



## Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 05:20 pm BST

PDB ID : 7NS2  
EMDB ID : EMD-12558  
Title : Virion of Leishmania RNA virus 1  
Authors : Prochazkova, M.; Grybchuk, D.; Fuzik, T.  
Deposited on : 2021-03-05  
Resolution : 3.63 Å(reported)  
Based on initial model : 6Y83

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

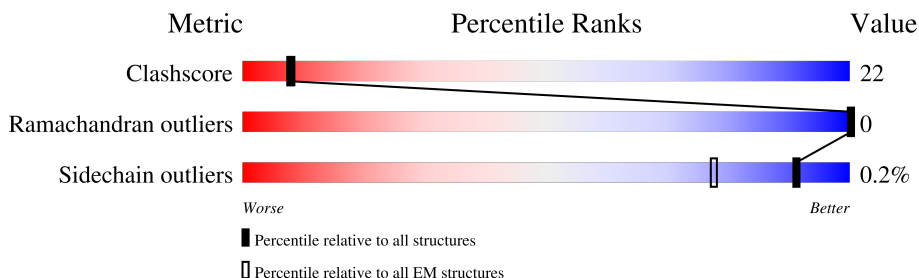
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.63 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	786	
1	B	786	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9575 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	605	Total	C	N	O	S	0	0
			4755	3010	823	888	34		
1	B	614	Total	C	N	O	S	0	0
			4820	3054	831	901	34		

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	432	ALA	THR	conflict	UNP L7XUU7
A	743	PRO	-	expression tag	UNP L7XUU7
A	744	ASP	-	expression tag	UNP L7XUU7
A	745	LEU	-	expression tag	UNP L7XUU7
A	746	GLY	-	expression tag	UNP L7XUU7
A	747	THR	-	expression tag	UNP L7XUU7
A	748	GLY	-	expression tag	UNP L7XUU7
A	749	GLY	-	expression tag	UNP L7XUU7
A	750	GLY	-	expression tag	UNP L7XUU7
A	751	SER	-	expression tag	UNP L7XUU7
A	752	GLY	-	expression tag	UNP L7XUU7
A	753	ILE	-	expression tag	UNP L7XUU7
A	754	GLU	-	expression tag	UNP L7XUU7
A	755	GLY	-	expression tag	UNP L7XUU7
A	756	ARG	-	expression tag	UNP L7XUU7
A	757	GLY	-	expression tag	UNP L7XUU7
A	758	SER	-	expression tag	UNP L7XUU7
A	759	MET	-	expression tag	UNP L7XUU7
A	760	ASP	-	expression tag	UNP L7XUU7
A	761	ILE	-	expression tag	UNP L7XUU7
A	762	GLY	-	expression tag	UNP L7XUU7
A	763	ASP	-	expression tag	UNP L7XUU7
A	764	PRO	-	expression tag	UNP L7XUU7
A	765	ASN	-	expression tag	UNP L7XUU7
A	766	SER	-	expression tag	UNP L7XUU7
A	767	VAL	-	expression tag	UNP L7XUU7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	768	GLN	-	expression tag	UNP L7XUU7
A	769	ALA	-	expression tag	UNP L7XUU7
A	770	LEU	-	expression tag	UNP L7XUU7
A	771	ALA	-	expression tag	UNP L7XUU7
A	772	ARG	-	expression tag	UNP L7XUU7
A	773	LEU	-	expression tag	UNP L7XUU7
A	774	GLN	-	expression tag	UNP L7XUU7
A	775	ALA	-	expression tag	UNP L7XUU7
A	776	SER	-	expression tag	UNP L7XUU7
A	777	SER	-	expression tag	UNP L7XUU7
A	778	VAL	-	expression tag	UNP L7XUU7
A	779	ASP	-	expression tag	UNP L7XUU7
A	780	LYS	-	expression tag	UNP L7XUU7
A	781	LEU	-	expression tag	UNP L7XUU7
A	782	ALA	-	expression tag	UNP L7XUU7
A	783	ALA	-	expression tag	UNP L7XUU7
A	784	ALA	-	expression tag	UNP L7XUU7
A	785	LEU	-	expression tag	UNP L7XUU7
A	786	GLU	-	expression tag	UNP L7XUU7
B	432	ALA	THR	conflict	UNP L7XUU7
B	743	PRO	-	expression tag	UNP L7XUU7
B	744	ASP	-	expression tag	UNP L7XUU7
B	745	LEU	-	expression tag	UNP L7XUU7
B	746	GLY	-	expression tag	UNP L7XUU7
B	747	THR	-	expression tag	UNP L7XUU7
B	748	GLY	-	expression tag	UNP L7XUU7
B	749	GLY	-	expression tag	UNP L7XUU7
B	750	GLY	-	expression tag	UNP L7XUU7
B	751	SER	-	expression tag	UNP L7XUU7
B	752	GLY	-	expression tag	UNP L7XUU7
B	753	ILE	-	expression tag	UNP L7XUU7
B	754	GLU	-	expression tag	UNP L7XUU7
B	755	GLY	-	expression tag	UNP L7XUU7
B	756	ARG	-	expression tag	UNP L7XUU7
B	757	GLY	-	expression tag	UNP L7XUU7
B	758	SER	-	expression tag	UNP L7XUU7
B	759	MET	-	expression tag	UNP L7XUU7
B	760	ASP	-	expression tag	UNP L7XUU7
B	761	ILE	-	expression tag	UNP L7XUU7
B	762	GLY	-	expression tag	UNP L7XUU7
B	763	ASP	-	expression tag	UNP L7XUU7
B	764	PRO	-	expression tag	UNP L7XUU7

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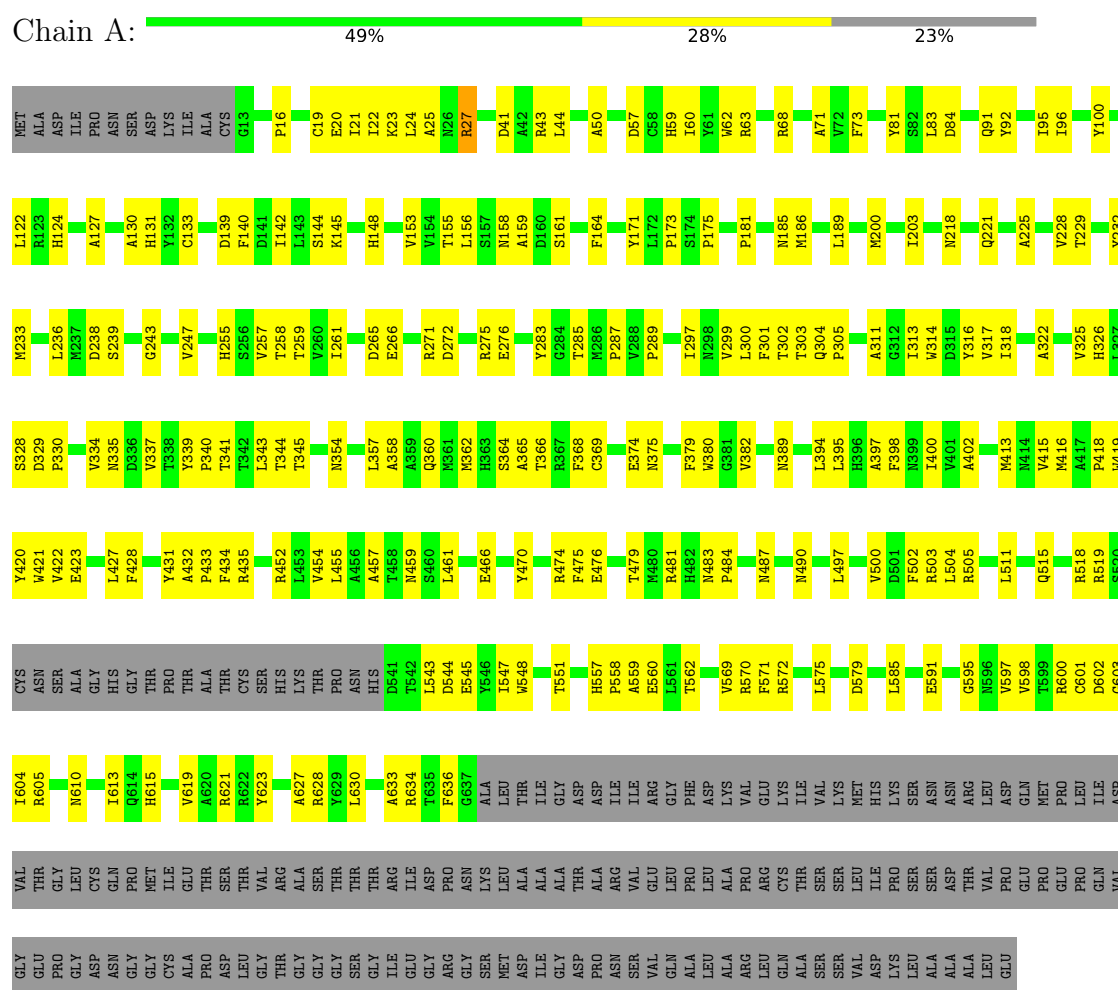
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Chain	Residue	Modelled	Actual	Comment	Reference
B	765	ASN	-	expression tag	UNP L7XUU7
B	766	SER	-	expression tag	UNP L7XUU7
B	767	VAL	-	expression tag	UNP L7XUU7
B	768	GLN	-	expression tag	UNP L7XUU7
B	769	ALA	-	expression tag	UNP L7XUU7
B	770	LEU	-	expression tag	UNP L7XUU7
B	771	ALA	-	expression tag	UNP L7XUU7
B	772	ARG	-	expression tag	UNP L7XUU7
B	773	LEU	-	expression tag	UNP L7XUU7
B	774	GLN	-	expression tag	UNP L7XUU7
B	775	ALA	-	expression tag	UNP L7XUU7
B	776	SER	-	expression tag	UNP L7XUU7
B	777	SER	-	expression tag	UNP L7XUU7
B	778	VAL	-	expression tag	UNP L7XUU7
B	779	ASP	-	expression tag	UNP L7XUU7
B	780	LYS	-	expression tag	UNP L7XUU7
B	781	LEU	-	expression tag	UNP L7XUU7
B	782	ALA	-	expression tag	UNP L7XUU7
B	783	ALA	-	expression tag	UNP L7XUU7
B	784	ALA	-	expression tag	UNP L7XUU7
B	785	LEU	-	expression tag	UNP L7XUU7
B	786	GLU	-	expression tag	UNP L7XUU7

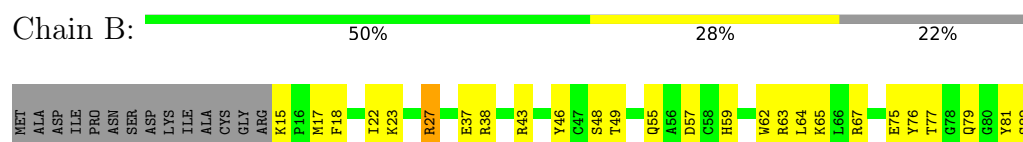
### 3 Residue-property plots

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: Capsid protein



#### • Molecule 1: Capsid protein



PRO	THR	G595	R518	L427	L319	Y92
ASP	SER	N596	R519	Y431	A322	T93
LEU	THR	V597	SER	R436	H326	Y100
GLY	VAL	C601	ASN	S436	H327	H103
THR	ARG	D602	SER	I438	D329	M117
GLY	ALA	K611	ALA	Y443	P330	V118
GLY	SER	R621	HIS	Q446	G331	L119
GLY	THR	R625	GLY	C447	M332	L122
GLY	THR	M626	THR	Y449	N335	G126
ILE	ARG	Y629	THR	L455	P340	I129
GLU	ILE	L630	CYS	A456	T341	A130
GLY	ASP	A631	SER	A457	T349	H131
ARG	PRO	R634	HIS	T458	R353	T135
GLY	ASN	I641	LYS	L461	N354	G136
GLY	THR	I645	THR	E462	A358	K137
PRO	ALA	I646	ASN	F463	S364	I138
ALA	ARG	F649	HIS	E466	A365	D141
ASN	VAL	LYS	T542	Y473	T258	S144
SER	GLU	LEU	E545	R474	V260	K145
GLN	LEU	PRO	W548	F475	I261	K146
ALA	ALA	ALA	G549	E476	A262	K147
LEU	ARG	VAL	S550	W477	H263	H148
LEU	ARG	GLY	D554	T478	E266	L156
GLN	CYS	ILE	L555	T479	G267	A159
ALA	THR	VAL	F556	M480	E374	S163
SER	SER	VAL	H557	R481	D272	F164
SER	ILE	MET	P558	N483	T376	L165
ASP	PRO	HIS	A559	P484	F379	P166
LYS	LYS	LYS	E560	L485	W380	A169
LEU	SER	ASN	L561	F486	G381	L170
ALA	ASP	ARG	T562	N487	V382	L172
ALA	THR	LEU	R570	I488	N389	P173
LEU	PRO	ASP	F571	L489	A402	L176
GLU	GLU	GLN	R572	G496	M413	M186
PRO	PRO	MET	L575	D501	M416	L187
GLU	PRO	PRO	S576	F502	A417	C192
PRO	PRO	PRO	G577	R503	W419	A193
GLN	VAL	ILE	A578	L504	Y420	G194
VAL	GLY	VAL	R583	P506	W421	D195
GLY	THR	THR	T589	W510	E423	I198
PRO	GLY	GLY	R590	L511	S424	D201
ASP	ASN	CYS	E591	E512	G514	
GLY	GLY	PRO	V592	E513	S425	
GLY	GLY	ILE	I593	Q515	A426	
CYS	CYS	GLU	E594			
ALA	ALA					

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	3768	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 ( $e^-/\text{\AA}^2$ )	1.3	Depositor
Minimum defocus (nm)	3500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	482.40002, 482.40002, 482.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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	0.41	0/4874	0.52	0/6636
1	B	0.41	0/4940	0.50	0/6728
All	All	0.41	0/9814	0.51	0/13364

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	4755	0	4603	223	0
1	B	4820	0	4663	214	0
All	All	9575	0	9266	416	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 22.

All (416) 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:322:ALA:HB1	1:A:421:TRP:CD1	1.44	1.52
1:A:322:ALA:CB	1:A:421:TRP:HE1	1.23	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ALA:HB1	1:A:421:TRP:NE1	1.20	1.47
1:A:322:ALA:CB	1:A:421:TRP:NE1	1.77	1.41
1:A:511:LEU:HD11	1:A:562:THR:CG2	1.59	1.31
1:A:300:LEU:CD2	1:B:165:LEU:HA	1.69	1.21
1:A:322:ALA:CB	1:A:421:TRP:CD1	2.21	1.20
1:B:83:LEU:CD2	1:B:245:ASP:OD2	1.92	1.17
1:B:243:GLY:O	1:B:247:VAL:HG23	1.45	1.14
1:A:322:ALA:HB2	1:A:421:TRP:HE1	1.05	1.13
1:B:83:LEU:HD22	1:B:245:ASP:OD2	1.44	1.12
1:A:511:LEU:HD11	1:A:562:THR:HG22	1.15	1.11
1:A:300:LEU:HD23	1:B:165:LEU:CA	1.81	1.10
1:A:300:LEU:HD23	1:B:165:LEU:HA	1.09	1.07
1:A:322:ALA:CA	1:A:421:TRP:CD1	2.47	0.96
1:B:327:LEU:O	1:B:436:SER:HB2	1.66	0.95
1:A:100:TYR:CD1	1:A:159:ALA:O	2.22	0.93
1:B:327:LEU:O	1:B:436:SER:CB	2.16	0.93
1:A:300:LEU:HB2	1:B:163:SER:HB3	1.52	0.92
1:B:461:LEU:HD11	1:B:473:TYR:HB3	1.52	0.91
1:A:271:ARG:HB2	1:A:421:TRP:CZ3	2.06	0.91
1:B:340:PRO:HG2	1:B:559:ALA:HB2	1.53	0.90
1:B:83:LEU:CD1	1:B:245:ASP:OD2	2.20	0.90
1:B:247:VAL:HG21	1:B:382:VAL:HG21	1.53	0.90
1:A:511:LEU:CD1	1:A:562:THR:CG2	2.48	0.89
1:A:511:LEU:CD1	1:A:562:THR:HG22	2.02	0.89
1:B:122:LEU:HD23	1:B:246:ALA:O	1.73	0.88
1:A:328:SER:HB3	1:A:375:ASN:HD22	1.39	0.88
1:B:237:MET:HG3	1:B:246:ALA:CB	2.04	0.87
1:A:100:TYR:HD1	1:A:159:ALA:O	1.58	0.87
1:A:322:ALA:O	1:A:421:TRP:CD1	2.30	0.84
1:A:62:TRP:CH2	1:A:427:LEU:HD11	2.14	0.82
1:A:62:TRP:CZ2	1:A:427:LEU:HD11	2.14	0.82
1:A:300:LEU:CD2	1:B:165:LEU:CA	2.50	0.81
1:B:83:LEU:HD13	1:B:245:ASP:OD2	1.80	0.81
1:A:551:THR:HG21	1:A:615:HIS:HB3	1.63	0.80
1:A:325:VAL:HG11	1:A:421:TRP:HB2	1.64	0.79
1:B:335:ASN:ND2	1:B:641:ILE:O	2.14	0.78
1:A:271:ARG:HB2	1:A:421:TRP:HZ3	1.45	0.78
1:B:119:LEU:CD2	1:B:246:ALA:HA	2.14	0.78
1:A:322:ALA:C	1:A:421:TRP:CD1	2.58	0.77
1:A:186:MET:HB3	1:A:229:THR:HG21	1.64	0.77
1:A:300:LEU:HB3	1:B:164:PHE:H	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:LEU:CD2	1:B:246:ALA:O	2.32	0.77
1:A:479:THR:HG23	1:A:562:THR:HB	1.69	0.75
1:A:504:LEU:O	1:A:504:LEU:HD23	1.86	0.75
1:B:458:THR:HA	1:B:483:ASN:HB2	1.68	0.75
1:A:511:LEU:HD12	1:A:511:LEU:O	1.86	0.75
1:B:327:LEU:O	1:B:436:SER:HB3	1.86	0.74
1:B:22:ILE:HB	1:B:316:TYR:HB2	1.71	0.72
1:B:83:LEU:HD22	1:B:245:ASP:CG	2.10	0.71
1:A:519:ARG:HH22	1:A:545:GLU:HG3	1.55	0.71
1:A:243:GLY:HA3	1:A:382:VAL:HG21	1.73	0.71
1:B:354:ASN:ND2	1:B:413:MET:O	2.24	0.71
1:B:480:MET:HB2	1:B:561:LEU:HB2	1.70	0.70
1:B:272:ASP:O	1:B:276:GLU:HG2	1.91	0.70
1:B:144:SER:HA	1:B:193:ALA:HB2	1.74	0.70
1:A:322:ALA:CA	1:A:421:TRP:NE1	2.49	0.70
1:B:237:MET:HG3	1:B:246:ALA:HB2	1.71	0.70
1:A:22:ILE:HB	1:A:316:TYR:HB2	1.73	0.69
1:A:511:LEU:HD12	1:A:511:LEU:C	2.13	0.69
1:A:247:VAL:HG21	1:A:380:TRP:CD1	2.28	0.69
1:A:300:LEU:CB	1:B:163:SER:HB3	2.23	0.68
1:A:325:VAL:CG1	1:A:421:TRP:HB2	2.22	0.68
1:A:344:THR:HG23	1:A:415:VAL:HG22	1.75	0.68
1:A:511:LEU:HD11	1:A:562:THR:HG23	1.69	0.68
1:A:155:THR:HB	1:A:203:ILE:HB	1.76	0.68
1:A:452:ARG:HG2	1:A:600:ARG:HB3	1.76	0.68
1:B:243:GLY:C	1:B:247:VAL:HG23	2.13	0.68
1:A:300:LEU:HD23	1:B:165:LEU:N	2.09	0.67
1:A:322:ALA:C	1:A:421:TRP:HD1	1.98	0.67
1:A:455:LEU:HD13	1:A:484:PRO:HG3	1.76	0.67
1:A:470:TYR:OH	1:A:572:ARG:NH1	2.28	0.67
1:A:503:ARG:HB2	1:A:570:ARG:HH11	1.60	0.67
1:A:20:GLU:OE1	1:A:20:GLU:N	2.19	0.66
1:A:511:LEU:HD21	1:A:562:THR:HG23	1.77	0.66
1:A:300:LEU:HB3	1:B:164:PHE:N	2.10	0.66
1:B:119:LEU:HD22	1:B:246:ALA:HA	1.78	0.66
1:A:100:TYR:CE1	1:A:159:ALA:O	2.47	0.66
1:B:242:TYR:HB3	1:B:245:ASP:HB3	1.77	0.66
1:A:421:TRP:HD1	1:A:422:VAL:HG22	1.61	0.65
1:A:337:VAL:HG23	1:A:339:TYR:HE2	1.60	0.65
1:B:548:TRP:CE3	1:B:560:GLU:HG2	2.31	0.65
1:A:153:VAL:HG11	1:A:200:MET:HE2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:MET:HE2	1:B:246:ALA:HB2	1.78	0.64
1:A:171:TYR:HD2	1:A:285:THR:HG23	1.63	0.64
1:B:244:ASP:HA	1:B:247:VAL:HB	1.80	0.64
1:A:365:ALA:HA	1:A:368:PHE:HB3	1.79	0.64
1:B:327:LEU:HD11	1:B:431:TYR:HE1	1.62	0.64
1:B:83:LEU:CG	1:B:245:ASP:OD2	2.45	0.64
1:B:171:TYR:HB3	1:B:285:THR:HG22	1.79	0.64
1:B:63:ARG:HB2	1:B:261:ILE:HB	1.80	0.64
1:A:218:ASN:H	1:A:221:GLN:NE2	1.96	0.64
1:A:300:LEU:HD21	1:B:165:LEU:HA	1.74	0.63
1:A:466:GLU:OE1	1:A:466:GLU:N	2.33	0.62
1:B:511:LEU:HB2	1:B:626:MET:HG2	1.81	0.62
1:B:518:ARG:NE	1:B:545:GLU:OE1	2.33	0.62
1:B:83:LEU:HD21	1:B:245:ASP:OD2	1.96	0.62
1:A:236:LEU:O	1:A:239:SER:OG	2.17	0.62
1:B:327:LEU:HD11	1:B:431:TYR:CE1	2.35	0.62
1:A:271:ARG:HB2	1:A:421:TRP:CH2	2.35	0.61
1:A:300:LEU:HD23	1:B:164:PHE:C	2.21	0.61
1:A:511:LEU:CG	1:A:562:THR:HG23	2.30	0.61
1:B:488:ILE:HD11	1:B:597:VAL:HG21	1.81	0.61
1:A:358:ALA:HB1	1:A:402:ALA:HB1	1.82	0.61
1:A:300:LEU:O	1:A:300:LEU:HD12	2.00	0.61
1:A:374:GLU:OE1	1:A:435:ARG:NH2	2.30	0.61
1:B:371:ILE:HG12	1:B:435:ARG:HH22	1.65	0.61
1:A:266:GLU:HG3	1:A:416:MET:HB2	1.83	0.61
1:B:165:LEU:HD12	1:B:166:PRO:HD2	1.83	0.61
1:B:176:LEU:HA	1:B:288:VAL:HG12	1.82	0.61
1:A:144:SER:OG	1:A:148:HIS:N	2.34	0.61
1:A:322:ALA:O	1:A:421:TRP:HD1	1.79	0.60
1:A:81:TYR:OH	1:A:389:ASN:OD1	2.20	0.60
1:A:322:ALA:HB1	1:A:421:TRP:HD1	1.50	0.60
1:B:458:THR:HA	1:B:483:ASN:CB	2.29	0.60
1:B:518:ARG:HD2	1:B:545:GLU:HB3	1.82	0.60
1:B:248:LEU:C	1:B:248:LEU:HD23	2.21	0.60
1:A:364:SER:HB2	1:A:419:TRP:HH2	1.67	0.60
1:B:18:PHE:HB2	1:B:316:TYR:HE2	1.65	0.60
1:B:353:ARG:NH2	1:B:402:ALA:O	2.35	0.59
1:B:365:ALA:HA	1:B:368:PHE:HB3	1.84	0.59
1:A:43:ARG:HD3	1:B:79:GLN:HB3	1.85	0.59
1:A:497:LEU:HD11	1:A:543:LEU:HD23	1.84	0.59
1:B:248:LEU:HD23	1:B:248:LEU:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ASN:OD1	1:A:483:ASN:OD1	2.21	0.59
1:B:266:GLU:OE2	1:B:621:ARG:NE	2.27	0.59
1:B:237:MET:CG	1:B:246:ALA:CB	2.79	0.59
1:A:454:VAL:HG22	1:A:598:VAL:HG22	1.85	0.58
1:A:299:VAL:HG21	1:A:313:ILE:HD11	1.85	0.58
1:B:82:SER:HB3	1:B:280:THR:HG21	1.85	0.58
1:A:156:LEU:HB2	1:A:161:SER:HB2	1.86	0.58
1:B:501:ASP:HB3	1:B:542:THR:HA	1.86	0.58
1:A:325:VAL:CG1	1:A:421:TRP:CB	2.82	0.58
1:B:135:THR:HG23	1:B:137:LYS:H	1.67	0.58
1:A:161:SER:O	1:A:164:PHE:HB2	2.04	0.58
1:A:20:GLU:O	1:A:24:LEU:HG	2.04	0.57
1:B:46:TYR:HB3	1:B:488:ILE:HG12	1.85	0.57
1:A:328:SER:HB3	1:A:375:ASN:ND2	2.14	0.57
1:A:421:TRP:CD1	1:A:422:VAL:HG22	2.40	0.57
1:B:237:MET:CG	1:B:246:ALA:HB2	2.35	0.57
1:A:470:TYR:HA	1:A:571:PHE:O	2.05	0.57
1:A:474:ARG:NH2	1:A:476:GLU:OE2	2.38	0.56
1:A:502:PHE:HE1	1:A:569:VAL:HG12	1.71	0.56
1:B:377:SER:OG	1:B:382:VAL:O	2.23	0.56
1:A:81:TYR:HE2	1:A:83:LEU:HB2	1.70	0.56
1:A:461:LEU:HD22	1:A:475:PHE:HE1	1.70	0.56
1:B:27:ARG:H	1:B:27:ARG:HD2	1.71	0.56
1:B:575:LEU:HB2	1:B:583:ARG:HG2	1.88	0.56
1:A:322:ALA:HA	1:A:421:TRP:CD1	2.37	0.56
1:B:237:MET:HG3	1:B:246:ALA:HB1	1.85	0.56
1:A:44:LEU:HD11	1:A:60:ILE:HD11	1.87	0.56
1:A:366:THR:HG22	1:A:395:LEU:HD11	1.87	0.56
1:B:503:ARG:HD3	1:B:570:ARG:HD3	1.89	0.55
1:A:457:ALA:HB2	1:A:595:GLY:O	2.07	0.55
1:B:329:ASP:CG	1:B:419:TRP:HB2	2.27	0.54
1:B:46:TYR:O	1:B:55:GLN:HA	2.07	0.54
1:B:76:TYR:O	1:B:77:THR:HG22	2.07	0.54
1:B:455:LEU:HD11	1:B:484:PRO:HG3	1.90	0.54
1:B:43:ARG:HG3	1:B:602:ASP:HB2	1.90	0.54
1:A:515:GLN:OE1	1:A:518:ARG:NH1	2.37	0.54
1:B:122:LEU:HD21	1:B:234:LEU:HD12	1.90	0.54
1:A:131:HIS:HB2	1:A:257:VAL:HG21	1.90	0.53
1:A:343:LEU:HB3	1:A:360:GLN:HG2	1.89	0.53
1:B:548:TRP:HZ2	1:B:557:HIS:H	1.54	0.53
1:B:631:ALA:HA	1:B:634:ARG:NH1	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:PRO:HG2	1:A:297:ILE:HG22	1.90	0.53
1:A:427:LEU:HD12	1:A:427:LEU:N	2.24	0.53
1:B:624:CYS:SG	1:B:625:MET:N	2.81	0.53
1:A:334:VAL:HG13	1:A:633:ALA:HB1	1.90	0.53
1:A:511:LEU:CD2	1:A:562:THR:HG23	2.38	0.53
1:B:243:GLY:O	1:B:247:VAL:CG2	2.38	0.53
1:B:413:MET:HG2	1:B:621:ARG:HD3	1.90	0.53
1:B:186:MET:HB3	1:B:229:THR:HG21	1.91	0.53
1:B:330:PRO:O	1:B:341:THR:OG1	2.19	0.53
1:B:413:MET:SD	1:B:621:ARG:HD3	2.49	0.53
1:B:170:LEU:HD23	1:B:198:ILE:HG22	1.91	0.53
1:A:20:GLU:H	1:A:20:GLU:CD	2.08	0.53
1:A:20:GLU:HB2	1:A:23:LYS:HB3	1.89	0.53
1:A:221:GLN:HB3	1:A:304:GLN:HG2	1.91	0.53
1:B:130:ALA:HB1	1:B:258:THR:HG23	1.90	0.52
1:A:124:HIS:CD2	1:A:145:LYS:HE3	2.44	0.52
1:A:329:ASP:HB2	1:A:419:TRP:CE3	2.44	0.52
1:A:603:GLY:HA3	1:B:79:GLN:HA	1.90	0.52
1:B:48:SER:HA	1:B:597:VAL:HA	1.92	0.52
1:B:221:GLN:HG3	1:B:304:GLN:HB3	1.91	0.52
1:B:59:HIS:N	1:B:554:ASP:OD1	2.43	0.52
1:B:325:VAL:HG23	1:B:368:PHE:CE1	2.45	0.52
1:A:300:LEU:HB3	1:B:164:PHE:O	2.10	0.52
1:B:438:ILE:HG13	1:B:443:TYR:HB2	1.92	0.52
1:B:67:ARG:HE	1:B:275:ARG:HD3	1.74	0.52
1:B:65:LYS:HE3	1:B:261:ILE:HD11	1.92	0.52
1:A:20:GLU:O	1:A:20:GLU:HG2	2.11	0.51
1:B:220:LEU:HB3	1:B:304:GLN:HB2	1.92	0.51
1:A:345:THR:HG21	1:A:354:ASN:HD21	1.76	0.51
1:A:369:CYS:SG	1:A:394:LEU:HD22	2.50	0.51
1:A:73:PHE:CZ	1:A:142:ILE:HD13	2.45	0.51
1:A:619:VAL:HG23	1:A:621:ARG:HD2	1.91	0.51
1:A:341:THR:O	1:A:418:PRO:HD2	2.11	0.51
1:A:344:THR:HG21	1:A:627:ALA:HB1	1.91	0.51
1:B:515:GLN:O	1:B:519:ARG:NH2	2.44	0.51
1:A:133:CYS:SG	1:A:314:TRP:HB2	2.51	0.51
1:B:589:THR:O	1:B:593:ILE:HD12	2.10	0.51
1:A:50:ALA:HB1	1:A:591:GLU:HG2	1.91	0.51
1:B:481:ARG:HD2	1:B:558:PRO:HG3	1.93	0.51
1:A:100:TYR:HA	1:A:158:ASN:O	2.11	0.51
1:A:511:LEU:CD1	1:A:562:THR:HG23	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:LYS:NZ	1:B:309:GLN:HB3	2.26	0.51
1:A:133:CYS:SG	1:A:311:ALA:HA	2.50	0.50
1:B:148:HIS:HA	1:B:192:CYS:SG	2.51	0.50
1:B:237:MET:CB	1:B:246:ALA:CB	2.90	0.50
1:A:181:PRO:O	1:A:185:ASN:ND2	2.41	0.50
1:A:271:ARG:O	1:A:275:ARG:HG2	2.11	0.50
1:A:476:GLU:N	1:A:476:GLU:OE1	2.44	0.50
1:A:457:ALA:HA	1:A:597:VAL:HG23	1.93	0.50
1:A:500:VAL:HG22	1:A:571:PHE:CD1	2.47	0.50
1:B:505:ARG:HB3	1:B:506:PRO:HD2	1.94	0.50
1:A:364:SER:HB2	1:A:419:TRP:CH2	2.47	0.50
1:A:487:ASN:HA	1:A:490:ASN:HB3	1.94	0.50
1:B:131:HIS:O	1:B:135:THR:HG22	2.11	0.50
1:B:38:ARG:NH2	1:B:315:ASP:OD2	2.45	0.49
1:A:572:ARG:HH21	1:A:575:LEU:HG	1.76	0.49
1:A:479:THR:HG21	1:A:559:ALA:HA	1.92	0.49
1:A:272:ASP:O	1:A:276:GLU:HG2	2.12	0.49
1:A:258:THR:HG21	1:A:318:ILE:HD13	1.95	0.49
1:B:138:ILE:HG13	1:B:222:LEU:HD23	1.93	0.49
1:A:218:ASN:HB2	1:A:221:GLN:OE1	2.12	0.49
1:B:187:LEU:HD13	1:B:286:MET:HG3	1.94	0.49
1:A:122:LEU:HD21	1:A:233:MET:HB2	1.95	0.49
1:A:420:TYR:OH	1:A:423:GLU:HG2	2.12	0.49
1:B:218:ASN:OD1	1:B:218:ASN:N	2.42	0.49
1:B:449:TYR:HA	1:B:601:CYS:SG	2.53	0.49
1:A:330:PRO:O	1:A:341:THR:OG1	2.31	0.48
1:A:379:PHE:HB2	1:A:434:PHE:HE1	1.78	0.48
1:A:397:ALA:O	1:A:400:ILE:HG22	2.13	0.48
1:B:591:GLU:O	1:B:595:GLY:N	2.45	0.48
1:B:23:LYS:HZ1	1:B:309:GLN:HB3	1.77	0.48
1:B:559:ALA:HA	1:B:562:THR:HG23	1.95	0.48
1:A:300:LEU:HB3	1:B:164:PHE:C	2.34	0.48
1:A:322:ALA:HB2	1:A:421:TRP:NE1	1.84	0.48
1:B:327:LEU:HD13	1:B:431:TYR:HD1	1.78	0.48
1:A:155:THR:CB	1:A:203:ILE:HB	2.42	0.48
1:A:20:GLU:HB3	1:A:299:VAL:HG23	1.96	0.48
1:B:49:THR:HG22	1:B:596:ASN:O	2.13	0.48
1:A:325:VAL:HG23	1:A:368:PHE:CZ	2.49	0.48
1:B:370:ASP:OD1	1:B:371:ILE:N	2.46	0.48
1:A:502:PHE:HB3	1:A:505:ARG:HG3	1.96	0.48
1:B:463:PHE:HZ	1:B:466:GLU:HB2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:LEU:HD23	1:B:561:LEU:HA	1.66	0.48
1:A:601:CYS:O	1:B:82:SER:OG	2.28	0.48
1:B:575:LEU:HG	1:B:576:SER:H	1.79	0.48
1:A:302:THR:HA	1:B:159:ALA:HA	1.96	0.47
1:B:341:THR:O	1:B:418:PRO:HD2	2.13	0.47
1:A:314:TRP:HA	1:A:317:VAL:HG12	1.95	0.47
1:A:156:LEU:HD13	1:A:159:ALA:HA	1.95	0.47
1:B:237:MET:HB2	1:B:246:ALA:HB3	1.96	0.47
1:B:457:ALA:HA	1:B:484:PRO:HD2	1.97	0.47
1:B:461:LEU:HD13	1:B:475:PHE:CD1	2.49	0.47
1:B:371:ILE:HG12	1:B:435:ARG:NH2	2.30	0.47
1:A:139:ASP:OD1	1:A:139:ASP:N	2.46	0.47
1:A:41:ASP:HB3	1:A:605:ARG:HG2	1.95	0.47
1:A:92:TYR:O	1:A:96:ILE:HG12	2.15	0.47
1:B:243:GLY:O	1:B:247:VAL:N	2.48	0.47
1:A:173:PRO:HB2	1:A:175:PRO:HD2	1.96	0.47
1:A:452:ARG:NH1	1:B:81:TYR:OH	2.48	0.47
1:A:579:ASP:OD1	1:A:579:ASP:N	2.43	0.47
1:B:236:LEU:O	1:B:239:SER:OG	2.31	0.47
1:B:548:TRP:NE1	1:B:550:SER:HB2	2.29	0.47
1:A:432:ALA:N	1:A:433:PRO:HD2	2.30	0.46
1:B:266:GLU:HB3	1:B:416:MET:HG2	1.97	0.46
1:B:631:ALA:HA	1:B:634:ARG:HH12	1.80	0.46
1:A:130:ALA:HB3	1:A:257:VAL:CG1	2.45	0.46
1:A:255:HIS:O	1:A:275:ARG:NE	2.40	0.46
1:A:511:LEU:HD21	1:A:562:THR:CG2	2.46	0.46
1:B:358:ALA:HB1	1:B:402:ALA:HB1	1.97	0.46
1:B:510:TRP:HB3	1:B:513:GLU:HB3	1.97	0.46
1:A:63:ARG:HD3	1:A:613:ILE:HG22	1.96	0.46
1:A:459:ASN:CG	1:A:483:ASN:OD1	2.54	0.46
1:B:237:MET:CB	1:B:246:ALA:HB3	2.45	0.46
1:B:325:VAL:HG11	1:B:421:TRP:HB3	1.97	0.46
1:B:503:ARG:HD2	1:B:503:ARG:HA	1.65	0.46
1:B:119:LEU:HD22	1:B:245:ASP:O	2.16	0.46
1:B:126:GLY:O	1:B:129:ILE:HG22	2.16	0.46
1:B:374:GLU:HG2	1:B:435:ARG:HE	1.81	0.46
1:A:127:ALA:O	1:A:257:VAL:HG11	2.16	0.46
1:A:300:LEU:CB	1:B:164:PHE:H	2.21	0.46
1:B:64:LEU:HD21	1:B:319:LEU:HD21	1.97	0.46
1:B:425:SER:HB3	1:B:446:GLN:H	1.81	0.46
1:B:542:THR:HG23	1:B:545:GLU:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:TYR:OH	1:B:389:ASN:ND2	2.38	0.45
1:A:325:VAL:HG23	1:A:368:PHE:CE1	2.51	0.45
1:B:267:GLY:HA3	1:B:420:TYR:O	2.16	0.45
1:A:92:TYR:HD1	1:A:287:PRO:HG3	1.81	0.45
1:A:337:VAL:HG23	1:A:339:TYR:CE2	2.46	0.45
1:A:497:LEU:O	1:A:544:ASP:HB2	2.16	0.45
1:A:19:CYS:CB	1:A:21:ILE:HG13	2.46	0.45
1:A:600:ARG:NH1	1:A:602:ASP:OD1	2.49	0.45
1:B:224:HIS:HB2	1:B:305:PRO:HD2	1.97	0.45
1:A:44:LEU:O	1:A:57:ASP:HA	2.16	0.45
1:A:68:ARG:H	1:A:71:ALA:HB2	1.81	0.45
1:B:483:ASN:O	1:B:483:ASN:OD1	2.35	0.45
1:A:20:GLU:HB2	1:A:23:LYS:HD3	1.98	0.45
1:A:300:LEU:HD23	1:B:164:PHE:O	2.17	0.45
1:A:500:VAL:HG22	1:A:571:PHE:CE1	2.52	0.45
1:B:75:GLU:H	1:B:75:GLU:CD	2.19	0.45
1:B:170:LEU:O	1:B:198:ILE:HA	2.17	0.45
1:B:426:ALA:HB2	1:B:447:CYS:SG	2.56	0.45
1:A:16:PRO:HB3	1:A:380:TRP:O	2.17	0.44
1:B:364:SER:HB3	1:B:419:TRP:HE1	1.81	0.44
1:B:195:ASP:OD1	1:B:195:ASP:N	2.49	0.44
1:A:43:ARG:HB2	1:A:602:ASP:HB2	2.00	0.44
1:B:328:SER:O	1:B:368:PHE:CD1	2.70	0.44
1:A:297:ILE:O	1:B:164:PHE:HB3	2.17	0.44
1:A:623:TYR:CE2	1:A:628:ARG:HB3	2.53	0.44
1:A:634:ARG:HD2	1:A:636:PHE:HD1	1.81	0.44
1:B:88:TYR:HB3	1:B:92:TYR:HB2	2.00	0.44
1:B:171:TYR:OH	1:B:201:ASP:OD1	2.16	0.44
1:A:301:PHE:CD1	1:A:305:PRO:HG3	2.52	0.44
1:A:413:MET:HE1	1:A:621:ARG:CZ	2.47	0.44
1:B:15:LYS:N	1:B:381:GLY:HA3	2.33	0.44
1:B:260:VAL:O	1:B:261:ILE:C	2.55	0.44
1:B:481:ARG:NH1	1:B:556:PHE:O	2.50	0.44
1:B:328:SER:HB3	1:B:372:PHE:HA	2.00	0.44
1:A:159:ALA:HB2	1:A:171:TYR:CZ	2.53	0.44
1:A:547:ILE:HG23	1:A:548:TRP:O	2.18	0.44
1:B:89:PRO:HG3	1:B:239:SER:HB2	1.99	0.44
1:B:145:LYS:HB2	1:B:147:LYS:HE3	2.00	0.44
1:B:171:TYR:O	1:B:173:PRO:HD3	2.18	0.44
1:B:166:PRO:HG2	1:B:169:ALA:HB2	2.00	0.43
1:A:23:LYS:HB2	1:A:313:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:HIS:HB3	1:A:560:GLU:HB2	1.99	0.43
1:A:610:ASN:OD1	1:A:613:ILE:HG13	2.18	0.43
1:B:122:LEU:HD21	1:B:246:ALA:O	2.14	0.43
1:A:322:ALA:HA	1:A:421:TRP:NE1	2.31	0.43
1:A:518:ARG:NE	1:A:545:GLU:OE2	2.51	0.43
1:B:92:TYR:CE1	1:B:290:ILE:HG12	2.53	0.43
1:A:379:PHE:HB2	1:A:434:PHE:CE1	2.54	0.43
1:A:428:PHE:HB2	1:A:431:TYR:CZ	2.54	0.43
1:B:263:HIS:CE1	1:B:423:GLU:H	2.37	0.43
1:A:63:ARG:HB2	1:A:261:ILE:HG12	2.00	0.43
1:B:300:LEU:HD13	1:B:305:PRO:HG3	2.00	0.43
1:B:100:TYR:HE1	1:B:285:THR:HG21	1.84	0.43
1:A:322:ALA:O	1:A:325:VAL:HG12	2.18	0.43
1:A:326:HIS:CD2	1:A:420:TYR:HD1	2.36	0.43
1:A:357:LEU:HD21	1:A:416:MET:HG2	2.00	0.43
1:B:248:LEU:C	1:B:248:LEU:CD2	2.85	0.43
1:A:71:ALA:HB3	1:A:257:VAL:HG23	2.01	0.43
1:B:57:ASP:OD1	1:B:57:ASP:N	2.49	0.43
1:B:83:LEU:HB3	1:B:117:ASN:OD1	2.19	0.43
1:B:413:MET:CG	1:B:621:ARG:HD3	2.49	0.43
1:B:479:THR:HG21	1:B:559:ALA:H	1.83	0.43
1:A:325:VAL:HG13	1:A:326:HIS:N	2.34	0.42
1:A:340:PRO:HG2	1:A:558:PRO:O	2.19	0.42
1:A:84:ASP:HA	1:A:283:TYR:OH	2.19	0.42
1:B:89:PRO:O	1:B:93:THR:HG23	2.19	0.42
1:B:119:LEU:CD2	1:B:246:ALA:CA	2.93	0.42
1:B:266:GLU:HB3	1:B:417:ALA:H	1.84	0.42
1:B:484:PRO:HG2	1:B:597:VAL:HG11	2.01	0.42
1:A:43:ARG:HG2	1:A:59:HIS:CE1	2.53	0.42
1:B:62:TRP:CH2	1:B:427:LEU:HG	2.54	0.42
1:B:100:TYR:CE2	1:B:165:LEU:HD23	2.54	0.42
1:B:611:LYS:HA	1:B:611:LYS:HD2	1.86	0.42
1:A:63:ARG:HD3	1:A:613:ILE:CG2	2.50	0.42
1:B:266:GLU:CD	1:B:621:ARG:HE	2.20	0.42
1:B:322:ALA:O	1:B:325:VAL:HG12	2.19	0.42
1:B:329:ASP:OD1	1:B:330:PRO:HD2	2.19	0.42
1:B:489:LEU:O	1:B:496:GLY:HA2	2.19	0.42
1:B:548:TRP:CE3	1:B:548:TRP:N	2.87	0.42
1:B:332:MET:HB2	1:B:341:THR:HA	2.01	0.42
1:A:325:VAL:HG11	1:A:421:TRP:CB	2.42	0.42
1:A:357:LEU:HD12	1:A:357:LEU:HA	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:LEU:HD23	1:B:504:LEU:HA	1.83	0.42
1:A:236:LEU:HD12	1:A:236:LEU:HA	1.89	0.42
1:B:236:LEU:HA	1:B:236:LEU:HD12	1.83	0.42
1:A:140:PHE:CD1	1:A:189:LEU:HD11	2.55	0.42
1:B:548:TRP:CZ3	1:B:560:GLU:HG2	2.55	0.42
1:B:572:ARG:HH11	1:B:575:LEU:HD12	1.85	0.42
1:A:335:ASN:H	1:A:634:ARG:HB3	1.85	0.41
1:A:455:LEU:CD1	1:A:484:PRO:HG3	2.49	0.41
1:B:81:TYR:HH	1:B:389:ASN:HD22	1.61	0.41
1:B:349:THR:HA	1:B:354:ASN:OD1	2.20	0.41
1:B:477:TRP:NE1	1:B:561:LEU:O	2.43	0.41
1:B:485:LEU:HD11	1:B:592:VAL:HG12	2.02	0.41
1:A:225:ALA:HA	1:A:228:VAL:HG12	2.02	0.41
1:B:330:PRO:HD2	1:B:419:TRP:CD1	2.55	0.41
1:A:232:TYR:CD1	1:A:289:PRO:HB3	2.55	0.41
1:B:461:LEU:HD23	1:B:594:GLU:HG2	2.02	0.41
1:B:503:ARG:HD3	1:B:570:ARG:HH11	1.85	0.41
1:A:140:PHE:HD1	1:A:189:LEU:HD11	1.85	0.41
1:B:629:TYR:CE2	1:B:645:ILE:HG23	2.56	0.41
1:A:259:THR:HG23	1:A:271:ARG:HD2	2.03	0.41
1:A:297:ILE:HG13	1:A:299:VAL:O	2.21	0.41
1:A:303:THR:HG22	1:A:304:GLN:HG3	2.00	0.41
1:B:17:MET:HB2	1:B:379:PHE:O	2.21	0.41
1:A:25:ALA:O	1:A:27:ARG:NH1	2.54	0.41
1:A:266:GLU:OE2	1:A:418:PRO:HA	2.21	0.41
1:B:478:THR:HG23	1:B:479:THR:N	2.35	0.41
1:A:585:LEU:HA	1:A:585:LEU:HD23	1.86	0.41
1:A:630:LEU:HA	1:A:633:ALA:HB2	2.03	0.41
1:B:483:ASN:OD1	1:B:486:PHE:CD2	2.74	0.41
1:A:41:ASP:O	1:A:604:ILE:HA	2.21	0.41
1:A:265:ASP:HB2	1:A:621:ARG:NH1	2.36	0.41
1:A:413:MET:HE2	1:A:416:MET:HB3	2.02	0.41
1:B:37:GLU:HB3	1:B:65:LYS:HB3	2.03	0.41
1:B:103:HIS:CD2	1:B:156:LEU:HG	2.55	0.41
1:A:91:GLN:O	1:A:95:ILE:HG13	2.21	0.41
1:A:158:ASN:O	1:A:159:ALA:C	2.59	0.41
1:A:423:GLU:OE2	1:A:481:ARG:NH1	2.39	0.41
1:B:510:TRP:CE3	1:B:561:LEU:HD22	2.55	0.41
1:B:141:ASP:HA	1:B:146:LYS:HA	2.02	0.40
1:A:362:MET:SD	1:A:398:PHE:HB3	2.61	0.40
1:B:463:PHE:CD1	1:B:590:ARG:HD3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:ILE:H	1:B:646:ILE:HG12	1.74	0.40
1:A:238:ASP:CG	1:A:382:VAL:HG23	2.41	0.40
1:A:247:VAL:HG21	1:A:380:TRP:CG	2.54	0.40
1:B:135:THR:HG23	1:B:137:LYS:HG2	2.03	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	601/786 (76%)	556 (92%)	45 (8%)	0	100	100
1	B	610/786 (78%)	552 (90%)	58 (10%)	0	100	100
All	All	1211/1572 (77%)	1108 (92%)	103 (8%)	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	512/658 (78%)	511 (100%)	1 (0%)	92	96
1	B	518/658 (79%)	517 (100%)	1 (0%)	92	96
All	All	1030/1316 (78%)	1028 (100%)	2 (0%)	91	96

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

Mol	Chain	Res	Type
1	A	27	ARG
1	B	27	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

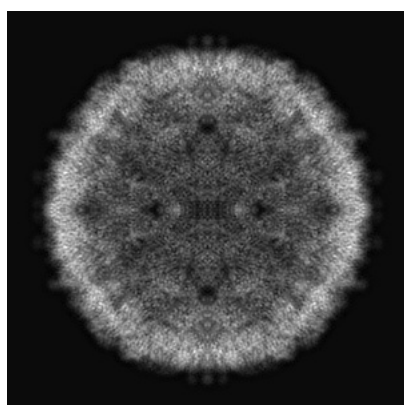
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12558. These allow visual inspection of the internal detail of the map and identification of artifacts.

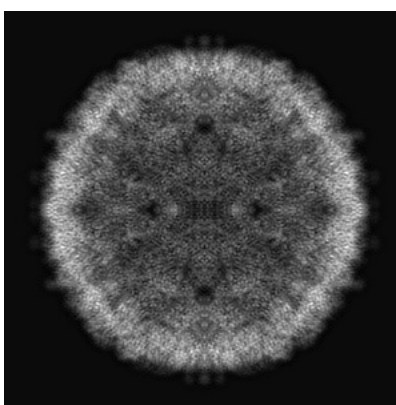
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

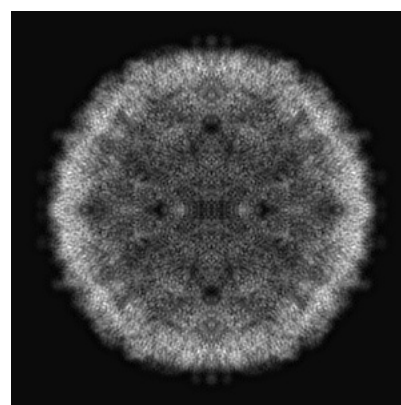
#### 6.1.1 Primary map



X



Y

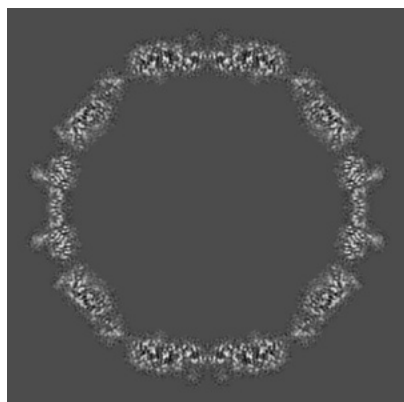


Z

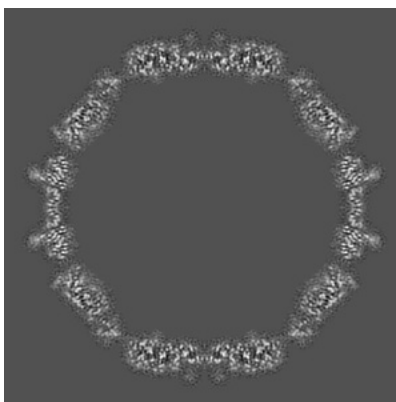
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

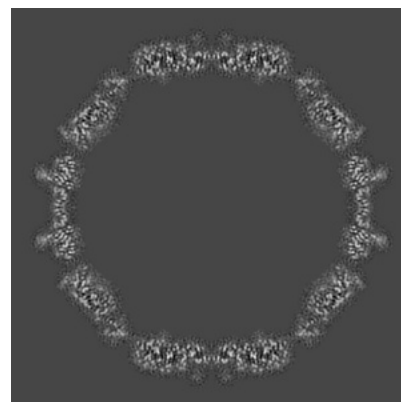
#### 6.2.1 Primary map



X Index: 180



Y Index: 180



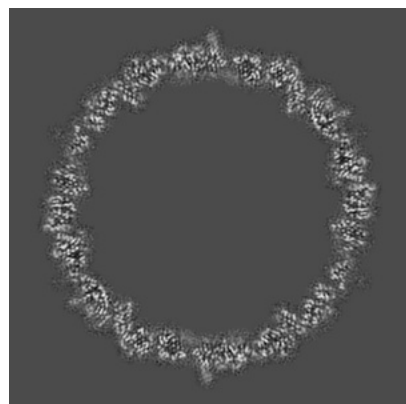
Z Index: 180



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

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

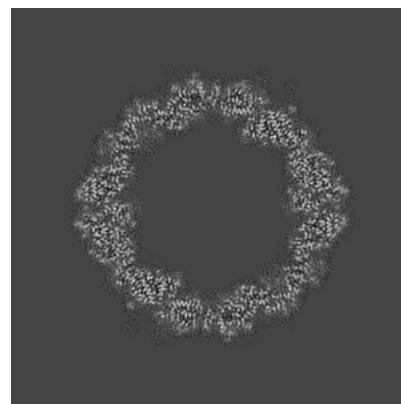
### 6.3.1 Primary map



X Index: 212



Y Index: 84

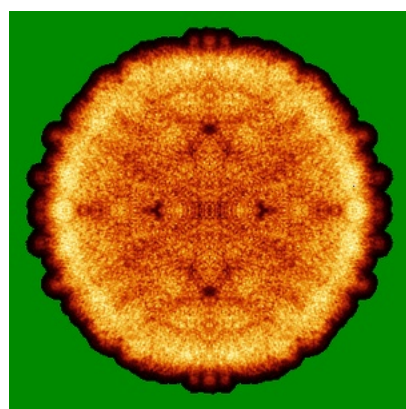


Z Index: 84

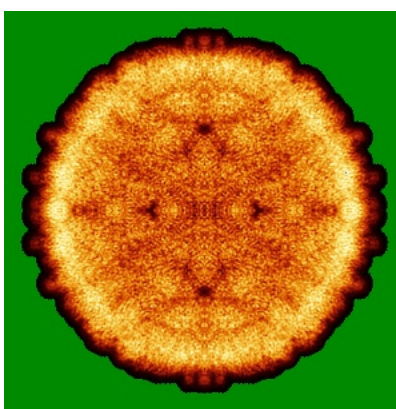
The images above show the largest variance slices of the map in three orthogonal directions.

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

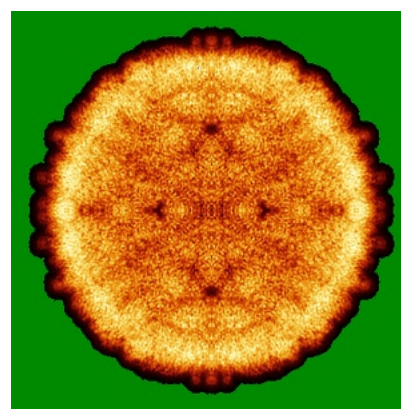
### 6.4.1 Primary map



X



Y

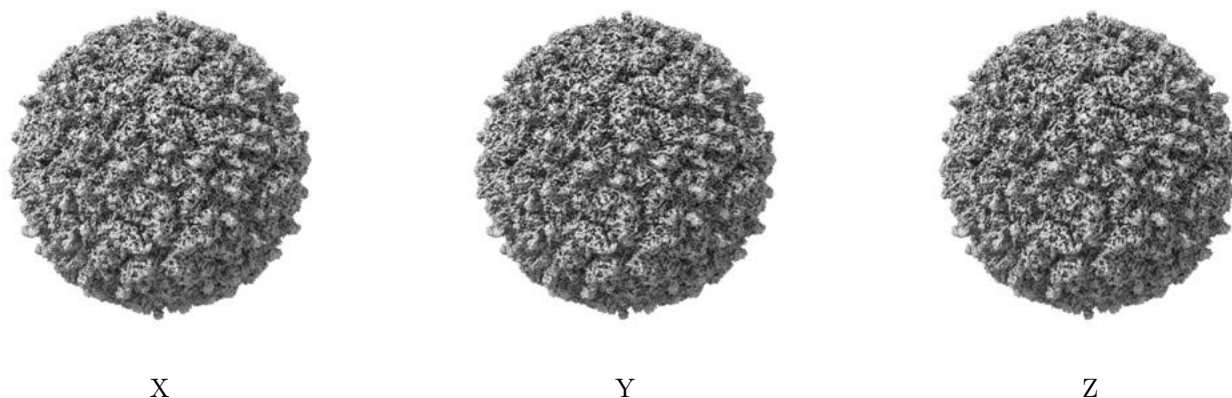


Z

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 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

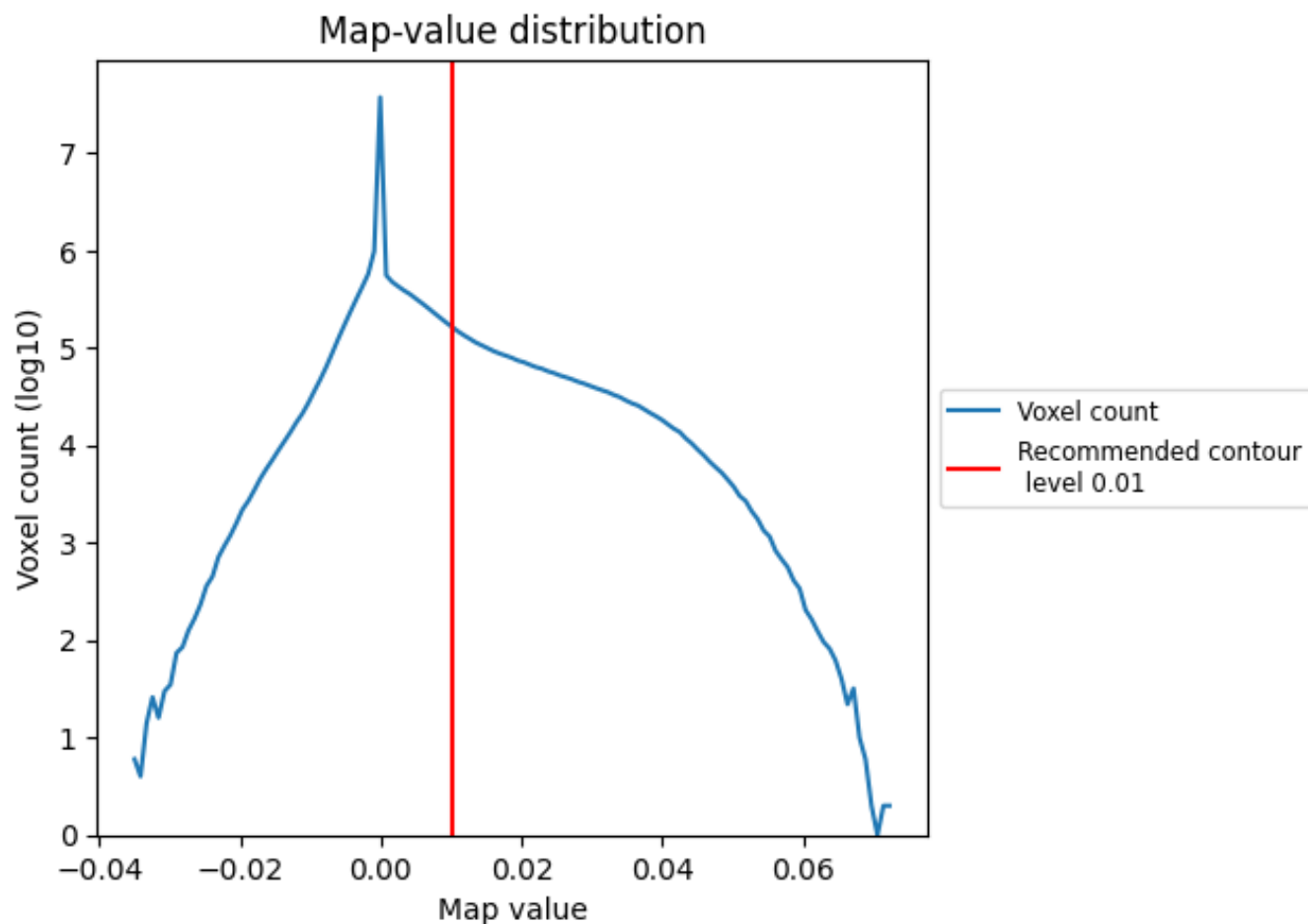
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

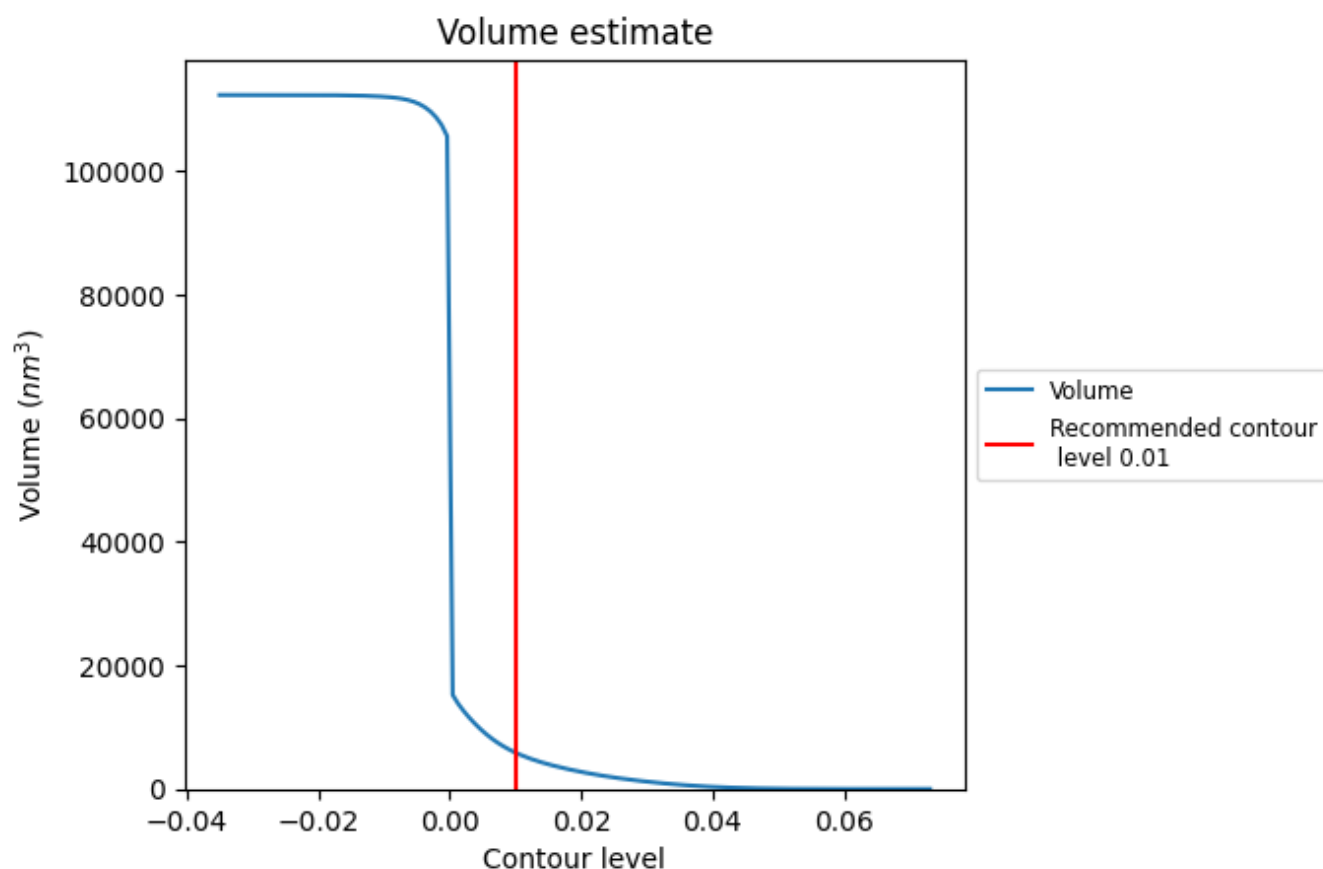
This section contains the results of statistical analysis of the map.

### 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.

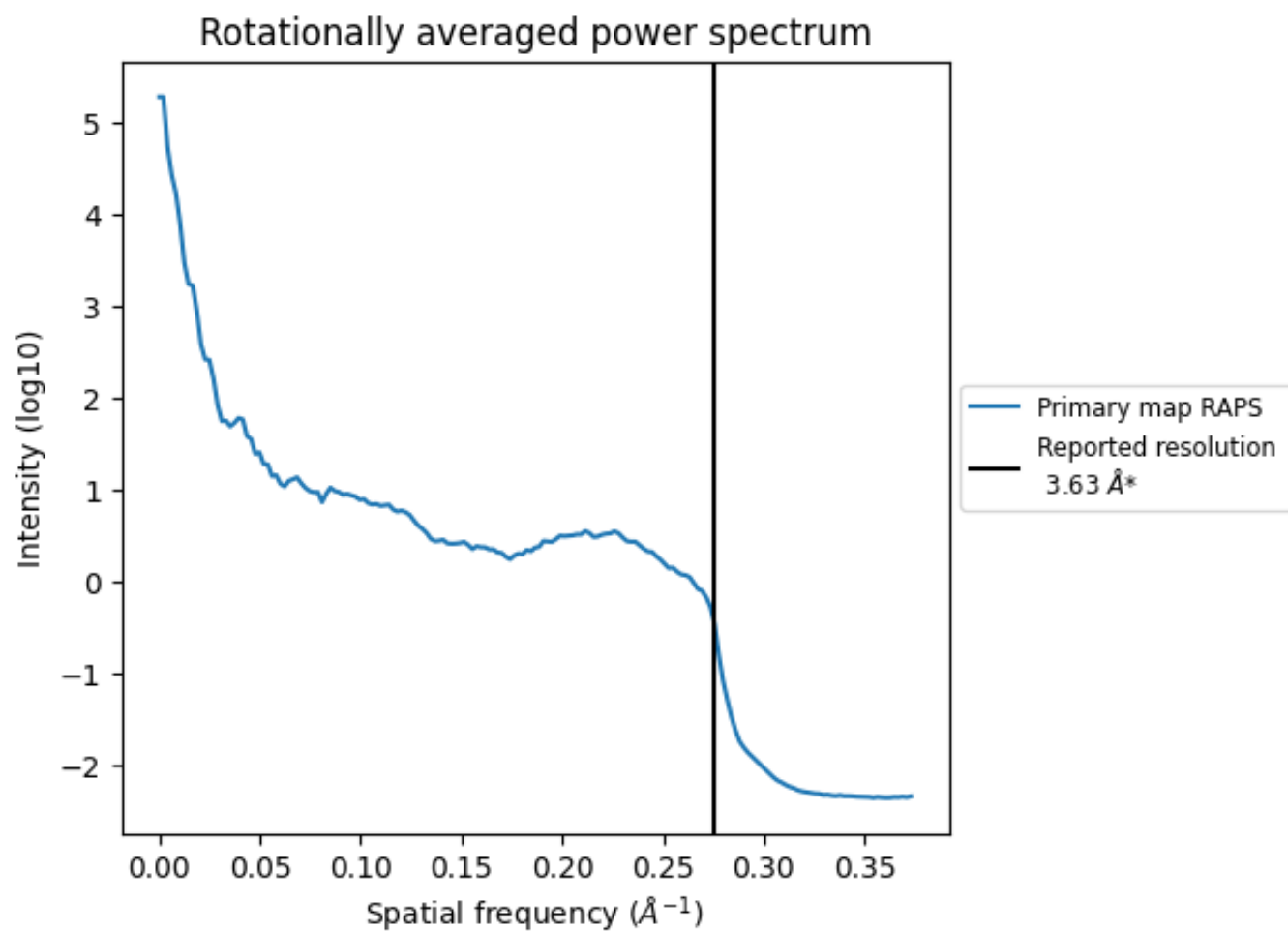
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5895  $\text{nm}^3$ ; this corresponds to an approximate mass of 5325 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 ⓘ

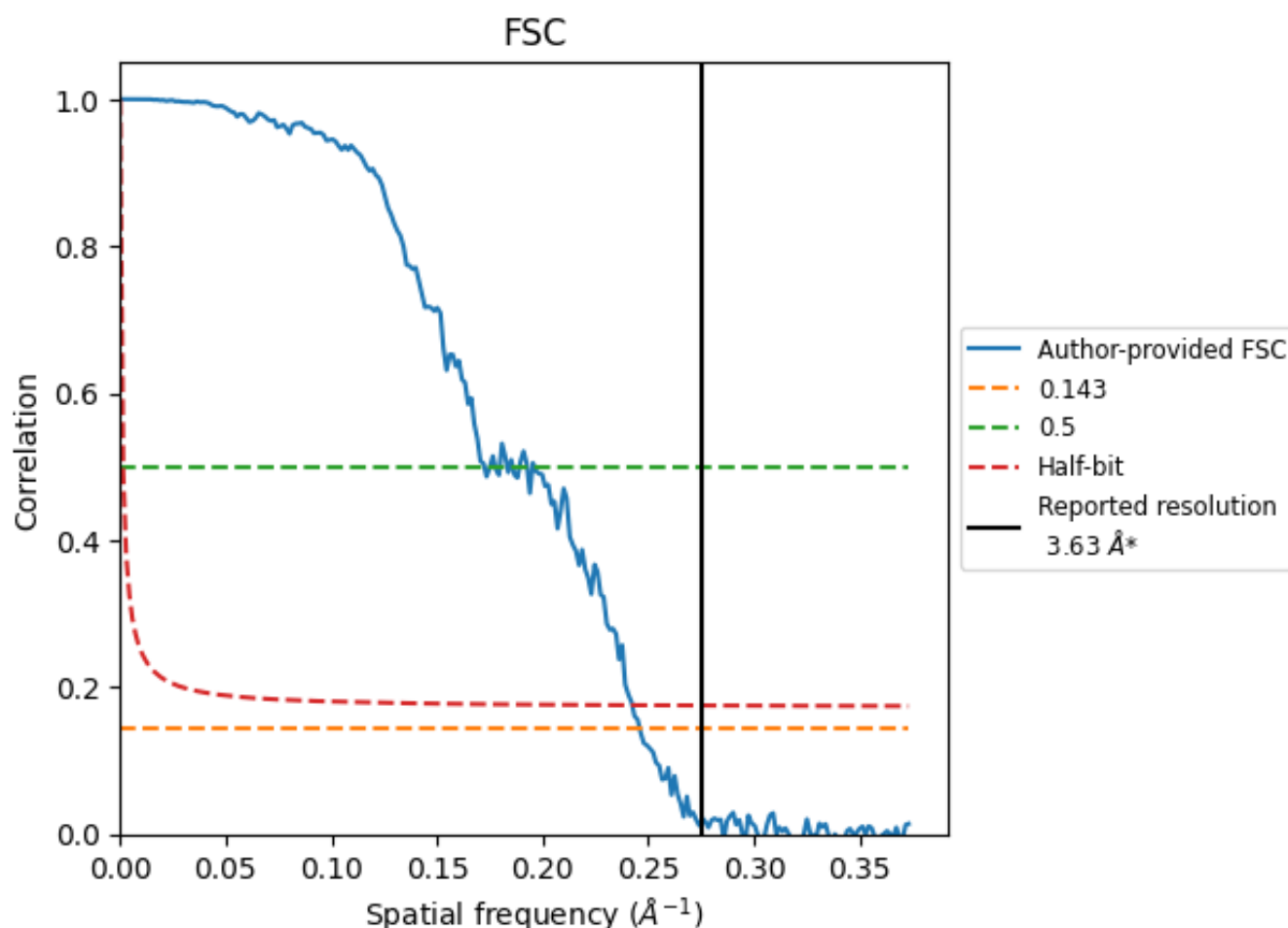


\*Reported resolution corresponds to spatial frequency of 0.275 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.275 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.63	-	-
Author-provided FSC curve	4.07	5.80	4.13
Unmasked-calculated*	-	-	-

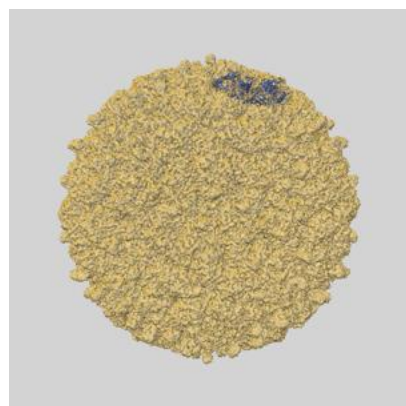
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.07 differs from the reported value 3.63 by more than 10 %

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

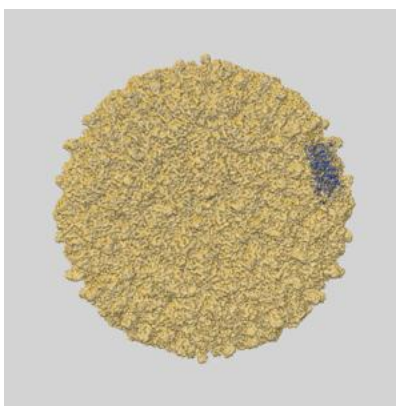
This section contains information regarding the fit between EMDB map EMD-12558 and PDB model 7NS2. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlays

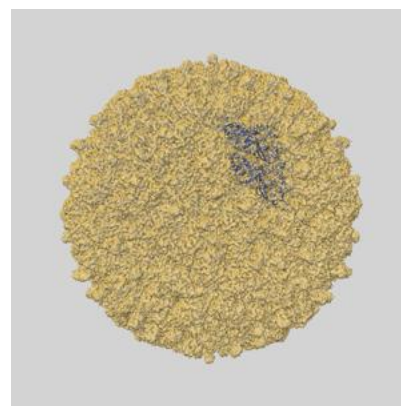
#### 9.1.1 Map-model overlay [i](#)



X

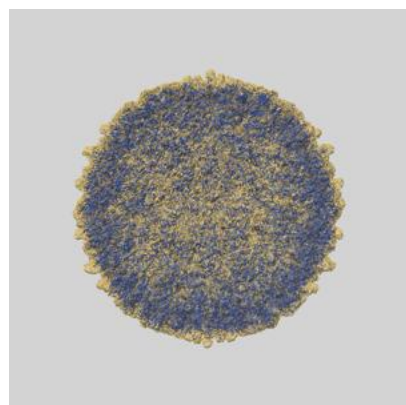


Y

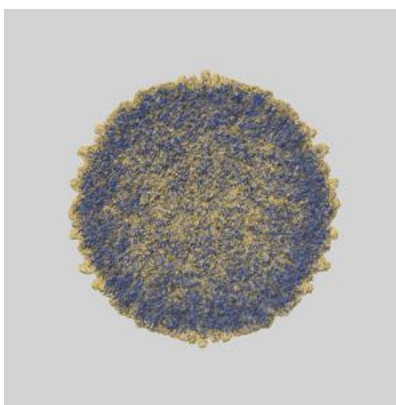


Z

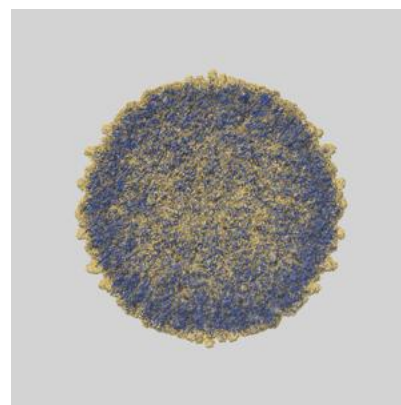
#### 9.1.2 Map-model assembly overlay [i](#)



X



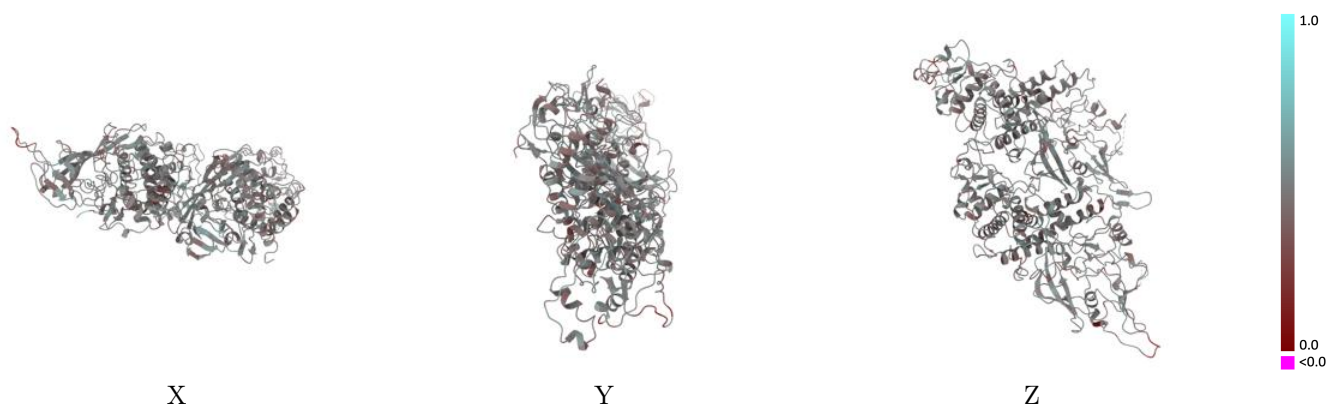
Y



Z

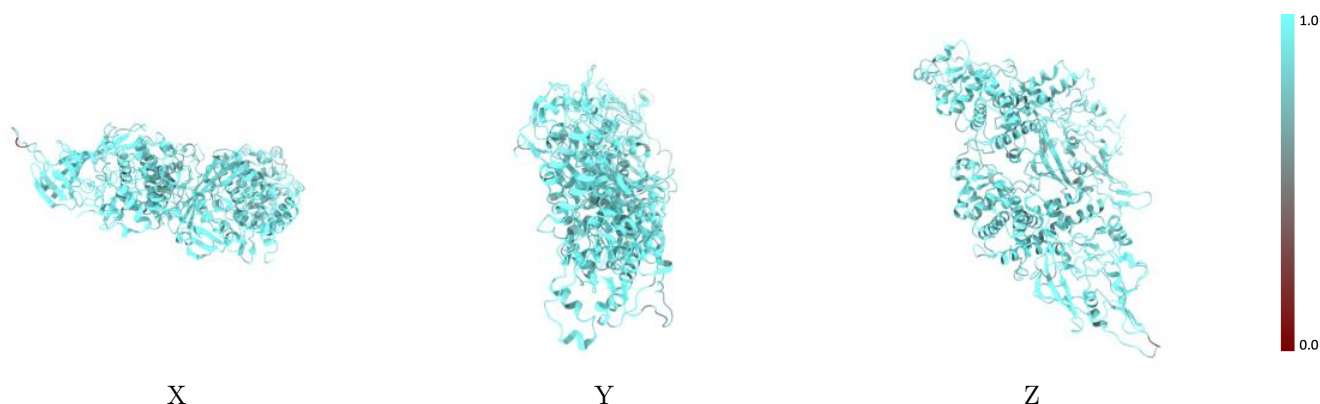
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



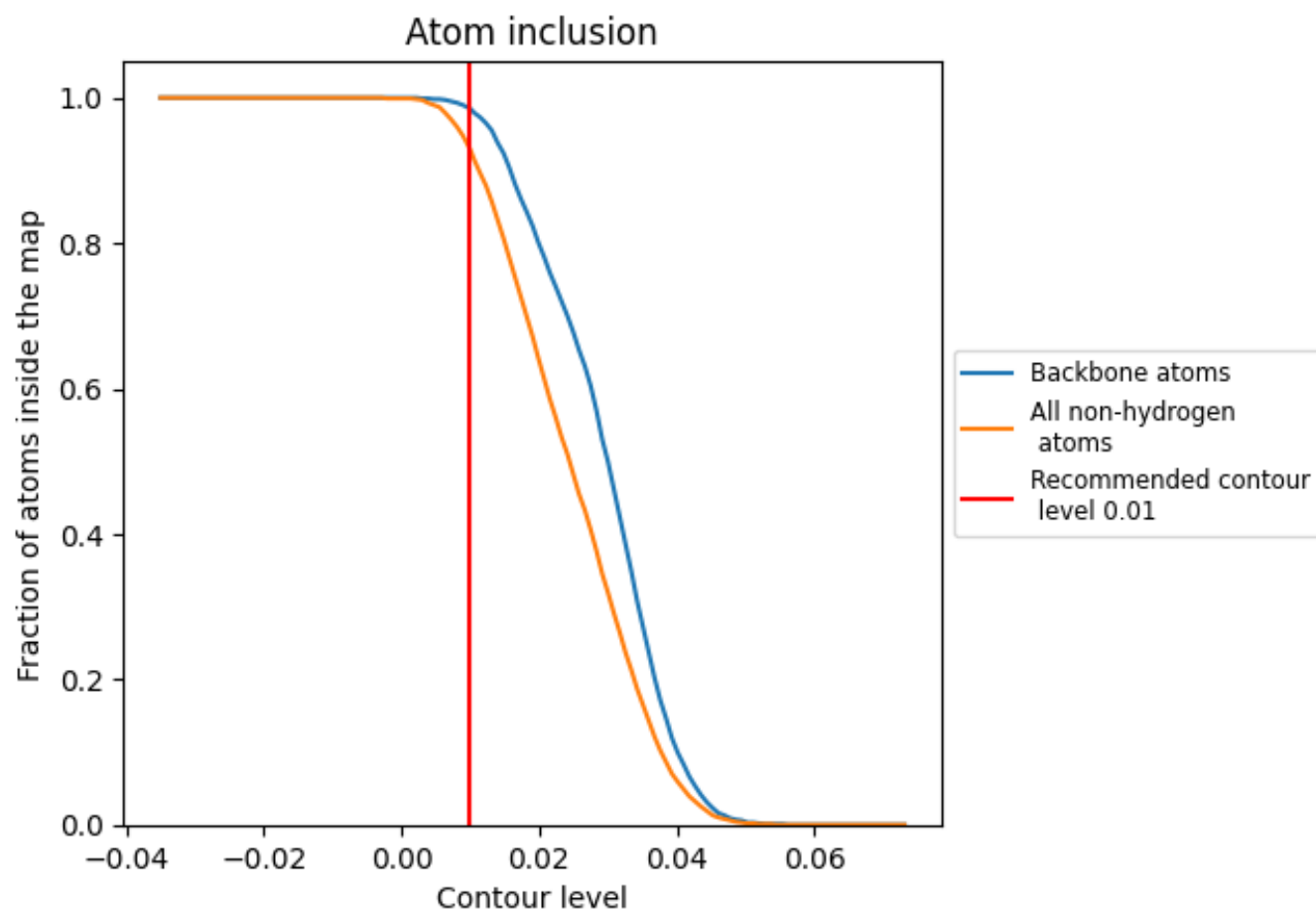
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 93% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9290	<div></div> 0.4630
A	<div></div> 0.9310	<div></div> 0.4650
B	<div></div> 0.9270	<div></div> 0.4620

