:A:304:LYS:HG2	2.07	0.54
1:A:355:LEU:HD11	1:A:411:VAL:HG23	1.90	0.54
3:C:20:ILE:HD11	3:C:413:VAL:HG11	1.89	0.54
4:D:287:ILE:O	4:D:291:VAL:HG23	2.07	0.54
2:B:64:LEU:HD11	2:B:161:ILE:HD11	1.90	0.54
2:B:165:LEU:O	2:B:170:LYS:HB3	2.08	0.54
1:A:689:THR:O	1:A:693:ARG:HG2	2.07	0.53
2:B:270:PRO:HB2	2:B:488:LEU:HD13	1.90	0.53
2:B:387:PHE:HE2	2:B:389:GLN:HE21	1.56	0.53
3:C:138:LEU:HD12	3:C:138:LEU:H	1.71	0.53
1:A:308:CYS:HB3	1:A:313:ARG:HD2	1.89	0.53
1:A:781:LEU:O	1:A:785:ARG:N	2.33	0.53
4:D:76:LEU:HD12	4:D:92:ILE:HD12	1.90	0.53
1:A:66:GLN:OE1	1:A:111:ARG:NE	2.37	0.53
3:C:66:ILE:HB	3:C:92:MET:HG2	1.89	0.53
3:C:248:LEU:HD21	3:C:389:PHE:CD2	2.43	0.53
4:D:545:ILE:O	4:D:549:VAL:HG23	2.09	0.53
2:B:454:PHE:HA	2:B:457:VAL:HG12	1.91	0.53
4:D:154:VAL:O	4:D:158:HIS:ND1	2.30	0.53
4:D:316:PHE:O	4:D:320:THR:HG23	2.09	0.53
1:A:635:VAL:HG12	1:A:698:VAL:HG21	1.91	0.52
3:C:13:GLN:HG3	3:C:439:ALA:HA	1.90	0.52
1:A:216:GLN:HA	1:A:219:ASN:HD21	1.74	0.52
1:A:496:GLN:NE2	1:A:500:GLU:OE2	2.43	0.52
2:B:255:LEU:O	2:B:258:SER:OG	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:PHE:CE2	3:C:158:VAL:HB	2.43	0.52
4:D:614:LEU:HD23	4:D:618:LEU:HD23	1.92	0.52
1:A:647:ASP:O	1:A:651:ARG:NH1	2.43	0.52
1:A:655:LEU:HG	1:A:703:PHE:HE1	1.74	0.52
4:D:164:HIS:O	4:D:168:ASN:ND2	2.43	0.52
2:B:413:GLY:HA2	2:B:441:MET:SD	2.50	0.52
3:C:157:HIS:HA	3:C:391:ALA:HB3	1.91	0.52
3:C:200:LEU:O	3:C:410:VAL:HA	2.09	0.52
3:C:207:ALA:HB3	3:C:419:LYS:HB3	1.91	0.52
4:D:405:SER:OG	4:D:408:PHE:HB3	2.09	0.52
4:D:718:GLN:HA	4:D:721:ILE:HD12	1.90	0.52
4:D:289:HIS:O	4:D:292:SER:OG	2.27	0.52
1:A:558:GLU:OE2	1:A:559:SER:N	2.43	0.52
1:A:512:PRO:HB3	2:B:315:TYR:CD1	2.45	0.51
4:D:73:VAL:HG11	4:D:110:ILE:HD13	1.90	0.51
1:A:636:ALA:HA	1:A:698:VAL:HG23	1.90	0.51
2:B:165:LEU:HD13	2:B:166:PRO:HD2	1.92	0.51
2:B:379:ILE:HD11	4:D:841:LEU:HD22	1.92	0.51
4:D:815:GLU:O	4:D:817:ILE:N	2.44	0.51
1:A:12:LEU:HA	1:A:15:VAL:HG12	1.93	0.51
1:A:124:ILE:HD11	1:A:152:LEU:HD11	1.92	0.51
4:D:151:LEU:HD12	4:D:173:LEU:HD21	1.93	0.51
4:D:663:TYR:CG	4:D:811:LEU:HD22	2.45	0.51
2:B:217:GLY:HA2	2:B:247:PRO:HB2	1.91	0.51
3:C:157:HIS:O	3:C:158:VAL:HG13	2.11	0.51
4:D:165:GLY:HA2	4:D:168:ASN:HD22	1.76	0.51
4:D:415:PHE:O	4:D:419:MET:HG2	2.10	0.51
1:A:569:MET:HB3	1:A:592:LEU:HD11	1.93	0.51
2:B:5:CYS:SG	2:B:499:TYR:HB2	2.51	0.51
2:B:34:SER:HB2	2:B:84:CYS:HB2	1.93	0.51
3:C:246:GLN:HG2	3:C:278:TYR:HD2	1.76	0.51
4:D:616:GLN:HA	4:D:619:GLU:HG3	1.93	0.50
1:A:26:ASP:OD1	1:A:27:THR:N	2.41	0.50
2:B:497:MET:HE1	2:B:508:PRO:HD3	1.93	0.50
4:D:486:LEU:HD21	4:D:547:VAL:HG12	1.93	0.50
4:D:148:GLN:HB2	4:D:149:MET:HE2	1.93	0.50
4:D:716:ASN:O	4:D:720:VAL:HG23	2.11	0.50
1:A:796:GLU:OE1	1:A:796:GLU:N	2.40	0.50
3:C:75:GLY:HA2	3:C:104:LEU:HD21	1.93	0.50
1:A:784:LEU:HA	1:A:787:THR:HG22	1.92	0.50
2:B:123:VAL:HG23	2:B:194:ILE:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:157:HIS:CD2	3:C:178:ASP:HB2	2.46	0.50
4:D:159:LEU:HD11	4:D:174:LEU:HD21	1.92	0.50
4:D:555:ALA:HA	4:D:561:MET:HE2	1.93	0.50
1:A:83:PHE:HB3	1:A:93:LEU:HD11	1.93	0.50
4:D:163:SER:HB3	4:D:166:VAL:HG22	1.94	0.50
4:D:436:ARG:NH2	4:D:887:PRO:HD3	2.26	0.50
2:B:25:MET:HE1	2:B:93:LEU:HD11	1.92	0.50
4:D:389:GLU:N	4:D:389:GLU:OE2	2.45	0.50
1:A:713:ARG:NH2	3:C:373:GLU:OE2	2.45	0.50
1:A:308:CYS:SG	1:A:313:ARG:HG3	2.52	0.49
1:A:710:ASP:OD1	1:A:711:CYS:N	2.44	0.49
4:D:505:LYS:O	4:D:508:LYS:HB3	2.13	0.49
2:B:290:ARG:NH2	2:B:319:ALA:O	2.46	0.49
4:D:123:SER:OG	4:D:124:HIS:N	2.45	0.49
2:B:26:LEU:HB3	2:B:236:TYR:CE2	2.48	0.49
2:B:236:TYR:CE1	2:B:238:SER:HB3	2.48	0.49
2:B:400:LEU:O	2:B:436:TYR:OH	2.18	0.49
1:A:522:GLU:O	1:A:526:GLN:HG2	2.13	0.49
2:B:217:GLY:O	2:B:241:SER:OG	2.30	0.49
4:D:134:LEU:HD12	4:D:151:LEU:HD11	1.94	0.49
4:D:577:ARG:NH2	4:D:649:LEU:O	2.46	0.49
1:A:478:LEU:HB3	1:A:531:TRP:HH2	1.78	0.49
2:B:269:ILE:HD13	2:B:447:PRO:HG2	1.95	0.49
1:A:74:SER:OG	1:A:78:ARG:NH2	2.43	0.49
1:A:127:LEU:HD13	1:A:130:LEU:HD21	1.95	0.49
3:C:35:MET:HG2	3:C:36:HIS:N	2.28	0.48
4:D:636:LEU:HB2	4:D:668:LEU:HD12	1.94	0.48
4:D:656:VAL:HB	4:D:813:LEU:HD12	1.95	0.48
1:A:662:LEU:HD12	1:A:695:LEU:HD21	1.94	0.48
3:C:94:HIS:HD2	3:C:137:HIS:CE1	2.31	0.48
3:C:165:GLN:HE21	3:C:167:LYS:HD2	1.78	0.48
4:D:468:HIS:HB3	4:D:506:CYS:SG	2.53	0.48
3:C:179:TYR:OH	3:C:398:ILE:HG12	2.13	0.48
3:C:274:LYS:HE3	3:C:277:HIS:CD2	2.48	0.48
3:C:438:PRO:HB3	3:C:444:VAL:HG21	1.94	0.48
4:D:456:LEU:HD23	4:D:492:ASN:HB2	1.96	0.48
4:D:413:LEU:HD22	4:D:442:ILE:HB	1.95	0.48
3:C:110:ILE:HD11	3:C:325:PRO:O	2.14	0.48
4:D:523:PRO:HG3	4:D:564:LEU:HD21	1.96	0.48
1:A:688:LEU:HG	1:A:692:LEU:HD23	1.96	0.48
2:B:69:LYS:O	2:B:75:VAL:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:GLU:O	2:B:342:ILE:HG12	2.14	0.48
4:D:615:GLN:O	4:D:618:LEU:HG	2.14	0.48
4:D:721:ILE:HG23	4:D:809:LEU:HD23	1.95	0.48
1:A:321:LEU:HD23	1:A:372:LEU:HD21	1.96	0.47
1:A:521:LEU:HD13	1:A:565:ALA:HA	1.95	0.47
4:D:917:TYR:CZ	4:D:944:GLY:HA3	2.49	0.47
1:A:36:PHE:HA	1:A:39:VAL:HG12	1.96	0.47
2:B:52:LEU:HD22	2:B:71:CYS:HB2	1.97	0.47
4:D:864:GLN:HB2	4:D:914:LEU:HD12	1.96	0.47
1:A:264:LEU:HG	1:A:268:ARG:HH21	1.78	0.47
3:C:321:VAL:HG21	3:C:340:TRP:HH2	1.79	0.47
4:D:478:THR:HG23	4:D:481:GLY:N	2.28	0.47
3:C:274:LYS:HE3	3:C:277:HIS:HD2	1.79	0.47
4:D:486:LEU:HD22	4:D:550:LEU:HD23	1.96	0.47
4:D:837:PHE:HZ	4:D:903:TRP:HB2	1.77	0.47
1:A:472:GLN:O	1:A:476:ARG:HG3	2.15	0.47
1:A:713:ARG:HB2	3:C:113:ASP:OD1	2.14	0.47
2:B:306:TYR:HH	2:B:336:SER:HG	1.50	0.47
2:B:393:VAL:HG11	2:B:408:PHE:CE2	2.49	0.47
4:D:293:ASP:OD1	4:D:294:GLY:N	2.48	0.47
4:D:632:ALA:O	4:D:635:LEU:HG	2.15	0.47
4:D:721:ILE:HD13	4:D:811:LEU:HD12	1.97	0.47
2:B:401:ARG:NH2	2:B:435:PRO:HG2	2.30	0.47
3:C:32:ASP:CG	3:C:73:HIS:HD1	2.22	0.47
3:C:266:TYR:HE1	3:C:306:LYS:HB2	1.80	0.47
3:C:423:LEU:O	3:C:427:ILE:HG13	2.15	0.47
1:A:251:ASP:HB3	1:A:252:PRO:HD3	1.96	0.47
1:A:433:LEU:HD22	1:A:453:LEU:HD21	1.96	0.47
3:C:308:PHE:CZ	3:C:313:ALA:HB2	2.50	0.47
3:C:338:ARG:HB2	3:C:372:MET:HE3	1.97	0.47
2:B:245:THR:OG1	2:B:247:PRO:HD2	2.14	0.47
2:B:393:VAL:HG12	2:B:395:THR:HG22	1.96	0.47
4:D:698:LYS:O	4:D:702:GLU:HG2	2.15	0.47
3:C:36:HIS:ND1	3:C:37:MET:O	2.48	0.46
4:D:197:GLN:HE22	4:D:230:HIS:HB2	1.80	0.46
3:C:16:GLY:HA3	3:C:36:HIS:HD2	1.79	0.46
3:C:101:PRO:HG3	3:C:130:MET:HG3	1.96	0.46
4:D:387:MET:HE3	4:D:387:MET:HA	1.97	0.46
2:B:420:VAL:HG23	2:B:441:MET:HE2	1.98	0.46
4:D:387:MET:O	4:D:390:VAL:HG22	2.15	0.46
4:D:536:GLU:OE2	4:D:572:HIS:NE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:632:ALA:O	4:D:636:LEU:HG	2.16	0.46
1:A:6:ALA:HA	1:A:9:LEU:HG	1.98	0.46
2:B:472:PRO:HG3	2:B:499:TYR:OH	2.15	0.46
1:A:564:SER:HA	1:A:567:THR:HG22	1.97	0.46
2:B:130:VAL:HG21	2:B:194:ILE:HG21	1.98	0.46
2:B:139:GLU:HG3	2:B:140:LEU:N	2.30	0.46
2:B:199:TYR:OH	2:B:221:GLY:HA2	2.15	0.46
2:B:329:ILE:HD11	2:B:383:PHE:CE1	2.51	0.46
3:C:206:TYR:HH	3:C:390:SER:HG	1.63	0.46
4:D:445:ARG:NH2	4:D:447:ASP:OD2	2.49	0.46
4:D:456:LEU:HD23	4:D:492:ASN:HD22	1.81	0.46
1:A:162:SER:O	1:A:166:GLN:HG2	2.15	0.46
4:D:249:ARG:HB2	4:D:298:VAL:HG11	1.97	0.46
2:B:6:LEU:HD22	2:B:87:GLU:HB2	1.97	0.46
3:C:217:ARG:HB3	3:C:389:PHE:CE1	2.51	0.46
3:C:223:LYS:HD3	3:C:223:LYS:HA	1.81	0.46
4:D:866:LEU:HB3	4:D:910:GLU:HB3	1.98	0.46
1:A:605:GLU:O	1:A:609:ARG:NH1	2.49	0.46
2:B:100:LEU:HD13	2:B:225:TRP:CD2	2.50	0.46
2:B:305:ILE:HG12	2:B:328:PHE:HE2	1.81	0.46
4:D:459:SER:O	4:D:464:ARG:NH1	2.49	0.46
1:A:450:LEU:HB3	1:A:497:PHE:CE1	2.51	0.46
4:D:269:PRO:HA	4:D:276:GLU:HA	1.98	0.46
1:A:271:VAL:O	1:A:274:SER:OG	2.31	0.45
1:A:478:LEU:HB3	1:A:531:TRP:CH2	2.51	0.45
4:D:400:MET:HE3	4:D:400:MET:O	2.16	0.45
1:A:506:GLN:NE2	1:A:545:GLU:HB3	2.31	0.45
2:B:8:GLY:H	2:B:501:ARG:HG3	1.81	0.45
3:C:83:MET:HG2	3:C:125:MET:HE1	1.98	0.45
3:C:153:TYR:HH	3:C:193:ASP:CG	2.24	0.45
3:C:256:TRP:CH2	3:C:263:VAL:HB	2.46	0.45
1:A:287:LEU:HD11	1:A:299:ALA:HB2	1.97	0.45
1:A:395:VAL:HG12	1:A:452:VAL:HG11	1.98	0.45
4:D:252:ALA:O	4:D:256:ILE:HG13	2.17	0.45
1:A:370:ALA:O	1:A:373:GLU:HG3	2.16	0.45
4:D:769:LEU:HA	4:D:772:LEU:HG	1.99	0.45
3:C:17:ARG:HA	3:C:35:MET:O	2.16	0.45
4:D:257:TRP:CG	4:D:305:LEU:HD22	2.51	0.45
1:A:147:ASP:OD1	1:A:147:ASP:N	2.49	0.45
1:A:216:GLN:HA	1:A:219:ASN:ND2	2.32	0.45
1:A:512:PRO:HB3	2:B:315:TYR:HD1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:LEU:HD22	1:A:577:LEU:HB2	1.97	0.45
1:A:707:ALA:O	1:A:710:ASP:HB2	2.17	0.45
2:B:281:PHE:CZ	2:B:308:LEU:HD21	2.51	0.45
2:B:296:LEU:O	2:B:298:PRO:HD3	2.17	0.45
4:D:553:ASN:OD1	4:D:585:PRO:HD3	2.17	0.45
4:D:567:ASP:OD1	4:D:568:HIS:N	2.48	0.45
4:D:572:HIS:O	4:D:576:LEU:HG	2.17	0.45
4:D:715:GLU:O	4:D:719:VAL:HG23	2.16	0.45
1:A:544:SER:OG	1:A:545:GLU:N	2.49	0.45
1:A:711:CYS:HB3	3:C:331:GLY:O	2.16	0.45
1:A:780:ASP:OD1	1:A:781:LEU:N	2.49	0.45
2:B:425:PRO:HG3	2:B:449:ASP:OD1	2.17	0.45
3:C:325:PRO:HG3	3:C:332:GLN:H	1.80	0.45
4:D:76:LEU:HD12	4:D:92:ILE:HG23	1.97	0.45
3:C:147:GLU:O	3:C:168:VAL:HA	2.16	0.45
3:C:217:ARG:HB3	3:C:389:PHE:HE1	1.81	0.45
3:C:236:LEU:HB3	3:C:348:VAL:HG12	1.98	0.45
4:D:244:ASP:HA	4:D:249:ARG:HH12	1.81	0.45
1:A:116:VAL:O	1:A:119:VAL:HG12	2.17	0.45
4:D:507:LEU:HD12	4:D:546:ALA:HB1	1.99	0.45
4:D:721:ILE:HD13	4:D:811:LEU:HA	1.99	0.45
1:A:708:LEU:HD21	1:A:784:LEU:HD23	1.99	0.44
1:A:818:ALA:HA	3:C:353:TYR:CD1	2.52	0.44
3:C:156:GLY:C	3:C:158:VAL:H	2.25	0.44
3:C:246:GLN:N	3:C:246:GLN:OE1	2.50	0.44
4:D:97:GLY:O	4:D:100:SER:OG	2.33	0.44
4:D:268:VAL:HG21	4:D:279:LEU:HD13	1.99	0.44
4:D:559:PRO:C	4:D:562:PRO:HD2	2.42	0.44
4:D:646:LEU:HA	4:D:649:LEU:HD12	1.99	0.44
2:B:11:THR:HG21	2:B:268:GLN:HG3	1.99	0.44
2:B:85:LEU:HD11	2:B:112:TYR:CG	2.52	0.44
2:B:110:LEU:O	2:B:114:THR:HG22	2.17	0.44
3:C:203:GLU:HA	3:C:413:VAL:O	2.16	0.44
1:A:206:LEU:HD21	1:A:218:LEU:HD12	1.99	0.44
1:A:729:LYS:HA	1:A:729:LYS:HD2	1.62	0.44
4:D:458:ASP:OD1	4:D:459:SER:N	2.47	0.44
4:D:826:GLU:HB3	4:D:848:ASP:HB3	1.99	0.44
3:C:412:LEU:HD11	3:C:423:LEU:HD23	2.00	0.44
2:B:9:HIS:CE1	2:B:12:LEU:HD23	2.52	0.44
2:B:503:GLU:HG3	2:B:504:VAL:H	1.83	0.44
1:A:610:ARG:HD3	1:A:649:GLU:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ARG:NH1	1:A:112:ALA:H	2.15	0.44
1:A:515:GLU:OE1	1:A:515:GLU:N	2.43	0.44
1:A:821:TYR:CE2	3:C:37:MET:HB2	2.52	0.44
2:B:321:LEU:HD23	2:B:321:LEU:HA	1.87	0.44
4:D:127:LEU:HD12	4:D:127:LEU:H	1.83	0.44
1:A:128:ARG:CZ	1:A:166:GLN:HB3	2.48	0.44
1:A:432:PHE:O	1:A:435:THR:N	2.51	0.44
1:A:630:ASP:N	1:A:630:ASP:OD1	2.51	0.44
4:D:206:ASP:OD1	4:D:207:GLN:N	2.47	0.44
4:D:616:GLN:O	4:D:620:ARG:HG3	2.18	0.44
1:A:381:ARG:HD2	1:A:385:TRP:CD2	2.53	0.43
2:B:19:PHE:CG	2:B:20:LYS:N	2.84	0.43
3:C:328:LEU:HD12	3:C:360:GLY:HA2	2.00	0.43
4:D:436:ARG:HH22	4:D:887:PRO:HD3	1.83	0.43
1:A:212:PRO:O	1:A:216:GLN:HG2	2.18	0.43
2:B:269:ILE:HD11	2:B:449:ASP:HB2	1.99	0.43
4:D:155:ALA:O	4:D:159:LEU:N	2.51	0.43
1:A:365:LEU:HD23	1:A:365:LEU:HA	1.86	0.43
1:A:548:GLN:HG2	1:A:579:ALA:HB1	1.99	0.43
4:D:290:MET:HE3	4:D:293:ASP:HB2	1.98	0.43
4:D:312:VAL:CG1	4:D:317:LEU:HD21	2.48	0.43
4:D:449:LEU:HA	4:D:452:VAL:HG12	2.00	0.43
1:A:799:PRO:O	1:A:803:LEU:HG	2.18	0.43
3:C:24:ILE:HG22	3:C:25:ALA:H	1.83	0.43
4:D:414:ASP:N	4:D:414:ASP:OD1	2.51	0.43
1:A:600:LEU:HD21	1:A:613:MET:HE1	2.00	0.43
2:B:253:ALA:O	2:B:256:LYS:HG3	2.18	0.43
2:B:263:LEU:HD21	2:B:457:VAL:HG21	2.00	0.43
3:C:150:ILE:HA	3:C:165:GLN:O	2.18	0.43
4:D:479:LYS:HG2	4:D:517:LEU:HA	2.00	0.43
4:D:863:VAL:CG1	4:D:875:ILE:HB	2.49	0.43
1:A:793:ASP:HB2	1:A:796:GLU:HG2	2.01	0.43
3:C:138:LEU:HD11	3:C:285:TRP:CZ2	2.53	0.43
3:C:171:GLU:OE1	3:C:171:GLU:N	2.51	0.43
3:C:224:LYS:O	3:C:228:THR:HG22	2.18	0.43
2:B:201:GLN:HG2	2:B:203:ILE:HD11	2.01	0.43
2:B:202:LYS:HB3	2:B:210:GLN:HE21	1.83	0.43
4:D:568:HIS:HD2	4:D:572:HIS:CE1	2.37	0.43
2:B:408:PHE:O	2:B:411:LEU:N	2.50	0.43
4:D:846:ASP:OD1	4:D:895:GLN:HG2	2.19	0.43
1:A:689:THR:OG1	1:A:690:GLU:OE1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:MET:SD	2:B:133:GLY:HA3	2.58	0.43
2:B:277:MET:HE3	2:B:447:PRO:HD2	2.01	0.43
3:C:269:THR:HG22	3:C:272:THR:H	1.84	0.43
3:C:328:LEU:HG	3:C:350:MET:HE1	2.01	0.43
4:D:70:GLU:O	4:D:74:ARG:HG2	2.17	0.43
4:D:132:ASP:HB2	4:D:169:LYS:NZ	2.33	0.43
4:D:839:SER:HB2	4:D:960:PRO:HA	2.00	0.43
1:A:256:ALA:O	1:A:260:VAL:HG23	2.18	0.43
1:A:639:LEU:HD23	1:A:639:LEU:HA	1.82	0.43
2:B:298:PRO:HG3	2:B:405:VAL:HG21	2.01	0.43
3:C:13:GLN:NE2	3:C:437:MET:HE3	2.33	0.43
3:C:14:ASP:OD1	3:C:15:VAL:N	2.50	0.43
4:D:696:ALA:O	4:D:700:ILE:HG12	2.19	0.43
4:D:765:PHE:HB3	4:D:768:ASP:OD1	2.18	0.43
1:A:236:LEU:O	1:A:240:LEU:HG	2.18	0.42
1:A:347:ASP:OD1	1:A:348:ALA:N	2.52	0.42
2:B:127:GLU:O	2:B:130:VAL:HG12	2.18	0.42
2:B:143:PHE:CD1	2:B:403:GLY:HA2	2.53	0.42
3:C:12:GLY:HA3	3:C:440:ASN:HA	2.01	0.42
3:C:308:PHE:HZ	3:C:313:ALA:HB2	1.84	0.42
3:C:340:TRP:CD1	3:C:340:TRP:N	2.87	0.42
4:D:577:ARG:HA	4:D:577:ARG:HD2	1.82	0.42
1:A:446:VAL:HG11	1:A:481:SER:OG	2.19	0.42
2:B:67:GLU:CD	2:B:153:ALA:HB1	2.44	0.42
2:B:103:ASN:OD1	2:B:103:ASN:N	2.52	0.42
3:C:32:ASP:OD2	3:C:73:HIS:ND1	2.43	0.42
3:C:266:TYR:CE1	3:C:306:LYS:HB2	2.54	0.42
4:D:145:GLN:HA	4:D:148:GLN:HG2	2.01	0.42
4:D:869:ASP:OD1	4:D:870:GLY:N	2.51	0.42
1:A:365:LEU:HD12	1:A:419:LEU:HD11	2.01	0.42
1:A:427:ARG:HD2	1:A:469:LYS:HE2	2.01	0.42
2:B:127:GLU:HB3	2:B:128:PRO:HD3	2.01	0.42
4:D:447:ASP:OD1	4:D:448:GLN:N	2.53	0.42
2:B:379:ILE:HG23	4:D:842:VAL:HG21	2.01	0.42
3:C:274:LYS:HG2	3:C:277:HIS:CD2	2.54	0.42
4:D:293:ASP:OD1	4:D:295:SER:N	2.50	0.42
1:A:88:ASN:OD1	1:A:89:CYS:N	2.52	0.42
1:A:128:ARG:NH2	1:A:166:GLN:HB3	2.33	0.42
3:C:19:CYS:SG	3:C:30:MET:HE2	2.58	0.42
4:D:508:LYS:HA	4:D:553:ASN:HD21	1.85	0.42
2:B:267:THR:HG22	2:B:269:ILE:N	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:492:CYS:SG	2:B:496:ALA:HB2	2.60	0.42
4:D:77:LEU:HD11	4:D:117:ILE:HD11	2.02	0.42
1:A:175:SER:OG	1:A:176:MET:N	2.52	0.42
1:A:209:ALA:HA	1:A:250:ARG:HH12	1.85	0.42
1:A:226:GLY:H	1:A:229:GLN:NE2	2.18	0.42
2:B:205:LEU:HD23	2:B:205:LEU:HA	1.82	0.42
2:B:100:LEU:O	2:B:101:ILE:HG13	2.19	0.42
3:C:78:PRO:HG2	3:C:104:LEU:HD13	2.01	0.42
1:A:206:LEU:HD23	1:A:206:LEU:HA	1.73	0.42
3:C:4:ILE:O	3:C:446:LEU:HD23	2.20	0.42
3:C:157:HIS:HD2	3:C:158:VAL:HG22	1.84	0.42
3:C:248:LEU:HD23	3:C:248:LEU:HA	1.86	0.42
4:D:85:ASP:OD1	4:D:87:SER:OG	2.29	0.42
4:D:717:LYS:H	4:D:717:LYS:HG3	1.62	0.42
2:B:14:CYS:SG	2:B:28:CYS:HA	2.60	0.42
4:D:126:VAL:HG13	4:D:127:LEU:H	1.85	0.42
4:D:699:GLN:O	4:D:703:GLU:HG2	2.20	0.42
4:D:707:MET:HA	4:D:711:TYR:HD2	1.84	0.42
1:A:521:LEU:HD23	1:A:521:LEU:HA	1.84	0.41
2:B:15:ASN:OD1	2:B:15:ASN:N	2.49	0.41
2:B:266:LEU:HB2	2:B:475:TYR:CZ	2.54	0.41
4:D:720:VAL:HG13	4:D:768:ASP:OD2	2.20	0.41
4:D:753:LYS:O	4:D:757:GLU:HG2	2.19	0.41
2:B:135:LEU:HD21	2:B:336:SER:HB2	2.01	0.41
3:C:94:HIS:HB3	3:C:95:PRO:HD3	2.02	0.41
3:C:182:THR:O	3:C:184:ASP:N	2.53	0.41
4:D:618:LEU:O	4:D:621:VAL:HG12	2.21	0.41
4:D:918:ASN:OD1	4:D:918:ASN:N	2.52	0.41
2:B:48:ARG:HG2	2:B:49:LEU:HD23	2.01	0.41
4:D:613:PHE:O	4:D:616:GLN:HG3	2.19	0.41
4:D:821:SER:OG	4:D:852:GLU:OE2	2.38	0.41
2:B:4:TYR:CD1	2:B:504:VAL:HG12	2.56	0.41
2:B:4:TYR:CZ	2:B:18:LYS:HD2	2.55	0.41
2:B:180:ARG:HG2	2:B:181:CYS:N	2.35	0.41
3:C:221:PHE:HB2	3:C:389:PHE:HZ	1.84	0.41
1:A:805:ASP:OD1	3:C:362:LYS:HG2	2.20	0.41
2:B:38:PHE:CD1	2:B:77:VAL:HB	2.55	0.41
2:B:103:ASN:ND2	2:B:218:TYR:HD2	2.17	0.41
2:B:281:PHE:CD1	2:B:308:LEU:HD11	2.56	0.41
3:C:44:ARG:HH21	3:C:45:PHE:HE1	1.68	0.41
3:C:256:TRP:CH2	3:C:265:ILE:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:312:VAL:HG13	4:D:317:LEU:HD21	2.01	0.41
4:D:582:HIS:CE1	4:D:583:LEU:HG	2.55	0.41
2:B:31:ASP:O	2:B:84:CYS:HB3	2.20	0.41
4:D:619:GLU:HA	4:D:622:TYR:CD2	2.56	0.41
1:A:549:LEU:HD23	1:A:549:LEU:HA	1.85	0.41
1:A:576:GLY:O	1:A:577:LEU:HD23	2.21	0.41
2:B:38:PHE:HD1	2:B:77:VAL:HB	1.86	0.41
3:C:274:LYS:HB3	3:C:278:TYR:HB2	2.02	0.41
4:D:444:LEU:HD22	4:D:449:LEU:HD13	2.02	0.41
4:D:707:MET:HA	4:D:711:TYR:CD2	2.56	0.41
1:A:102:LEU:O	1:A:108:PRO:HD2	2.20	0.41
1:A:237:TRP:O	1:A:241:SER:OG	2.33	0.41
1:A:647:ASP:OD1	1:A:648:TRP:N	2.47	0.41
1:A:787:THR:HG23	1:A:788:LEU:HD22	2.02	0.41
1:A:800:GLN:O	1:A:804:GLN:HG3	2.21	0.41
1:A:221:LEU:HD23	1:A:221:LEU:HA	1.87	0.41
1:A:458:GLU:HB3	1:A:504:VAL:HG13	2.03	0.41
3:C:107:TYR:CE2	3:C:120:PHE:HZ	2.38	0.41
3:C:156:GLY:O	3:C:157:HIS:HB3	2.19	0.41
4:D:169:LYS:HA	4:D:169:LYS:HD3	1.72	0.41
4:D:577:ARG:O	4:D:581:SER:OG	2.22	0.41
4:D:723:HIS:HB3	4:D:761:PHE:HE1	1.85	0.41
4:D:900:HIS:CG	4:D:901:THR:H	2.38	0.41
4:D:914:LEU:HD22	4:D:945:THR:HB	2.01	0.41
1:A:58:LEU:O	1:A:62:VAL:HG13	2.21	0.41
1:A:175:SER:OG	1:A:195:ALA:HB2	2.20	0.41
2:B:1:MET:HG2	2:B:232:GLU:OE1	2.21	0.41
2:B:66:LYS:HD2	2:B:66:LYS:HA	1.81	0.41
3:C:328:LEU:HD23	3:C:328:LEU:HA	1.88	0.41
4:D:257:TRP:CD2	4:D:305:LEU:HD22	2.56	0.41
4:D:753:LYS:HA	4:D:753:LYS:HD2	1.92	0.41
1:A:37:LYS:HE2	1:A:37:LYS:HB3	1.89	0.40
1:A:177:ARG:HH11	1:A:177:ARG:HA	1.84	0.40
2:B:2:LYS:HZ3	4:D:90:LEU:HD13	1.86	0.40
2:B:236:TYR:CZ	2:B:238:SER:HB3	2.56	0.40
4:D:543:ALA:O	4:D:547:VAL:HG13	2.21	0.40
4:D:882:PHE:CZ	4:D:892:LEU:HD13	2.55	0.40
4:D:461:ARG:HH12	4:D:498:THR:HG1	1.62	0.40
1:A:62:VAL:HG12	1:A:68:LEU:HD11	2.02	0.40
1:A:116:VAL:HG22	1:A:118:THR:H	1.85	0.40
2:B:57:LEU:HD23	2:B:60:GLY:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:250:ILE:O	3:C:254:THR:HG22	2.20	0.40
2:B:100:LEU:HB3	2:B:225:TRP:NE1	2.36	0.40
2:B:289:VAL:CG1	2:B:324:VAL:HG11	2.52	0.40
4:D:413:LEU:O	4:D:417:VAL:HG22	2.22	0.40
4:D:416:LEU:HG	4:D:435:MET:CE	2.51	0.40
4:D:861:VAL:O	4:D:862:LYS:NZ	2.49	0.40
4:D:898:LEU:HD13	4:D:909:VAL:HG21	2.04	0.40
2:B:84:CYS:SG	2:B:85:LEU:N	2.92	0.40
2:B:288:THR:HG21	2:B:419:THR:OG1	2.21	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	698/827 (84%)	666 (95%)	32 (5%)	0	100	100
2	B	479/658 (73%)	427 (89%)	52 (11%)	0	100	100
3	C	423/612 (69%)	371 (88%)	52 (12%)	0	100	100
4	D	690/973 (71%)	665 (96%)	25 (4%)	0	100	100
All	All	2290/3070 (75%)	2129 (93%)	161 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	600/677 (89%)	600 (100%)	0	100	100
2	B	438/600 (73%)	438 (100%)	0	100	100
3	C	363/529 (69%)	363 (100%)	0	100	100
4	D	629/852 (74%)	629 (100%)	0	100	100
All	All	2030/2658 (76%)	2030 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	196	GLN
1	A	229	GLN
1	A	257	HIS
1	A	307	HIS
1	A	426	GLN
1	A	552	GLN
1	A	717	GLN
2	B	45	GLN
2	B	74	HIS
2	B	210	GLN
2	B	389	GLN
2	B	465	GLN
3	C	94	HIS
3	C	97	GLN
3	C	119	ASN
3	C	137	HIS
3	C	165	GLN
3	C	260	ASN
3	C	277	HIS
3	C	335	GLN
3	C	440	ASN
4	D	84	ASN
4	D	144	ASN
4	D	168	ASN
4	D	176	ASN
4	D	221	GLN
4	D	403	GLN
4	D	553	ASN
4	D	568	HIS

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Mol	Chain	Res	Type
4	D	582	HIS
4	D	633	GLN
4	D	724	HIS
4	D	810	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

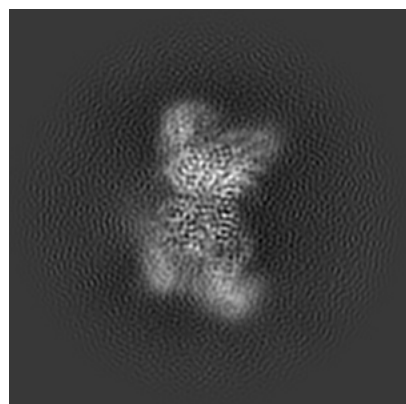
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18839. These allow visual inspection of the internal detail of the map and identification of artifacts.

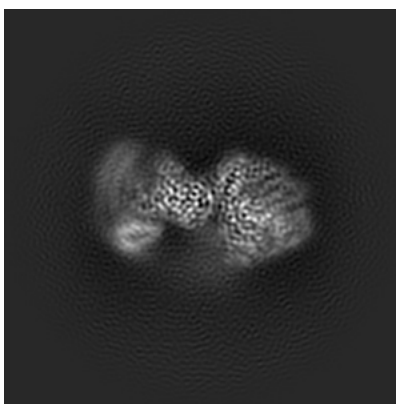
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

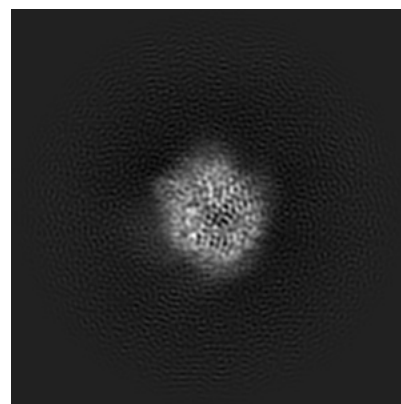
6.1.1 Primary map



X

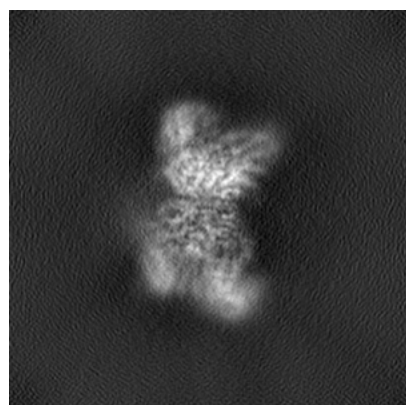


Y

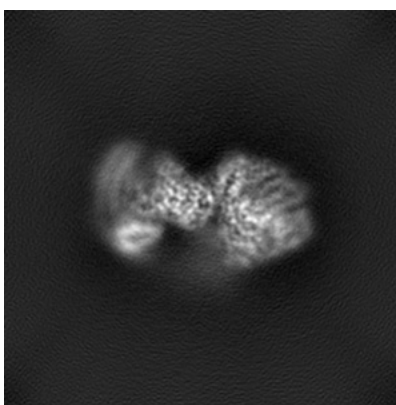


Z

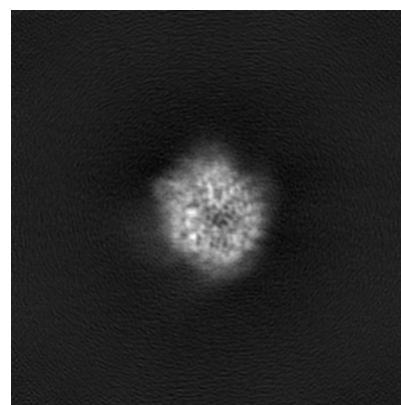
6.1.2 Raw map



X



Y

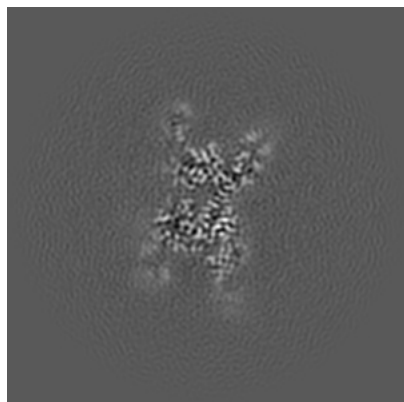


Z

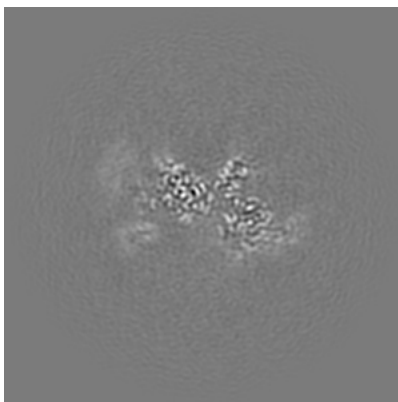
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

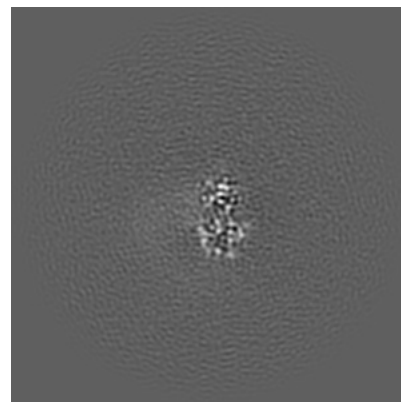
6.2.1 Primary map



X Index: 115

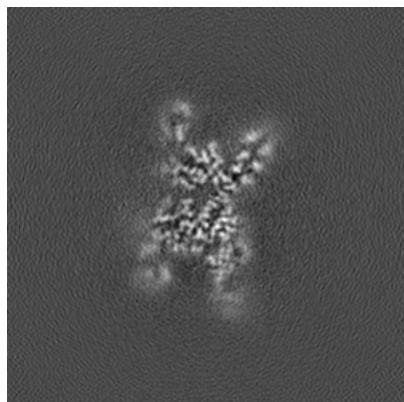


Y Index: 115

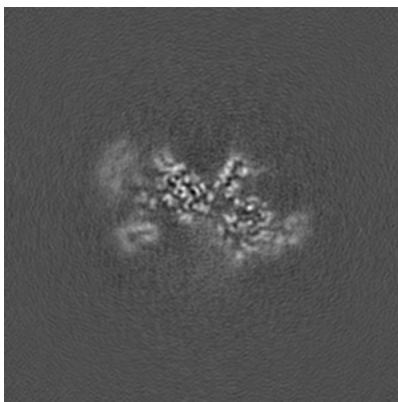


Z Index: 115

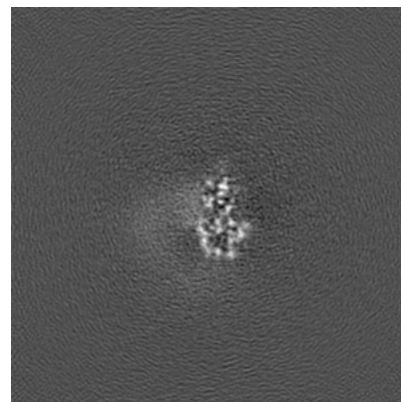
6.2.2 Raw map



X Index: 115



Y Index: 115

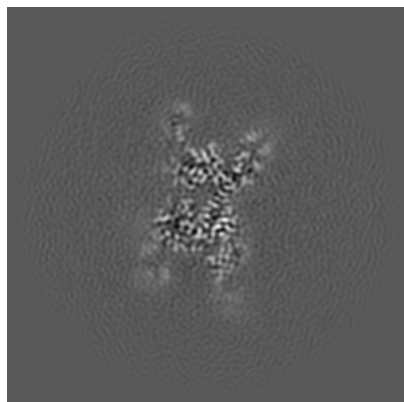


Z Index: 115

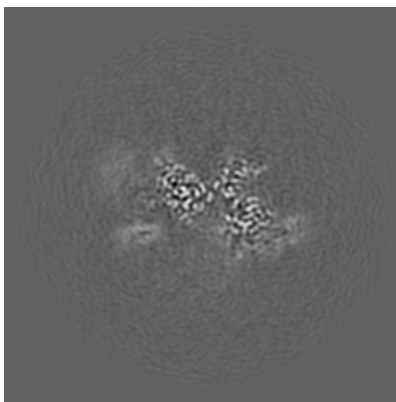
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

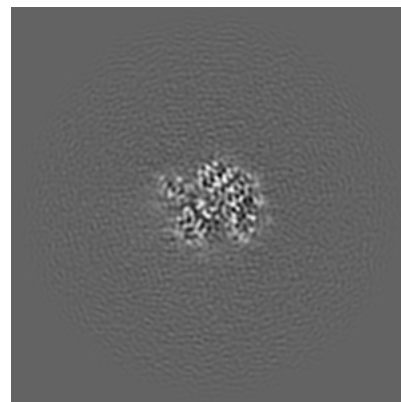
6.3.1 Primary map



X Index: 115

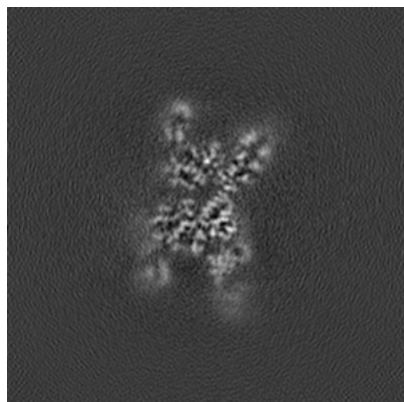


Y Index: 114

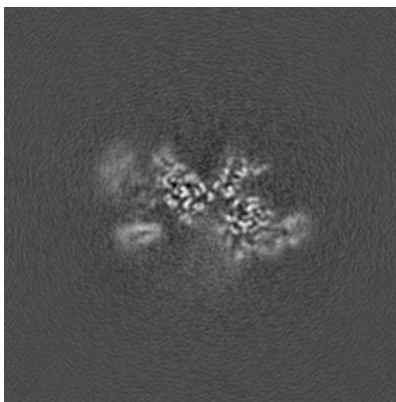


Z Index: 132

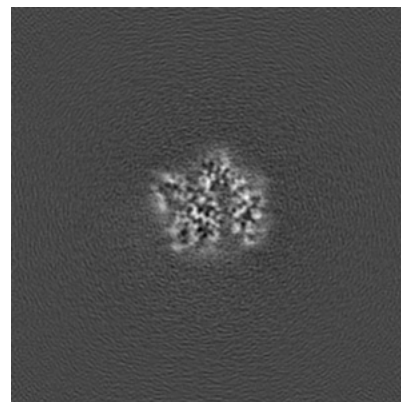
6.3.2 Raw map



X Index: 114



Y Index: 114

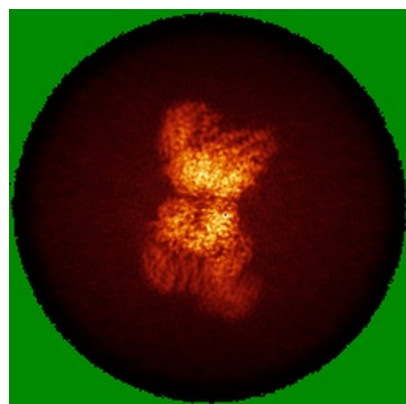


Z Index: 135

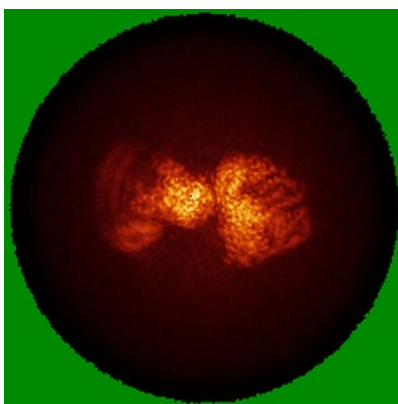
The images above show the largest variance slices of the map in three orthogonal directions.

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

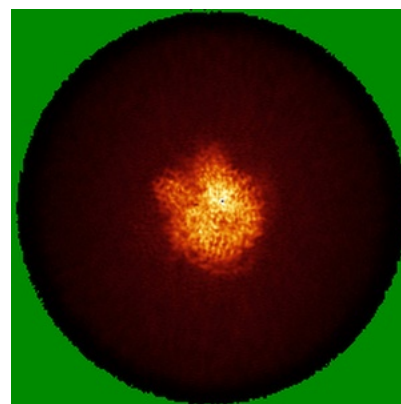
6.4.1 Primary map



X

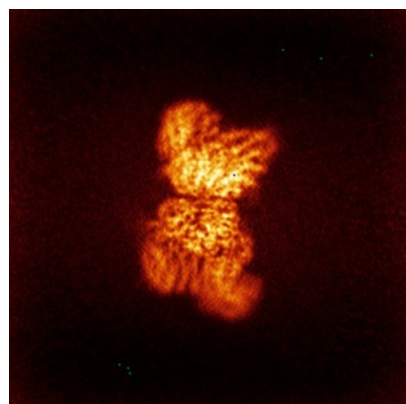


Y

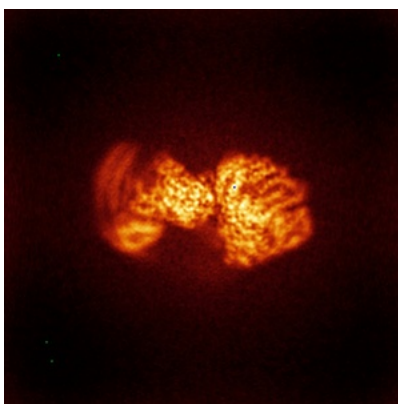


Z

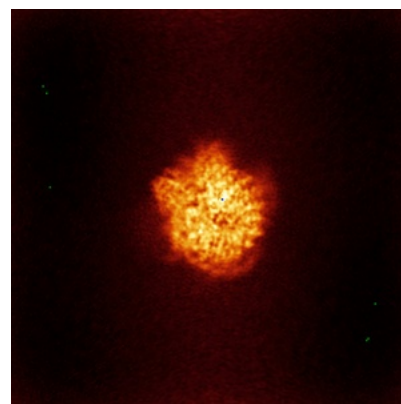
6.4.2 Raw map



X



Y

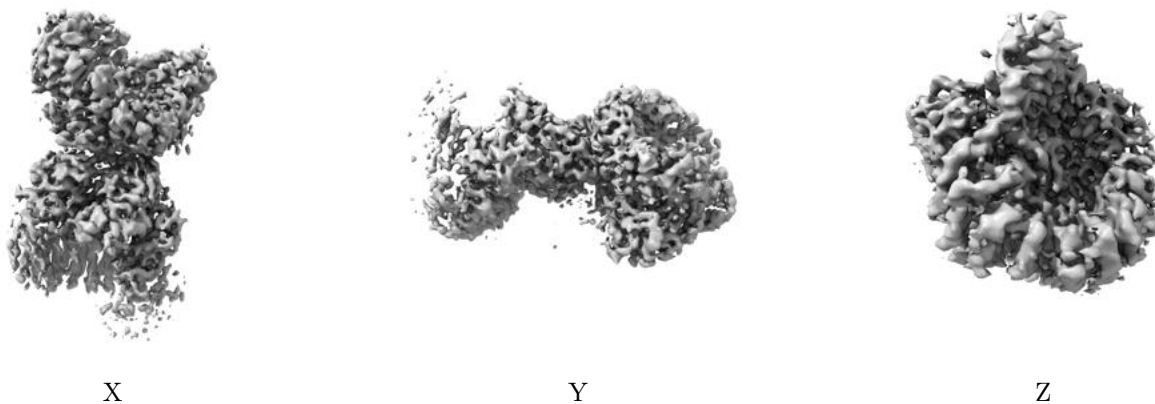


Z

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.

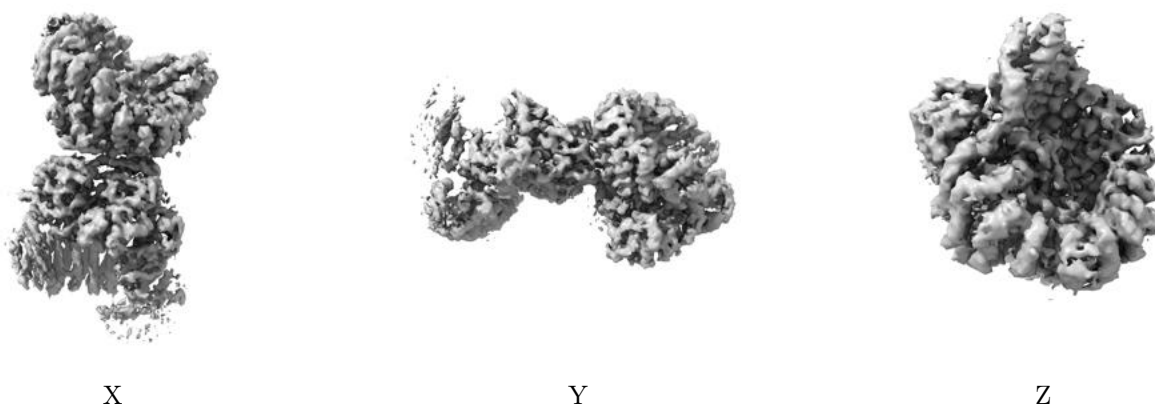
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.324. 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.

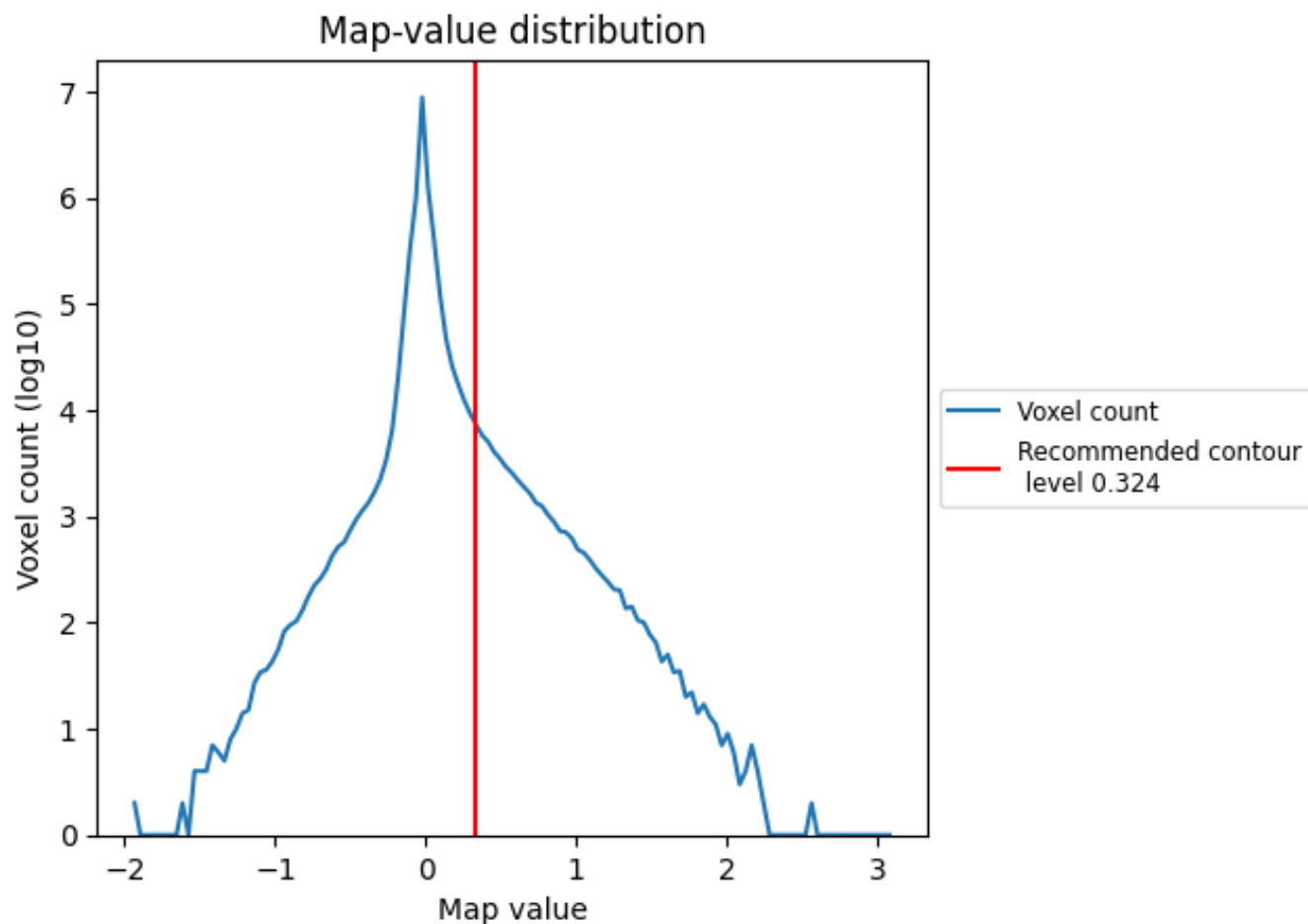
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

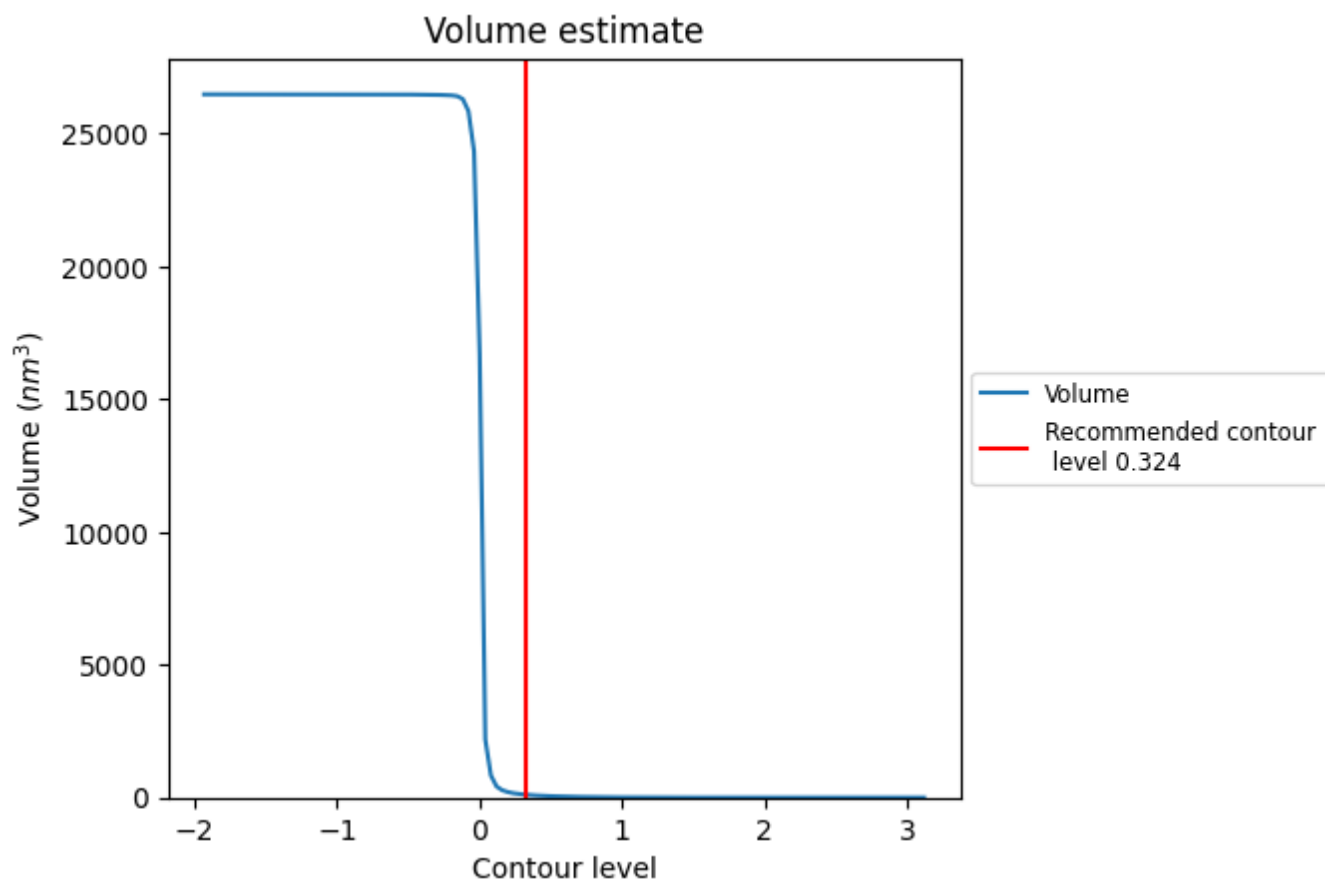
This section contains the results of statistical analysis of the map.

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.

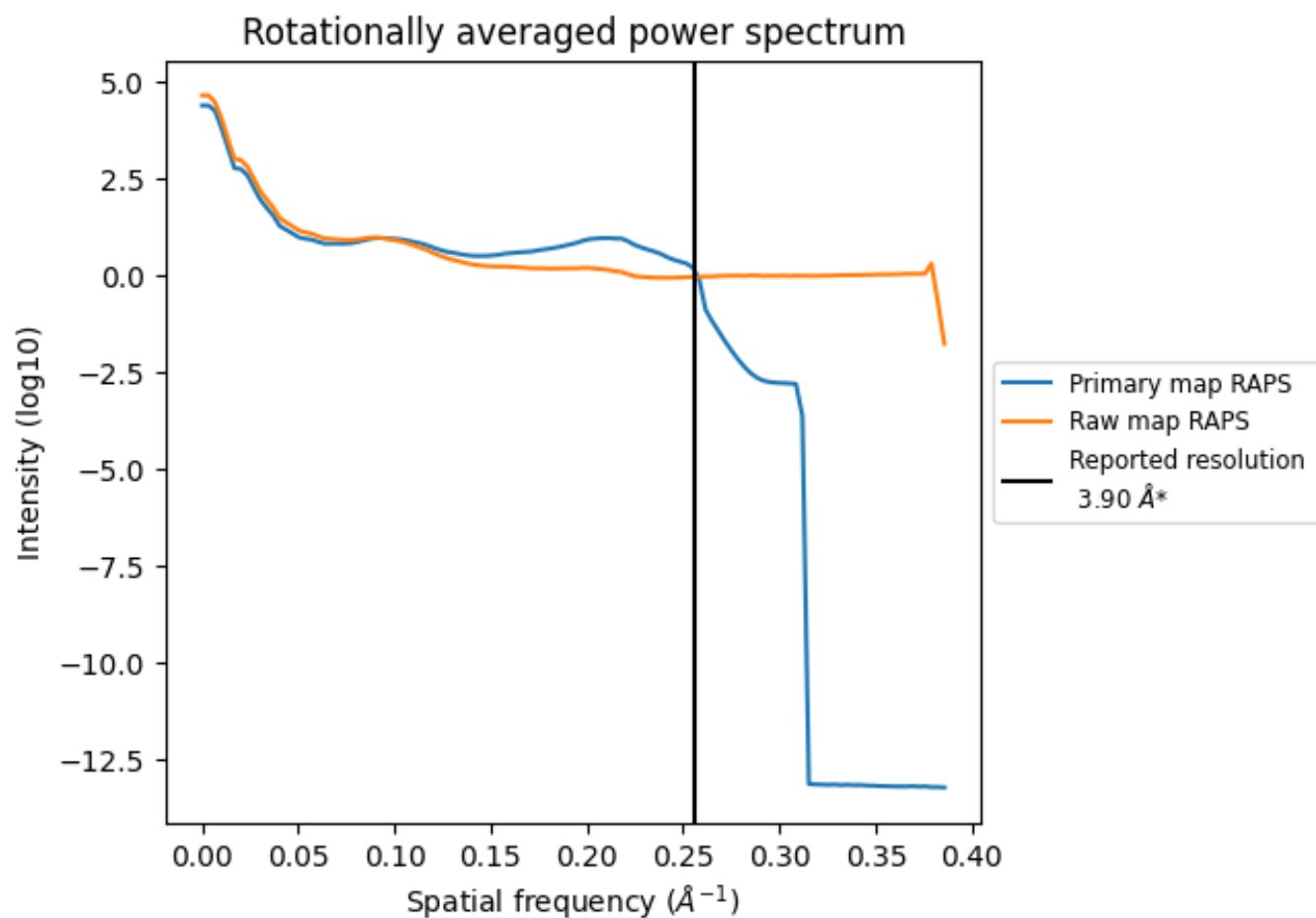
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 107 nm³; this corresponds to an approximate mass of 96 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 ⓘ

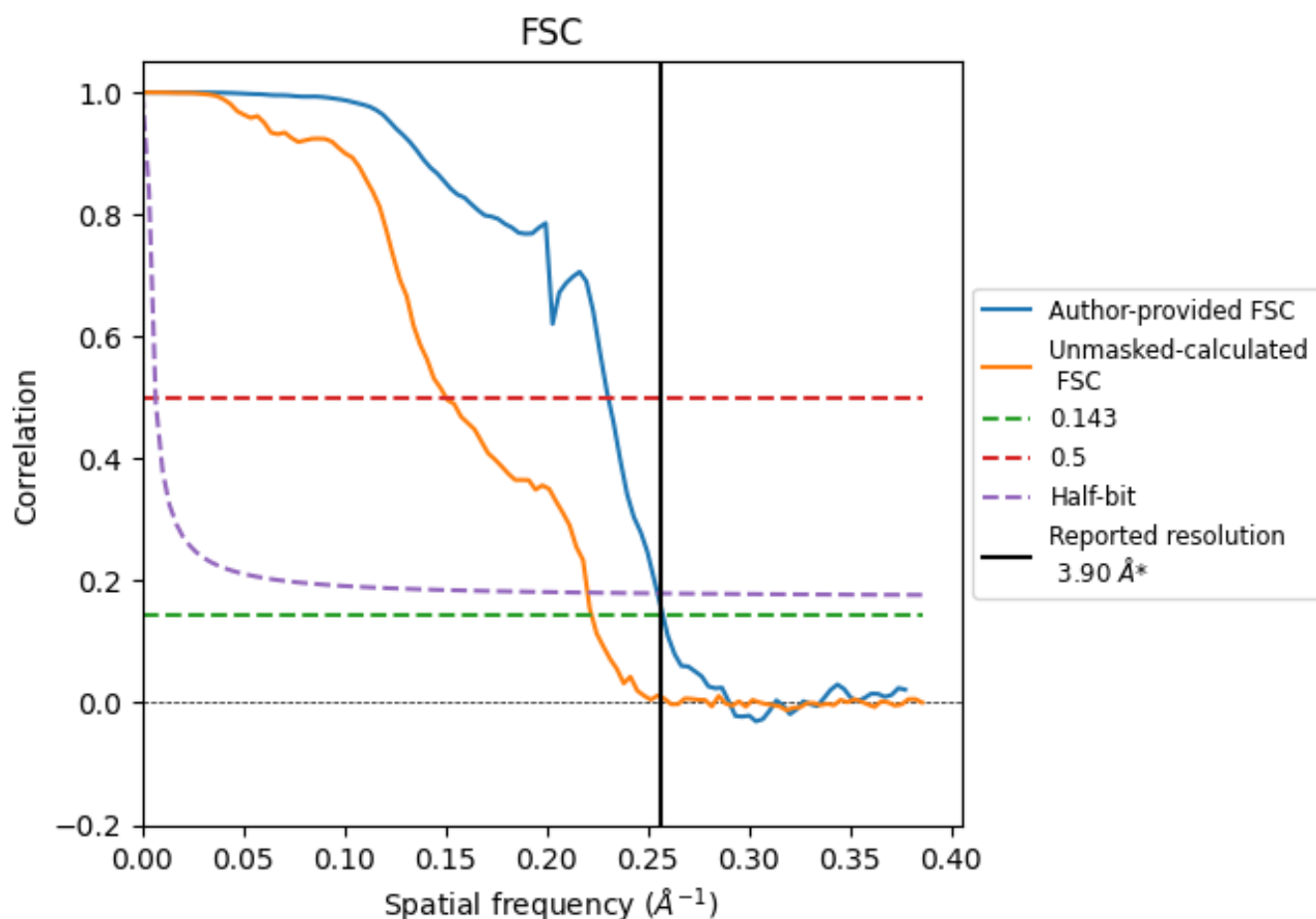


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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](#)

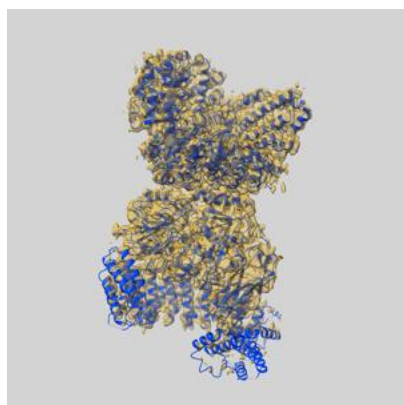
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.88	4.34	3.92
Unmasked-calculated*	4.50	6.65	4.54

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

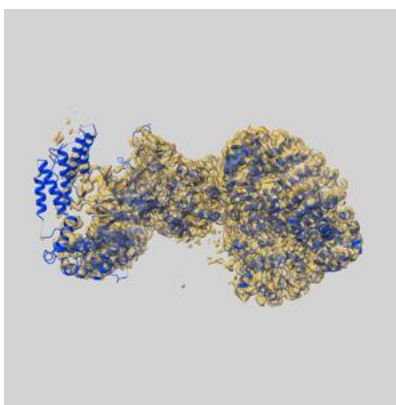
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18839 and PDB model 8R2D. Per-residue inclusion information can be found in section [3](#) on page [5](#).

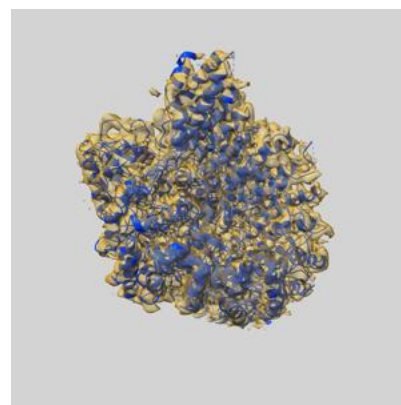
9.1 Map-model overlay [i](#)



X



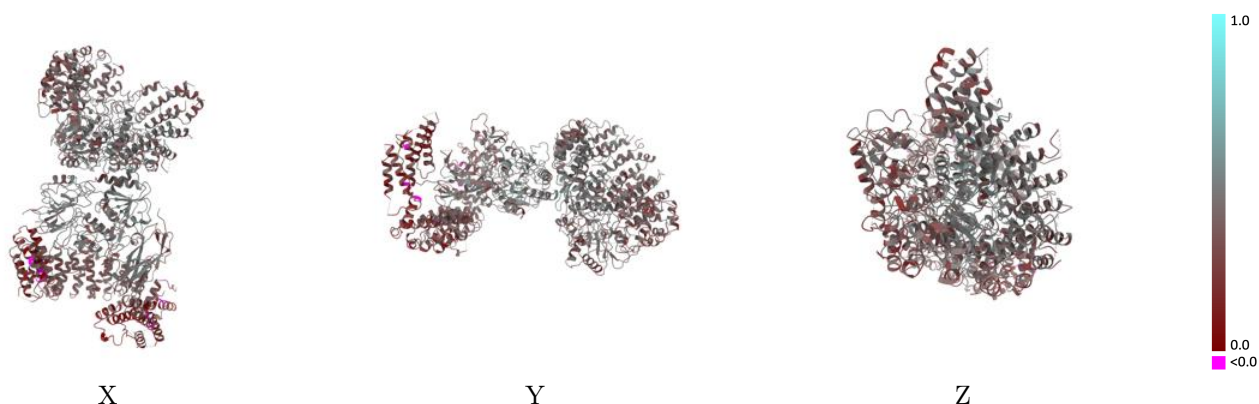
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.324 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](#)

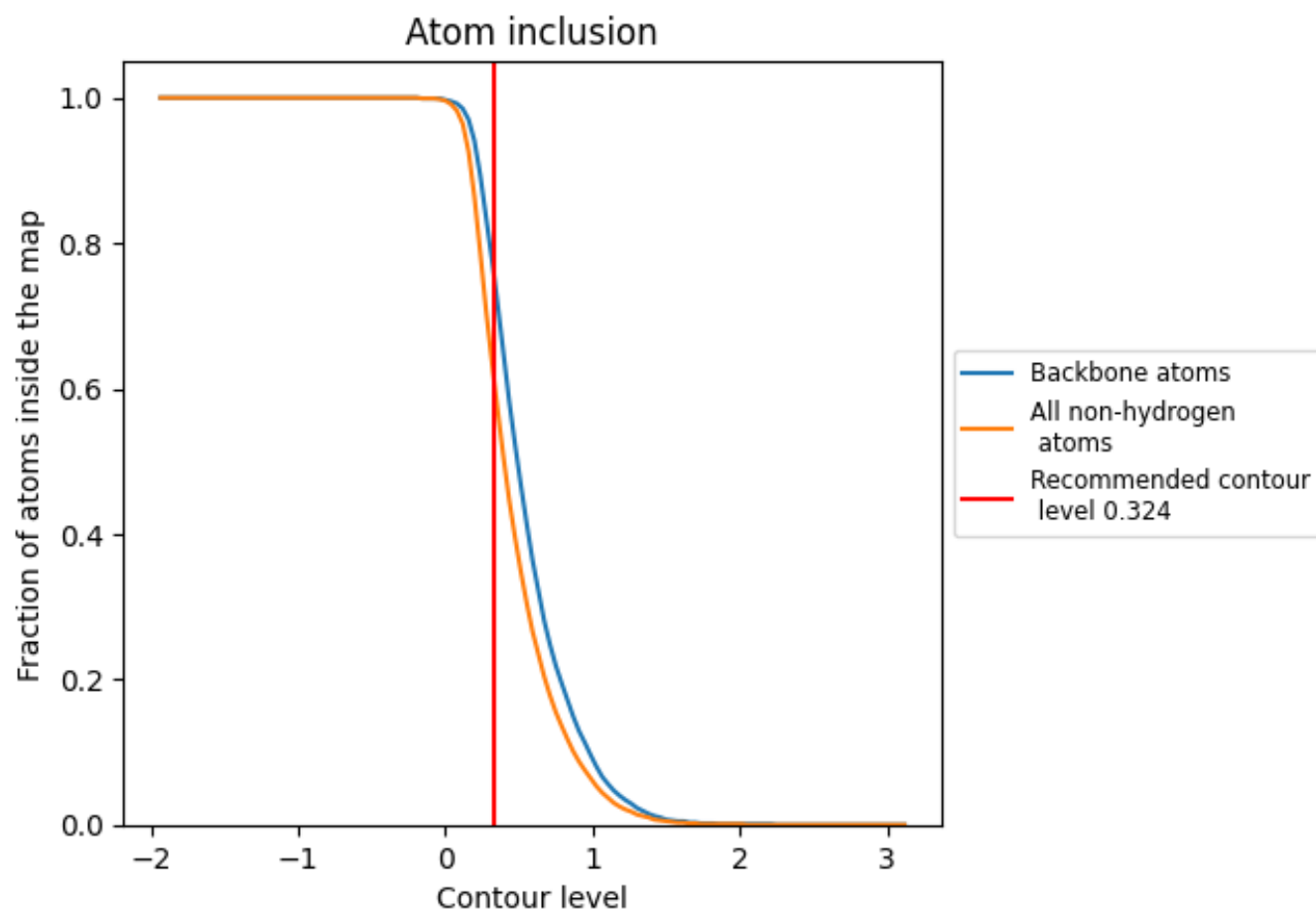


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 62% 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 (0.324) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6220	0.3890
A	0.7220	0.4090
B	0.7720	0.4570
C	0.7300	0.4260
D	0.3590	0.3010

