



Full wwPDB EM Validation Report ⓘ

May 13, 2025 – 11:18 PM EDT

PDB ID : 9B7T / pdb_00009b7t
EMDB ID : EMD-44323
Title : Fab3-3 in complex with the capsid of Adeno-associated virus type 9
Authors : Mietzsch, M.; McKenna, R.
Deposited on : 2024-03-27
Resolution : 3.56 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

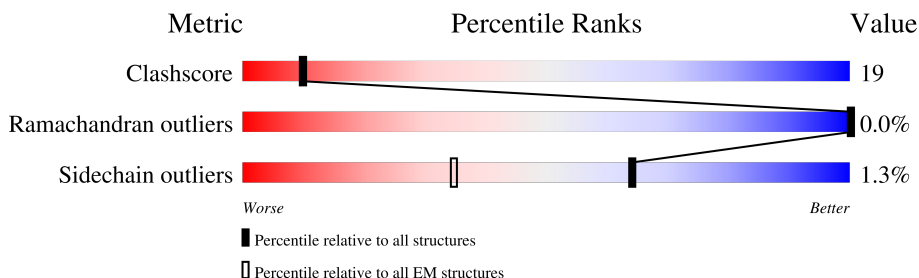
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

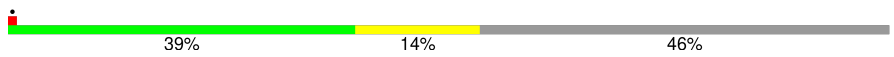
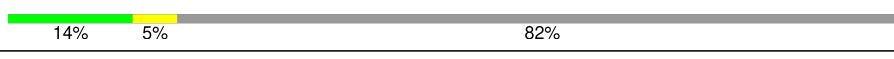

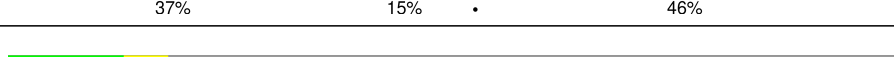

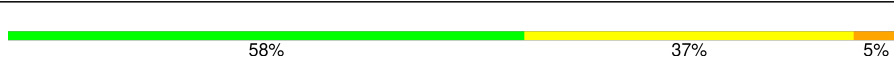


The reported resolution of this entry is 3.56 Å.

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 ≥ 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	736	
1	B	736	
1	C	736	
1	D	736	
1	E	736	
1	F	736	
2	H	123	
3	L	105	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18059 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 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	394	Total	C	N	O	S	0	0
			3116	1978	533	594	11		
1	B	134	Total	C	N	O	S	0	0
			1052	654	190	205	3		
1	C	499	Total	C	N	O	S	0	0
			3987	2516	695	762	14		
1	D	394	Total	C	N	O	S	0	0
			3116	1978	533	594	11		
1	E	134	Total	C	N	O	S	0	0
			1052	654	190	205	3		
1	F	499	Total	C	N	O	S	0	0
			3987	2516	695	762	14		

- Molecule 2 is a protein called Fab3-3 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	123	Total	C	N	O	S	0	0
			948	603	156	187	2		

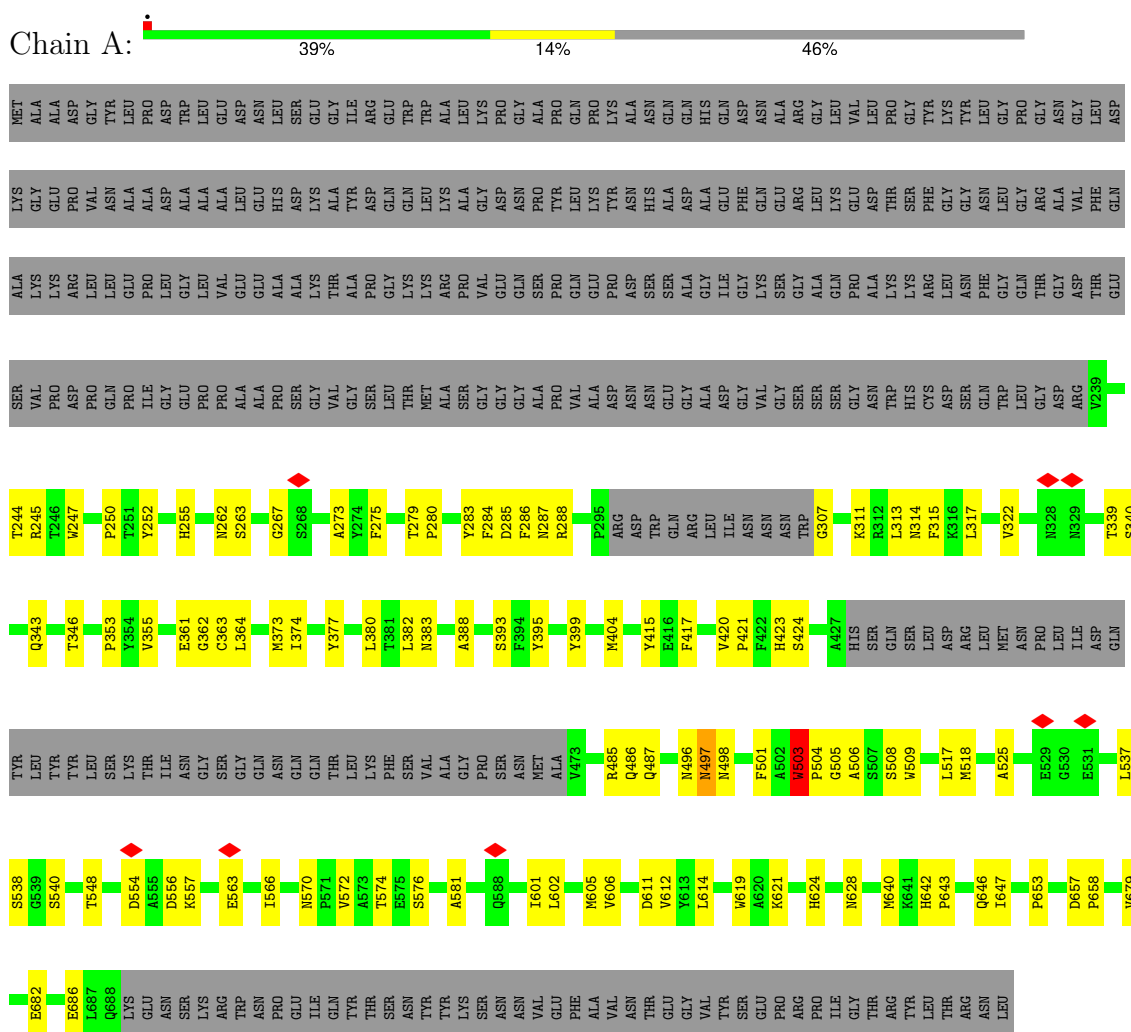
- Molecule 3 is a protein called Fab3-3 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	105	Total	C	N	O	S	0	0
			801	505	133	160	3		

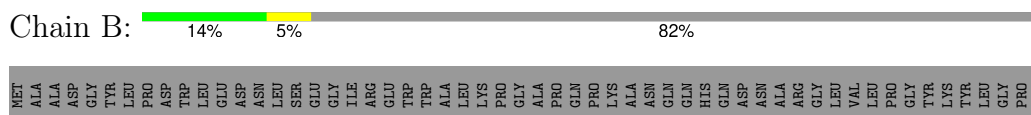
3 Residue-property plots

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

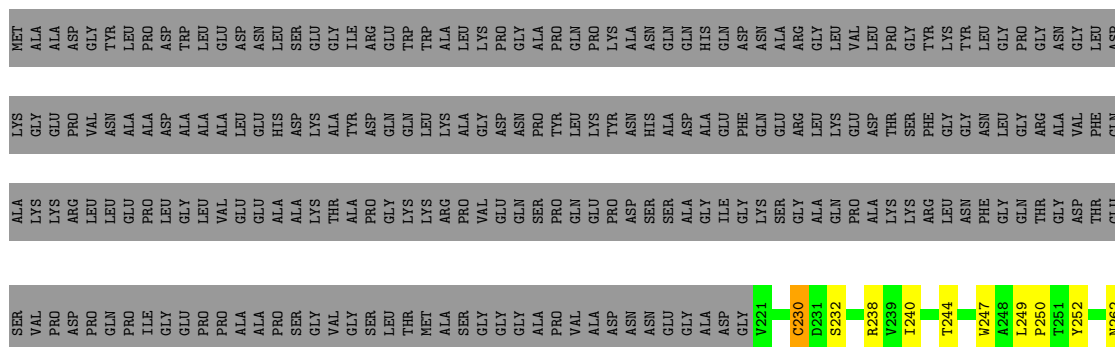
• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1



GLU	ASN	V880	ASN	H428	GLU	LEU	THR	SER	ALA	LYS	MET
PRO	LYS	AS81	ARG	S429	ILE	THR	THR	VAL	LYS	GLY	ALA
ARG	ASP	T582	GLY	Q430	CYS	ASN	SER	PRO	LYS	GLY	ALA
PRO	ASN	Q581	ASN	S431	LEU	ASN	THR	ARG	ASP	PRO	GLY
GLY	LEU	Q585	SER	LEU	PRO	TRP	THR	GLN	LEU	ASN	TYR
ASN	ASN	S586	LEU	PHE	PRO	PHE	TRP	PRO	GLU	LEU	GLY
SER	PHE	Q590	MET	P438	GLY	THR	THR	ALA	PRO	GLU	LEU
ARG	ILE	Q598	PRO	L439	ASN	ALA	ALA	ILE	PRO	ALA	PRO
LEU	THR	Q599	GLY	Q442	ARG	PRO	PRO	GLY	GLY	ASP	TRP
THR	GLN	Q599	GLY	Y443	VAL	VAL	LYS	THR	LEU	ALA	ALA
ARG	TYR	G600	ALA	PHE	PHE	ARG	TYR	PRO	VAL	ALA	GLU
ASN	SER	I601	MET	T450	MET	LEU	ASN	ALA	GLU	LEU	ASP
LEU	THR	V606	ALA	I451	ILE	ASN	ASN	ALA	GLU	GLY	ASN
	GLY	V606	SER	N452	PRO	PHE	HIS	PRO	ALA	HIS	ASN
	GLN		HIS		GLN	LEU	TYR	SER	ALA	ASP	GLY
	VAL	D609	LYS	N457	TYR	LEU	LEU	GLY	LYS	LYS	GLY
SER	SER	R610	GLU	Q459	PHE	PHE	GLN	VAL	THR	ALA	GLY
VAL	VAL	ASP	GLY	Q459	TYR	ASN	GLN	GLY	ALA	TYR	ILE
ILE	ILE	VAL	GLU	T460	ILE	ILE	ILE	SER	PRO	ASP	ARG
GLU	TYR	LEU	ASP	L461	THR	THR	ASN	LEU	LYS	GLN	TRP
TRP	GLU	LEU	ARG	K462	VAL	VAL	ASN	THR	ARG	LYS	TRP
GLU	TRP	GLN	PHE	F463	ASN	LYS	SER	ALA	LYS	LEU	TRP
LEU	GLY	GLY	PHE	S464	ASP	GLU	THR	ALA	ARG	ALA	LEU
GLN	GLN	ILE	PRO	V465	GLY	VAL	SER	SER	PRO	ALA	LEU
LYS	LYS	TRP	LEU	A466	THR	THR	GLY	GLY	VAL	GLY	LYS
ASN	ASN	ALA	GLY	M471	ALA	ASN	ASN	ALA	SER	PRO	PRO
LYS	LYS	ASP	SER	A472	VAL	ASN	SER	ALA	SER	PRO	ALA
SER	SER	I622	LEU	V473	GLY	GLY	ASN	PRO	PRO	TYR	PRO
LYS	LYS	GLY	ILE	Q474	ARG	VAL	ASN	VAL	GLU	LEU	GLN
TRP	ARG	L634	PHE	G475	SER	LYS	ASN	ALA	ALA	LYS	PRO
ASN	ASN	MET	GLY	R476	SER	ILE	TYR	ASN	ASP	TYR	LYS
PRO	PRO	GLY	GLN	N477	PHE	ALA	PHE	ASN	ASN	ASN	ASN
GLU	GLU	PHE	GLY	S483	CYS	ASN	GLY	GLU	SER	ALA	GLN
ILE	GLY	GLY	THR	T484	LEU	ASN	TYR	GLY	ALA	ASP	GLN
GLN	GLN	MET	GLY	R485	GLU	LEU	SER	ALA	GLY	ALA	HIS
TYR	TYR	LYS	ARG	THR	TYR	THR	THR	GLY	ILE	GLU	GLN
THR	THR	HIS	ASP	T491	PHE	SER	PRO	VAL	LYS	PHE	ASN
ASN	ASN	PRO	ASN	THR	PRO	THR	TRP	GLY	GLN	GLN	ASN
PRO	PRO	PRO	VAL	VAL	SER	VAL	GLY	GLY	SER	GLY	ALA
TYR	TYR	PRO	ASP	THR	GLN	GLN	TYR	SER	GLY	ARG	ARG
LYS	LYS	ILE	ALA	GLN	MET	VAL	PHE	SER	ALA	LEU	LEU
SER	SER	LEU	ASP	ASN	LEU	THR	ASP	SER	GLN	LYS	VAL
ASN	ASN	ILE	VAL	ASN	THR	THR	ASN	ASN	ALA	ASP	GLY
VAL	VAL	LYS	MET	SER	GLY	SER	ARG	TRP	LYS	THR	PRO
GLU	PHE	PRO	ILE	GLU	ASN	ASP	PHE	HIS	LYS	ARG	TYR
ALA	ALA	VAL	ASN	E563	GLN	LEU	HIS	GLN	GLY	GLY	TYR
ASN	ASN	PRO	THR	E564	PHE	PRO	PHE	GLN	ASN	ASN	TYR
THR	THR	THR	THR	TRP	GLN	LEU	THR	GLN	LYS	GLY	GLY
VAL	VAL	VAL	VAL	PRO	SER	THR	SER	TRP	PHE	ASN	LEU
THR	THR	ALA	ALA	GLY	THR	TYR	SER	GLY	GLY	LEU	GLY
GLU	GLU										



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	185536	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	14.684	Depositor
Minimum map value	-9.440	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2	Depositor
Map size (Å)	184.4, 184.4, 184.4	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.922, 0.922, 0.922	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	0.35	0/3212	0.76	5/4378 (0.1%)
1	B	0.36	0/1078	0.56	0/1467
1	C	0.41	0/4106	0.61	1/5593 (0.0%)
1	D	0.34	0/3212	0.62	4/4378 (0.1%)
1	E	0.35	0/1078	0.55	0/1467
1	F	0.39	0/4106	0.56	3/5593 (0.1%)
2	H	0.53	0/972	0.74	1/1321 (0.1%)
3	L	0.45	0/821	0.84	4/1116 (0.4%)
All	All	0.39	0/18585	0.64	18/25313 (0.1%)

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

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

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	503	TRP	CA-C-N	23.04	143.97	118.85
1	A	503	TRP	C-N-CA	23.04	143.97	118.85
1	D	503	TRP	CA-C-N	8.49	128.11	118.85
1	D	503	TRP	C-N-CA	8.49	128.11	118.85
2	H	120	GLY	N-CA-C	8.30	123.96	111.18
1	A	505	GLY	N-CA-C	8.25	122.63	112.73
3	L	80	VAL	CA-C-N	7.39	127.31	119.85
3	L	80	VAL	C-N-CA	7.39	127.31	119.85
1	D	539	GLY	N-CA-C	7.22	121.40	112.73
3	L	80	VAL	N-CA-C	7.09	115.61	109.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	565	GLU	N-CA-C	6.39	118.24	111.28
1	A	504	PRO	N-CA-C	6.01	121.46	113.40
1	A	540	SER	N-CA-C	5.69	117.84	109.24
1	D	272	ASN	N-CA-C	5.51	117.29	111.28
1	F	729	THR	CA-C-N	-5.19	115.08	123.23
1	F	729	THR	C-N-CA	-5.19	115.08	123.23
3	L	83	ARG	N-CA-C	5.10	117.50	111.33
1	F	565	GLU	N-CA-C	5.05	116.78	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	503	TRP	Peptide

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	3116	0	2930	110	0
1	B	1052	0	995	42	0
1	C	3987	0	3748	209	0
1	D	3116	0	2930	128	0
1	E	1052	0	995	50	0
1	F	3987	0	3746	158	0
2	H	948	0	909	81	0
3	L	801	0	763	57	0
All	All	18059	0	17016	669	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 19.

All (669) 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:D:490:SER:CB	1:D:534:PHE:CE1	1.77	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:525:ALA:CA	1:F:566:ILE:HD11	1.35	1.54
1:D:490:SER:HB2	1:D:534:PHE:CD1	1.39	1.53
3:L:43:ILE:CD1	3:L:124:THR:HG21	1.44	1.44
1:D:490:SER:CB	1:D:534:PHE:HE1	1.13	1.40
1:D:490:SER:HB2	1:D:534:PHE:CE1	0.86	1.39
1:A:496:ASN:O	1:C:459:GLN:HG2	1.30	1.30
1:B:429:SER:O	1:C:382:LEU:HG	1.31	1.30
1:E:585:GLN:OE1	1:F:501:PHE:CE1	1.84	1.30
3:L:43:ILE:CD1	3:L:124:THR:CG2	2.07	1.29
1:C:566:ILE:HD11	1:C:608:GLN:CB	1.62	1.28
1:F:525:ALA:N	1:F:566:ILE:HD11	1.53	1.24
3:L:43:ILE:HD13	3:L:124:THR:CG2	1.69	1.21
1:F:525:ALA:HA	1:F:566:ILE:HD11	1.18	1.15
1:F:529:GLU:OE1	1:F:567:LYS:NZ	1.77	1.14
3:L:43:ILE:HD11	3:L:124:THR:CG2	1.72	1.14
1:E:582:THR:O	1:F:485:ARG:NH1	1.81	1.14
1:F:525:ALA:CA	1:F:566:ILE:CD1	2.26	1.13
1:C:528:LYS:HE3	1:C:575:GLU:OE2	1.47	1.12
1:C:705:TYR:CE1	1:D:389:VAL:HB	1.84	1.12
1:F:525:ALA:N	1:F:566:ILE:CD1	2.12	1.11
1:F:525:ALA:HB2	1:F:566:ILE:HD12	1.28	1.11
1:A:288:ARG:HD3	1:A:363:CYS:SG	1.93	1.08
1:A:288:ARG:NH1	1:C:443:TYR:CE2	2.22	1.07
3:L:24:ILE:HG23	3:L:48:SER:OG	1.54	1.07
1:A:288:ARG:NH1	1:C:443:TYR:CD2	2.21	1.06
1:C:532:ASP:OD2	2:H:75:LEU:HB2	1.55	1.05
1:D:506:ALA:HB1	1:D:517:LEU:HD11	1.39	1.05
3:L:43:ILE:HD13	3:L:124:THR:HG21	1.09	1.05
1:A:287:ASN:OD1	1:A:619:TRP:CE2	2.11	1.03
1:D:490:SER:HB3	1:D:534:PHE:HE1	1.20	1.03
1:F:525:ALA:HB2	1:F:566:ILE:CD1	1.89	1.02
1:C:566:ILE:HD11	1:C:608:GLN:HB2	1.40	1.02
1:A:288:ARG:CD	1:A:363:CYS:SG	2.49	0.99
1:A:496:ASN:O	1:C:459:GLN:CG	2.11	0.99
1:C:566:ILE:HD11	1:C:608:GLN:HB3	1.41	0.99
3:L:43:ILE:HD13	3:L:124:THR:CB	1.93	0.98
1:A:382:LEU:HG	1:C:429:SER:O	1.65	0.96
1:C:566:ILE:CD1	1:C:608:GLN:CB	2.45	0.94
1:F:525:ALA:CB	1:F:566:ILE:CD1	2.44	0.94
1:C:528:LYS:CE	1:C:575:GLU:OE2	2.17	0.93
1:C:566:ILE:CD1	1:C:608:GLN:HB2	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:502:ALA:HB2	1:F:450:THR:HG23	1.51	0.93
2:H:121:ALA:HB3	2:H:124:TYR:CE2	2.04	0.93
3:L:51:ILE:HD11	3:L:93:PHE:CE2	2.04	0.92
1:C:705:TYR:HE1	1:D:389:VAL:HB	1.35	0.92
1:D:490:SER:CB	1:D:534:PHE:CD1	2.20	0.92
1:F:525:ALA:CB	1:F:566:ILE:HD11	1.99	0.92
1:F:712:GLU:OE2	1:F:725:ARG:NH2	2.02	0.91
1:E:585:GLN:OE1	1:F:501:PHE:CD1	2.23	0.91
2:H:60:GLN:O	2:H:112:ALA:HB1	1.70	0.91
3:L:43:ILE:HD11	3:L:124:THR:HG21	1.38	0.91
3:L:43:ILE:HD11	3:L:124:THR:HG22	1.50	0.90
3:L:51:ILE:HA	3:L:114:ASN:HD22	1.36	0.90
1:A:417:PHE:CD1	1:A:640:MET:HE1	2.08	0.89
3:L:80:VAL:CG2	3:L:81:PRO:HD2	2.01	0.89
1:C:528:LYS:CE	1:C:575:GLU:CD	2.45	0.89
1:C:704:ASN:CB	1:C:706:TYR:HE2	1.86	0.87
1:C:566:ILE:CG1	1:C:608:GLN:HB2	2.04	0.87
1:D:420:VAL:HB	1:D:421:PRO:HD2	1.57	0.86
2:H:58:ILE:HG22	2:H:68:PHE:HA	1.56	0.85
2:H:35:GLU:O	2:H:106:VAL:HG23	1.76	0.85
1:C:704:ASN:CB	1:C:706:TYR:CE2	2.59	0.84
3:L:80:VAL:HG22	3:L:81:PRO:HD2	1.58	0.84
1:A:498:ASN:O	1:C:451:ILE:HG21	1.77	0.84
1:E:585:GLN:CD	1:F:501:PHE:CE1	2.55	0.84
1:D:503:TRP:HB3	1:D:504:PRO:HD3	1.60	0.83
2:H:121:ALA:CB	2:H:124:TYR:CE2	2.62	0.82
1:B:429:SER:O	1:C:382:LEU:CG	2.23	0.82
1:A:417:PHE:HD1	1:A:640:MET:HE1	1.43	0.81
2:H:54:TYR:HB2	2:H:119:HIS:HB3	1.62	0.81
2:H:71:ASN:HD22	2:H:119:HIS:CD2	1.98	0.81
1:E:450:THR:HG21	1:F:501:PHE:CE2	2.15	0.81
3:L:43:ILE:CD1	3:L:124:THR:CB	2.56	0.81
1:A:250:PRO:HG3	1:A:373:MET:HE3	1.62	0.81
1:D:498:ASN:HB2	1:F:459:GLN:NE2	1.95	0.80
1:F:325:VAL:HG22	1:F:334:ILE:HG12	1.63	0.80
1:D:506:ALA:CB	1:D:517:LEU:HD11	2.10	0.80
2:H:121:ALA:CB	2:H:124:TYR:CZ	2.66	0.78
1:C:529:GLU:CG	1:C:567:LYS:CE	2.61	0.78
1:C:262:ASN:HD22	1:C:273:ALA:HA	1.48	0.78
1:C:529:GLU:CD	1:C:567:LYS:HE2	2.07	0.78
1:A:286:PHE:CE1	1:A:619:TRP:HH2	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:490:SER:CA	1:D:534:PHE:CD1	2.67	0.77
1:C:704:ASN:HB3	1:C:706:TYR:CE2	2.18	0.77
1:E:450:THR:HB	1:F:501:PHE:HE2	1.50	0.77
1:B:590:GLN:HG2	1:C:497:ASN:HD21	1.51	0.76
1:C:529:GLU:CG	1:C:567:LYS:HE2	2.15	0.76
1:F:525:ALA:N	1:F:566:ILE:HD13	1.98	0.76
1:B:566:ILE:HD12	1:B:570:ASN:HD22	1.51	0.76
1:D:262:ASN:HB2	1:D:273:ALA:HA	1.68	0.76
1:B:590:GLN:HA	1:C:497:ASN:ND2	2.01	0.75
2:H:60:GLN:C	2:H:112:ALA:HB1	2.11	0.75
1:D:566:ILE:HD12	1:D:570:ASN:HD22	1.51	0.75
1:D:490:SER:CA	1:D:534:PHE:HD1	1.99	0.75
1:C:528:LYS:HE3	1:C:575:GLU:CD	2.10	0.75
1:C:566:ILE:CD1	1:C:608:GLN:HB3	2.13	0.75
1:D:599:GLN:OE1	1:E:598:ASN:ND2	2.20	0.75
1:A:262:ASN:HD22	1:A:273:ALA:HA	1.51	0.74
1:D:269:SER:HB3	1:D:272:ASN:HB2	1.69	0.74
1:E:585:GLN:OE1	1:F:501:PHE:HE1	1.67	0.74
2:H:61:PRO:HA	2:H:112:ALA:HB2	1.66	0.74
1:D:307:GLY:HA2	1:D:423:HIS:O	1.86	0.74
1:A:566:ILE:HD12	1:A:570:ASN:HD22	1.50	0.74
1:C:566:ILE:HD11	1:C:608:GLN:C	2.12	0.74
1:A:497:ASN:HD22	1:A:497:ASN:H	1.32	0.74
1:C:569:THR:HG22	1:C:736:LEU:HD21	1.71	0.73
1:A:353:PRO:HB3	1:C:430:GLN:HE22	1.54	0.73
1:C:343:GLN:HG2	1:C:404:MET:HG2	1.68	0.73
1:C:542:ILE:HG12	1:C:560:ILE:HG23	1.70	0.73
1:C:705:TYR:HE1	1:D:389:VAL:CB	2.01	0.72
1:C:705:TYR:CE1	1:D:389:VAL:CB	2.69	0.72
1:D:501:PHE:CZ	1:F:585:GLN:OE1	2.43	0.72
2:H:48:ILE:HG13	2:H:97:ASN:OD1	1.90	0.72
1:C:290:HIS:HD2	1:C:615:GLN:HA	1.53	0.72
1:E:585:GLN:NE2	1:F:496:ASN:OD1	2.23	0.72
2:H:128:PHE:CZ	3:L:55:LEU:O	2.42	0.72
1:C:704:ASN:HB2	1:C:706:TYR:CE2	2.25	0.72
1:E:599:GLN:OE1	1:F:598:ASN:ND2	2.22	0.71
1:A:286:PHE:HE1	1:A:619:TRP:HH2	1.37	0.71
1:A:506:ALA:HB1	1:A:517:LEU:CD1	2.20	0.71
1:A:498:ASN:OD1	1:C:459:GLN:OE1	2.09	0.71
1:E:485:ARG:NH2	1:E:576:SER:OG	2.24	0.71
1:F:415:TYR:OH	1:F:642:HIS:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:54:TYR:CE1	2:H:73:TYR:CD1	2.78	0.71
1:D:490:SER:HA	1:D:534:PHE:HD1	1.56	0.71
1:C:528:LYS:HE2	1:C:575:GLU:CD	2.16	0.70
1:F:485:ARG:NH2	1:F:576:SER:OG	2.24	0.70
1:B:590:GLN:HA	1:C:497:ASN:HD22	1.55	0.70
1:A:417:PHE:HD1	1:A:640:MET:CE	2.05	0.70
1:C:503:TRP:H	1:C:504:PRO:CD	2.05	0.70
1:A:497:ASN:HD22	1:A:497:ASN:N	1.88	0.69
1:C:532:ASP:OD2	2:H:75:LEU:HD12	1.92	0.69
1:C:562:ASN:ND2	2:H:75:LEU:CD1	2.56	0.69
1:E:564:GLU:O	1:E:567:LYS:NZ	2.26	0.69
1:A:346:THR:HG22	1:A:647:ILE:HG12	1.75	0.69
1:C:532:ASP:OD2	2:H:75:LEU:CB	2.35	0.69
1:D:501:PHE:CE2	1:F:585:GLN:OE1	2.45	0.69
1:D:537:LEU:C	1:D:537:LEU:HD23	2.17	0.69
1:E:462:LYS:NZ	1:F:554:ASP:OD1	2.17	0.69
2:H:127:LEU:HG	3:L:113:ALA:HB1	1.73	0.69
1:D:262:ASN:ND2	1:D:273:ALA:HB2	2.07	0.68
1:C:533:ARG:HH22	2:H:79:TYR:CB	2.06	0.68
1:F:275:PHE:HB3	1:F:383:ASN:HB3	1.76	0.68
1:C:566:ILE:HD11	1:C:608:GLN:CA	2.24	0.68
3:L:55:LEU:HD22	3:L:93:PHE:CD1	2.28	0.68
1:D:485:ARG:HH21	1:D:576:SER:N	1.92	0.68
3:L:76:LEU:HD22	3:L:80:VAL:HG11	1.76	0.68
1:B:477:ASN:ND2	1:C:357:GLY:O	2.25	0.67
1:A:284:PHE:CE1	1:A:679:VAL:HG21	2.30	0.67
1:E:450:THR:CB	1:F:501:PHE:HE2	2.06	0.67
3:L:59:GLN:HB2	3:L:69:LEU:HD11	1.76	0.67
1:C:503:TRP:N	1:C:504:PRO:CD	2.56	0.67
1:F:313:LEU:HB3	1:F:415:TYR:HB3	1.76	0.67
3:L:43:ILE:CD1	3:L:124:THR:HB	2.24	0.67
3:L:28:GLN:HG2	3:L:45:CYS:HB3	1.77	0.67
1:E:450:THR:CB	1:F:501:PHE:CE2	2.78	0.67
1:F:288:ARG:HD3	1:F:363:CYS:SG	2.35	0.67
2:H:119:HIS:CE1	2:H:129:PHE:HE1	2.13	0.66
1:A:399:TYR:O	1:F:230:CYS:O	2.13	0.66
1:C:562:ASN:ND2	2:H:75:LEU:HD13	2.10	0.66
1:F:525:ALA:HA	1:F:566:ILE:CD1	2.09	0.66
2:H:121:ALA:HB3	2:H:124:TYR:CZ	2.31	0.66
2:H:121:ALA:HB3	2:H:124:TYR:CD2	2.30	0.66
1:C:325:VAL:HG22	1:C:334:ILE:HG12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:ASP:OD1	1:C:462:LYS:NZ	2.22	0.66
1:D:497:ASN:HD22	1:F:590:GLN:HA	1.60	0.66
2:H:106:VAL:CG1	2:H:140:VAL:HG21	2.25	0.66
1:A:288:ARG:HD3	1:A:363:CYS:CB	2.25	0.66
1:C:533:ARG:NH2	2:H:79:TYR:HB2	2.11	0.65
1:C:611:ASP:OD1	1:C:612:VAL:N	2.30	0.65
1:A:509:TRP:HD1	1:A:518:MET:HE2	1.59	0.65
1:F:565:GLU:OE1	1:F:565:GLU:N	2.20	0.65
1:C:529:GLU:HG2	1:C:567:LYS:HE3	1.79	0.65
1:D:343:GLN:HG2	1:D:404:MET:HG2	1.77	0.65
1:D:353:PRO:HB3	1:F:430:GLN:HE22	1.62	0.65
3:L:51:ILE:HD11	3:L:93:PHE:CZ	2.31	0.65
1:F:712:GLU:OE1	1:F:725:ARG:NH1	2.29	0.65
1:A:621:LYS:HB2	1:A:643:PRO:HG3	1.78	0.65
1:C:525:ALA:HB2	1:C:567:LYS:HA	1.79	0.64
1:D:496:ASN:OD1	1:F:585:GLN:NE2	2.30	0.64
1:F:466:ALA:HB1	1:F:474:GLN:HG2	1.78	0.64
1:C:705:TYR:CD1	1:D:389:VAL:HB	2.30	0.64
1:D:262:ASN:HB2	1:D:274:TYR:H	1.62	0.64
1:A:287:ASN:OD1	1:A:619:TRP:CZ2	2.51	0.64
1:D:537:LEU:HD23	1:D:537:LEU:O	1.98	0.64
1:E:450:THR:CG2	1:F:501:PHE:CE2	2.81	0.64
3:L:52:ASN:C	3:L:52:ASN:HD22	2.06	0.64
1:F:525:ALA:H	1:F:566:ILE:CD1	2.07	0.63
1:E:585:GLN:CD	1:F:501:PHE:HE1	2.02	0.63
1:D:262:ASN:ND2	1:D:273:ALA:CB	2.62	0.63
1:A:537:LEU:C	1:A:537:LEU:HD23	2.24	0.63
1:A:252:TYR:OH	1:A:374:ILE:O	2.14	0.63
1:C:487:GLN:HE21	1:C:487:GLN:HA	1.64	0.62
1:D:312:ARG:NH1	1:D:684:GLU:OE1	2.29	0.62
1:F:725:ARG:HB2	1:F:726:PRO:HD2	1.80	0.62
1:C:323:LYS:NZ	1:C:336:ASN:OD1	2.25	0.62
3:L:24:ILE:HG23	3:L:48:SER:HG	1.59	0.62
1:C:423:HIS:NE2	1:C:612:VAL:HG22	2.14	0.62
1:F:611:ASP:OD1	1:F:612:VAL:N	2.32	0.62
1:C:529:GLU:HG2	1:C:567:LYS:CE	2.28	0.62
1:E:483:SER:OG	1:E:577:TYR:HB2	1.98	0.62
1:F:247:TRP:CD1	1:F:679:VAL:HG23	2.35	0.62
1:D:250:PRO:HG3	1:D:373:MET:HE3	1.80	0.62
1:A:288:ARG:HD2	1:A:363:CYS:SG	2.39	0.62
1:D:290:HIS:HD2	1:D:615:GLN:HA	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:TYR:OH	1:C:642:HIS:O	2.16	0.61
1:E:590:GLN:HA	1:F:497:ASN:ND2	2.15	0.61
3:L:54:TRP:HB3	3:L:113:ALA:HB3	1.81	0.61
1:B:485:ARG:NH2	1:B:576:SER:OG	2.33	0.61
1:D:554:ASP:OD1	1:F:462:LYS:NZ	2.27	0.61
1:F:250:PRO:HG3	1:F:373:MET:HE3	1.81	0.61
1:F:298:TRP:HE1	1:F:727:ILE:HG22	1.66	0.61
1:D:485:ARG:NH2	1:D:576:SER:OG	2.33	0.61
1:B:585:GLN:OE1	1:C:501:PHE:CZ	2.54	0.61
1:C:262:ASN:ND2	1:C:273:ALA:HA	2.15	0.61
1:C:621:LYS:HB2	1:C:643:PRO:HG3	1.82	0.61
1:E:485:ARG:HH21	1:E:576:SER:N	1.99	0.61
1:D:490:SER:O	1:D:496:ASN:ND2	2.32	0.60
1:B:458:GLN:NE2	3:L:72:SER:OG	2.33	0.60
1:C:361:GLU:HG3	1:C:362:GLY:H	1.67	0.60
1:C:533:ARG:HH22	2:H:79:TYR:HB2	1.65	0.60
1:E:457:ASN:N	1:F:498:ASN:OD1	2.35	0.60
1:E:459:GLN:HG2	1:F:496:ASN:O	2.02	0.60
1:C:562:ASN:HD21	2:H:75:LEU:CD1	2.15	0.60
1:D:272:ASN:OD1	1:F:471:MET:N	2.33	0.60
1:C:459:GLN:OE1	1:C:459:GLN:N	2.34	0.60
1:C:533:ARG:NH2	2:H:79:TYR:CB	2.65	0.60
1:A:244:THR:O	1:A:245:ARG:NH2	2.31	0.60
1:A:485:ARG:HH21	1:A:576:SER:N	2.00	0.60
1:A:506:ALA:HB1	1:A:517:LEU:HD11	1.83	0.60
1:C:490:SER:HB2	1:C:534:PHE:CD1	2.37	0.60
3:L:55:LEU:HD22	3:L:93:PHE:CG	2.36	0.60
1:C:247:TRP:CD1	1:C:679:VAL:HG23	2.37	0.59
2:H:35:GLU:O	2:H:106:VAL:CG2	2.47	0.59
1:C:250:PRO:HG3	1:C:373:MET:HE3	1.84	0.59
1:C:707:LYS:O	1:C:707:LYS:HG3	2.02	0.59
1:A:255:HIS:CG	1:A:653:PRO:HB3	2.38	0.59
1:C:566:ILE:HG23	1:C:566:ILE:O	2.00	0.59
2:H:111:THR:HG23	2:H:111:THR:O	2.03	0.59
3:L:80:VAL:HG23	3:L:81:PRO:HD2	1.83	0.59
3:L:34:SER:HA	3:L:127:ASP:HB2	1.84	0.59
1:D:358:SER:O	1:F:442:GLN:NE2	2.36	0.59
2:H:71:ASN:HB3	2:H:119:HIS:HD2	1.68	0.59
1:C:532:ASP:HB3	2:H:77:SER:HB2	1.83	0.58
1:C:712:GLU:CD	1:C:725:ARG:HH22	2.11	0.58
1:F:232:SER:HA	1:F:240:ILE:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:37:LEU:HD11	2:H:138:VAL:HG11	1.86	0.58
1:A:247:TRP:CD1	1:A:679:VAL:HG23	2.38	0.58
1:C:529:GLU:CD	1:C:567:LYS:CE	2.75	0.58
1:C:563:GLU:OE1	1:C:563:GLU:HA	2.04	0.58
1:C:485:ARG:HH21	1:C:576:SER:N	2.02	0.58
1:C:528:LYS:HE2	1:C:575:GLU:HG3	1.86	0.58
1:D:249:LEU:HB2	1:D:374:ILE:HD12	1.86	0.58
1:D:497:ASN:ND2	1:F:590:GLN:HA	2.19	0.58
1:F:290:HIS:HD2	1:F:615:GLN:HA	1.69	0.58
1:D:346:THR:HG22	1:D:647:ILE:HG12	1.86	0.57
1:D:490:SER:CB	1:D:534:PHE:HD1	2.03	0.57
2:H:128:PHE:CD1	3:L:56:ALA:HB2	2.38	0.57
1:C:288:ARG:HD3	1:C:363:CYS:SG	2.44	0.57
1:F:262:ASN:HD22	1:F:273:ALA:HA	1.68	0.57
1:F:425:SER:HB2	1:F:729:THR:O	2.04	0.57
2:H:106:VAL:HG12	2:H:140:VAL:HG21	1.85	0.57
1:B:581:ALA:O	1:C:485:ARG:HD2	2.04	0.57
1:E:585:GLN:NE2	1:F:501:PHE:CE1	2.73	0.57
1:D:493:VAL:HG12	1:F:461:LEU:HD13	1.86	0.57
1:C:228:TRP:CD1	1:D:402:SER:HG	2.22	0.57
1:C:290:HIS:CE1	1:C:366:PRO:HG3	2.40	0.57
1:C:704:ASN:O	1:D:390:GLY:HA3	2.04	0.57
1:A:361:GLU:HG3	1:A:362:GLY:H	1.70	0.57
1:C:332:LYS:NZ	1:D:657:ASP:OD2	2.27	0.57
1:A:339:THR:O	1:F:321:GLN:NE2	2.34	0.57
1:C:704:ASN:HB3	1:C:706:TYR:CD2	2.40	0.57
3:L:56:ALA:HB3	3:L:111:GLN:HB3	1.87	0.57
3:L:80:VAL:HG22	3:L:81:PRO:CD	2.31	0.56
1:F:355:VAL:H	1:F:646:GLN:NE2	2.03	0.56
1:A:275:PHE:HB3	1:A:383:ASN:HB3	1.88	0.56
1:C:528:LYS:HE2	1:C:575:GLU:CG	2.36	0.56
1:D:485:ARG:HD2	1:F:581:ALA:O	2.05	0.56
3:L:24:ILE:CG2	3:L:48:SER:OG	2.41	0.56
1:B:582:THR:O	1:C:485:ARG:NH1	2.38	0.56
1:C:252:TYR:HB2	1:C:280:PRO:HA	1.87	0.56
1:C:458:GLN:OE1	1:C:458:GLN:HA	2.05	0.56
1:D:503:TRP:CB	1:D:504:PRO:HD3	2.28	0.56
1:E:450:THR:HG21	1:F:501:PHE:CD2	2.40	0.56
1:A:420:VAL:HB	1:A:421:PRO:HD2	1.88	0.56
1:F:501:PHE:CD2	1:F:501:PHE:N	2.73	0.56
2:H:121:ALA:HB2	2:H:124:TYR:CZ	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:128:PHE:CE1	3:L:113:ALA:HB2	2.41	0.56
1:A:307:GLY:HA2	1:A:423:HIS:O	2.06	0.56
2:H:52:SER:HA	2:H:74:TYR:CD2	2.41	0.56
1:B:427:ALA:HB3	1:C:391:ARG:HD3	1.87	0.56
1:A:497:ASN:H	1:A:497:ASN:ND2	2.03	0.56
1:F:343:GLN:HG2	1:F:404:MET:HG2	1.88	0.56
1:A:285:ASP:O	1:A:363:CYS:HA	2.06	0.56
1:C:485:ARG:NH2	1:C:576:SER:OG	2.39	0.56
3:L:43:ILE:CG1	3:L:124:THR:HG21	2.31	0.56
1:D:581:ALA:O	1:E:485:ARG:HD2	2.06	0.55
1:F:424:SER:HB2	1:F:426:TYR:CE2	2.41	0.55
1:B:420:VAL:HB	1:B:421:PRO:HD2	1.88	0.55
1:D:288:ARG:HH21	1:D:615:GLN:HB3	1.72	0.55
1:D:415:TYR:OH	1:D:642:HIS:O	2.22	0.55
1:E:606:VAL:HG12	1:F:628:ASN:HB3	1.88	0.55
1:C:548:THR:CG2	1:C:553:VAL:HG11	2.36	0.55
1:B:485:ARG:HG2	1:B:486:GLN:N	2.21	0.55
2:H:25:GLU:OE2	2:H:133:GLY:HA3	2.06	0.55
1:C:569:THR:HG22	1:C:736:LEU:CD2	2.36	0.55
1:C:284:PHE:CE1	1:C:679:VAL:HG21	2.41	0.55
1:C:298:TRP:CG	1:C:614:LEU:HD12	2.42	0.55
1:D:626:ASP:OD1	1:F:424:SER:OG	2.10	0.55
1:A:566:ILE:HD12	1:A:570:ASN:ND2	2.21	0.55
2:H:87:ARG:NH1	2:H:110:ASP:OD1	2.40	0.55
1:F:690:GLU:HG3	1:F:732:LEU:HD13	1.88	0.54
1:B:443:TYR:HB3	1:C:361:GLU:OE1	2.07	0.54
2:H:49:SER:OG	2:H:94:THR:OG1	2.13	0.54
2:H:54:TYR:CE1	2:H:73:TYR:HD1	2.22	0.54
1:A:611:ASP:OD1	1:A:612:VAL:N	2.40	0.54
1:C:322:VAL:HG11	1:C:673:GLN:HE21	1.72	0.54
1:F:712:GLU:CD	1:F:725:ARG:HH22	2.08	0.54
1:A:518:MET:O	1:A:538:SER:HB2	2.07	0.54
1:C:503:TRP:H	1:C:504:PRO:HD3	1.72	0.54
1:E:437:ASN:HB2	1:F:355:VAL:HB	1.88	0.54
1:C:459:GLN:CD	1:C:459:GLN:H	2.14	0.54
1:D:288:ARG:HD3	1:D:363:CYS:SG	2.47	0.54
1:A:313:LEU:HB3	1:A:415:TYR:HB3	1.89	0.54
1:C:229:HIS:O	1:C:244:THR:OG1	2.22	0.54
1:C:609:ASP:CG	1:C:630:HIS:HE2	2.15	0.54
1:A:485:ARG:NH2	1:A:576:SER:OG	2.40	0.54
1:A:501:PHE:C	1:A:501:PHE:CD1	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:THR:HG22	1:C:647:ILE:HG12	1.89	0.54
1:C:533:ARG:HH22	2:H:79:TYR:HB3	1.73	0.54
1:C:566:ILE:HG12	1:C:608:GLN:HB2	1.88	0.54
1:A:286:PHE:CE1	1:A:619:TRP:CH2	2.90	0.54
1:A:417:PHE:CE1	1:A:640:MET:HE1	2.43	0.54
1:B:585:GLN:HB3	1:C:487:GLN:OE1	2.07	0.54
1:C:426:TYR:CD1	1:C:426:TYR:C	2.86	0.54
1:A:485:ARG:HH21	1:A:576:SER:H	1.56	0.54
1:C:562:ASN:ND2	2:H:75:LEU:HD11	2.22	0.54
1:C:425:SER:HB2	1:C:729:THR:O	2.08	0.53
1:F:566:ILE:HD12	1:F:566:ILE:C	2.33	0.53
1:A:508:SER:O	1:C:578:GLY:HA3	2.08	0.53
1:D:309:ARG:NH1	1:D:420:VAL:O	2.38	0.53
1:D:392:SER:O	1:F:694:ARG:NH2	2.41	0.53
1:C:262:ASN:HB2	1:C:267:GLY:HA2	1.89	0.53
2:H:119:HIS:CE1	2:H:129:PHE:CE1	2.95	0.53
2:H:120:GLY:CA	2:H:125:SER:HA	2.39	0.53
1:A:501:PHE:CZ	1:C:450:THR:HG21	2.44	0.53
1:C:426:TYR:CE2	1:C:734:ARG:HD3	2.43	0.53
1:B:485:ARG:HH21	1:B:576:SER:N	2.06	0.53
2:H:113:VAL:CG2	2:H:115:TYR:CE1	2.92	0.53
1:A:658:PRO:HG2	1:F:250:PRO:HB3	1.91	0.53
1:C:566:ILE:CG1	1:C:608:GLN:CB	2.80	0.52
1:C:426:TYR:CD2	1:C:734:ARG:HD3	2.45	0.52
1:F:249:LEU:HB2	1:F:374:ILE:HD12	1.91	0.52
1:F:501:PHE:H	1:F:501:PHE:HD2	1.56	0.52
1:C:435:LEU:HD21	1:C:736:LEU:HB3	1.92	0.52
1:E:459:GLN:NE2	1:F:496:ASN:O	2.42	0.52
1:A:506:ALA:CB	1:A:517:LEU:CD1	2.86	0.52
1:A:572:VAL:HG12	1:A:574:THR:H	1.75	0.52
1:D:500:GLU:HA	1:D:500:GLU:OE1	2.08	0.52
1:A:581:ALA:O	1:B:485:ARG:HD2	2.09	0.52
1:B:426:TYR:CD1	1:B:426:TYR:C	2.87	0.52
1:B:434:ARG:NH2	1:C:271:ASP:O	2.39	0.52
1:D:621:LYS:HB2	1:D:643:PRO:HG3	1.92	0.52
2:H:58:ILE:HD11	2:H:132:TRP:CZ3	2.44	0.52
1:A:343:GLN:HG2	1:A:404:MET:HG2	1.91	0.52
1:C:487:GLN:HA	1:C:487:GLN:NE2	2.24	0.52
1:C:532:ASP:OD2	2:H:75:LEU:CD1	2.56	0.52
1:F:501:PHE:N	1:F:501:PHE:HD2	2.07	0.52
2:H:66:LEU:N	2:H:66:LEU:CD1	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:106:VAL:HG11	2:H:140:VAL:HG21	1.91	0.52
3:L:52:ASN:O	3:L:52:ASN:ND2	2.43	0.52
1:C:232:SER:OG	1:C:297:ASP:OD2	2.27	0.52
1:E:582:THR:HG22	1:F:597:GLN:HG3	1.93	0.52
1:F:358:SER:HB2	1:F:360:HIS:CD2	2.45	0.51
1:F:525:ALA:H	1:F:566:ILE:HD13	1.69	0.51
1:D:503:TRP:N	1:D:504:PRO:CD	2.73	0.51
1:D:274:TYR:HA	1:D:383:ASN:ND2	2.25	0.51
1:D:351:GLN:O	1:F:735:ASN:ND2	2.43	0.51
1:A:247:TRP:CZ2	1:A:317:LEU:HD11	2.46	0.51
1:C:488:ARG:O	1:C:488:ARG:HG3	2.09	0.51
1:B:428:HIS:HE1	1:C:624:HIS:O	1.93	0.51
1:C:529:GLU:HG3	1:C:567:LYS:HE2	1.92	0.51
1:E:477:ASN:ND2	1:F:357:GLY:O	2.43	0.51
3:L:28:GLN:HG2	3:L:45:CYS:CB	2.41	0.51
1:A:563:GLU:O	1:A:566:ILE:HG12	2.10	0.51
1:D:501:PHE:CD1	1:D:501:PHE:C	2.89	0.51
1:E:442:GLN:NE2	1:F:358:SER:O	2.44	0.51
1:D:283:TYR:HB3	1:D:648:LEU:HD13	1.92	0.51
1:A:275:PHE:CZ	1:A:388:ALA:HB2	2.46	0.51
1:A:283:TYR:HE1	1:A:285:ASP:HB2	1.76	0.51
1:A:287:ASN:OD1	1:A:619:TRP:CD2	2.61	0.51
1:C:296:ARG:HD2	1:C:296:ARG:O	2.11	0.51
1:C:698:GLU:HG2	1:F:296:ARG:NE	2.26	0.50
1:F:288:ARG:HH21	1:F:615:GLN:HB3	1.76	0.50
1:A:657:ASP:HB3	1:F:325:VAL:HG21	1.92	0.50
1:D:380:LEU:HD21	1:F:438:PRO:HB3	1.92	0.50
1:C:532:ASP:H	2:H:77:SER:HB2	1.75	0.50
1:A:395:TYR:OH	1:C:735:ASN:OD1	2.21	0.50
1:D:262:ASN:CB	1:D:273:ALA:HA	2.40	0.50
1:F:306:TRP:CE2	1:F:690:GLU:HG2	2.46	0.50
1:A:279:THR:OG1	1:A:377:TYR:O	2.23	0.50
1:A:287:ASN:OD1	1:A:619:TRP:NE1	2.45	0.50
1:C:355:VAL:H	1:C:646:GLN:NE2	2.10	0.50
1:D:309:ARG:NH1	1:D:419:ASN:OD1	2.45	0.50
1:F:262:ASN:OD1	1:F:263:SER:N	2.44	0.50
1:F:329:ASN:OD1	1:F:330:GLY:N	2.44	0.50
1:A:355:VAL:H	1:A:646:GLN:NE2	2.10	0.50
1:B:458:GLN:NE2	3:L:72:SER:HG	2.10	0.50
1:D:314:ASN:OD1	1:D:315:PHE:N	2.44	0.50
1:A:424:SER:HG	1:B:626:ASP:CG	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:GLN:HE22	3:L:72:SER:HG	1.57	0.50
1:E:429:SER:O	1:F:382:LEU:HG	2.11	0.49
2:H:54:TYR:CD2	2:H:126:GLY:CA	2.95	0.49
1:A:628:ASN:HB3	1:C:606:VAL:HG12	1.93	0.49
1:A:601:ILE:HD11	1:C:603:PRO:HD3	1.95	0.49
1:C:321:GLN:HE22	1:D:340:SER:HA	1.77	0.49
1:D:361:GLU:HG3	1:D:362:GLY:H	1.77	0.49
1:F:298:TRP:HE1	1:F:727:ILE:CG2	2.24	0.49
1:B:466:ALA:HB1	1:B:474:GLN:HG2	1.93	0.49
2:H:48:ILE:HG21	2:H:92:LEU:HD11	1.94	0.49
1:A:485:ARG:HD2	1:C:581:ALA:O	2.13	0.49
2:H:21:VAL:HG22	2:H:46:GLU:HG3	1.94	0.49
1:A:509:TRP:CD1	1:A:518:MET:HE2	2.45	0.49
1:D:316:LYS:HB2	1:D:680:SER:OG	2.12	0.49
3:L:88:GLY:HA3	3:L:93:PHE:CD1	2.47	0.49
1:A:262:ASN:OD1	1:A:263:SER:N	2.46	0.49
1:C:275:PHE:HB3	1:C:383:ASN:HB3	1.94	0.49
1:D:253:ASN:O	1:D:256:LEU:HB2	2.13	0.49
1:A:506:ALA:HB2	1:A:537:LEU:HD22	1.95	0.49
1:A:525:ALA:HB3	1:A:572:VAL:HA	1.93	0.49
1:C:244:THR:HA	1:C:679:VAL:O	2.13	0.49
1:A:497:ASN:N	1:A:497:ASN:ND2	2.60	0.48
1:D:247:TRP:CD1	1:D:679:VAL:HG23	2.47	0.48
1:E:461:LEU:HD13	1:F:493:VAL:HG12	1.95	0.48
1:A:288:ARG:CD	1:A:363:CYS:CB	2.90	0.48
1:D:424:SER:HB2	1:D:426:TYR:CE2	2.48	0.48
1:D:511:LEU:HD21	1:F:568:THR:O	2.12	0.48
2:H:106:VAL:HG11	2:H:140:VAL:CG2	2.43	0.48
1:A:283:TYR:CE1	1:A:285:ASP:HB2	2.48	0.48
1:A:314:ASN:OD1	1:A:315:PHE:N	2.46	0.48
1:C:230:CYS:SG	1:C:244:THR:N	2.82	0.48
1:F:306:TRP:CZ2	1:F:690:GLU:HG2	2.48	0.48
1:A:506:ALA:HB2	1:A:537:LEU:CD2	2.43	0.48
1:C:323:LYS:HZ1	1:D:337:ASN:HD21	1.61	0.48
1:F:611:ASP:OD1	1:F:729:THR:HG22	2.14	0.48
2:H:120:GLY:HA2	2:H:125:SER:HA	1.95	0.48
1:D:509:TRP:HD1	1:D:518:MET:HE2	1.78	0.48
1:E:452:ASN:ND2	1:E:460:THR:HG21	2.27	0.48
1:D:537:LEU:C	1:D:537:LEU:CD2	2.87	0.48
1:C:503:TRP:H	1:C:504:PRO:HD2	1.78	0.48
1:C:562:ASN:HD21	2:H:75:LEU:HD13	1.73	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:466:ALA:HB1	1:E:474:GLN:HG2	1.95	0.48
1:A:503:TRP:CD1	1:A:503:TRP:C	2.91	0.48
1:C:488:ARG:NH1	1:C:534:PHE:CD1	2.82	0.48
1:F:299:GLN:NE2	1:F:701:TYR:O	2.46	0.48
3:L:43:ILE:HD13	3:L:124:THR:HB	1.84	0.48
3:L:33:VAL:HG13	3:L:126:VAL:HG23	1.94	0.48
2:H:128:PHE:HE2	3:L:72:SER:H	1.58	0.48
1:C:249:LEU:HB2	1:C:374:ILE:HD12	1.96	0.47
1:F:563:GLU:HB3	1:F:566:ILE:CG1	2.44	0.47
2:H:54:TYR:CD2	2:H:126:GLY:HA3	2.49	0.47
1:C:707:LYS:HD2	1:D:384:ASP:OD2	2.15	0.47
1:F:316:LYS:HB2	1:F:680:SER:OG	2.14	0.47
1:C:303:ASN:HB3	1:C:700:GLN:NE2	2.30	0.47
1:F:563:GLU:HB3	1:F:566:ILE:HG13	1.95	0.47
2:H:124:TYR:CD2	2:H:124:TYR:N	2.82	0.47
3:L:76:LEU:HD22	3:L:80:VAL:CG1	2.45	0.47
1:C:313:LEU:HB3	1:C:415:TYR:HB3	1.97	0.47
1:D:255:HIS:CG	1:D:653:PRO:HB3	2.50	0.47
1:D:323:LYS:NZ	1:D:336:ASN:OD1	2.27	0.47
1:D:353:PRO:HB3	1:F:430:GLN:NE2	2.28	0.47
1:F:244:THR:HA	1:F:679:VAL:O	2.14	0.47
3:L:97:ILE:HG21	3:L:100:LEU:HD13	1.96	0.47
1:B:442:GLN:NE2	1:C:358:SER:O	2.47	0.47
1:F:312:ARG:HG2	1:F:416:GLU:OE1	2.15	0.47
1:B:433:ASP:OD1	1:B:433:ASP:N	2.46	0.47
1:E:580:VAL:HG23	1:F:484:TYR:CZ	2.50	0.47
1:C:503:TRP:HZ3	1:C:517:LEU:HB2	1.79	0.47
1:C:529:GLU:CG	1:C:567:LYS:HE3	2.39	0.47
1:E:473:VAL:HA	1:F:517:LEU:HB3	1.96	0.47
1:C:450:THR:HA	1:C:460:THR:O	2.15	0.46
1:C:548:THR:HG23	1:C:553:VAL:HG11	1.97	0.46
1:F:283:TYR:HB3	1:F:648:LEU:HD13	1.97	0.46
2:H:113:VAL:HG21	2:H:115:TYR:CE1	2.51	0.46
3:L:44:THR:HB	3:L:94:THR:HG22	1.96	0.46
1:C:531:GLU:O	1:C:531:GLU:HG3	2.15	0.46
1:F:712:GLU:CD	1:F:725:ARG:NH2	2.70	0.46
1:A:380:LEU:HD21	1:C:438:PRO:HB3	1.98	0.46
1:C:705:TYR:HE1	1:D:389:VAL:CG2	2.28	0.46
1:D:400:PHE:CE1	1:F:693:LYS:HG3	2.50	0.46
1:F:361:GLU:HG3	1:F:362:GLY:H	1.79	0.46
1:F:452:ASN:ND2	1:F:460:THR:HG21	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:699:ILE:HG12	1:F:703:SER:O	2.15	0.46
1:F:238:ARG:NH1	1:F:684:GLU:OE2	2.48	0.46
1:F:481:GLY:HA3	1:F:607:TRP:HB3	1.98	0.46
1:A:487:GLN:NE2	1:C:591:ALA:HB1	2.30	0.46
2:H:54:TYR:CD1	2:H:73:TYR:HD1	2.33	0.46
1:D:501:PHE:HZ	1:F:585:GLN:HE22	1.64	0.46
1:D:271:ASP:OD1	1:D:271:ASP:N	2.44	0.46
1:A:602:LEU:N	1:A:605:MET:SD	2.87	0.46
1:D:490:SER:OG	1:D:534:PHE:CE1	2.57	0.46
1:A:322:VAL:HG11	1:A:340:SER:HB2	1.98	0.46
1:A:322:VAL:HG11	1:A:340:SER:CB	2.46	0.46
1:C:232:SER:CB	1:C:297:ASP:OD2	2.64	0.46
1:A:262:ASN:HB2	1:A:267:GLY:HA2	1.98	0.45
1:B:443:TYR:CZ	1:C:359:ALA:HB1	2.51	0.45
1:C:283:TYR:HB3	1:C:648:LEU:HD13	1.97	0.45
1:C:509:TRP:N	1:C:516:SER:O	2.48	0.45
1:F:322:VAL:HG11	1:F:673:GLN:HE21	1.81	0.45
1:C:503:TRP:N	1:C:504:PRO:HD2	2.31	0.45
1:C:704:ASN:N	1:C:704:ASN:ND2	2.60	0.45
1:F:379:TYR:OH	1:F:395:TYR:N	2.42	0.45
1:B:568:THR:O	1:C:511:LEU:HD21	2.16	0.45
1:C:361:GLU:HG3	1:C:362:GLY:N	2.30	0.45
1:E:428:HIS:CE1	1:F:624:HIS:O	2.69	0.45
1:E:464:SER:OG	1:F:552:ASN:N	2.42	0.45
1:A:286:PHE:O	1:A:286:PHE:HD1	2.00	0.45
1:A:606:VAL:HG12	1:B:628:ASN:HB3	1.98	0.45
1:B:428:HIS:NE2	1:B:608:GLN:NE2	2.65	0.45
1:C:286:PHE:CE1	1:C:619:TRP:HH2	2.34	0.45
3:L:104:ASP:OD1	3:L:104:ASP:N	2.47	0.45
1:F:418:GLU:OE2	1:F:641:LYS:N	2.48	0.45
1:E:450:THR:HB	1:F:501:PHE:CE2	2.38	0.45
1:B:572:VAL:HG12	1:B:574:THR:H	1.82	0.45
1:C:276:GLY:HA3	1:C:380:LEU:HD23	1.98	0.45
1:C:313:LEU:O	1:C:415:TYR:N	2.48	0.45
1:D:482:PRO:HB2	1:F:602:LEU:HD22	1.98	0.45
1:F:417:PHE:HD1	1:F:640:MET:HE1	1.82	0.45
1:B:447:LEU:HD11	1:B:461:LEU:HD12	1.99	0.45
1:D:313:LEU:HB2	1:D:417:PHE:CE2	2.52	0.45
1:A:574:THR:O	1:C:584:HIS:NE2	2.48	0.45
1:C:712:GLU:OE1	1:C:725:ARG:NH2	2.49	0.44
1:D:501:PHE:CD1	1:D:501:PHE:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:51:ILE:CA	3:L:114:ASN:HD22	2.17	0.44
1:A:286:PHE:O	1:A:286:PHE:CD1	2.70	0.44
1:F:276:GLY:HA3	1:F:380:LEU:HD23	1.99	0.44
3:L:69:LEU:HD22	3:L:80:VAL:HG21	1.99	0.44
1:A:503:TRP:CD1	1:A:503:TRP:O	2.70	0.44
1:B:483:SER:OG	1:B:577:TYR:HB2	2.18	0.44
1:C:375:PRO:HA	1:D:662:PHE:CD1	2.52	0.44
1:E:450:THR:HG1	1:F:501:PHE:HD2	1.64	0.44
1:E:590:GLN:HA	1:F:497:ASN:HD21	1.82	0.44
1:C:426:TYR:CD1	1:C:426:TYR:O	2.70	0.44
1:D:326:THR:OG1	1:D:333:THR:HB	2.17	0.44
1:A:624:HIS:O	1:C:428:HIS:HE1	1.99	0.44
1:B:608:GLN:HE22	1:C:625:THR:HA	1.81	0.44
1:C:703:SER:O	1:F:699:ILE:HG12	2.17	0.44
1:D:279:THR:OG1	1:D:377:TYR:O	2.30	0.44
1:E:471:MET:O	1:E:476:ARG:NH2	2.49	0.44
1:F:541:LEU:O	1:F:561:THR:HG23	2.17	0.44
1:A:509:TRP:O	1:A:509:TRP:CE3	2.70	0.44
2:H:58:ILE:HD11	2:H:132:TRP:CH2	2.53	0.44
3:L:26:MET:CE	3:L:112:GLN:HB3	2.47	0.44
1:C:529:GLU:OE1	1:C:567:LYS:CE	2.66	0.44
1:D:511:LEU:HD11	1:F:567:LYS:O	2.17	0.44
3:L:60:GLN:O	3:L:106:ALA:HB1	2.18	0.44
1:A:424:SER:OG	1:B:626:ASP:OD2	2.35	0.43
1:D:485:ARG:HH21	1:D:576:SER:H	1.65	0.43
2:H:66:LEU:HB2	3:L:120:PHE:CD2	2.53	0.43
2:H:129:PHE:N	2:H:129:PHE:CD1	2.85	0.43
1:D:244:THR:HA	1:D:679:VAL:O	2.17	0.43
1:F:694:ARG:HD3	1:F:698:GLU:OE2	2.18	0.43
2:H:50:SER:O	2:H:50:SER:OG	2.34	0.43
3:L:120:PHE:N	3:L:120:PHE:CD1	2.86	0.43
1:D:290:HIS:CD2	1:D:615:GLN:HA	2.49	0.43
1:A:415:TYR:OH	1:A:642:HIS:O	2.36	0.43
1:D:507:SER:O	1:D:518:MET:HB3	2.19	0.43
2:H:54:TYR:HD2	2:H:126:GLY:N	2.16	0.43
2:H:60:GLN:C	2:H:112:ALA:CB	2.86	0.43
1:A:382:LEU:HG	1:C:429:SER:C	2.40	0.43
1:C:308:PHE:HA	1:C:686:GLU:O	2.18	0.43
1:C:490:SER:HB2	1:C:534:PHE:CE1	2.54	0.43
1:F:250:PRO:HG2	1:F:252:TYR:CZ	2.54	0.43
1:F:694:ARG:NH1	1:F:698:GLU:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:61:PRO:CA	2:H:112:ALA:HB2	2.42	0.43
3:L:47:ALA:HB2	3:L:51:ILE:HD13	2.00	0.43
1:D:485:ARG:HG2	1:D:486:GLN:N	2.33	0.43
1:E:439:LEU:HD11	1:F:278:SER:HB2	2.01	0.43
1:E:585:GLN:O	1:E:586:SER:OG	2.34	0.43
3:L:37:VAL:HG21	3:L:102:PRO:HG3	2.01	0.43
1:A:503:TRP:O	1:A:503:TRP:HD1	2.00	0.43
1:C:490:SER:HB2	1:C:534:PHE:HD1	1.80	0.43
1:D:252:TYR:OH	1:D:374:ILE:O	2.33	0.43
1:F:423:HIS:HB2	1:F:638:PHE:CE1	2.53	0.43
1:A:556:ASP:OD1	1:A:557:LYS:N	2.51	0.43
1:C:306:TRP:CZ2	1:C:690:GLU:HG2	2.54	0.43
1:C:559:MET:SD	1:C:726:PRO:HD3	2.59	0.43
1:D:601:ILE:O	1:E:601:ILE:HG12	2.18	0.43
1:A:311:LYS:HD3	1:A:686:GLU:OE1	2.19	0.42
1:C:425:SER:CB	1:C:729:THR:HG22	2.48	0.42
1:F:322:VAL:CG1	1:F:673:GLN:HE21	2.31	0.42
1:C:257:TYR:OH	1:C:397:LEU:N	2.49	0.42
1:C:569:THR:CG2	1:C:736:LEU:HD21	2.46	0.42
1:E:580:VAL:HG11	1:F:597:GLN:HB3	2.00	0.42
1:F:716:ASN:O	1:F:719:GLY:N	2.50	0.42
1:A:314:ASN:HB3	1:A:682:GLU:HB3	2.00	0.42
1:D:536:PRO:CG	1:D:539:GLY:HA3	2.49	0.42
2:H:32:LYS:HB2	2:H:35:GLU:HG3	2.01	0.42
2:H:66:LEU:HD13	2:H:66:LEU:H	1.84	0.42
1:D:243:SER:O	1:D:680:SER:HA	2.19	0.42
1:D:501:PHE:CZ	1:F:585:GLN:NE2	2.88	0.42
1:C:528:LYS:CE	1:C:575:GLU:CG	2.95	0.42
1:C:704:ASN:N	1:C:704:ASN:HD22	2.17	0.42
1:A:548:THR:HG23	1:A:557:LYS:HB3	2.02	0.42
1:D:260:ILE:HD11	1:F:438:PRO:CG	2.50	0.42
1:D:601:ILE:HG12	1:F:601:ILE:O	2.19	0.42
1:C:306:TRP:CE2	1:C:690:GLU:HG2	2.54	0.42
1:C:548:THR:HG22	1:C:553:VAL:HG11	2.01	0.42
1:C:696:ASN:HB2	1:C:697:PRO:HD2	2.01	0.42
2:H:37:LEU:HB3	2:H:103:VAL:CG1	2.50	0.42
3:L:55:LEU:HD12	3:L:111:GLN:O	2.19	0.42
1:C:361:GLU:HG2	1:D:664:LYS:HD2	2.01	0.42
1:D:355:VAL:H	1:D:646:GLN:NE2	2.18	0.42
1:F:361:GLU:HG3	1:F:362:GLY:N	2.35	0.42
1:F:427:ALA:O	1:F:733:THR:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:238:ARG:HD2	1:F:684:GLU:OE2	2.20	0.42
2:H:28:PRO:HD2	2:H:38:SER:O	2.19	0.42
2:H:130:ASP:OD1	2:H:131:TYR:N	2.53	0.42
1:C:302:ILE:HG22	1:C:729:THR:HG23	2.00	0.41
1:D:351:GLN:HE21	1:F:691:ASN:ND2	2.18	0.41
1:C:302:ILE:HG22	1:C:729:THR:HA	2.02	0.41
1:D:313:LEU:HD13	1:D:314:ASN:N	2.34	0.41
1:D:501:PHE:O	1:D:501:PHE:HD1	2.04	0.41
2:H:60:GLN:HG3	2:H:66:LEU:HD12	2.02	0.41
1:D:255:HIS:CD2	1:D:653:PRO:HB3	2.55	0.41
1:D:503:TRP:CE3	1:D:503:TRP:O	2.73	0.41
1:C:704:ASN:CG	1:C:706:TYR:HE2	2.28	0.41
1:D:418:GLU:OE2	1:D:641:LYS:N	2.54	0.41
1:E:443:TYR:CE2	1:F:288:ARG:HD2	2.55	0.41
1:F:308:PHE:HA	1:F:686:GLU:O	2.21	0.41
2:H:113:VAL:HG21	2:H:115:TYR:CZ	2.54	0.41
1:C:367:PHE:CE2	1:C:369:ALA:HB3	2.56	0.41
1:A:485:ARG:HG2	1:A:486:GLN:N	2.35	0.41
1:B:590:GLN:HG2	1:C:497:ASN:ND2	2.29	0.41
1:C:509:TRP:O	1:C:516:SER:HB2	2.21	0.41
1:C:569:THR:CG2	1:C:736:LEU:CD2	2.98	0.41
1:D:498:ASN:HA	1:F:459:GLN:HG3	2.01	0.41
1:D:501:PHE:CZ	1:F:585:GLN:CD	2.99	0.41
3:L:55:LEU:HA	3:L:111:GLN:O	2.20	0.41
1:A:286:PHE:HB3	1:A:364:LEU:HD13	2.02	0.41
1:D:259:GLN:NE2	1:D:275:PHE:HE1	2.19	0.41
1:D:328:ASN:O	1:D:329:ASN:OD1	2.39	0.41
1:C:488:ARG:HB3	1:C:574:THR:HB	2.02	0.41
1:C:618:ILE:O	1:C:637:GLY:HA3	2.21	0.41
1:C:696:ASN:ND2	1:F:711:VAL:HG11	2.36	0.41
1:E:438:PRO:HB3	1:F:380:LEU:HD21	2.02	0.41
1:E:568:THR:O	1:F:511:LEU:HD21	2.21	0.41
2:H:37:LEU:CD1	2:H:138:VAL:HG11	2.49	0.41
2:H:71:ASN:ND2	2:H:119:HIS:CD2	2.79	0.41
2:H:71:ASN:CB	2:H:119:HIS:HD2	2.31	0.41
2:H:113:VAL:CG2	2:H:115:TYR:CZ	3.03	0.41
1:C:711:VAL:HG11	1:F:696:ASN:ND2	2.36	0.41
1:B:427:ALA:CB	1:C:391:ARG:HD3	2.50	0.40
1:C:479:ILE:O	1:C:605:MET:HA	2.21	0.40
1:D:257:TYR:CD1	1:D:279:THR:HG22	2.56	0.40
1:D:487:GLN:O	1:D:536:PRO:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:506:ALA:CB	1:D:517:LEU:CD1	2.90	0.40
1:F:285:ASP:HB3	1:F:363:CYS:HA	2.03	0.40
1:F:588:GLN:OE1	1:F:588:GLN:N	2.55	0.40
1:C:417:PHE:HD1	1:C:640:MET:HE1	1.85	0.40
1:C:425:SER:HB2	1:C:729:THR:HG22	2.02	0.40
1:A:423:HIS:CE1	1:A:612:VAL:HG13	2.56	0.40
1:B:483:SER:HB3	1:B:571:PRO:CG	2.52	0.40
1:B:585:GLN:OE1	1:C:501:PHE:CE1	2.75	0.40
1:D:286:PHE:CE1	1:D:619:TRP:HH2	2.39	0.40
1:C:368:PRO:HB2	1:D:398:GLU:HB2	2.03	0.40
1:A:252:TYR:HB2	1:A:280:PRO:HA	2.04	0.40
1:B:443:TYR:CE2	1:C:359:ALA:HB1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	388/736 (53%)	376 (97%)	12 (3%)	0	100	100
1	B	128/736 (17%)	123 (96%)	5 (4%)	0	100	100
1	C	495/736 (67%)	480 (97%)	15 (3%)	0	100	100
1	D	388/736 (53%)	377 (97%)	11 (3%)	0	100	100
1	E	128/736 (17%)	123 (96%)	5 (4%)	0	100	100
1	F	495/736 (67%)	483 (98%)	12 (2%)	0	100	100
2	H	121/123 (98%)	118 (98%)	2 (2%)	1 (1%)	16	51
3	L	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
All	All	2246/4644 (48%)	2179 (97%)	66 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	86	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	341/615 (55%)	338 (99%)	3 (1%)	75	87
1	B	116/615 (19%)	116 (100%)	0	100	100
1	C	437/615 (71%)	432 (99%)	5 (1%)	70	84
1	D	341/615 (55%)	336 (98%)	5 (2%)	60	78
1	E	116/615 (19%)	114 (98%)	2 (2%)	56	76
1	F	437/615 (71%)	433 (99%)	4 (1%)	75	87
2	H	105/105 (100%)	99 (94%)	6 (6%)	17	46
3	L	89/89 (100%)	88 (99%)	1 (1%)	70	84
All	All	1982/3884 (51%)	1956 (99%)	26 (1%)	64	82

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	393	SER
1	A	497	ASN
1	A	614	LEU
1	C	313	LEU
1	C	459	GLN
1	C	560	ILE
1	C	566	ILE
1	C	708	SER
1	D	262	ASN
1	D	264	THR
1	D	271	ASP
1	D	507	SER
1	D	614	LEU
1	E	431	SER
1	E	580	VAL

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Mol	Chain	Res	Type
1	F	230	CYS
1	F	500	GLU
1	F	501	PHE
1	F	725	ARG
2	H	66	LEU
2	H	106	VAL
2	H	107	THR
2	H	113	VAL
2	H	119	HIS
2	H	125	SER
3	L	43	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	487	GLN
1	A	497	ASN
1	A	546	GLN
1	A	624	HIS
1	A	642	HIS
1	A	646	GLN
1	A	651	ASN
1	A	673	GLN
1	B	458	GLN
1	B	585	GLN
1	B	608	GLN
1	C	229	HIS
1	C	321	GLN
1	C	430	GLN
1	C	452	ASN
1	C	456	GLN
1	C	562	ASN
1	C	608	GLN
1	C	624	HIS
1	C	646	GLN
1	C	651	ASN
1	C	673	GLN
1	C	700	GLN
1	C	704	ASN
1	D	262	ASN
1	D	423	HIS
1	D	495	GLN

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Mol	Chain	Res	Type
1	D	498	ASN
1	D	624	HIS
1	D	642	HIS
1	D	646	GLN
1	D	673	GLN
1	E	442	GLN
1	E	452	ASN
1	E	608	GLN
1	F	430	GLN
1	F	452	ASN
1	F	546	GLN
1	F	585	GLN
1	F	624	HIS
1	F	642	HIS
1	F	646	GLN
1	F	673	GLN
1	F	691	ASN
1	F	700	GLN
1	F	704	ASN
2	H	119	HIS
3	L	114	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

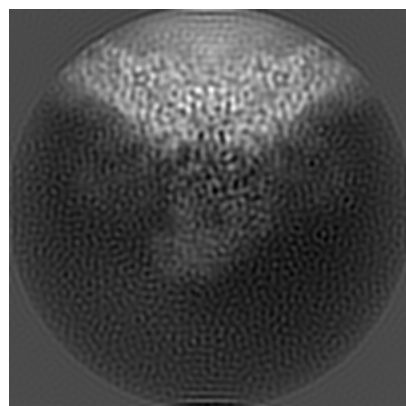
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44323. These allow visual inspection of the internal detail of the map and identification of artifacts.

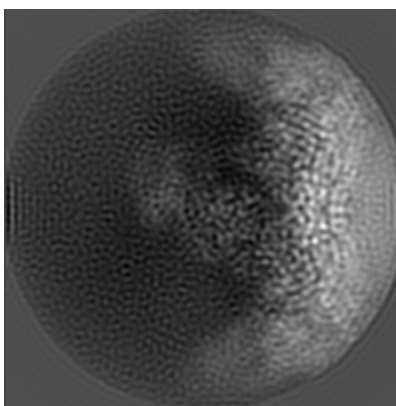
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

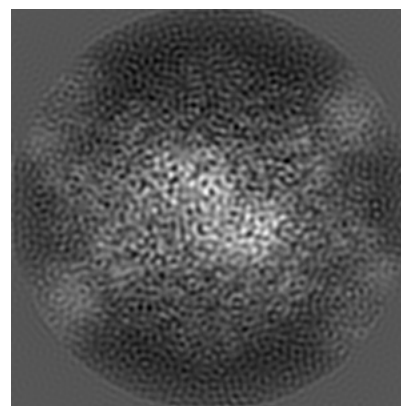
6.1.1 Primary map



X

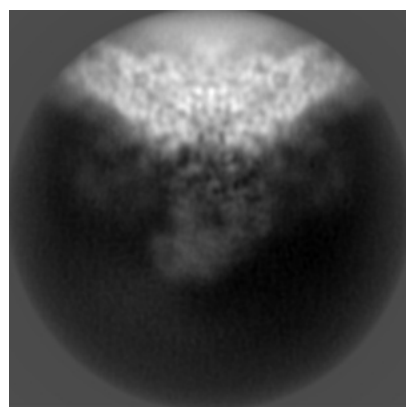


Y

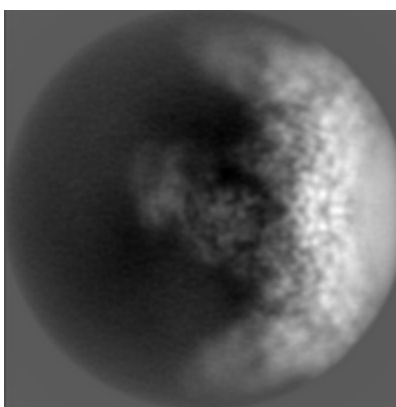


Z

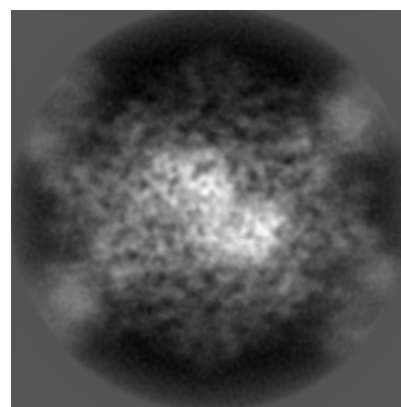
6.1.2 Raw map



X



Y

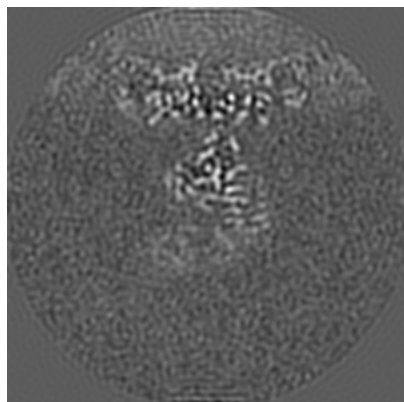


Z

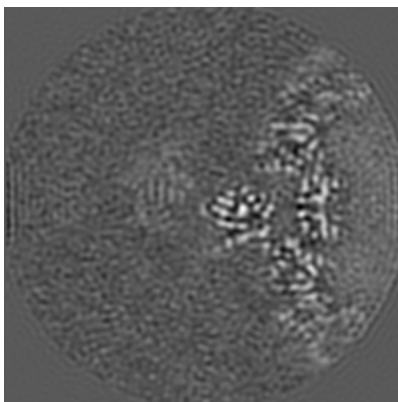
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

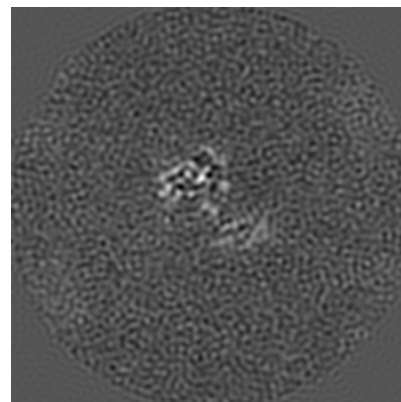
6.2.1 Primary map



X Index: 100

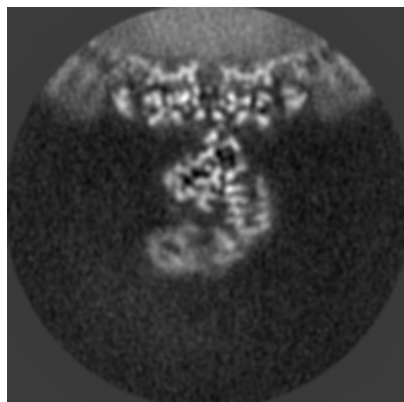


Y Index: 100

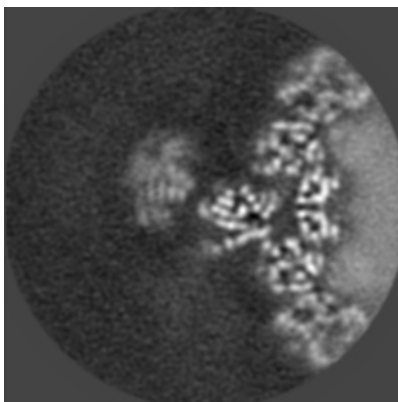


Z Index: 100

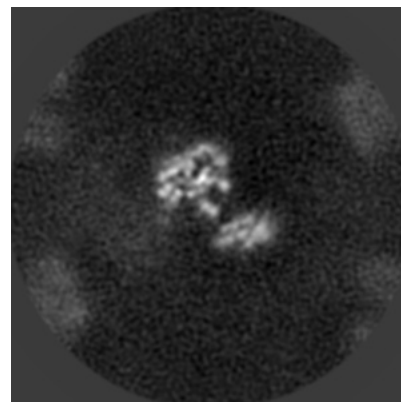
6.2.2 Raw map



X Index: 100



Y Index: 100

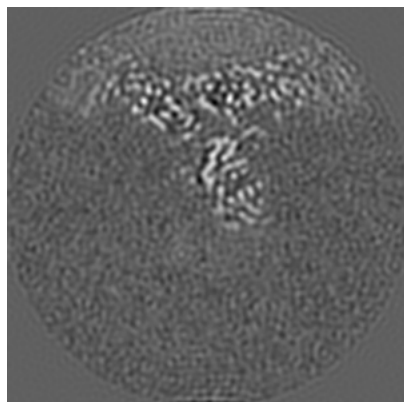


Z Index: 100

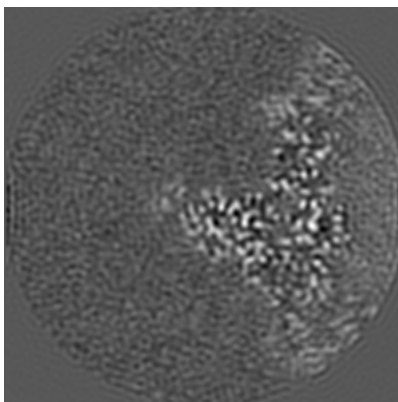
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

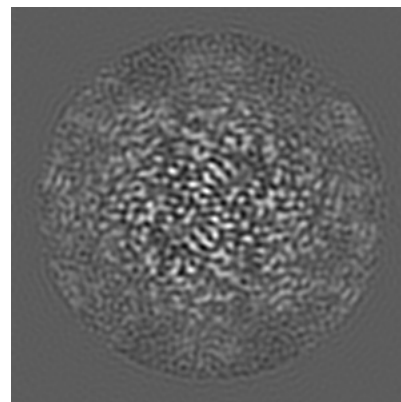
6.3.1 Primary map



X Index: 90

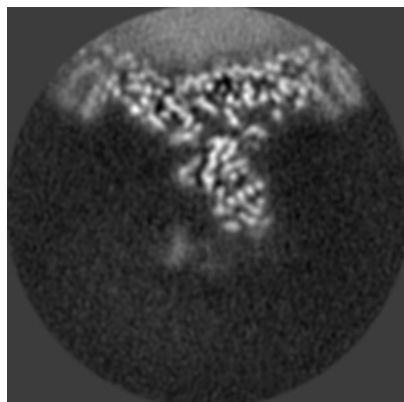


Y Index: 111

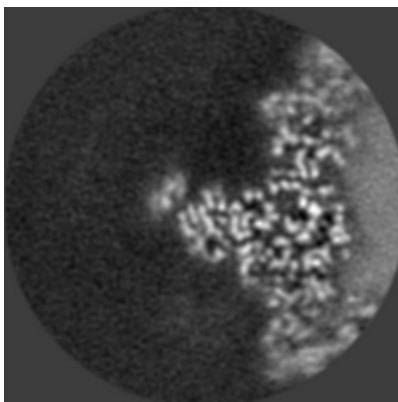


Z Index: 153

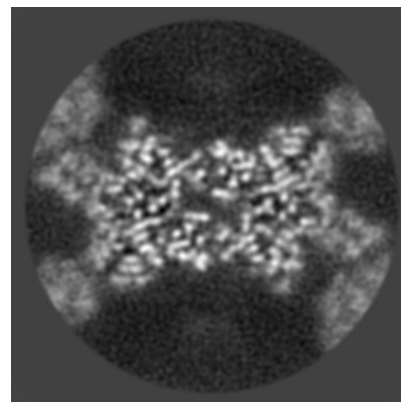
6.3.2 Raw map



X Index: 90



Y Index: 112

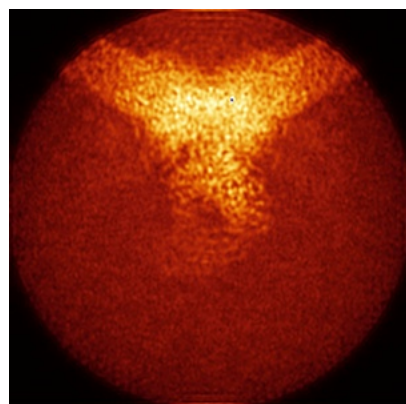


Z Index: 140

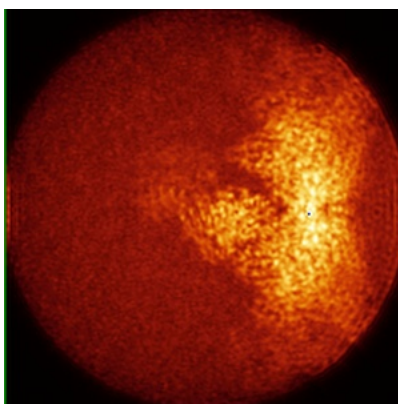
The images above show the largest variance slices of the map in three orthogonal directions.

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

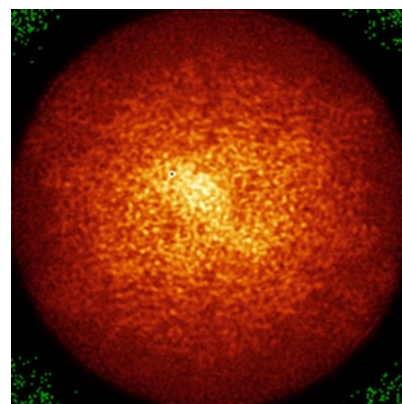
6.4.1 Primary map



X

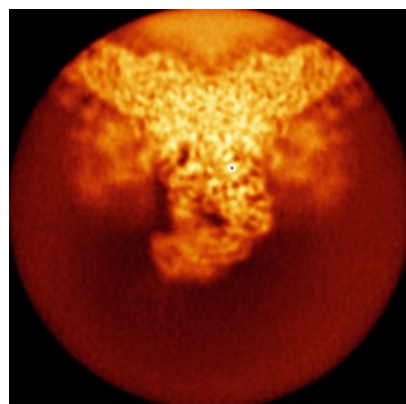


Y

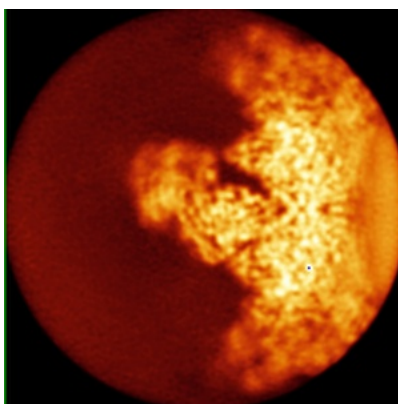


Z

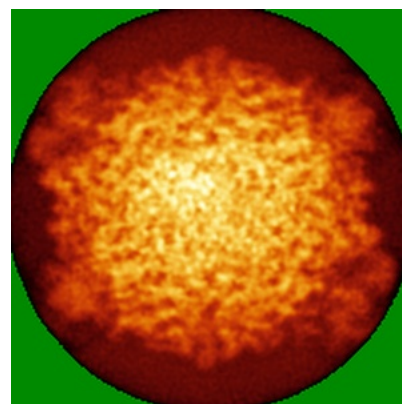
6.4.2 Raw map



X



Y

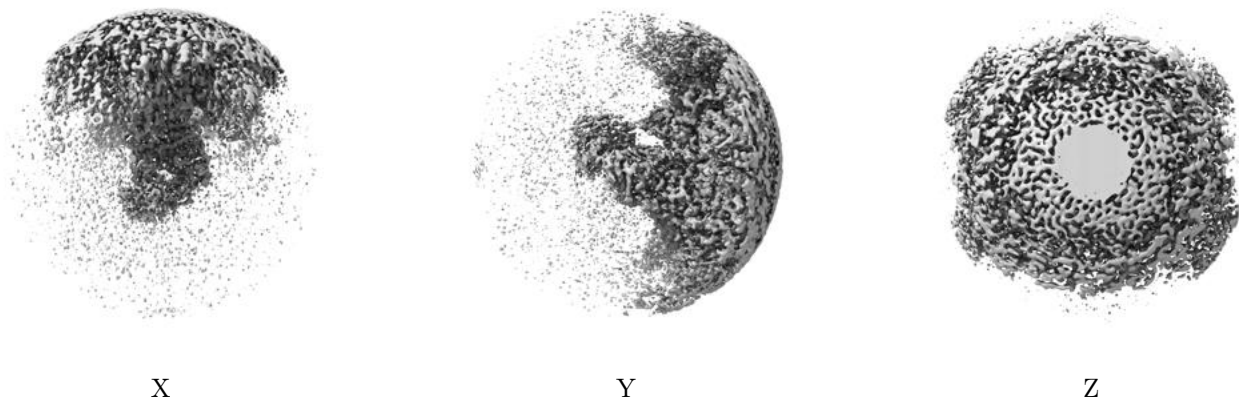


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

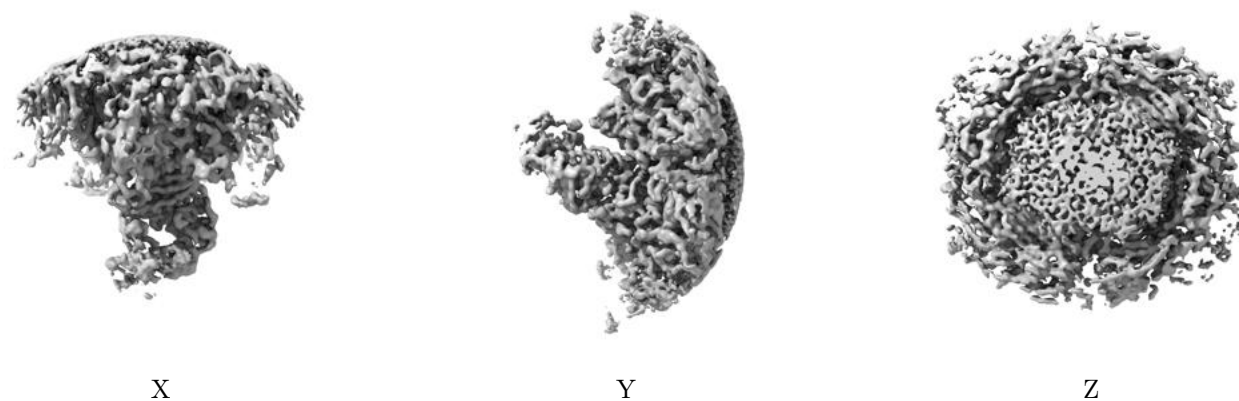
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

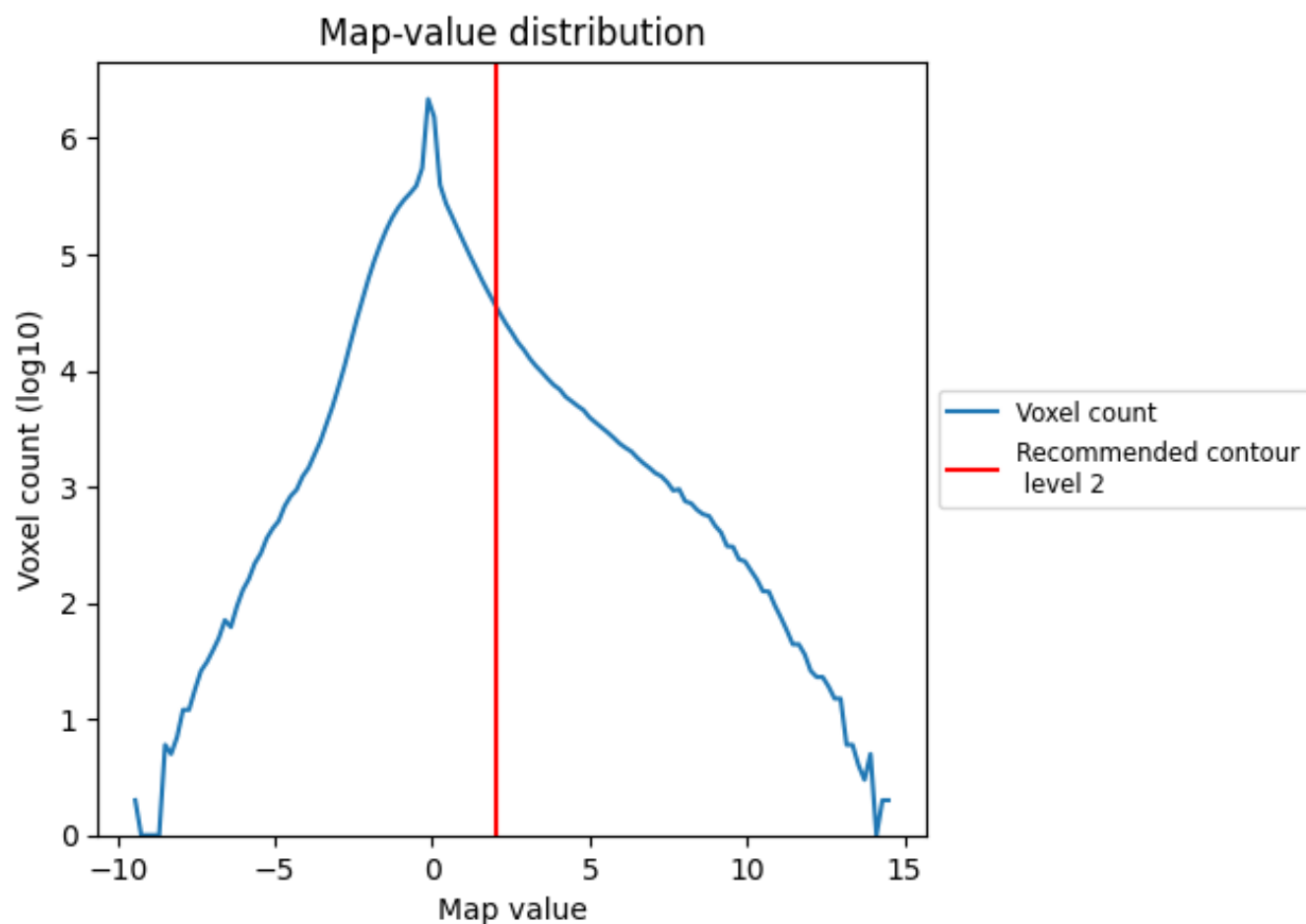
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

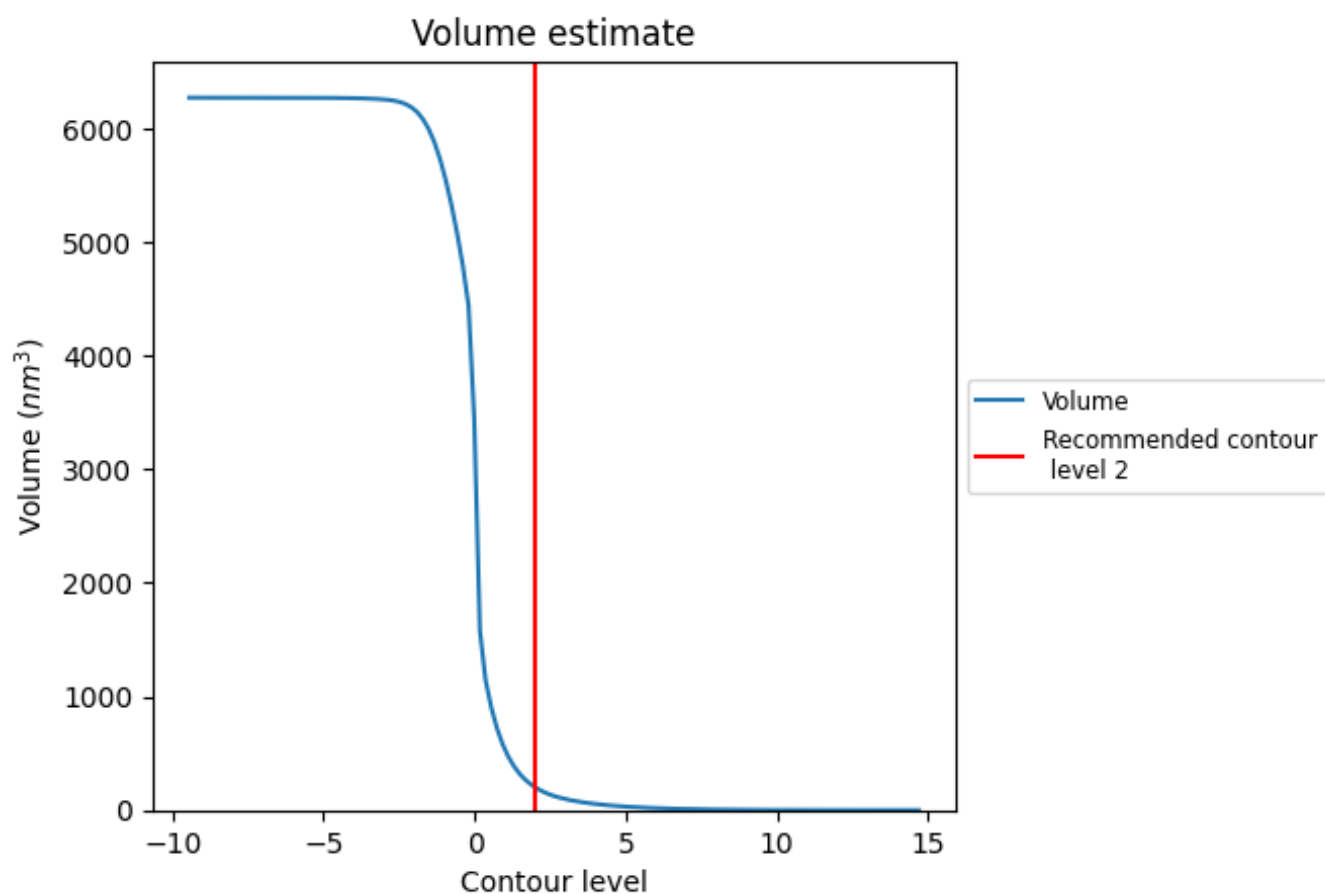
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

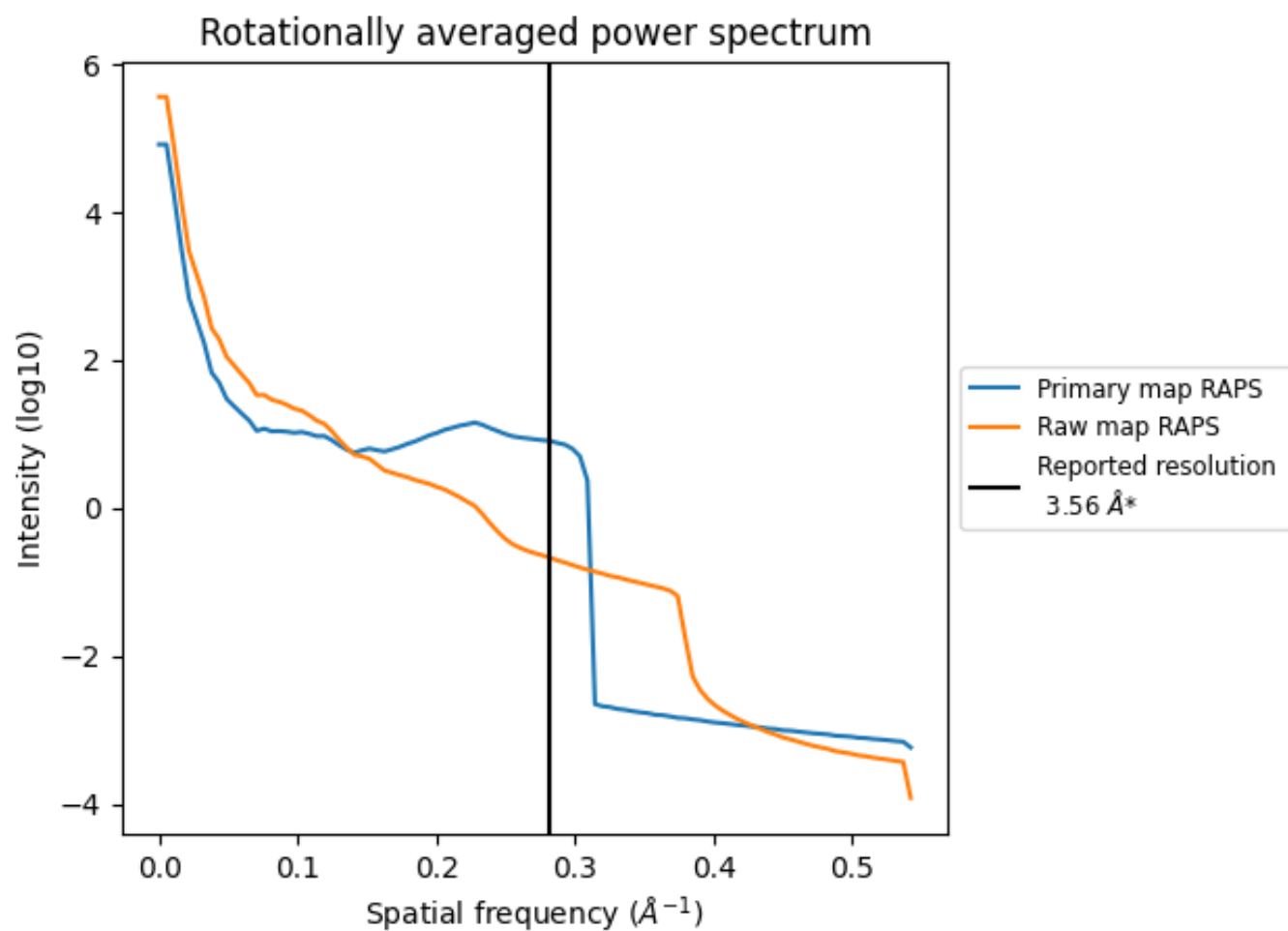
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 201 nm³; this corresponds to an approximate mass of 182 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 ⓘ

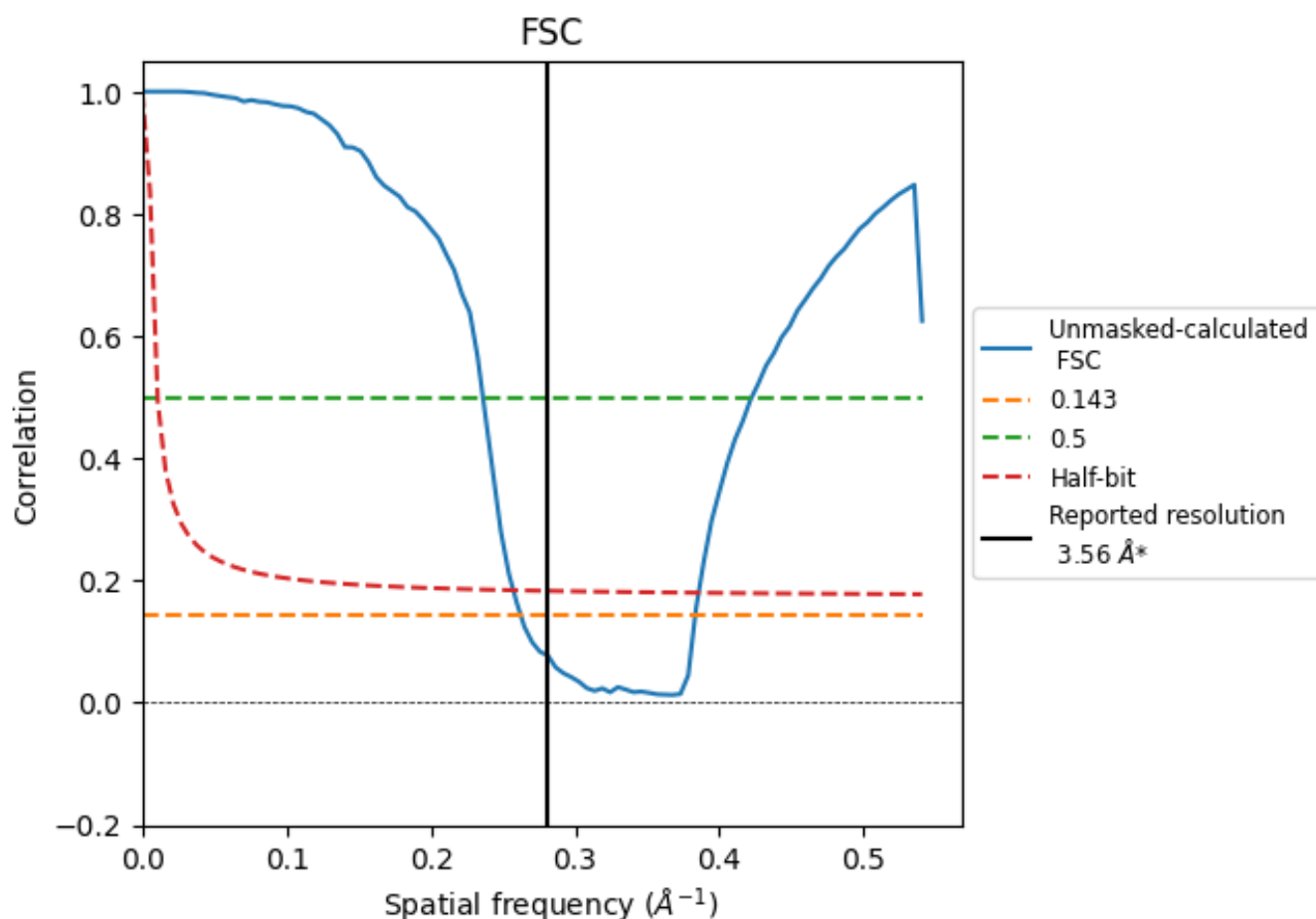


*Reported resolution corresponds to spatial frequency of 0.281 \AA^{-1}

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 0.281 Å⁻¹

8.2 Resolution estimates [i](#)

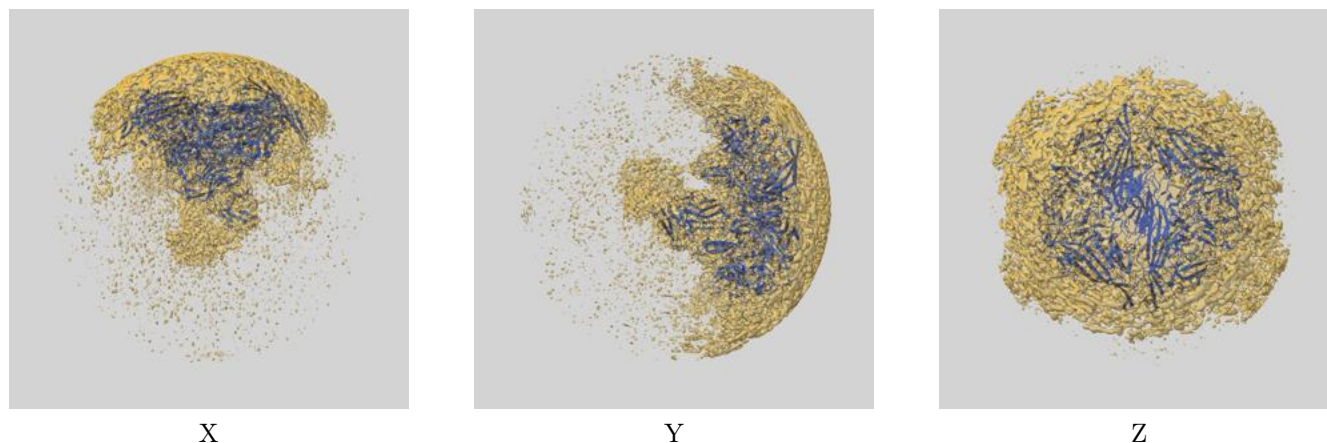
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.56	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.81	4.23	3.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

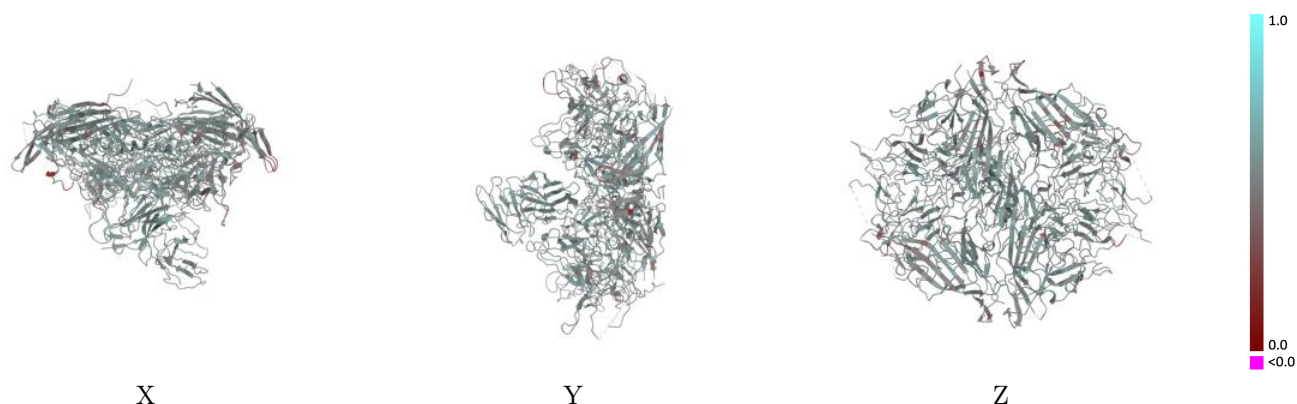
This section contains information regarding the fit between EMDB map EMD-44323 and PDB model 9B7T. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



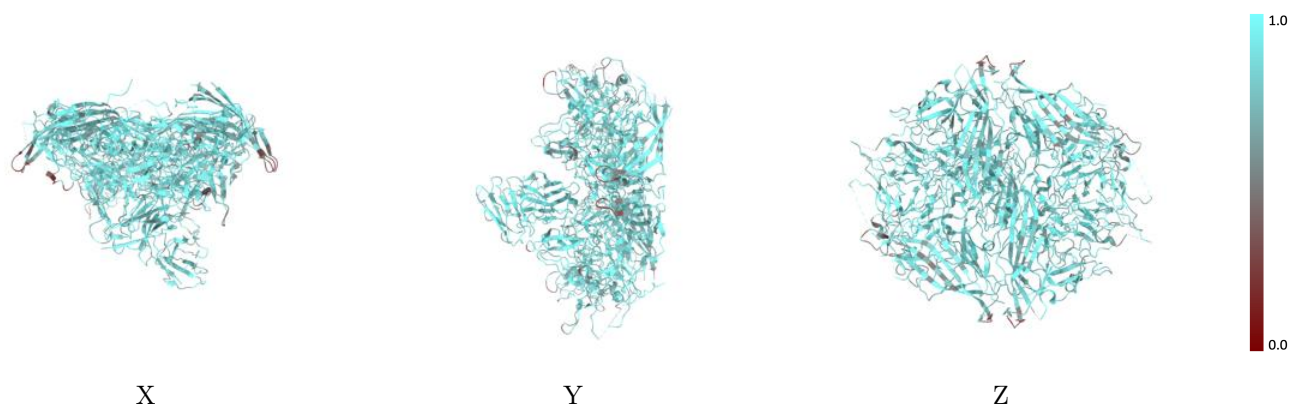
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



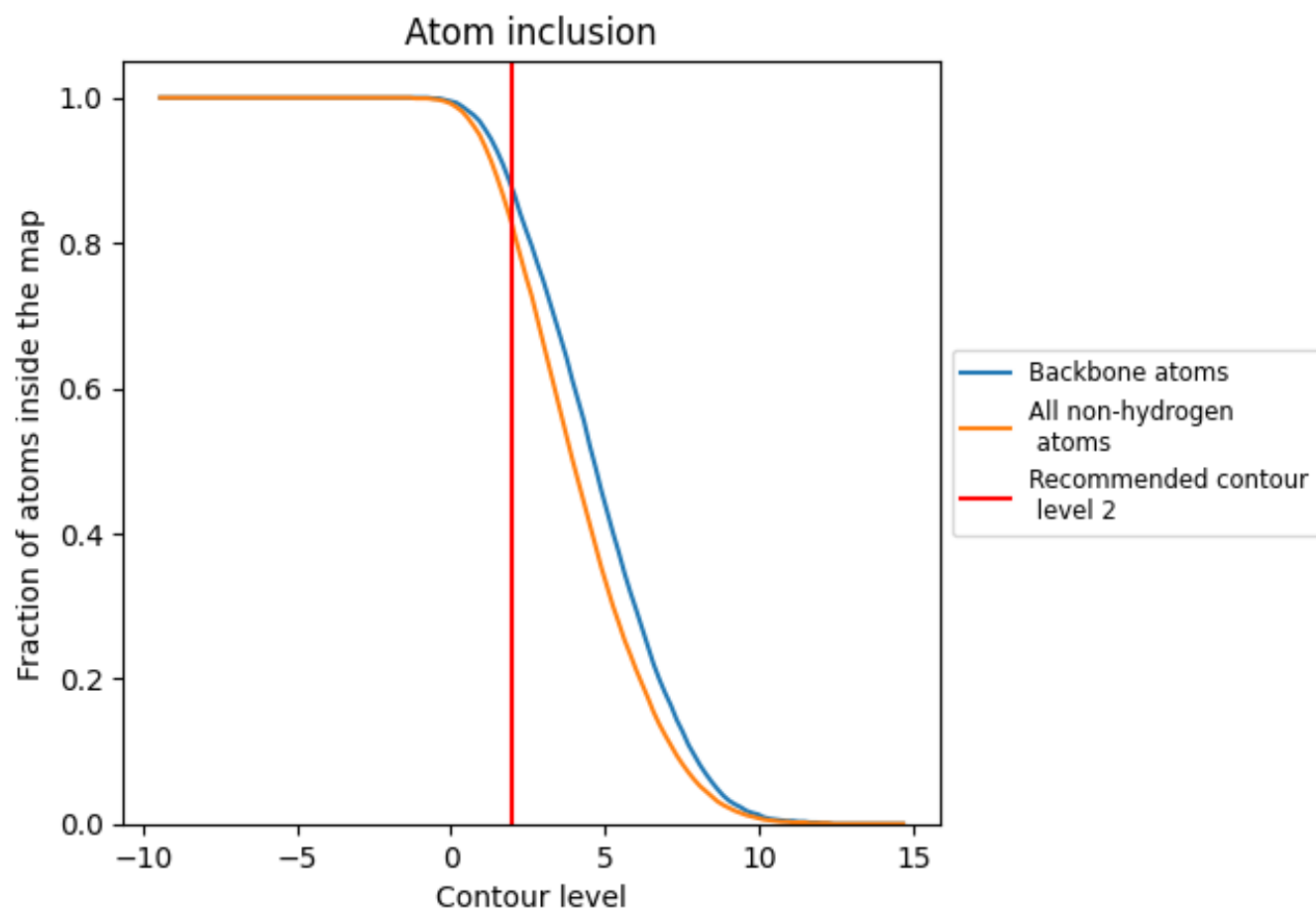
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 82% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8230	<div><div></div></div> 0.5200
A	<div><div></div></div> 0.8110	<div><div></div></div> 0.5130
B	<div><div></div></div> 0.8290	<div><div></div></div> 0.5190
C	<div><div></div></div> 0.8310	<div><div></div></div> 0.5230
D	<div><div></div></div> 0.8020	<div><div></div></div> 0.5120
E	<div><div></div></div> 0.8230	<div><div></div></div> 0.5140
F	<div><div></div></div> 0.8310	<div><div></div></div> 0.5240
H	<div><div></div></div> 0.8580	<div><div></div></div> 0.5480
L	<div><div></div></div> 0.8210	<div><div></div></div> 0.5200

1.0

0.0

<0.0