



Full wwPDB EM Validation Report ⓘ

Apr 4, 2024 – 10:49 AM EDT

PDB ID : 8V7O
EMDB ID : EMD-43008
Title : Fab fragment of human mAb #58 in complex with computationally optimized broadly reactive H1 influenza hemagglutinin X6
Authors : Nagashima, K.A.; Mousa, J.J.
Deposited on : 2023-12-04
Resolution : 3.57 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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.1

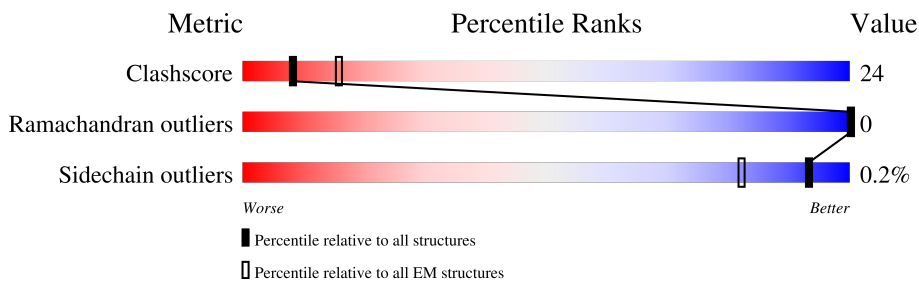
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.57 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.



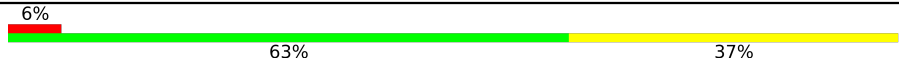
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	555	18% 49% 37% 13%
1	B	555	17% 50% 37% 13%
1	C	555	18% 50% 37% 13%
2	H	125	18% 58% 40% ..
2	I	125	19% 58% 40% ..
2	J	125	18% 56% 42% ..
3	L	109	6% 63% 37%
3	M	109	6% 61% 39%

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Mol	Chain	Length	Quality of chain
3	N	109	 <p>6% 63% 37%</p>

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 16452 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	482	3771	2377	649	727	18	0	0
1	B	482	3771	2377	649	727	18	0	0
1	C	482	3771	2377	649	727	18	0	0

There are 162 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	208	LYS	ARG	conflict	UNP Q00Q05
A	503	GLY	-	expression tag	UNP Q00Q05
A	504	THR	-	expression tag	UNP Q00Q05
A	505	GLY	-	expression tag	UNP Q00Q05
A	506	TYR	-	expression tag	UNP Q00Q05
A	507	ILE	-	expression tag	UNP Q00Q05
A	508	PRO	-	expression tag	UNP Q00Q05
A	509	GLU	-	expression tag	UNP Q00Q05
A	510	ALA	-	expression tag	UNP Q00Q05
A	511	PRO	-	expression tag	UNP Q00Q05
A	512	ARG	-	expression tag	UNP Q00Q05
A	513	ASP	-	expression tag	UNP Q00Q05
A	514	GLY	-	expression tag	UNP Q00Q05
A	515	GLN	-	expression tag	UNP Q00Q05
A	516	ALA	-	expression tag	UNP Q00Q05
A	517	TYR	-	expression tag	UNP Q00Q05
A	518	VAL	-	expression tag	UNP Q00Q05
A	519	ARG	-	expression tag	UNP Q00Q05
A	520	LYS	-	expression tag	UNP Q00Q05
A	521	ASP	-	expression tag	UNP Q00Q05
A	522	GLY	-	expression tag	UNP Q00Q05
A	523	GLU	-	expression tag	UNP Q00Q05
A	524	TRP	-	expression tag	UNP Q00Q05
A	525	VAL	-	expression tag	UNP Q00Q05

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Chain	Residue	Modelled	Actual	Comment	Reference
A	526	LEU	-	expression tag	UNP Q00Q05
A	527	LEU	-	expression tag	UNP Q00Q05
A	528	SER	-	expression tag	UNP Q00Q05
A	529	THR	-	expression tag	UNP Q00Q05
A	530	PHE	-	expression tag	UNP Q00Q05
A	531	LEU	-	expression tag	UNP Q00Q05
A	532	GLY	-	expression tag	UNP Q00Q05
A	533	SER	-	expression tag	UNP Q00Q05
A	534	GLY	-	expression tag	UNP Q00Q05
A	535	LEU	-	expression tag	UNP Q00Q05
A	536	ASN	-	expression tag	UNP Q00Q05
A	537	ASP	-	expression tag	UNP Q00Q05
A	538	ILE	-	expression tag	UNP Q00Q05
A	539	PHE	-	expression tag	UNP Q00Q05
A	540	GLU	-	expression tag	UNP Q00Q05
A	541	ALA	-	expression tag	UNP Q00Q05
A	542	GLN	-	expression tag	UNP Q00Q05
A	543	LYS	-	expression tag	UNP Q00Q05
A	544	ILE	-	expression tag	UNP Q00Q05
A	545	GLU	-	expression tag	UNP Q00Q05
A	546	TRP	-	expression tag	UNP Q00Q05
A	547	HIS	-	expression tag	UNP Q00Q05
A	548	GLU	-	expression tag	UNP Q00Q05
A	549	GLY	-	expression tag	UNP Q00Q05
A	550	HIS	-	expression tag	UNP Q00Q05
A	551	HIS	-	expression tag	UNP Q00Q05
A	552	HIS	-	expression tag	UNP Q00Q05
A	553	HIS	-	expression tag	UNP Q00Q05
A	554	HIS	-	expression tag	UNP Q00Q05
A	555	HIS	-	expression tag	UNP Q00Q05
B	208	LYS	ARG	conflict	UNP Q00Q05
B	503	GLY	-	expression tag	UNP Q00Q05
B	504	THR	-	expression tag	UNP Q00Q05
B	505	GLY	-	expression tag	UNP Q00Q05
B	506	TYR	-	expression tag	UNP Q00Q05
B	507	ILE	-	expression tag	UNP Q00Q05
B	508	PRO	-	expression tag	UNP Q00Q05
B	509	GLU	-	expression tag	UNP Q00Q05
B	510	ALA	-	expression tag	UNP Q00Q05
B	511	PRO	-	expression tag	UNP Q00Q05
B	512	ARG	-	expression tag	UNP Q00Q05
B	513	ASP	-	expression tag	UNP Q00Q05

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Chain	Residue	Modelled	Actual	Comment	Reference
B	514	GLY	-	expression tag	UNP Q00Q05
B	515	GLN	-	expression tag	UNP Q00Q05
B	516	ALA	-	expression tag	UNP Q00Q05
B	517	TYR	-	expression tag	UNP Q00Q05
B	518	VAL	-	expression tag	UNP Q00Q05
B	519	ARG	-	expression tag	UNP Q00Q05
B	520	LYS	-	expression tag	UNP Q00Q05
B	521	ASP	-	expression tag	UNP Q00Q05
B	522	GLY	-	expression tag	UNP Q00Q05
B	523	GLU	-	expression tag	UNP Q00Q05
B	524	TRP	-	expression tag	UNP Q00Q05
B	525	VAL	-	expression tag	UNP Q00Q05
B	526	LEU	-	expression tag	UNP Q00Q05
B	527	LEU	-	expression tag	UNP Q00Q05
B	528	SER	-	expression tag	UNP Q00Q05
B	529	THR	-	expression tag	UNP Q00Q05
B	530	PHE	-	expression tag	UNP Q00Q05
B	531	LEU	-	expression tag	UNP Q00Q05
B	532	GLY	-	expression tag	UNP Q00Q05
B	533	SER	-	expression tag	UNP Q00Q05
B	534	GLY	-	expression tag	UNP Q00Q05
B	535	LEU	-	expression tag	UNP Q00Q05
B	536	ASN	-	expression tag	UNP Q00Q05
B	537	ASP	-	expression tag	UNP Q00Q05
B	538	ILE	-	expression tag	UNP Q00Q05
B	539	PHE	-	expression tag	UNP Q00Q05
B	540	GLU	-	expression tag	UNP Q00Q05
B	541	ALA	-	expression tag	UNP Q00Q05
B	542	GLN	-	expression tag	UNP Q00Q05
B	543	LYS	-	expression tag	UNP Q00Q05
B	544	ILE	-	expression tag	UNP Q00Q05
B	545	GLU	-	expression tag	UNP Q00Q05
B	546	TRP	-	expression tag	UNP Q00Q05
B	547	HIS	-	expression tag	UNP Q00Q05
B	548	GLU	-	expression tag	UNP Q00Q05
B	549	GLY	-	expression tag	UNP Q00Q05
B	550	HIS	-	expression tag	UNP Q00Q05
B	551	HIS	-	expression tag	UNP Q00Q05
B	552	HIS	-	expression tag	UNP Q00Q05
B	553	HIS	-	expression tag	UNP Q00Q05
B	554	HIS	-	expression tag	UNP Q00Q05
B	555	HIS	-	expression tag	UNP Q00Q05

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Chain	Residue	Modelled	Actual	Comment	Reference
C	208	LYS	ARG	conflict	UNP Q00Q05
C	503	GLY	-	expression tag	UNP Q00Q05
C	504	THR	-	expression tag	UNP Q00Q05
C	505	GLY	-	expression tag	UNP Q00Q05
C	506	TYR	-	expression tag	UNP Q00Q05
C	507	ILE	-	expression tag	UNP Q00Q05
C	508	PRO	-	expression tag	UNP Q00Q05
C	509	GLU	-	expression tag	UNP Q00Q05
C	510	ALA	-	expression tag	UNP Q00Q05
C	511	PRO	-	expression tag	UNP Q00Q05
C	512	ARG	-	expression tag	UNP Q00Q05
C	513	ASP	-	expression tag	UNP Q00Q05
C	514	GLY	-	expression tag	UNP Q00Q05
C	515	GLN	-	expression tag	UNP Q00Q05
C	516	ALA	-	expression tag	UNP Q00Q05
C	517	TYR	-	expression tag	UNP Q00Q05
C	518	VAL	-	expression tag	UNP Q00Q05
C	519	ARG	-	expression tag	UNP Q00Q05
C	520	LYS	-	expression tag	UNP Q00Q05
C	521	ASP	-	expression tag	UNP Q00Q05
C	522	GLY	-	expression tag	UNP Q00Q05
C	523	GLU	-	expression tag	UNP Q00Q05
C	524	TRP	-	expression tag	UNP Q00Q05
C	525	VAL	-	expression tag	UNP Q00Q05
C	526	LEU	-	expression tag	UNP Q00Q05
C	527	LEU	-	expression tag	UNP Q00Q05
C	528	SER	-	expression tag	UNP Q00Q05
C	529	THR	-	expression tag	UNP Q00Q05
C	530	PHE	-	expression tag	UNP Q00Q05
C	531	LEU	-	expression tag	UNP Q00Q05
C	532	GLY	-	expression tag	UNP Q00Q05
C	533	SER	-	expression tag	UNP Q00Q05
C	534	GLY	-	expression tag	UNP Q00Q05
C	535	LEU	-	expression tag	UNP Q00Q05
C	536	ASN	-	expression tag	UNP Q00Q05
C	537	ASP	-	expression tag	UNP Q00Q05
C	538	ILE	-	expression tag	UNP Q00Q05
C	539	PHE	-	expression tag	UNP Q00Q05
C	540	GLU	-	expression tag	UNP Q00Q05
C	541	ALA	-	expression tag	UNP Q00Q05
C	542	GLN	-	expression tag	UNP Q00Q05
C	543	LYS	-	expression tag	UNP Q00Q05

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Chain	Residue	Modelled	Actual	Comment	Reference
C	544	ILE	-	expression tag	UNP Q00Q05
C	545	GLU	-	expression tag	UNP Q00Q05
C	546	TRP	-	expression tag	UNP Q00Q05
C	547	HIS	-	expression tag	UNP Q00Q05
C	548	GLU	-	expression tag	UNP Q00Q05
C	549	GLY	-	expression tag	UNP Q00Q05
C	550	HIS	-	expression tag	UNP Q00Q05
C	551	HIS	-	expression tag	UNP Q00Q05
C	552	HIS	-	expression tag	UNP Q00Q05
C	553	HIS	-	expression tag	UNP Q00Q05
C	554	HIS	-	expression tag	UNP Q00Q05
C	555	HIS	-	expression tag	UNP Q00Q05

- Molecule 2 is a protein called #58 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	123	928	591	157	177	3	0	0
2	I	123	928	591	157	177	3	0	0
2	J	123	928	591	157	177	3	0	0

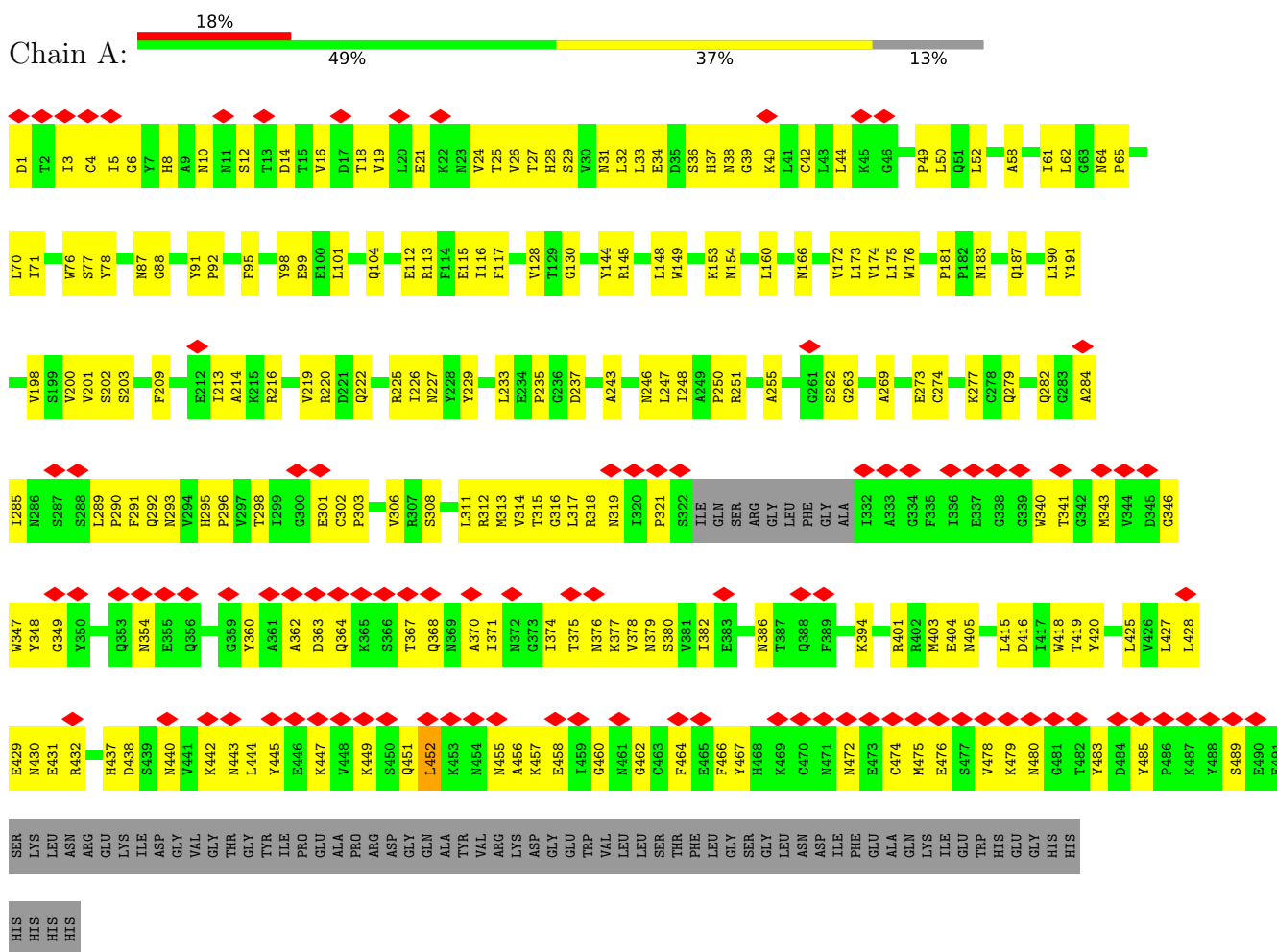
- Molecule 3 is a protein called #58 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	109	785	499	137	147	2	0	0
3	M	109	785	499	137	147	2	0	0
3	N	109	785	499	137	147	2	0	0

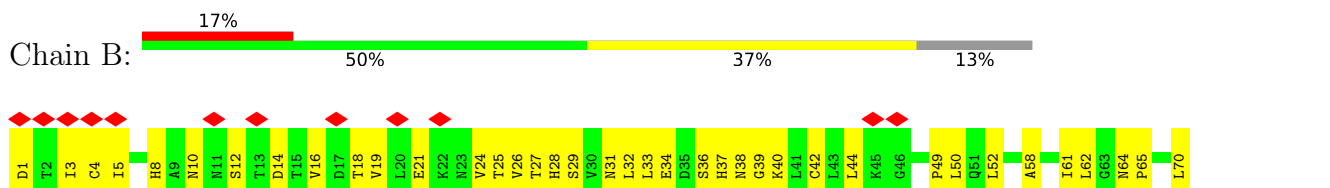
3 Residue-property plots

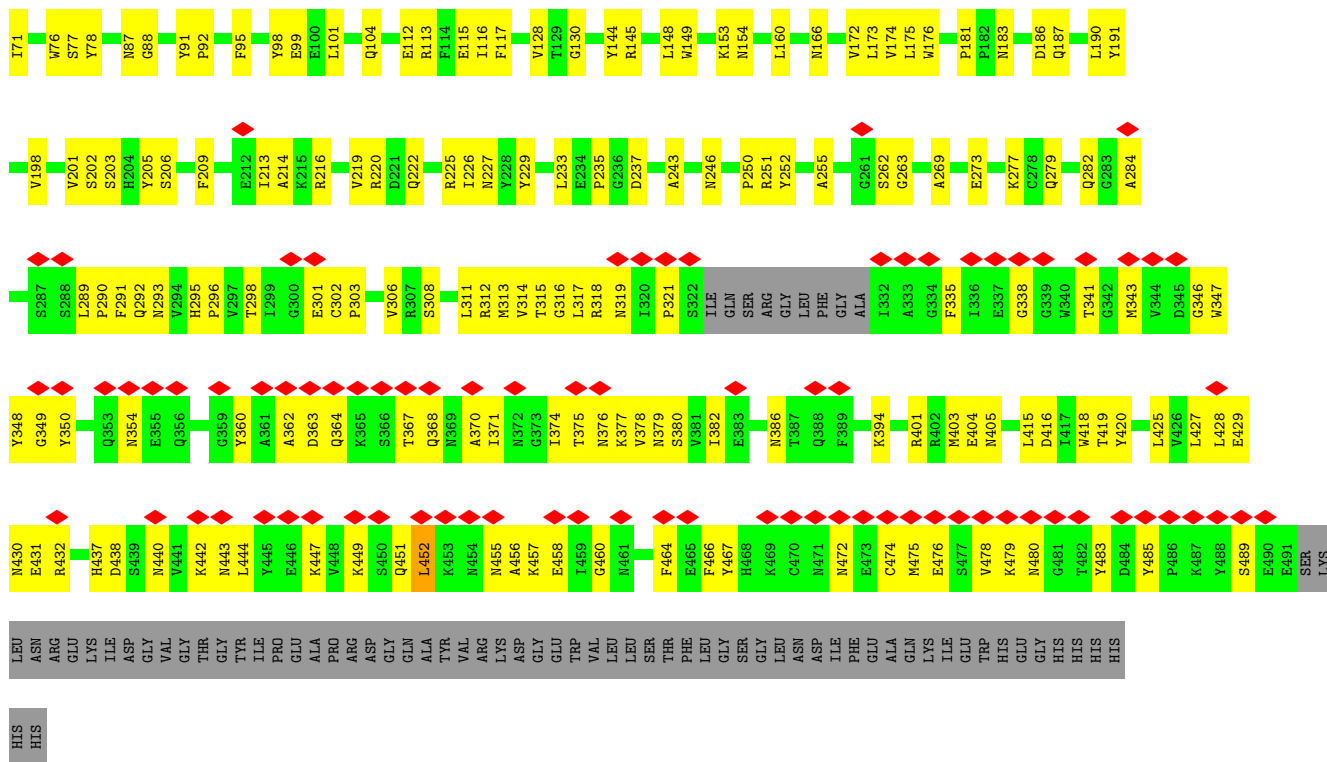
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

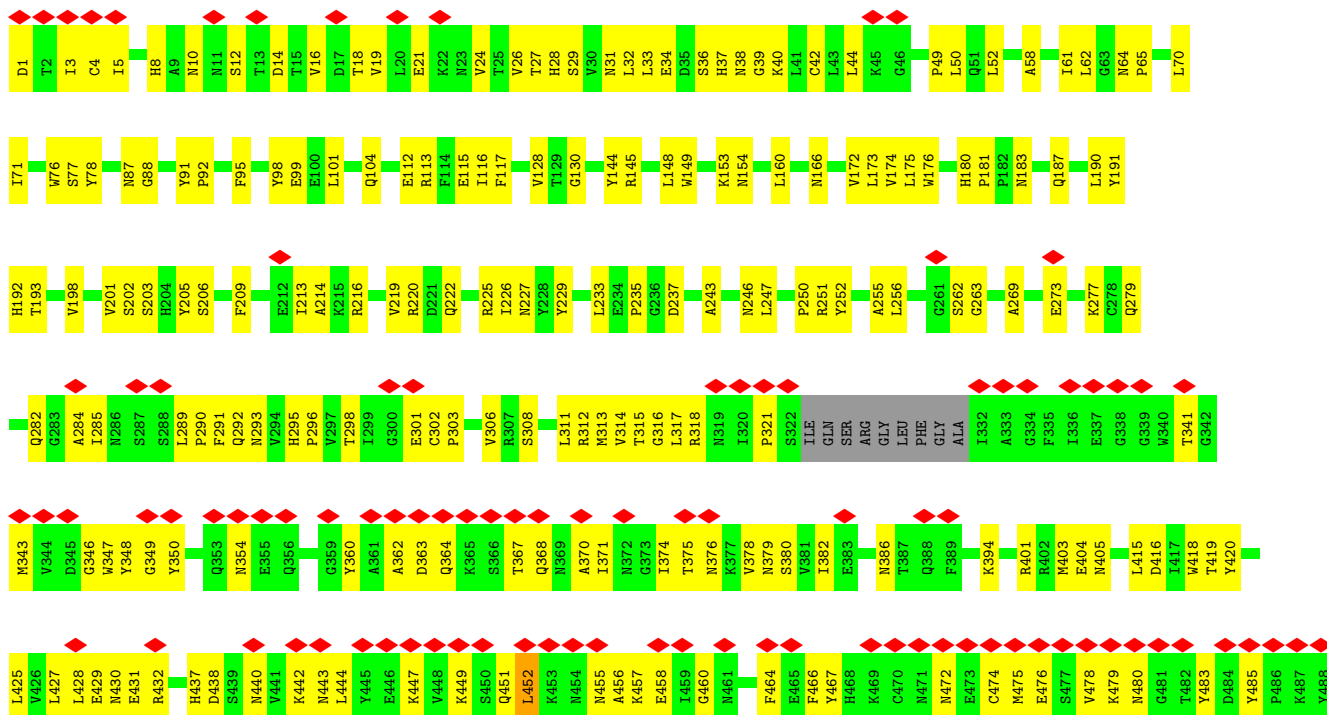


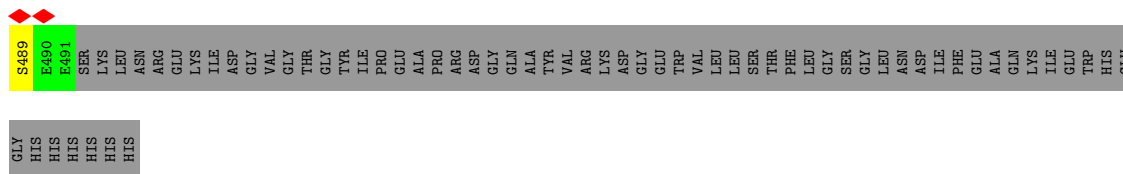
- Molecule 1: Hemagglutinin



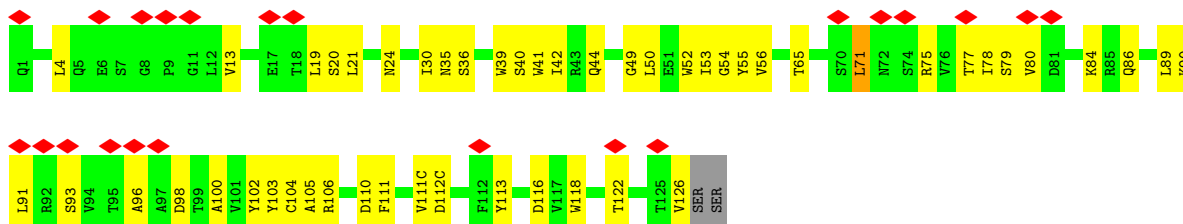


• Molecule 1: Hemagglutinin

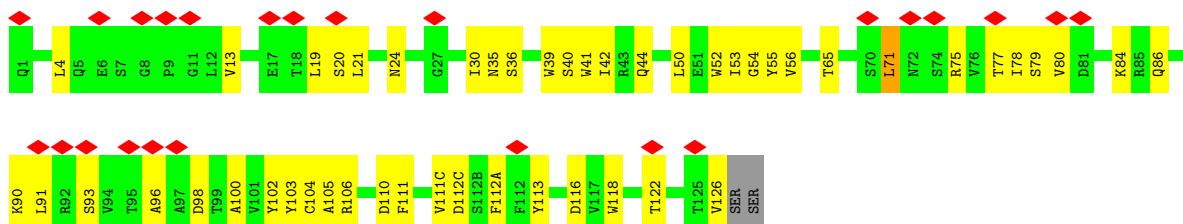




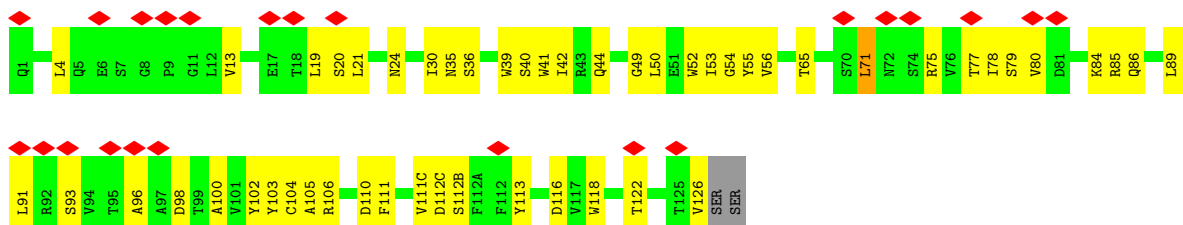
• Molecule 2: #58 heavy chain



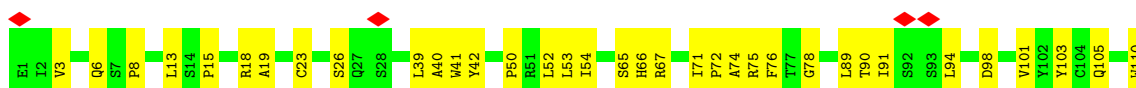
• Molecule 2: #58 heavy chain



• Molecule 2: #58 heavy chain

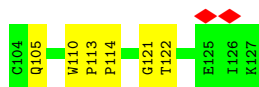


• Molecule 3: #58 light chain

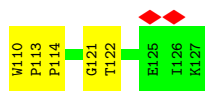
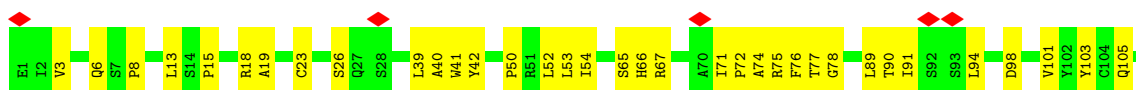




- Molecule 3: #58 light chain



- Molecule 3: #58 light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	110051	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57.22	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.602	Depositor
Minimum map value	-0.414	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.12	Depositor
Map size (\AA)	315.6, 315.6, 315.6	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.526, 0.526, 0.526	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	0.38	0/3862	0.60	1/5245 (0.0%)
1	B	0.38	0/3862	0.60	1/5245 (0.0%)
1	C	0.38	0/3862	0.60	1/5245 (0.0%)
2	H	0.40	0/954	0.62	1/1306 (0.1%)
2	I	0.40	0/954	0.62	1/1306 (0.1%)
2	J	0.40	0/954	0.62	1/1306 (0.1%)
3	L	0.35	0/807	0.61	0/1109
3	M	0.35	0/807	0.61	0/1109
3	N	0.36	0/807	0.61	0/1109
All	All	0.38	0/16869	0.60	6/22980 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	452	LEU	CA-CB-CG	7.45	132.43	115.30
1	A	452	LEU	CA-CB-CG	7.44	132.42	115.30
1	B	452	LEU	CA-CB-CG	7.43	132.40	115.30
2	I	71	LEU	CA-CB-CG	6.66	130.61	115.30
2	H	71	LEU	CA-CB-CG	6.64	130.58	115.30
2	J	71	LEU	CA-CB-CG	6.64	130.57	115.30

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	3771	0	3593	190	0
1	B	3771	0	3593	194	0
1	C	3771	0	3593	192	0
2	H	928	0	849	53	0
2	I	928	0	849	53	0
2	J	928	0	849	54	0
3	L	785	0	741	37	0
3	M	785	0	741	39	0
3	N	785	0	741	41	0
All	All	16452	0	15549	781	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 24.

All (781) 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:B:348:TYR:OH	1:B:437:HIS:ND1	2.10	0.85
1:C:348:TYR:OH	1:C:437:HIS:ND1	2.10	0.85
1:A:348:TYR:OH	1:A:437:HIS:ND1	2.10	0.85
3:N:41:TRP:HZ3	3:N:89:LEU:HB2	1.43	0.84
3:M:41:TRP:HZ3	3:M:89:LEU:HB2	1.43	0.83
1:A:149:TRP:HH2	2:H:111(C):VAL:HG21	1.43	0.83
1:C:149:TRP:HH2	2:J:111(C):VAL:HG21	1.43	0.83
2:H:50:LEU:HD13	3:L:103:TYR:HE1	1.44	0.82
1:C:4:CYS:HB3	1:C:464:PHE:H	1.45	0.82
3:N:41:TRP:CZ3	3:N:89:LEU:HB2	2.15	0.82
3:L:41:TRP:CZ3	3:L:89:LEU:HB2	2.15	0.82
3:L:41:TRP:HZ3	3:L:89:LEU:HB2	1.43	0.82
2:J:50:LEU:HD13	3:N:103:TYR:HE1	1.44	0.81
3:M:41:TRP:CZ3	3:M:89:LEU:HB2	2.15	0.80
1:B:4:CYS:HB3	1:B:464:PHE:H	1.44	0.80
2:I:50:LEU:HD13	3:M:103:TYR:HE1	1.45	0.80
1:A:4:CYS:HB3	1:A:464:PHE:H	1.45	0.80
1:A:153:LYS:HD3	1:A:154:ASN:HB2	1.65	0.78
1:C:153:LYS:HD3	1:C:154:ASN:HB2	1.65	0.78
1:C:61:ILE:HG22	1:C:175:LEU:HD11	1.67	0.77
2:J:110:ASP:OD2	2:J:111:PHE:N	2.18	0.77
1:A:61:ILE:HG22	1:A:175:LEU:HD11	1.67	0.77
1:A:149:TRP:CH2	2:H:111(C):VAL:HG21	2.19	0.77
1:B:61:ILE:HG22	1:B:175:LEU:HD11	1.67	0.76
1:B:71:ILE:HG12	1:B:113:ARG:HH12	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:110:ASP:OD2	2:H:111:PHE:N	2.18	0.76
1:A:71:ILE:HG12	1:A:113:ARG:HH12	1.49	0.76
1:B:440:ASN:HA	1:B:443:ASN:HD22	1.50	0.76
1:C:149:TRP:CH2	2:J:111(C):VAL:HG21	2.19	0.76
2:I:110:ASP:OD2	2:I:111:PHE:N	2.18	0.76
1:B:153:LYS:HD3	1:B:154:ASN:HB2	1.65	0.75
1:A:440:ASN:HA	1:A:443:ASN:HD22	1.50	0.75
1:C:71:ILE:HG12	1:C:113:ARG:HH12	1.49	0.74
1:C:440:ASN:HA	1:C:443:ASN:HD22	1.50	0.74
1:B:363:ASP:OD1	1:B:364:GLN:N	2.20	0.74
1:B:401:ARG:HH22	1:C:104:GLN:HE22	1.35	0.74
1:A:363:ASP:OD1	1:A:364:GLN:N	2.20	0.74
1:A:430:ASN:OD1	1:A:431:GLU:N	2.21	0.74
1:C:363:ASP:OD1	1:C:364:GLN:N	2.20	0.74
1:C:430:ASN:OD1	1:C:431:GLU:N	2.21	0.73
1:B:183:ASN:HD21	3:M:110:TRP:HB2	1.53	0.73
3:L:6:GLN:NE2	3:L:23:CYS:SG	2.62	0.73
1:B:430:ASN:OD1	1:B:431:GLU:N	2.21	0.72
1:C:183:ASN:HD21	3:N:110:TRP:HB2	1.53	0.72
3:M:6:GLN:NE2	3:M:23:CYS:SG	2.62	0.72
3:N:6:GLN:NE2	3:N:23:CYS:SG	2.62	0.72
1:B:64:ASN:ND2	1:B:88:GLY:O	2.23	0.72
1:C:64:ASN:ND2	1:C:88:GLY:O	2.23	0.71
1:B:38:ASN:ND2	1:B:42:CYS:SG	2.63	0.71
1:C:198:VAL:HB	1:C:209:PHE:HB2	1.73	0.71
1:B:8:HIS:ND1	1:B:346:GLY:O	2.21	0.71
1:B:214:ALA:O	1:B:216:ARG:NH1	2.24	0.71
1:A:64:ASN:ND2	1:A:88:GLY:O	2.23	0.71
1:A:104:GLN:HE22	1:C:401:ARG:HH22	1.38	0.71
1:A:214:ALA:O	1:A:216:ARG:NH1	2.24	0.71
1:A:183:ASN:HD21	3:L:110:TRP:HB2	1.53	0.70
1:A:198:VAL:HB	1:A:209:PHE:HB2	1.73	0.70
1:A:38:ASN:ND2	1:A:42:CYS:SG	2.63	0.70
1:C:8:HIS:ND1	1:C:346:GLY:O	2.21	0.70
1:C:38:ASN:ND2	1:C:42:CYS:SG	2.63	0.70
2:J:96:ALA:HA	2:J:126:VAL:HG21	1.73	0.70
2:H:96:ALA:HA	2:H:126:VAL:HG21	1.73	0.70
1:C:214:ALA:O	1:C:216:ARG:NH1	2.24	0.70
3:M:41:TRP:HE3	3:M:89:LEU:HD12	1.57	0.70
1:B:198:VAL:HB	1:B:209:PHE:HB2	1.73	0.70
3:L:41:TRP:HE3	3:L:89:LEU:HD12	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:67:ARG:HG2	3:L:71:ILE:HB	1.74	0.69
3:N:41:TRP:HE3	3:N:89:LEU:HD12	1.57	0.69
1:B:401:ARG:HH12	1:C:104:GLN:CD	1.95	0.69
1:C:476:GLU:O	1:C:480:ASN:ND2	2.26	0.69
2:I:96:ALA:HA	2:I:126:VAL:HG21	1.73	0.69
1:A:32:LEU:HD23	1:A:313:MET:HB2	1.74	0.69
3:M:67:ARG:HG2	3:M:71:ILE:HB	1.74	0.69
1:A:8:HIS:ND1	1:A:346:GLY:O	2.21	0.69
1:B:476:GLU:O	1:B:480:ASN:ND2	2.26	0.68
2:H:40:SER:HA	2:H:55:TYR:HB3	1.75	0.68
1:A:401:ARG:HH22	1:B:104:GLN:HE22	1.39	0.68
1:B:290:PRO:HG3	1:B:382:ILE:HG22	1.75	0.68
1:A:476:GLU:O	1:A:480:ASN:ND2	2.26	0.68
2:I:40:SER:HA	2:I:55:TYR:HB3	1.75	0.68
1:A:401:ARG:HH12	1:B:104:GLN:CD	1.96	0.68
1:A:478:VAL:HG12	1:A:483:TYR:HB2	1.76	0.68
1:B:32:LEU:HD23	1:B:313:MET:HB2	1.74	0.68
1:A:293:ASN:ND2	1:A:308:SER:O	2.26	0.68
1:B:293:ASN:ND2	1:B:308:SER:O	2.26	0.68
1:A:290:PRO:HG3	1:A:382:ILE:HG22	1.75	0.68
3:N:67:ARG:HG2	3:N:71:ILE:HB	1.74	0.68
1:B:478:VAL:HG12	1:B:483:TYR:HB2	1.76	0.68
1:C:315:THR:HG22	1:C:347:TRP:HH2	1.59	0.68
1:C:19:VAL:HB	1:C:427:LEU:HD11	1.77	0.67
1:C:293:ASN:ND2	1:C:308:SER:O	2.26	0.67
1:C:478:VAL:HG12	1:C:483:TYR:HB2	1.76	0.67
2:J:40:SER:HA	2:J:55:TYR:HB3	1.75	0.67
1:A:34:GLU:OE2	1:A:36:SER:N	2.28	0.67
1:C:32:LEU:HD23	1:C:313:MET:HB2	1.74	0.67
1:B:149:TRP:HH2	2:I:111(C):VAL:HG21	1.59	0.66
1:B:19:VAL:HB	1:B:427:LEU:HD11	1.76	0.66
1:B:16:VAL:HG11	1:B:314:VAL:HB	1.78	0.66
1:A:16:VAL:HG11	1:A:314:VAL:HB	1.78	0.66
1:B:34:GLU:OE2	1:B:36:SER:N	2.28	0.66
2:H:111(C):VAL:HG22	2:H:111(C):VAL:O	1.96	0.66
1:C:290:PRO:HG3	1:C:382:ILE:HG22	1.75	0.66
2:J:111(C):VAL:HG22	2:J:111(C):VAL:O	1.96	0.66
1:A:19:VAL:HB	1:A:427:LEU:HD11	1.77	0.65
1:A:104:GLN:CD	1:C:401:ARG:HH12	1.98	0.65
1:A:315:THR:HG22	1:A:347:TRP:HH2	1.59	0.65
1:B:315:THR:HG22	1:B:347:TRP:HH2	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:VAL:HG11	1:C:314:VAL:HB	1.78	0.65
1:C:34:GLU:OE2	1:C:36:SER:N	2.28	0.64
2:I:111(C):VAL:O	2:I:111(C):VAL:HG22	1.96	0.64
1:A:295:HIS:ND1	1:A:296:PRO:HD2	2.13	0.64
1:C:95:PHE:HE1	1:C:101:LEU:HD23	1.63	0.64
1:C:440:ASN:HA	1:C:443:ASN:ND2	2.13	0.64
1:C:44:LEU:HD23	1:C:77:SER:HB2	1.80	0.63
2:J:118:TRP:NE1	3:N:50:PRO:O	2.31	0.63
1:B:44:LEU:HD23	1:B:77:SER:HB2	1.81	0.63
1:B:95:PHE:HE1	1:B:101:LEU:HD23	1.63	0.63
1:C:295:HIS:ND1	1:C:296:PRO:HD2	2.13	0.63
1:B:354:ASN:ND2	1:B:475:MET:SD	2.71	0.63
1:C:354:ASN:ND2	1:C:475:MET:SD	2.71	0.63
1:A:354:ASN:ND2	1:A:475:MET:SD	2.71	0.63
1:B:295:HIS:ND1	1:B:296:PRO:HD2	2.13	0.63
1:A:34:GLU:HB2	1:A:289:LEU:HD12	1.80	0.63
2:H:118:TRP:NE1	3:L:50:PRO:O	2.31	0.63
1:A:440:ASN:HA	1:A:443:ASN:ND2	2.13	0.63
1:A:95:PHE:HE1	1:A:101:LEU:HD23	1.63	0.63
1:A:44:LEU:HD23	1:A:77:SER:HB2	1.80	0.63
3:L:6:GLN:OE1	3:L:121:GLY:N	2.22	0.62
1:C:37:HIS:ND1	1:C:282:GLN:O	2.28	0.62
2:I:118:TRP:NE1	3:M:50:PRO:O	2.32	0.62
1:B:440:ASN:HA	1:B:443:ASN:ND2	2.13	0.62
3:M:72:PRO:HB2	3:M:75:ARG:HG3	1.81	0.62
3:N:72:PRO:HB2	3:N:75:ARG:HG3	1.81	0.62
3:M:67:ARG:NH2	3:M:76:PHE:O	2.33	0.62
3:N:6:GLN:OE1	3:N:121:GLY:N	2.22	0.62
1:B:34:GLU:HB2	1:B:289:LEU:HD12	1.81	0.62
1:A:202:SER:OG	1:A:237:ASP:OD2	2.18	0.61
3:L:72:PRO:HB2	3:L:75:ARG:HG3	1.81	0.61
1:B:202:SER:OG	1:B:237:ASP:OD2	2.18	0.61
3:L:67:ARG:NH2	3:L:76:PHE:O	2.33	0.61
3:N:67:ARG:NH2	3:N:76:PHE:O	2.33	0.61
1:C:202:SER:OG	1:C:237:ASP:OD2	2.18	0.61
1:C:34:GLU:HB2	1:C:289:LEU:HD12	1.80	0.61
3:M:18:ARG:NH1	3:M:90:THR:OG1	2.34	0.61
3:L:18:ARG:NH1	3:L:90:THR:OG1	2.34	0.61
1:C:14:ASP:OD2	1:C:29:SER:OG	2.18	0.61
3:N:18:ARG:NH1	3:N:90:THR:OG1	2.34	0.61
1:B:458:GLU:OE1	1:B:460:GLY:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:41:TRP:CE2	2:H:89:LEU:HB2	2.37	0.60
1:B:371:ILE:O	1:B:375:THR:HG23	2.02	0.60
1:C:371:ILE:O	1:C:375:THR:HG23	2.02	0.60
2:J:50:LEU:HD13	3:N:103:TYR:CE1	2.33	0.59
1:C:8:HIS:CE1	1:C:10:ASN:HD22	2.20	0.59
1:B:16:VAL:HG12	1:B:312:ARG:HB3	1.84	0.59
2:H:53:ILE:HD12	2:H:53:ILE:H	1.68	0.59
1:A:8:HIS:CE1	1:A:10:ASN:HD22	2.20	0.59
2:I:41:TRP:CE2	2:I:89:LEU:HB2	2.37	0.59
1:B:401:ARG:NH2	1:C:104:GLN:HE22	2.00	0.59
1:B:8:HIS:CE1	1:B:10:ASN:HD22	2.20	0.59
1:A:371:ILE:O	1:A:375:THR:HG23	2.02	0.59
1:A:458:GLU:OE1	1:A:460:GLY:N	2.33	0.59
1:B:14:ASP:OD2	1:B:312:ARG:NH1	2.36	0.59
2:J:41:TRP:CE2	2:J:89:LEU:HB2	2.37	0.59
1:C:292:GLN:NE2	1:C:303:PRO:O	2.36	0.59
1:A:292:GLN:NE2	1:A:303:PRO:O	2.36	0.59
1:B:367:THR:O	1:B:371:ILE:HG12	2.03	0.59
1:B:27:THR:OG1	1:B:28:HIS:ND1	2.23	0.58
1:B:452:LEU:HG	1:B:456:ALA:HB3	1.85	0.58
1:A:71:ILE:HG12	1:A:113:ARG:NH1	2.18	0.58
2:I:50:LEU:HD13	3:M:103:TYR:CE1	2.32	0.58
1:C:172:VAL:HG12	1:C:233:LEU:HB2	1.86	0.58
1:C:14:ASP:OD2	1:C:312:ARG:NH1	2.36	0.58
1:C:27:THR:OG1	1:C:28:HIS:ND1	2.23	0.58
2:J:53:ILE:HD12	2:J:53:ILE:H	1.68	0.58
1:C:367:THR:O	1:C:371:ILE:HG12	2.03	0.58
1:C:458:GLU:OE1	1:C:460:GLY:N	2.33	0.58
1:A:16:VAL:HG12	1:A:312:ARG:HB3	1.84	0.58
1:C:452:LEU:HG	1:C:456:ALA:HB3	1.84	0.58
1:A:367:THR:O	1:A:371:ILE:HG12	2.03	0.58
2:I:53:ILE:HD12	2:I:53:ILE:H	1.68	0.58
1:B:183:ASN:ND2	3:M:110:TRP:HB2	2.19	0.57
1:C:16:VAL:HG12	1:C:312:ARG:HB3	1.84	0.57
1:A:183:ASN:ND2	3:L:110:TRP:HB2	2.19	0.57
1:A:452:LEU:HG	1:A:456:ALA:HB3	1.85	0.57
1:B:31:ASN:OD1	1:B:32:LEU:N	2.38	0.57
1:B:172:VAL:HG12	1:B:233:LEU:HB2	1.86	0.57
1:B:292:GLN:NE2	1:B:303:PRO:O	2.36	0.57
1:C:183:ASN:ND2	3:N:110:TRP:HB2	2.19	0.57
1:A:95:PHE:CE1	1:A:101:LEU:HD23	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ASN:OD1	1:A:32:LEU:N	2.38	0.57
1:B:37:HIS:ND1	1:B:282:GLN:O	2.28	0.57
2:H:118:TRP:HH2	3:L:42:TYR:CE1	2.23	0.57
1:A:172:VAL:HG12	1:A:233:LEU:HB2	1.86	0.57
1:B:149:TRP:CH2	2:I:111(C):VAL:HG21	2.38	0.57
1:B:216:ARG:HG2	1:C:201:VAL:HG11	1.86	0.57
2:J:118:TRP:HH2	3:N:42:TYR:CE1	2.23	0.57
1:A:14:ASP:OD2	1:A:312:ARG:NH1	2.36	0.57
1:C:95:PHE:CE1	1:C:101:LEU:HD23	2.40	0.57
1:C:31:ASN:OD1	1:C:32:LEU:N	2.38	0.57
2:H:44:GLN:HB3	2:H:50:LEU:HG	1.86	0.57
1:B:71:ILE:HG12	1:B:113:ARG:NH1	2.18	0.56
3:M:6:GLN:OE1	3:M:121:GLY:N	2.22	0.56
1:A:27:THR:OG1	1:A:28:HIS:ND1	2.23	0.56
2:J:44:GLN:HB3	2:J:50:LEU:HG	1.86	0.56
1:A:19:VAL:O	1:B:376:ASN:ND2	2.38	0.56
1:A:401:ARG:NH2	1:B:104:GLN:HE22	2.03	0.56
1:C:176:TRP:HE1	1:C:209:PHE:HE2	1.53	0.56
1:C:306:VAL:HG13	1:C:419:THR:HA	1.88	0.56
1:C:378:VAL:O	1:C:382:ILE:HG12	2.05	0.56
1:A:370:ALA:O	1:A:374:ILE:HG12	2.05	0.56
1:A:378:VAL:O	1:A:382:ILE:HG12	2.05	0.56
1:B:32:LEU:HD11	1:B:311:LEU:HB2	1.88	0.56
1:A:14:ASP:OD2	1:A:29:SER:OG	2.17	0.56
1:A:32:LEU:HD11	1:A:311:LEU:HB2	1.88	0.56
1:B:26:VAL:HG22	1:B:318:ARG:HA	1.88	0.56
1:B:378:VAL:O	1:B:382:ILE:HG12	2.05	0.56
2:I:44:GLN:HB3	2:I:50:LEU:HG	1.86	0.56
1:A:149:TRP:CH2	2:H:111(C):VAL:CG2	2.88	0.56
1:A:216:ARG:HG2	1:B:201:VAL:HG11	1.87	0.56
1:C:370:ALA:O	1:C:374:ILE:HG12	2.05	0.56
1:A:306:VAL:HG13	1:A:419:THR:HA	1.88	0.56
1:B:370:ALA:O	1:B:374:ILE:HG12	2.05	0.56
1:B:176:TRP:HE1	1:B:209:PHE:HE2	1.53	0.55
1:C:29:SER:OG	1:C:312:ARG:NH1	2.40	0.55
1:C:149:TRP:CH2	2:J:111(C):VAL:CG2	2.88	0.55
2:I:102:TYR:O	2:I:122:THR:N	2.37	0.55
1:B:95:PHE:CE1	1:B:101:LEU:HD23	2.40	0.55
1:B:5:ILE:HG21	1:B:444:LEU:HD22	1.89	0.55
1:B:29:SER:OG	1:B:312:ARG:NH1	2.40	0.55
1:A:176:TRP:HE1	1:A:209:PHE:HE2	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:PRO:HG2	1:B:291:PHE:HD2	1.71	0.55
2:I:35:ASN:HA	2:I:84:LYS:NZ	2.22	0.55
2:J:35:ASN:HA	2:J:84:LYS:NZ	2.22	0.55
1:A:29:SER:OG	1:A:312:ARG:NH1	2.40	0.55
1:B:306:VAL:HG13	1:B:419:THR:HA	1.88	0.55
1:A:37:HIS:ND1	1:A:282:GLN:O	2.28	0.55
1:A:201:VAL:HG11	1:C:216:ARG:HG2	1.89	0.55
2:H:35:ASN:HA	2:H:84:LYS:NZ	2.22	0.55
1:B:432:ARG:HA	1:B:432:ARG:NE	2.22	0.55
1:C:290:PRO:HG2	1:C:291:PHE:HD2	1.71	0.55
1:C:432:ARG:HA	1:C:432:ARG:NE	2.22	0.55
1:C:447:LYS:NZ	1:C:451:GLN:HE22	2.05	0.55
2:H:50:LEU:HD13	3:L:103:TYR:CE1	2.33	0.55
1:A:432:ARG:HA	1:A:432:ARG:NE	2.22	0.55
1:B:474:CYS:O	1:B:478:VAL:HG22	2.07	0.55
1:C:32:LEU:HD11	1:C:311:LEU:HB2	1.88	0.55
1:A:290:PRO:HG2	1:A:291:PHE:HD2	1.71	0.54
1:C:26:VAL:HG22	1:C:318:ARG:HA	1.88	0.54
1:A:26:VAL:HG22	1:A:318:ARG:HA	1.88	0.54
1:B:62:LEU:HB3	1:B:144:TYR:CD2	2.43	0.54
1:C:474:CYS:O	1:C:478:VAL:HG22	2.07	0.54
1:A:447:LYS:NZ	1:A:451:GLN:HE22	2.05	0.54
1:A:104:GLN:HE22	1:C:401:ARG:NH2	2.04	0.54
1:A:376:ASN:ND2	1:C:19:VAL:O	2.40	0.54
1:C:62:LEU:HB3	1:C:144:TYR:CD2	2.43	0.54
1:C:71:ILE:HG12	1:C:113:ARG:NH1	2.18	0.54
2:J:102:TYR:O	2:J:122:THR:N	2.37	0.54
3:M:67:ARG:NH1	3:M:74:ALA:HA	2.23	0.54
1:A:474:CYS:O	1:A:478:VAL:HG22	2.07	0.54
3:L:67:ARG:NH1	3:L:74:ALA:HA	2.23	0.54
1:A:5:ILE:HG21	1:A:444:LEU:HD22	1.89	0.54
1:B:447:LYS:NZ	1:B:451:GLN:HE22	2.05	0.54
2:H:39:TRP:O	2:H:55:TYR:HB2	2.08	0.54
1:C:92:PRO:HG3	1:C:219:VAL:HG21	1.91	0.53
2:H:102:TYR:O	2:H:122:THR:N	2.37	0.53
3:N:39:LEU:HD12	3:N:105:GLN:O	2.08	0.53
1:A:160:LEU:HD21	1:A:243:ALA:HB3	1.91	0.53
1:A:418:TRP:HZ2	1:C:416:ASP:OD2	1.92	0.53
1:C:5:ILE:HG21	1:C:444:LEU:HD22	1.89	0.53
1:B:19:VAL:O	1:C:376:ASN:ND2	2.40	0.53
1:C:62:LEU:HD21	1:C:95:PHE:HE2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:110:TRP:HB3	3:L:113:PRO:HD3	1.91	0.53
3:N:67:ARG:NH1	3:N:74:ALA:HA	2.23	0.53
2:I:39:TRP:O	2:I:55:TYR:HB2	2.08	0.53
1:A:62:LEU:HB3	1:A:144:TYR:CD2	2.43	0.53
3:L:39:LEU:HD12	3:L:105:GLN:O	2.08	0.53
3:M:89:LEU:HD23	3:M:90:THR:N	2.24	0.53
2:I:110:ASP:O	2:I:113:TYR:HB2	2.09	0.53
1:C:38:ASN:OD1	1:C:40:LYS:N	2.40	0.52
1:C:77:SER:HG	1:C:78:TYR:HD2	1.57	0.52
2:J:118:TRP:NE1	3:N:50:PRO:HD2	2.25	0.52
3:M:39:LEU:HD12	3:M:105:GLN:O	2.08	0.52
1:B:160:LEU:HD21	1:B:243:ALA:HB3	1.91	0.52
3:L:89:LEU:HD23	3:L:90:THR:N	2.24	0.52
3:N:89:LEU:HD23	3:N:90:THR:N	2.24	0.52
2:J:39:TRP:O	2:J:55:TYR:HB2	2.08	0.52
3:N:110:TRP:HB3	3:N:113:PRO:HD3	1.91	0.52
1:B:92:PRO:HG3	1:B:219:VAL:HG21	1.91	0.52
1:B:62:LEU:HD21	1:B:95:PHE:HE2	1.73	0.52
1:B:416:ASP:OD2	1:C:418:TRP:HZ2	1.92	0.52
1:A:62:LEU:HD21	1:A:95:PHE:HE2	1.73	0.52
2:H:110:ASP:O	2:H:113:TYR:HB2	2.09	0.52
2:H:118:TRP:NE1	3:L:50:PRO:HD2	2.25	0.52
1:A:92:PRO:HG3	1:A:219:VAL:HG21	1.91	0.52
1:C:160:LEU:HD21	1:C:243:ALA:HB3	1.91	0.52
1:C:216:ARG:HG3	1:C:216:ARG:HH11	1.75	0.52
2:J:110:ASP:O	2:J:113:TYR:HB2	2.09	0.52
1:C:27:THR:OG1	1:C:28:HIS:N	2.43	0.52
3:M:110:TRP:HB3	3:M:113:PRO:HD3	1.91	0.52
1:B:1:ASP:O	1:B:466:PHE:N	2.38	0.52
1:B:27:THR:OG1	1:B:28:HIS:N	2.43	0.51
2:I:39:TRP:CZ3	2:I:106:ARG:HB2	2.45	0.51
2:J:39:TRP:CZ3	2:J:106:ARG:HB2	2.45	0.51
1:B:77:SER:HG	1:B:78:TYR:HD2	1.57	0.51
1:B:216:ARG:HG3	1:B:216:ARG:HH11	1.75	0.51
1:B:14:ASP:OD2	1:B:29:SER:OG	2.17	0.51
1:B:405:ASN:HB3	1:C:394:LYS:NZ	2.25	0.51
1:C:262:SER:OG	1:C:263:GLY:N	2.43	0.51
1:B:262:SER:OG	1:B:263:GLY:N	2.43	0.51
1:C:175:LEU:O	1:C:250:PRO:HB3	2.11	0.51
1:A:262:SER:OG	1:A:263:GLY:N	2.43	0.51
1:A:416:ASP:OD2	1:B:418:TRP:HZ2	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LEU:O	1:B:250:PRO:HB3	2.11	0.51
2:H:39:TRP:CZ3	2:H:106:ARG:HB2	2.45	0.51
2:J:77:THR:H	2:J:90:LYS:HB3	1.76	0.51
2:I:118:TRP:HH2	3:M:42:TYR:CE1	2.28	0.51
1:A:216:ARG:HH11	1:A:216:ARG:HG3	1.75	0.50
1:A:27:THR:OG1	1:A:28:HIS:N	2.43	0.50
1:A:175:LEU:O	1:A:250:PRO:HB3	2.11	0.50
1:B:403:MET:CE	1:C:403:MET:HE3	2.42	0.50
1:C:1:ASP:O	1:C:466:PHE:N	2.38	0.50
2:H:77:THR:H	2:H:90:LYS:HB3	1.76	0.50
2:H:98:ASP:OD1	2:H:98:ASP:N	2.44	0.50
2:I:98:ASP:N	2:I:98:ASP:OD1	2.44	0.50
1:A:77:SER:HG	1:A:78:TYR:HD2	1.58	0.50
1:A:394:LYS:NZ	1:C:405:ASN:HB3	2.27	0.50
1:B:314:VAL:HG12	1:B:430:ASN:HB2	1.94	0.50
2:I:77:THR:H	2:I:90:LYS:HB3	1.76	0.50
1:A:314:VAL:HG12	1:A:430:ASN:HB2	1.94	0.50
1:B:403:MET:HE3	1:C:403:MET:HE3	1.93	0.50
1:C:314:VAL:HG12	1:C:430:ASN:HB2	1.94	0.50
2:J:41:TRP:HD1	2:J:78:ILE:HD13	1.77	0.50
2:I:41:TRP:HD1	2:I:78:ILE:HD13	1.77	0.50
2:H:35:ASN:HA	2:H:84:LYS:HZ1	1.75	0.49
2:I:19:LEU:HB3	2:I:91:LEU:HB3	1.93	0.49
2:I:71:LEU:HD23	2:I:71:LEU:O	2.12	0.49
1:A:296:PRO:HB3	1:A:415:LEU:HD11	1.94	0.49
2:J:71:LEU:O	2:J:71:LEU:HD23	2.12	0.49
1:A:316:GLY:C	1:A:317:LEU:HD12	2.32	0.49
1:B:316:GLY:C	1:B:317:LEU:HD12	2.32	0.49
2:J:19:LEU:HB3	2:J:91:LEU:HB3	1.93	0.49
1:C:316:GLY:C	1:C:317:LEU:HD12	2.33	0.49
2:H:71:LEU:HD23	2:H:71:LEU:O	2.12	0.49
2:I:35:ASN:OD1	2:I:36:SER:N	2.46	0.49
2:I:41:TRP:CD1	2:I:89:LEU:HD13	2.48	0.49
2:J:35:ASN:HA	2:J:84:LYS:HZ1	1.77	0.49
1:C:472:ASN:HA	1:C:475:MET:HE2	1.95	0.49
2:H:35:ASN:OD1	2:H:36:SER:N	2.46	0.49
2:I:13:VAL:HG13	2:I:126:VAL:HG23	1.95	0.49
2:J:98:ASP:OD1	2:J:98:ASP:N	2.44	0.49
1:B:455:ASN:HD21	1:B:489:SER:HB3	1.78	0.49
2:H:100:ALA:HB3	2:H:102:TYR:HE1	1.78	0.49
1:A:38:ASN:OD1	1:A:40:LYS:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:VAL:HG23	1:A:220:ARG:H	1.78	0.49
1:B:296:PRO:HB3	1:B:415:LEU:HD11	1.94	0.49
1:C:455:ASN:HD21	1:C:489:SER:HB3	1.78	0.49
1:A:190:LEU:HD23	1:A:191:TYR:HE2	1.78	0.49
1:C:447:LYS:HZ1	1:C:451:GLN:HE22	1.58	0.49
2:J:35:ASN:OD1	2:J:36:SER:N	2.46	0.49
1:A:457:LYS:HE2	1:A:467:TYR:CD1	2.48	0.48
1:B:38:ASN:OD1	1:B:40:LYS:N	2.40	0.48
3:M:65:SER:HB2	3:M:66:HIS:CD2	2.49	0.48
1:B:314:VAL:CG1	1:B:430:ASN:HB2	2.43	0.48
1:B:401:ARG:HH22	1:C:104:GLN:NE2	2.09	0.48
1:B:457:LYS:HE2	1:B:467:TYR:CD1	2.48	0.48
1:C:314:VAL:CG1	1:C:430:ASN:HB2	2.43	0.48
1:C:371:ILE:HA	1:C:374:ILE:HG12	1.95	0.48
2:J:100:ALA:HB3	2:J:102:TYR:HE1	1.78	0.48
3:N:3:VAL:HG12	3:N:26:SER:HB3	1.96	0.48
1:B:49:PRO:HB3	1:B:78:TYR:CE2	2.48	0.48
1:B:452:LEU:HD23	1:B:452:LEU:O	2.13	0.48
1:C:219:VAL:HG23	1:C:220:ARG:H	1.78	0.48
2:H:41:TRP:HD1	2:H:78:ILE:HD13	1.77	0.48
2:J:41:TRP:CD1	2:J:89:LEU:HD13	2.48	0.48
2:J:106:ARG:O	2:J:116:ASP:HA	2.14	0.48
1:A:314:VAL:CG1	1:A:430:ASN:HB2	2.43	0.48
2:I:19:LEU:HD11	2:I:21:LEU:HD22	1.96	0.48
3:M:52:LEU:HD23	3:M:53:LEU:N	2.28	0.48
3:N:52:LEU:HD23	3:N:53:LEU:N	2.28	0.48
1:A:405:ASN:HB3	1:B:394:LYS:NZ	2.29	0.48
1:A:455:ASN:HD21	1:A:489:SER:HB3	1.78	0.48
1:C:190:LEU:HD23	1:C:191:TYR:HE2	1.78	0.48
1:C:348:TYR:O	1:C:363:ASP:N	2.38	0.48
1:C:457:LYS:HE2	1:C:467:TYR:CD1	2.48	0.48
2:H:13:VAL:HG13	2:H:126:VAL:HG23	1.95	0.48
2:J:13:VAL:HG13	2:J:126:VAL:HG23	1.95	0.48
2:H:19:LEU:HD11	2:H:21:LEU:HD22	1.96	0.48
2:H:41:TRP:CD1	2:H:89:LEU:HD13	2.48	0.48
2:J:100:ALA:HB3	2:J:102:TYR:CE1	2.49	0.48
1:A:321:PRO:O	1:A:341:THR:OG1	2.32	0.48
2:H:19:LEU:HB3	2:H:91:LEU:HB3	1.93	0.48
2:I:100:ALA:HB3	2:I:102:TYR:HE1	1.78	0.48
1:A:452:LEU:HD23	1:A:452:LEU:O	2.13	0.48
1:B:371:ILE:HA	1:B:374:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:ASP:OD2	1:C:1:ASP:N	2.46	0.48
1:C:296:PRO:HB3	1:C:415:LEU:HD11	1.94	0.48
2:I:100:ALA:HB3	2:I:102:TYR:CE1	2.49	0.48
2:I:106:ARG:O	2:I:116:ASP:HA	2.14	0.48
3:L:52:LEU:HD23	3:L:53:LEU:N	2.28	0.48
3:N:65:SER:HB2	3:N:66:HIS:CD2	2.49	0.48
1:B:219:VAL:HG23	1:B:220:ARG:H	1.78	0.48
1:B:321:PRO:O	1:B:341:THR:OG1	2.32	0.48
1:B:348:TYR:HH	1:B:437:HIS:CE1	2.30	0.48
1:C:49:PRO:HB3	1:C:78:TYR:CE2	2.48	0.48
3:L:53:LEU:HG	3:L:76:PHE:HE1	1.79	0.48
3:N:8:PRO:O	3:N:122:THR:HG21	2.14	0.48
1:A:222:GLN:NE2	2:H:112(C):ASP:OD1	2.44	0.47
1:A:447:LYS:HZ1	1:A:451:GLN:HE22	1.62	0.47
1:B:1:ASP:OD2	1:B:1:ASP:N	2.46	0.47
1:C:452:LEU:O	1:C:452:LEU:HD23	2.13	0.47
3:L:3:VAL:HG12	3:L:26:SER:HB3	1.96	0.47
3:L:8:PRO:O	3:L:122:THR:HG21	2.14	0.47
3:L:65:SER:HB2	3:L:66:HIS:CD2	2.49	0.47
1:A:49:PRO:HB3	1:A:78:TYR:CE2	2.48	0.47
1:A:1:ASP:OD2	1:A:1:ASP:N	2.46	0.47
1:B:317:LEU:HD11	1:B:348:TYR:OH	2.15	0.47
1:C:18:THR:OG1	1:C:21:GLU:N	2.48	0.47
2:H:52:TRP:CZ2	2:H:54:GLY:HA2	2.50	0.47
1:C:49:PRO:HB3	1:C:78:TYR:CZ	2.50	0.47
3:N:53:LEU:HG	3:N:76:PHE:HE1	1.79	0.47
1:A:371:ILE:HA	1:A:374:ILE:HG12	1.95	0.47
1:C:219:VAL:HG23	1:C:220:ARG:N	2.30	0.47
2:H:100:ALA:HB3	2:H:102:TYR:CE1	2.49	0.47
2:I:52:TRP:CZ2	2:I:54:GLY:HA2	2.50	0.47
2:J:19:LEU:HD11	2:J:21:LEU:HD22	1.96	0.47
3:M:3:VAL:HG12	3:M:26:SER:HB3	1.96	0.47
3:M:53:LEU:HG	3:M:76:PHE:HE1	1.79	0.47
1:A:91:TYR:HE2	1:A:222:GLN:OE1	1.97	0.47
1:B:190:LEU:HD23	1:B:191:TYR:HE2	1.78	0.47
2:H:106:ARG:O	2:H:116:ASP:HA	2.14	0.47
1:A:49:PRO:HB3	1:A:78:TYR:CZ	2.50	0.47
1:B:273:GLU:O	1:B:273:GLU:HG2	2.15	0.47
1:A:403:MET:HE3	1:C:403:MET:CE	2.45	0.47
2:J:75:ARG:NH1	2:J:93:SER:O	2.48	0.47
1:A:58:ALA:HB2	1:A:98:TYR:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:PRO:HG3	1:A:187:GLN:HE21	1.80	0.46
1:A:317:LEU:HD11	1:A:348:TYR:OH	2.15	0.46
1:B:18:THR:OG1	1:B:21:GLU:N	2.48	0.46
1:B:173:LEU:HD23	1:B:174:VAL:N	2.30	0.46
1:B:219:VAL:HG23	1:B:220:ARG:N	2.30	0.46
1:C:91:TYR:HE2	1:C:222:GLN:OE1	1.97	0.46
1:C:415:LEU:HD23	1:C:415:LEU:HA	1.78	0.46
2:H:75:ARG:NH1	2:H:93:SER:O	2.48	0.46
1:A:219:VAL:HG23	1:A:220:ARG:N	2.30	0.46
1:A:370:ALA:HB1	1:A:437:HIS:CE1	2.51	0.46
1:C:181:PRO:HG3	1:C:187:GLN:HE21	1.80	0.46
2:J:52:TRP:CZ2	2:J:54:GLY:HA2	2.50	0.46
3:M:8:PRO:O	3:M:122:THR:HG21	2.14	0.46
1:A:34:GLU:OE2	1:A:36:SER:OG	2.31	0.46
1:C:279:GLN:N	1:C:279:GLN:OE1	2.49	0.46
1:C:321:PRO:O	1:C:341:THR:OG1	2.32	0.46
1:A:415:LEU:HD23	1:A:415:LEU:HA	1.78	0.46
1:B:49:PRO:HB3	1:B:78:TYR:CZ	2.50	0.46
1:B:58:ALA:HB2	1:B:98:TYR:CZ	2.50	0.46
1:C:58:ALA:HB2	1:C:98:TYR:CZ	2.50	0.46
1:C:273:GLU:O	1:C:273:GLU:HG2	2.15	0.46
1:C:370:ALA:HB1	1:C:437:HIS:CE1	2.51	0.46
2:I:75:ARG:NH1	2:I:93:SER:O	2.48	0.46
1:A:472:ASN:HA	1:A:475:MET:HE2	1.98	0.46
1:B:279:GLN:N	1:B:279:GLN:OE1	2.49	0.46
1:A:173:LEU:HD23	1:A:174:VAL:N	2.30	0.46
1:A:279:GLN:N	1:A:279:GLN:OE1	2.49	0.46
1:A:18:THR:OG1	1:A:21:GLU:N	2.48	0.46
1:C:173:LEU:HD23	1:C:174:VAL:N	2.30	0.46
1:A:44:LEU:HB2	1:A:279:GLN:HE22	1.81	0.46
1:B:181:PRO:HG3	1:B:187:GLN:HE21	1.80	0.46
1:B:472:ASN:HA	1:B:475:MET:HE2	1.98	0.46
1:C:202:SER:OG	1:C:203:SER:N	2.49	0.46
3:N:101:VAL:HG12	3:N:103:TYR:HE2	1.81	0.46
1:B:44:LEU:HB2	1:B:279:GLN:HE22	1.81	0.46
1:B:91:TYR:HE2	1:B:222:GLN:OE1	1.97	0.46
1:B:279:GLN:HG3	1:B:284:ALA:HB2	1.98	0.46
1:B:370:ALA:HB1	1:B:437:HIS:CE1	2.51	0.46
1:C:438:ASP:O	1:C:442:LYS:HG2	2.16	0.46
1:C:44:LEU:HB2	1:C:279:GLN:HE22	1.81	0.46
3:M:15:PRO:HA	3:M:94:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:GLU:O	1:A:273:GLU:HG2	2.15	0.45
1:A:379:ASN:OD1	1:A:380:SER:N	2.49	0.45
1:B:29:SER:OG	1:B:29:SER:O	2.33	0.45
1:C:115:GLU:HA	1:C:251:ARG:O	2.16	0.45
1:C:222:GLN:NE2	2:J:112(C):ASP:OD1	2.44	0.45
1:C:317:LEU:HD11	1:C:348:TYR:OH	2.15	0.45
2:J:85:ARG:HE	2:J:85:ARG:HB3	1.60	0.45
1:B:438:ASP:O	1:B:442:LYS:HG2	2.16	0.45
3:N:15:PRO:HA	3:N:94:LEU:HD22	1.98	0.45
1:A:181:PRO:HG2	1:A:213:ILE:HD12	1.98	0.45
1:B:58:ALA:O	1:B:62:LEU:HD23	2.16	0.45
2:I:24:ASN:HA	2:I:86:GLN:HA	1.98	0.45
1:B:34:GLU:OE2	1:B:36:SER:OG	2.31	0.45
1:B:91:TYR:CD2	1:B:92:PRO:HD2	2.52	0.45
1:B:115:GLU:HA	1:B:251:ARG:O	2.16	0.45
1:B:190:LEU:HB3	1:B:191:TYR:CD2	2.52	0.45
1:C:3:ILE:O	1:C:464:PHE:HB2	2.16	0.45
1:C:58:ALA:O	1:C:62:LEU:HD23	2.16	0.45
1:C:190:LEU:HB3	1:C:191:TYR:CD2	2.52	0.45
1:C:379:ASN:OD1	1:C:380:SER:N	2.49	0.45
3:L:101:VAL:HG12	3:L:103:TYR:HE2	1.81	0.45
1:A:115:GLU:HA	1:A:251:ARG:O	2.16	0.45
1:B:26:VAL:HG13	1:B:317:LEU:O	2.17	0.45
1:B:202:SER:OG	1:B:203:SER:N	2.49	0.45
1:C:181:PRO:HG2	1:C:213:ILE:HD12	1.98	0.45
2:H:24:ASN:HA	2:H:86:GLN:HA	1.98	0.45
1:A:3:ILE:O	1:A:464:PHE:HB2	2.16	0.45
1:A:58:ALA:O	1:A:62:LEU:HD23	2.16	0.45
1:B:99:GLU:OE1	1:B:99:GLU:N	2.50	0.45
1:B:181:PRO:HG3	1:B:187:GLN:HB2	1.98	0.45
1:B:379:ASN:OD1	1:B:380:SER:N	2.49	0.45
3:M:101:VAL:HG12	3:M:103:TYR:HE2	1.81	0.45
1:A:29:SER:OG	1:A:29:SER:O	2.34	0.45
1:A:190:LEU:HB3	1:A:191:TYR:CD2	2.52	0.45
1:B:3:ILE:O	1:B:464:PHE:HB2	2.16	0.45
1:B:227:ASN:HB2	1:B:229:TYR:CE2	2.52	0.45
3:L:15:PRO:HA	3:L:94:LEU:HD22	1.98	0.45
1:C:279:GLN:HG3	1:C:284:ALA:HB2	1.98	0.45
2:J:42:ILE:HB	2:J:103:TYR:HB2	1.99	0.45
2:J:55:TYR:OH	3:N:114:PRO:HB3	2.17	0.45
1:A:1:ASP:O	1:A:466:PHE:N	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:SER:OG	1:A:203:SER:N	2.49	0.45
1:C:91:TYR:CD2	1:C:92:PRO:HD2	2.52	0.45
1:C:181:PRO:HG3	1:C:187:GLN:HB2	1.98	0.45
1:C:227:ASN:HB2	1:C:229:TYR:CE2	2.52	0.45
1:C:379:ASN:HA	1:C:382:ILE:HG12	1.99	0.45
1:C:401:ARG:HB2	1:C:404:GLU:HB3	1.99	0.45
2:I:118:TRP:NE1	3:M:50:PRO:HD2	2.33	0.45
3:M:67:ARG:CG	3:M:71:ILE:HB	2.46	0.45
1:A:438:ASP:O	1:A:442:LYS:HG2	2.16	0.44
1:A:445:TYR:OH	1:A:462:GLY:O	2.30	0.44
1:B:181:PRO:HG2	1:B:213:ILE:HD12	1.98	0.44
1:B:449:LYS:O	1:B:449:LYS:HD3	2.18	0.44
1:C:99:GLU:N	1:C:99:GLU:OE1	2.50	0.44
1:A:91:TYR:CD2	1:A:92:PRO:HD2	2.52	0.44
1:A:416:ASP:OD1	1:B:386:ASN:HB2	2.17	0.44
1:C:29:SER:OG	1:C:29:SER:O	2.34	0.44
1:C:298:THR:HB	1:C:302:CYS:SG	2.57	0.44
2:I:55:TYR:OH	3:M:114:PRO:HB3	2.17	0.44
1:A:181:PRO:HG3	1:A:187:GLN:HB2	1.98	0.44
1:A:420:TYR:OH	1:B:425:LEU:HD22	2.18	0.44
1:B:148:LEU:HD23	1:B:148:LEU:HA	1.84	0.44
1:B:447:LYS:HZ1	1:B:451:GLN:HE22	1.64	0.44
2:I:40:SER:HA	2:I:55:TYR:CB	2.47	0.44
1:A:99:GLU:N	1:A:99:GLU:OE1	2.50	0.44
1:A:425:LEU:HD22	1:C:420:TYR:OH	2.18	0.44
1:A:449:LYS:O	1:A:449:LYS:HD3	2.18	0.44
1:B:379:ASN:HA	1:B:382:ILE:HG12	1.99	0.44
2:J:24:ASN:HA	2:J:86:GLN:HA	1.98	0.44
1:A:26:VAL:HG13	1:A:317:LEU:O	2.17	0.44
1:A:279:GLN:HG3	1:A:284:ALA:HB2	1.98	0.44
1:C:26:VAL:HG13	1:C:317:LEU:O	2.17	0.44
1:C:62:LEU:HD21	1:C:95:PHE:CE2	2.52	0.44
1:C:449:LYS:O	1:C:449:LYS:HD3	2.18	0.44
2:H:40:SER:HA	2:H:55:TYR:CB	2.47	0.44
1:A:427:LEU:O	1:A:431:GLU:HG2	2.18	0.44
2:H:42:ILE:HB	2:H:103:TYR:HB2	1.99	0.44
2:H:55:TYR:OH	3:L:114:PRO:HB3	2.17	0.44
3:M:13:LEU:HD11	3:M:94:LEU:HD13	2.00	0.44
1:A:62:LEU:HD21	1:A:95:PHE:CE2	2.52	0.44
1:A:191:TYR:CE1	1:A:246:ASN:HA	2.53	0.44
1:A:298:THR:HB	1:A:302:CYS:SG	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:44:GLN:CB	2:H:50:LEU:HG	2.48	0.44
2:J:44:GLN:CB	2:J:50:LEU:HG	2.48	0.44
3:L:19:ALA:HB3	3:L:91:ILE:HG12	2.00	0.44
1:A:65:PRO:HB3	1:A:145:ARG:HH12	1.83	0.44
1:A:401:ARG:HB2	1:A:404:GLU:HB3	1.99	0.44
1:B:348:TYR:O	1:B:363:ASP:N	2.37	0.44
3:M:54:ILE:HD13	3:M:78:GLY:N	2.33	0.44
1:A:227:ASN:HB2	1:A:229:TYR:CE2	2.52	0.43
1:A:401:ARG:HH22	1:B:104:GLN:NE2	2.13	0.43
1:B:298:THR:HB	1:B:302:CYS:SG	2.57	0.43
1:B:455:ASN:ND2	1:B:485:TYR:O	2.51	0.43
1:C:65:PRO:HB3	1:C:145:ARG:HH12	1.83	0.43
2:I:42:ILE:HB	2:I:103:TYR:HB2	1.99	0.43
1:B:429:GLU:OE2	1:B:429:GLU:HA	2.19	0.43
1:A:12:SER:HB2	1:A:27:THR:HA	2.00	0.43
1:A:348:TYR:O	1:A:363:ASP:N	2.38	0.43
1:B:427:LEU:O	1:B:431:GLU:HG2	2.18	0.43
1:C:50:LEU:HD12	1:C:76:TRP:CD1	2.53	0.43
1:C:427:LEU:O	1:C:431:GLU:HG2	2.18	0.43
3:L:41:TRP:C	3:L:42:TYR:HD2	2.22	0.43
3:N:41:TRP:C	3:N:42:TYR:HD2	2.22	0.43
1:A:50:LEU:HD12	1:A:76:TRP:CD1	2.53	0.43
1:A:349:GLY:HA3	1:A:362:ALA:HA	2.00	0.43
1:A:379:ASN:HA	1:A:382:ILE:HG12	1.99	0.43
1:B:401:ARG:HB2	1:B:404:GLU:HB3	1.99	0.43
2:J:19:LEU:HD12	2:J:20:SER:N	2.34	0.43
3:N:19:ALA:HB3	3:N:91:ILE:HG12	2.00	0.43
1:A:403:MET:CE	1:B:403:MET:HE3	2.48	0.43
1:A:429:GLU:HA	1:A:429:GLU:OE2	2.19	0.43
1:B:12:SER:HB2	1:B:27:THR:HA	2.00	0.43
1:B:40:LYS:HA	1:B:269:ALA:HB1	2.01	0.43
1:C:191:TYR:CE1	1:C:246:ASN:HA	2.53	0.43
1:C:349:GLY:HA3	1:C:362:ALA:HA	2.00	0.43
1:C:429:GLU:HA	1:C:429:GLU:OE2	2.19	0.43
1:A:8:HIS:NE2	1:A:10:ASN:HB3	2.33	0.43
1:A:455:ASN:ND2	1:A:485:TYR:O	2.51	0.43
1:B:191:TYR:CE1	1:B:246:ASN:HA	2.53	0.43
1:C:348:TYR:HH	1:C:437:HIS:CE1	2.33	0.43
2:I:44:GLN:CB	2:I:50:LEU:HG	2.48	0.43
1:B:65:PRO:HB3	1:B:145:ARG:HH12	1.83	0.43
1:B:187:GLN:NE2	1:B:246:ASN:OD1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:TYR:HH	1:B:437:HIS:HD1	1.37	0.43
1:C:12:SER:HB2	1:C:27:THR:HA	2.00	0.43
1:C:455:ASN:ND2	1:C:485:TYR:O	2.51	0.43
2:H:19:LEU:HD12	2:H:20:SER:N	2.34	0.43
2:I:19:LEU:HD12	2:I:20:SER:N	2.34	0.43
1:B:428:LEU:HD13	1:C:428:LEU:HD21	2.01	0.43
2:J:4:LEU:HD21	2:J:104:CYS:HB2	2.00	0.43
3:L:54:ILE:HG21	3:L:78:GLY:HA3	2.01	0.43
3:L:67:ARG:CG	3:L:71:ILE:HB	2.46	0.43
3:M:41:TRP:C	3:M:42:TYR:HD2	2.22	0.43
1:B:416:ASP:OD1	1:C:386:ASN:HB2	2.18	0.43
1:C:190:LEU:HD23	1:C:191:TYR:CE2	2.54	0.43
1:A:95:PHE:HB3	1:A:98:TYR:HB2	2.01	0.43
1:A:190:LEU:HD23	1:A:191:TYR:CE2	2.54	0.43
1:A:379:ASN:HA	1:A:382:ILE:CG1	2.49	0.43
1:B:8:HIS:NE2	1:B:10:ASN:HB3	2.33	0.43
1:B:420:TYR:OH	1:C:425:LEU:HD22	2.18	0.43
1:C:8:HIS:NE2	1:C:10:ASN:HB3	2.33	0.43
1:C:52:LEU:HA	1:C:70:LEU:HD11	2.01	0.43
1:C:160:LEU:HD23	1:C:160:LEU:H	1.84	0.43
3:L:54:ILE:HD13	3:L:78:GLY:N	2.33	0.43
3:N:54:ILE:HD13	3:N:78:GLY:N	2.33	0.43
1:A:40:LYS:HA	1:A:269:ALA:HB1	2.00	0.42
1:A:160:LEU:H	1:A:160:LEU:HD23	1.84	0.42
1:A:386:ASN:HB2	1:C:416:ASP:OD1	2.19	0.42
1:B:50:LEU:HD12	1:B:76:TRP:CD1	2.53	0.42
1:B:52:LEU:HA	1:B:70:LEU:HD11	2.01	0.42
3:L:13:LEU:HD11	3:L:94:LEU:HD13	2.00	0.42
3:M:19:ALA:HB3	3:M:91:ILE:HG12	2.00	0.42
3:N:54:ILE:HG21	3:N:78:GLY:HA3	2.01	0.42
3:N:67:ARG:CG	3:N:71:ILE:HB	2.46	0.42
1:A:313:MET:HE3	1:A:377:LYS:HE2	2.01	0.42
1:B:112:GLU:HG3	1:B:255:ALA:HB3	2.01	0.42
1:B:476:GLU:O	1:B:479:LYS:HB2	2.19	0.42
3:N:76:PHE:O	3:N:77:THR:OG1	2.35	0.42
1:B:160:LEU:HD23	1:B:160:LEU:H	1.84	0.42
1:B:277:LYS:HE2	1:B:301:GLU:OE1	2.19	0.42
3:M:76:PHE:O	3:M:77:THR:OG1	2.35	0.42
1:A:42:CYS:HB3	1:A:274:CYS:HB2	1.46	0.42
1:A:70:LEU:HD23	1:A:70:LEU:HA	1.85	0.42
1:A:476:GLU:O	1:A:479:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:GLY:HA3	1:B:362:ALA:HA	2.00	0.42
1:C:10:ASN:HD21	1:C:28:HIS:HE1	1.68	0.42
1:C:112:GLU:HG3	1:C:255:ALA:HB3	2.01	0.42
1:C:277:LYS:HE2	1:C:301:GLU:OE1	2.19	0.42
2:J:30:ILE:HG13	2:J:39:TRP:CD1	2.55	0.42
3:N:75:ARG:HH12	3:N:98:ASP:CB	2.32	0.42
1:B:62:LEU:HD21	1:B:95:PHE:CE2	2.52	0.42
1:B:190:LEU:HD23	1:B:191:TYR:CE2	2.54	0.42
1:B:379:ASN:HA	1:B:382:ILE:CG1	2.49	0.42
3:M:75:ARG:HH12	3:M:98:ASP:CB	2.32	0.42
1:A:10:ASN:HD21	1:A:28:HIS:HE1	1.68	0.42
1:A:91:TYR:CE2	1:A:222:GLN:OE1	2.73	0.42
1:A:277:LYS:HE2	1:A:301:GLU:OE1	2.19	0.42
2:J:4:LEU:HD21	2:J:104:CYS:CB	2.50	0.42
1:A:52:LEU:HA	1:A:70:LEU:HD11	2.01	0.42
1:B:186:ASP:OD1	2:I:112(A):PHE:CE2	2.73	0.42
1:B:313:MET:HE3	1:B:377:LYS:HE2	2.00	0.42
2:I:4:LEU:HD21	2:I:104:CYS:HB2	2.01	0.42
1:A:247:LEU:HD12	1:A:247:LEU:HA	1.89	0.42
1:C:24:VAL:HG21	1:C:318:ARG:HG2	2.02	0.42
1:C:91:TYR:CE2	1:C:222:GLN:OE1	2.73	0.42
1:C:128:VAL:O	1:C:130:GLY:N	2.52	0.42
1:C:379:ASN:HA	1:C:382:ILE:CG1	2.49	0.42
2:H:4:LEU:HD21	2:H:104:CYS:HB2	2.00	0.42
2:H:111(C):VAL:O	2:H:111(C):VAL:CG2	2.67	0.42
3:L:75:ARG:HH12	3:L:98:ASP:CB	2.32	0.42
3:N:13:LEU:HD11	3:N:94:LEU:HD13	2.00	0.42
1:A:64:ASN:ND2	1:A:87:ASN:O	2.53	0.42
1:C:34:GLU:OE2	1:C:36:SER:OG	2.31	0.42
1:C:40:LYS:HA	1:C:269:ALA:HB1	2.00	0.42
2:H:30:ILE:HG13	2:H:39:TRP:CD1	2.55	0.42
1:A:112:GLU:HG3	1:A:255:ALA:HB3	2.01	0.42
1:A:128:VAL:O	1:A:130:GLY:N	2.52	0.42
1:A:219:VAL:HG11	1:A:225:ARG:CZ	2.50	0.42
1:C:95:PHE:HB3	1:C:98:TYR:HB2	2.01	0.42
2:I:56:VAL:HG23	2:I:65:THR:HA	2.02	0.42
2:J:79:SER:OG	2:J:80:VAL:N	2.53	0.42
3:M:54:ILE:HG21	3:M:78:GLY:HA3	2.01	0.42
1:A:38:ASN:OD1	1:A:39:GLY:N	2.53	0.41
1:A:166:ASN:ND2	1:A:235:PRO:HA	2.35	0.41
1:B:10:ASN:HD21	1:B:28:HIS:HE1	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ASN:OD1	1:B:39:GLY:N	2.53	0.41
1:B:64:ASN:ND2	1:B:87:ASN:O	2.53	0.41
1:C:64:ASN:ND2	1:C:87:ASN:O	2.53	0.41
1:C:476:GLU:O	1:C:479:LYS:HB2	2.19	0.41
1:C:219:VAL:HG11	1:C:225:ARG:CZ	2.50	0.41
2:J:56:VAL:HG23	2:J:65:THR:HA	2.02	0.41
3:N:71:ILE:HG23	3:N:72:PRO:HD2	2.02	0.41
1:C:116:ILE:HG12	1:C:117:PHE:CE2	2.55	0.41
1:C:187:GLN:NE2	1:C:246:ASN:OD1	2.50	0.41
1:A:148:LEU:HA	1:A:148:LEU:HD23	1.85	0.41
1:B:33:LEU:HD22	1:B:311:LEU:HD12	2.02	0.41
1:C:166:ASN:ND2	1:C:235:PRO:HA	2.35	0.41
2:H:4:LEU:HD21	2:H:104:CYS:CB	2.50	0.41
2:I:35:ASN:HA	2:I:84:LYS:HZ1	1.85	0.41
1:B:95:PHE:HB3	1:B:98:TYR:HB2	2.01	0.41
1:B:116:ILE:HG12	1:B:117:PHE:CE2	2.55	0.41
1:B:166:ASN:ND2	1:B:235:PRO:HA	2.35	0.41
1:C:247:LEU:HA	1:C:247:LEU:HD12	1.89	0.41
2:I:30:ILE:HG13	2:I:39:TRP:CD1	2.55	0.41
1:A:116:ILE:HG23	1:A:117:PHE:HD2	1.86	0.41
1:B:222:GLN:NE2	2:I:112(C):ASP:OD1	2.49	0.41
1:C:226:ILE:HG22	1:C:227:ASN:N	2.36	0.41
2:I:79:SER:OG	2:I:80:VAL:N	2.53	0.41
2:J:77:THR:N	2:J:90:LYS:HB3	2.35	0.41
1:A:24:VAL:HG21	1:A:318:ARG:HG2	2.02	0.41
1:B:91:TYR:CE2	1:B:222:GLN:OE1	2.73	0.41
1:C:180:HIS:NE2	1:C:227:ASN:ND2	2.69	0.41
2:J:30:ILE:HG12	2:J:30:ILE:O	2.21	0.41
3:M:37:THR:OG1	3:M:56:ASP:OD2	2.39	0.41
3:M:40:ALA:O	3:M:105:GLN:HB3	2.21	0.41
3:N:40:ALA:O	3:N:105:GLN:HB3	2.21	0.41
3:N:67:ARG:HH12	3:N:74:ALA:HA	1.86	0.41
1:A:343:MET:HG2	1:A:360:TYR:CD2	2.56	0.41
1:B:128:VAL:O	1:B:130:GLY:N	2.52	0.41
1:B:149:TRP:CH2	2:I:111(C):VAL:CG2	3.03	0.41
1:B:415:LEU:HA	1:B:415:LEU:HD23	1.78	0.41
2:I:40:SER:OG	2:I:105:ALA:HB3	2.21	0.41
2:J:40:SER:HA	2:J:55:TYR:CB	2.47	0.41
1:A:33:LEU:HD22	1:A:311:LEU:HD12	2.02	0.41
1:A:284:ALA:O	1:A:285:ILE:HD13	2.21	0.41
1:B:219:VAL:HG11	1:B:225:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ILE:HG22	1:B:227:ASN:N	2.36	0.41
1:B:335:PHE:HA	1:B:338:GLY:O	2.21	0.41
1:B:343:MET:HG2	1:B:360:TYR:CD2	2.56	0.41
1:B:350:TYR:HD2	1:B:479:LYS:HZ2	1.62	0.41
1:C:33:LEU:HD22	1:C:311:LEU:HD12	2.02	0.41
1:C:148:LEU:HD23	1:C:148:LEU:HA	1.84	0.41
1:C:192:HIS:O	1:C:193:THR:OG1	2.37	0.41
1:C:205:TYR:CD1	1:C:206:SER:N	2.89	0.41
1:C:284:ALA:O	1:C:285:ILE:HD13	2.21	0.41
2:H:30:ILE:O	2:H:30:ILE:HG12	2.21	0.41
3:L:40:ALA:O	3:L:105:GLN:HB3	2.21	0.41
3:N:67:ARG:HE	3:N:67:ARG:HB2	1.72	0.41
1:A:116:ILE:HG12	1:A:117:PHE:CE2	2.55	0.41
1:C:38:ASN:OD1	1:C:39:GLY:N	2.53	0.41
1:C:290:PRO:HG2	1:C:291:PHE:CD2	2.55	0.41
2:I:41:TRP:CZ2	2:I:89:LEU:HB2	2.56	0.41
2:I:77:THR:N	2:I:90:LYS:HB3	2.35	0.41
1:A:428:LEU:HD21	1:C:428:LEU:HD13	2.04	0.40
1:B:24:VAL:HG21	1:B:318:ARG:HG2	2.02	0.40
1:B:205:TYR:CD1	1:B:206:SER:N	2.89	0.40
1:C:350:TYR:HD2	1:C:479:LYS:HZ2	1.64	0.40
2:H:41:TRP:CZ2	2:H:89:LEU:HB2	2.56	0.40
2:I:4:LEU:HD21	2:I:104:CYS:CB	2.50	0.40
2:I:30:ILE:O	2:I:30:ILE:HG12	2.21	0.40
2:I:91:LEU:HD12	2:I:91:LEU:HA	1.88	0.40
1:B:27:THR:HG23	1:B:317:LEU:O	2.21	0.40
2:H:49:GLY:C	2:H:50:LEU:HD12	2.42	0.40
2:H:77:THR:N	2:H:90:LYS:HB3	2.35	0.40
2:H:79:SER:OG	2:H:80:VAL:N	2.53	0.40
2:J:40:SER:OG	2:J:105:ALA:HB3	2.21	0.40
2:J:41:TRP:CZ2	2:J:89:LEU:HB2	2.56	0.40
2:J:49:GLY:C	2:J:50:LEU:HD12	2.42	0.40
1:A:6:GLY:HA3	1:A:340:TRP:CE2	2.56	0.40
1:B:25:THR:HG21	1:B:319:ASN:HD22	1.87	0.40
1:B:101:LEU:O	1:B:104:GLN:HB2	2.21	0.40
1:B:116:ILE:HG23	1:B:117:PHE:HD2	1.86	0.40
1:B:148:LEU:HG	1:B:251:ARG:HB2	2.04	0.40
1:B:251:ARG:HD2	1:B:252:TYR:CD1	2.57	0.40
1:B:401:ARG:O	1:B:404:GLU:N	2.55	0.40
1:C:251:ARG:HD2	1:C:252:TYR:CD1	2.57	0.40
1:C:343:MET:HG2	1:C:360:TYR:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:56:VAL:HG23	2:H:65:THR:HA	2.02	0.40
3:L:105:GLN:HE21	3:L:116:LEU:CD1	2.35	0.40
3:M:71:ILE:HG23	3:M:72:PRO:HD2	2.02	0.40
1:A:25:THR:HG21	1:A:319:ASN:HD22	1.87	0.40
1:A:116:ILE:HG12	1:A:117:PHE:CD2	2.57	0.40
1:A:401:ARG:O	1:A:404:GLU:N	2.55	0.40
1:B:377:LYS:O	1:B:380:SER:OG	2.35	0.40
1:C:27:THR:HG23	1:C:317:LEU:O	2.22	0.40
1:C:101:LEU:O	1:C:104:GLN:HB2	2.21	0.40
1:C:256:LEU:HD12	1:C:256:LEU:HA	1.90	0.40
2:J:112(B):SER:O	2:J:112(B):SER:OG	2.39	0.40
3:N:101:VAL:HG12	3:N:103:TYR:CE2	2.57	0.40
1:A:148:LEU:HG	1:A:251:ARG:HB2	2.04	0.40
1:A:176:TRP:CZ2	1:A:200:VAL:HG21	2.57	0.40
1:A:226:ILE:HG22	1:A:227:ASN:N	2.36	0.40
1:A:248:ILE:HG23	1:A:248:ILE:HD12	1.84	0.40
1:C:148:LEU:HG	1:C:251:ARG:HB2	2.04	0.40
2:H:40:SER:OG	2:H:105:ALA:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	478/555 (86%)	426 (89%)	52 (11%)	0	100	100
1	B	478/555 (86%)	425 (89%)	53 (11%)	0	100	100
1	C	478/555 (86%)	427 (89%)	51 (11%)	0	100	100
2	H	121/125 (97%)	102 (84%)	19 (16%)	0	100	100
2	I	121/125 (97%)	102 (84%)	19 (16%)	0	100	100
2	J	121/125 (97%)	102 (84%)	19 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	107/109 (98%)	85 (79%)	22 (21%)	0	100	100
3	M	107/109 (98%)	85 (79%)	22 (21%)	0	100	100
3	N	107/109 (98%)	85 (79%)	22 (21%)	0	100	100
All	All	2118/2367 (90%)	1839 (87%)	279 (13%)	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	410/480 (85%)	409 (100%)	1 (0%)	93	98
1	B	410/480 (85%)	409 (100%)	1 (0%)	93	98
1	C	410/480 (85%)	409 (100%)	1 (0%)	93	98
2	H	95/111 (86%)	95 (100%)	0	100	100
2	I	95/111 (86%)	95 (100%)	0	100	100
2	J	95/111 (86%)	95 (100%)	0	100	100
3	L	78/90 (87%)	78 (100%)	0	100	100
3	M	78/90 (87%)	78 (100%)	0	100	100
3	N	78/90 (87%)	78 (100%)	0	100	100
All	All	1749/2043 (86%)	1746 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	GLN
1	B	368	GLN
1	C	368	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	187	GLN
1	A	246	ASN
1	A	353	GLN
1	A	443	ASN
1	A	455	ASN
1	A	480	ASN
1	B	10	ASN
1	B	187	GLN
1	B	246	ASN
1	B	443	ASN
1	B	455	ASN
1	B	480	ASN
1	C	10	ASN
1	C	187	GLN
1	C	246	ASN
1	C	443	ASN
1	C	455	ASN
1	C	480	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 monosaccharides 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

There are no chain breaks in this entry.

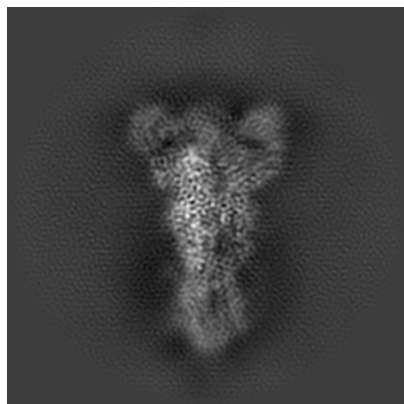
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43008. These allow visual inspection of the internal detail of the map and identification of artifacts.

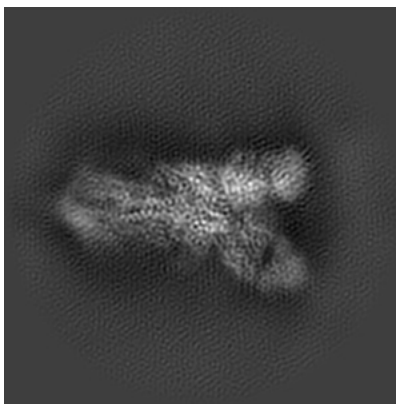
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

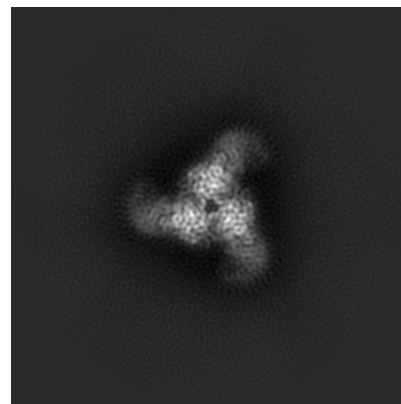
6.1.1 Primary map



X

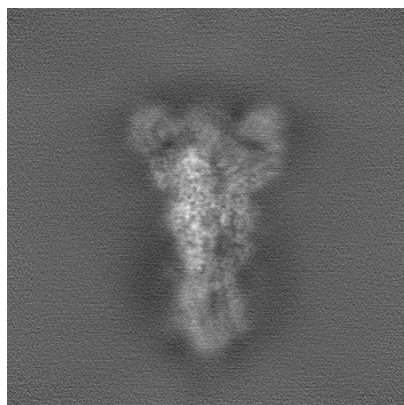


Y

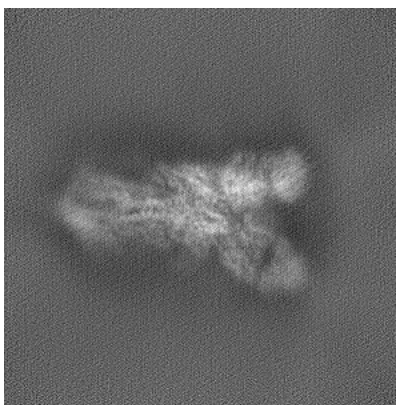


Z

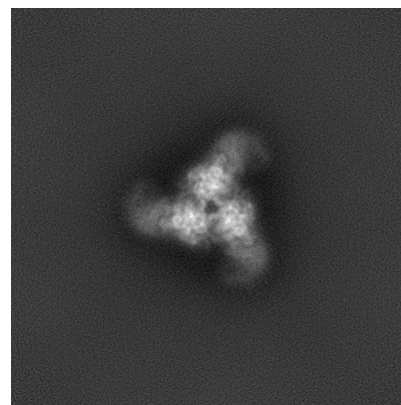
6.1.2 Raw map



X



Y

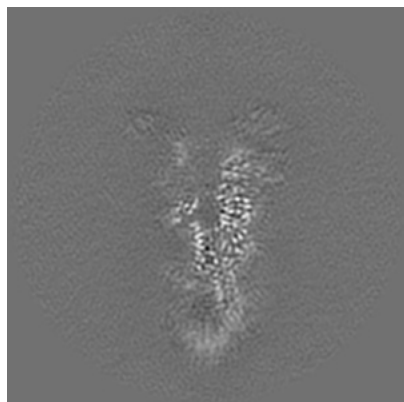


Z

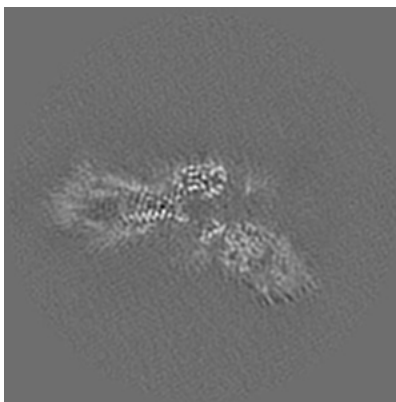
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

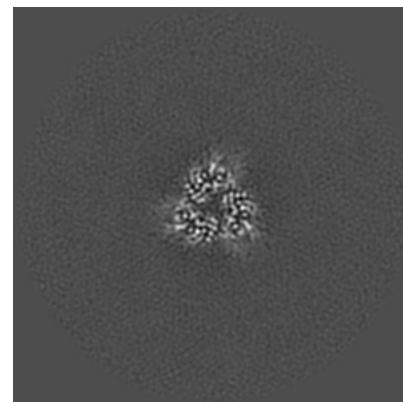
6.2.1 Primary map



X Index: 300

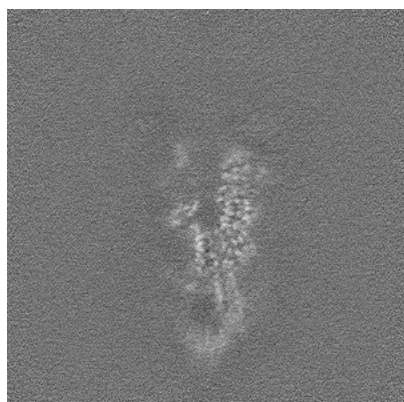


Y Index: 300

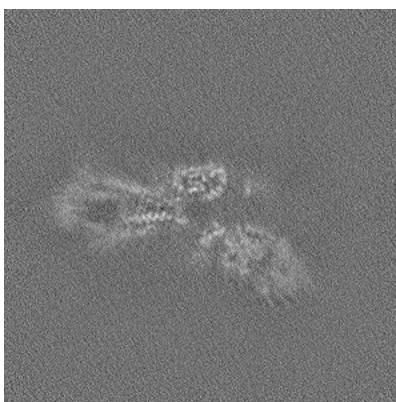


Z Index: 300

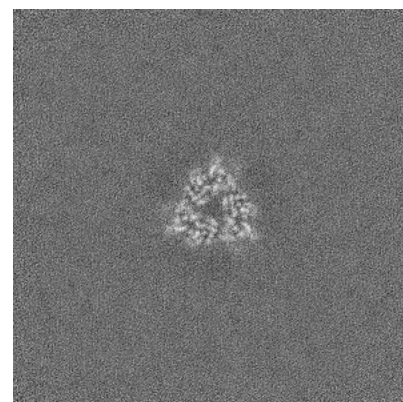
6.2.2 Raw map



X Index: 300



Y Index: 300

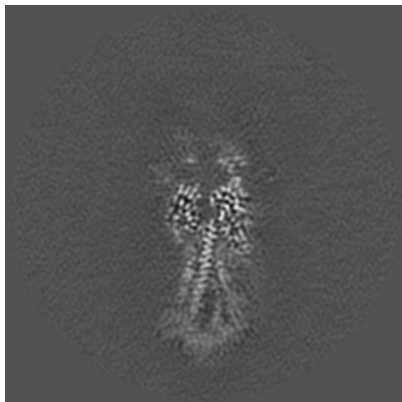


Z Index: 300

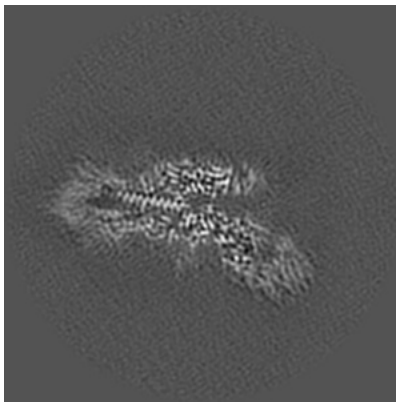
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

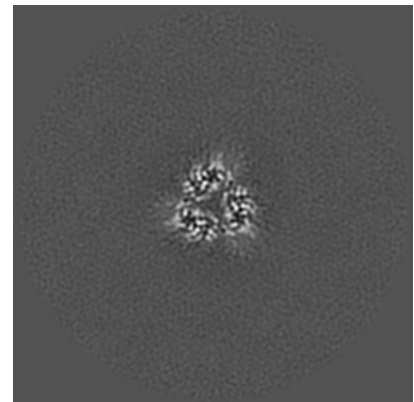
6.3.1 Primary map



X Index: 287

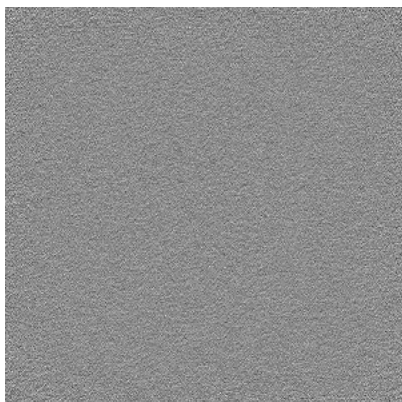


Y Index: 286

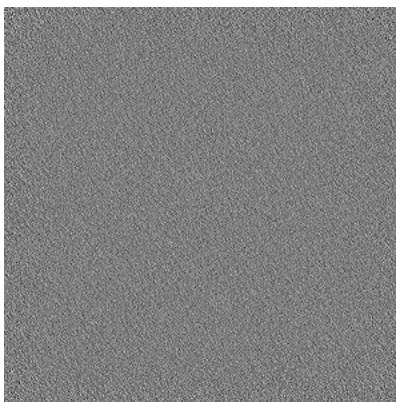


Z Index: 298

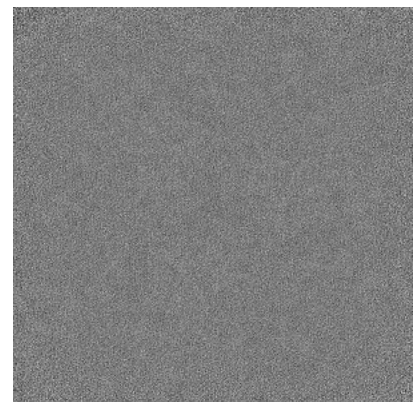
6.3.2 Raw map



X Index: 0



Y Index: 0

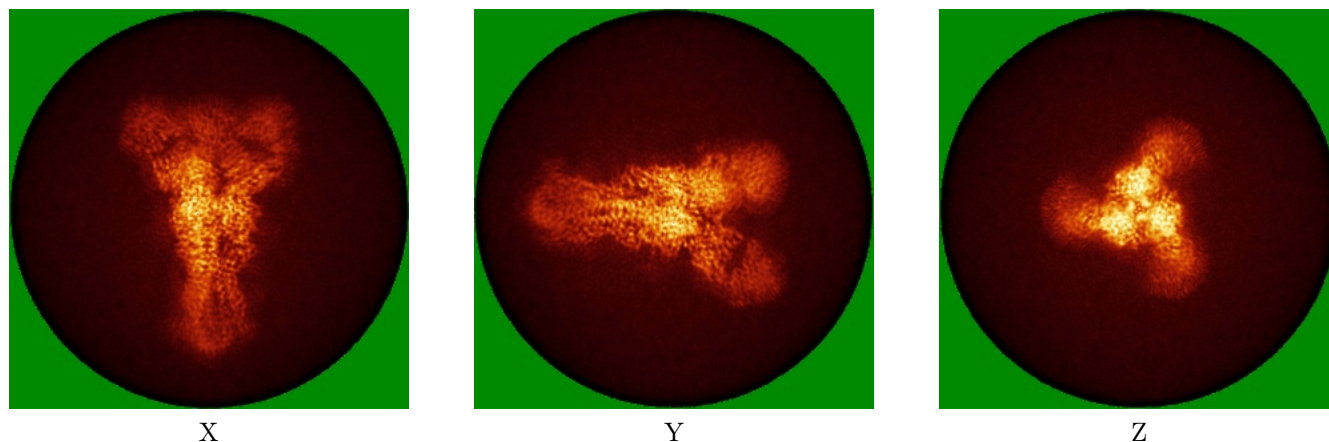


Z Index: 599

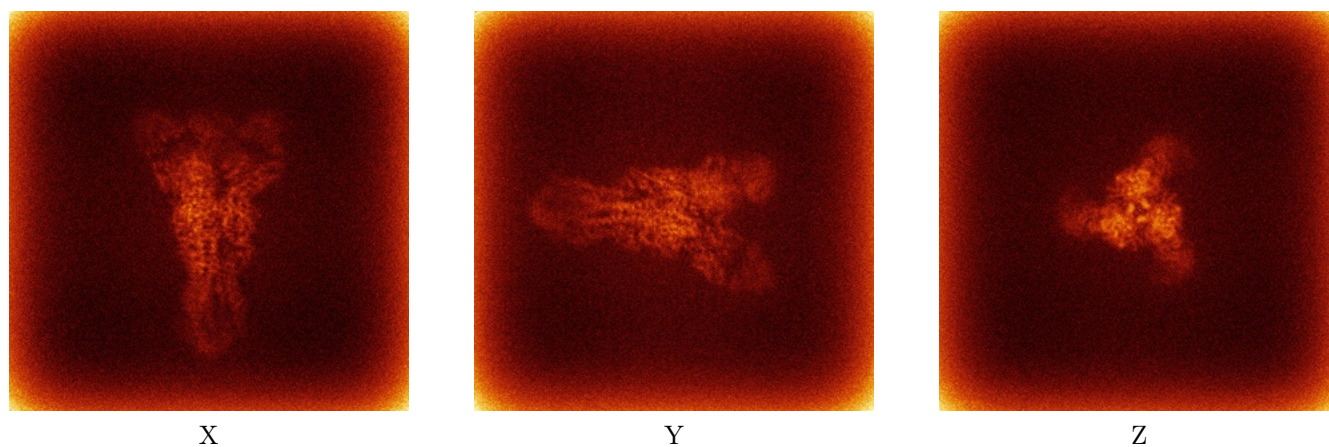
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



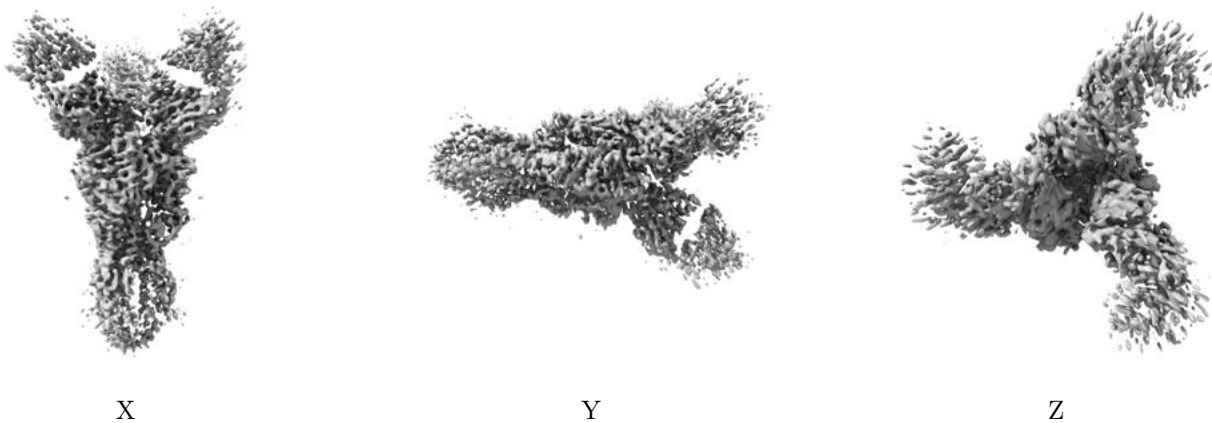
6.4.2 Raw map



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.

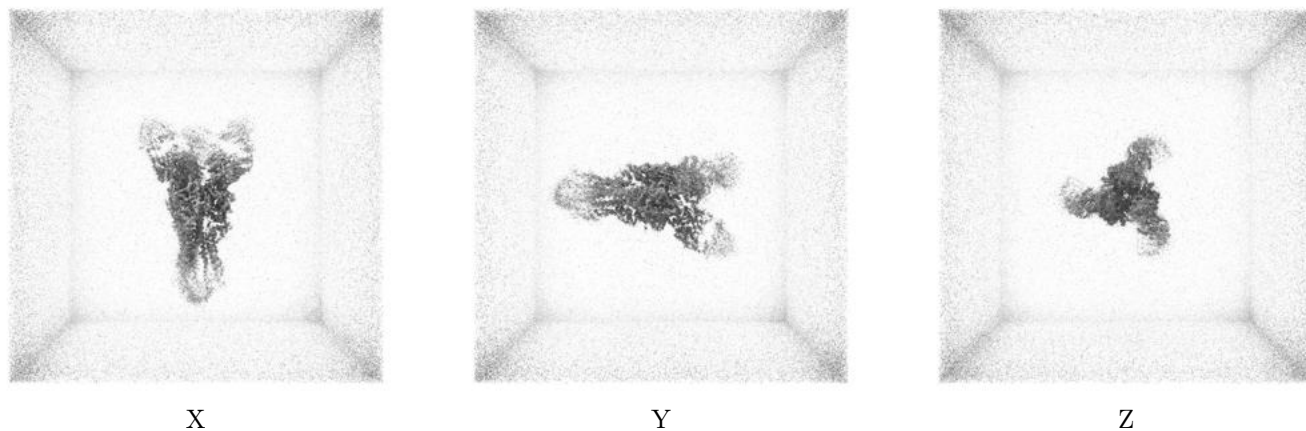
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

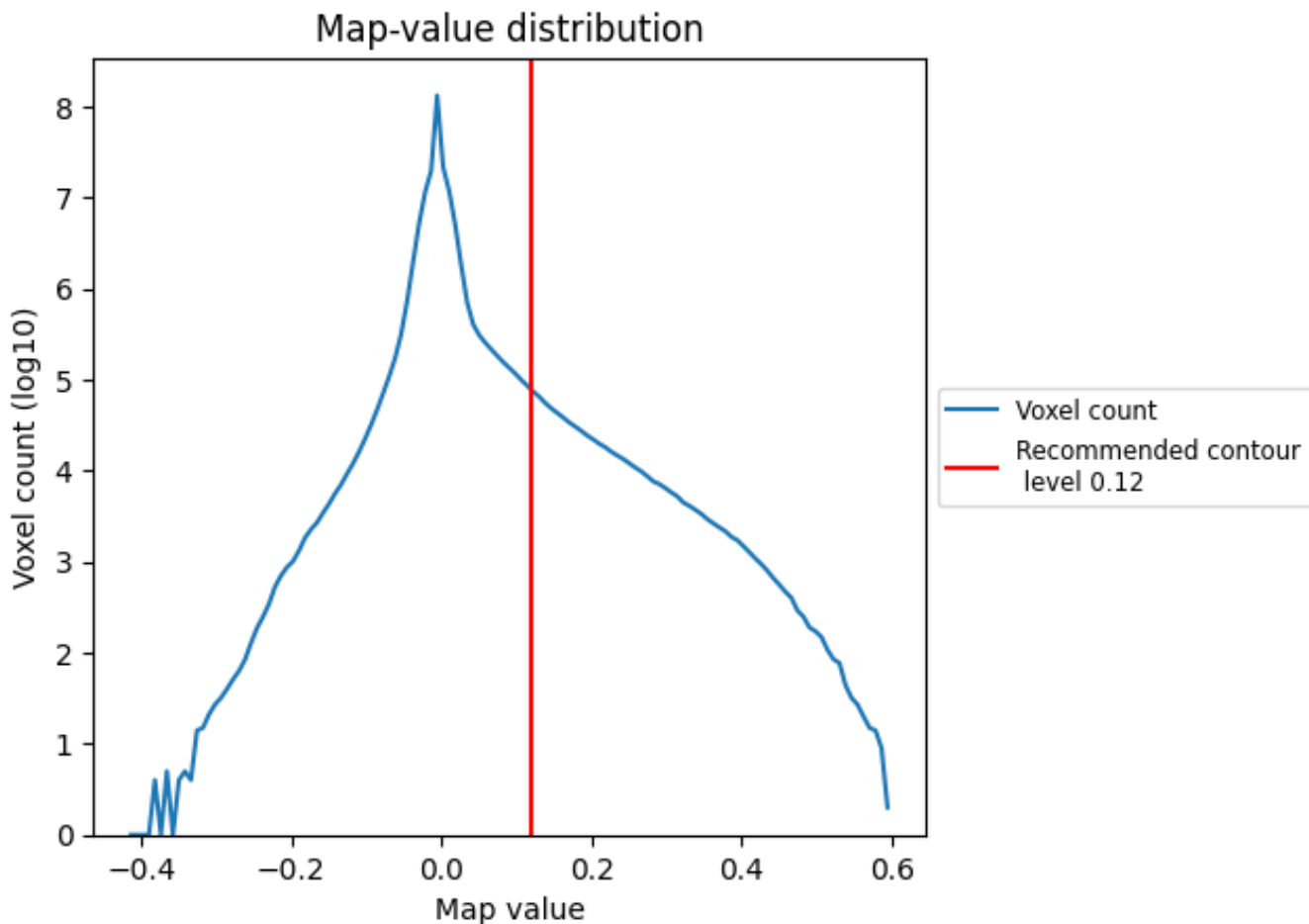
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

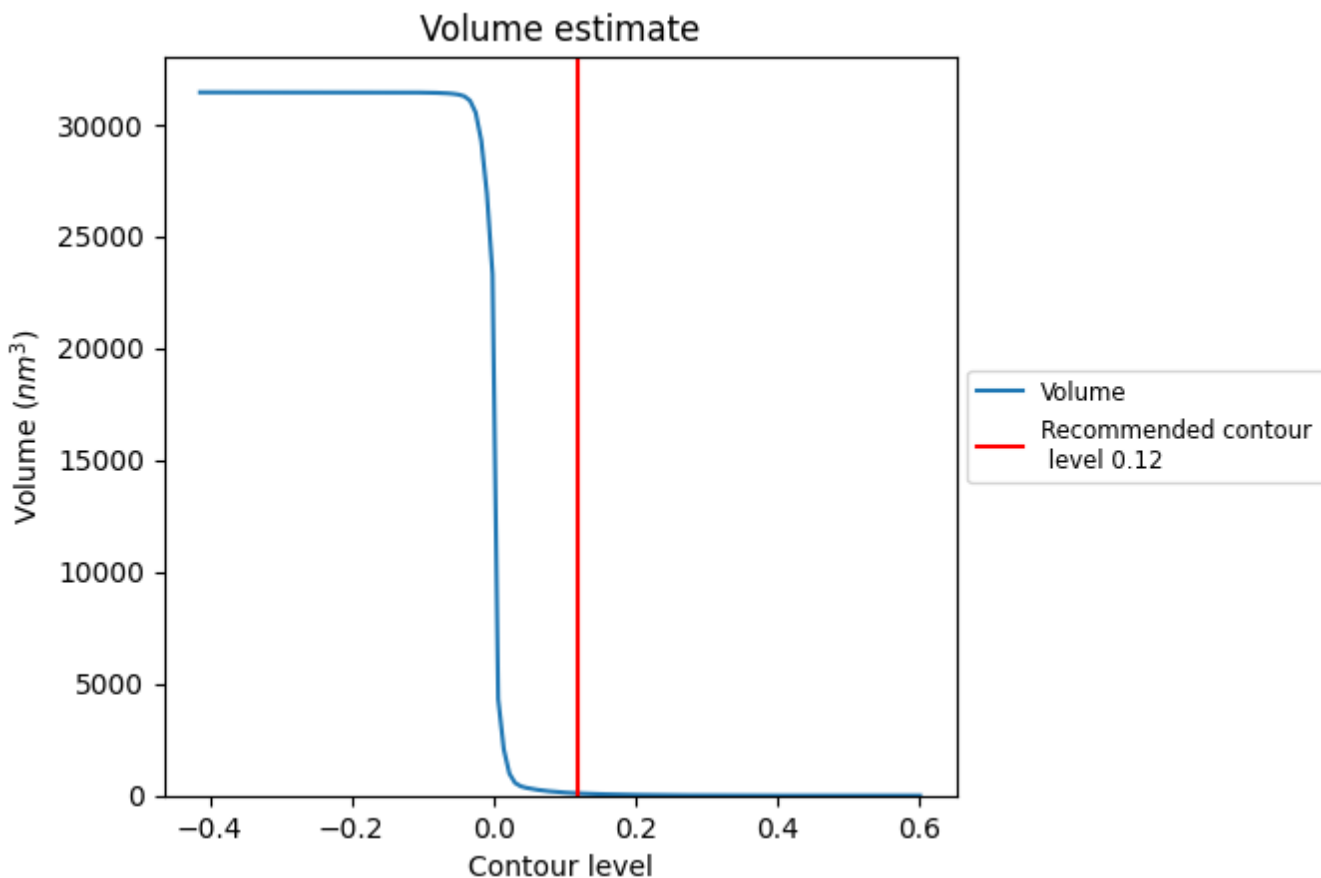
This section contains the results of statistical analysis of the map.

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.

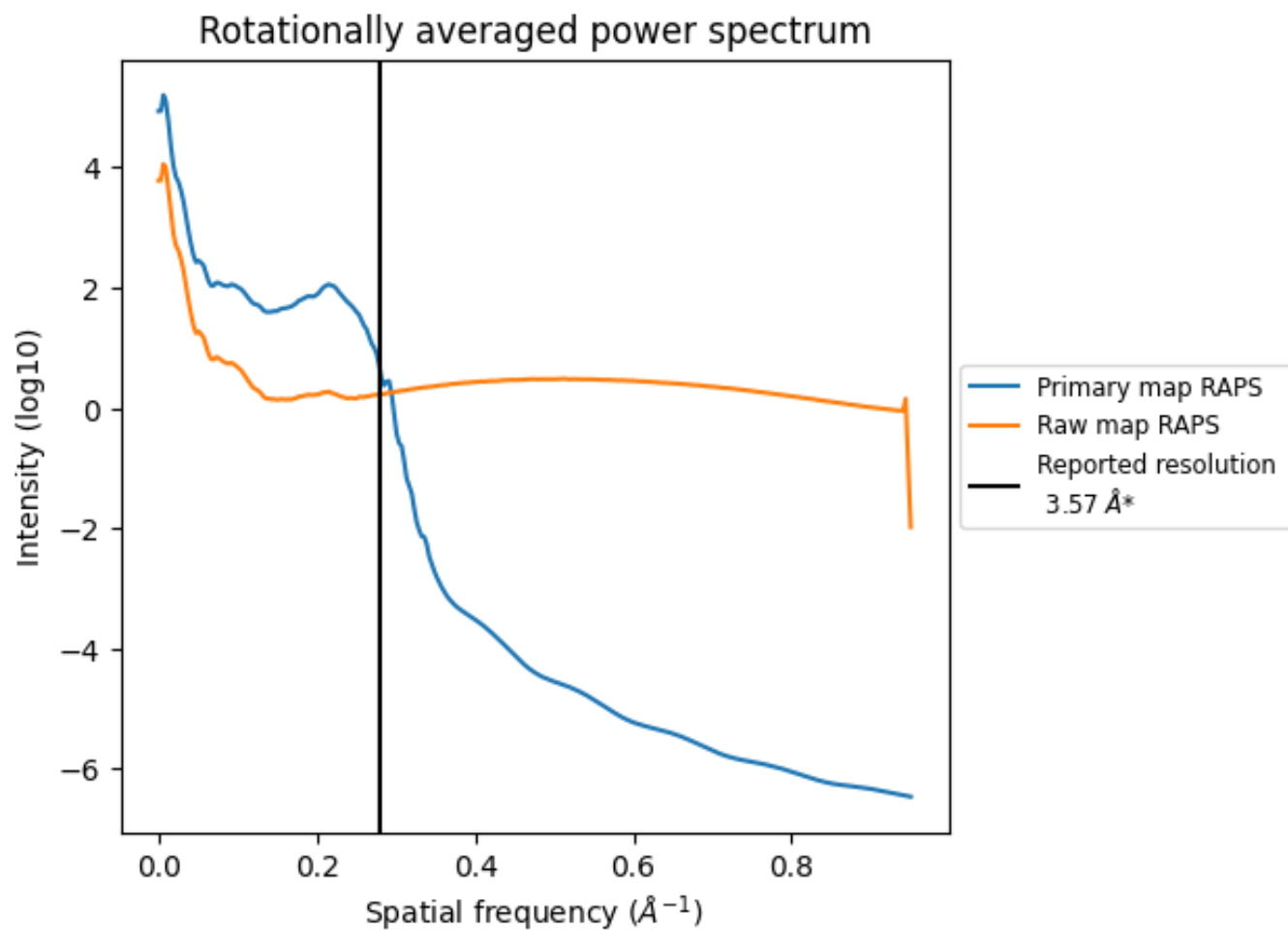
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 99 nm³; this corresponds to an approximate mass of 89 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 [i](#)

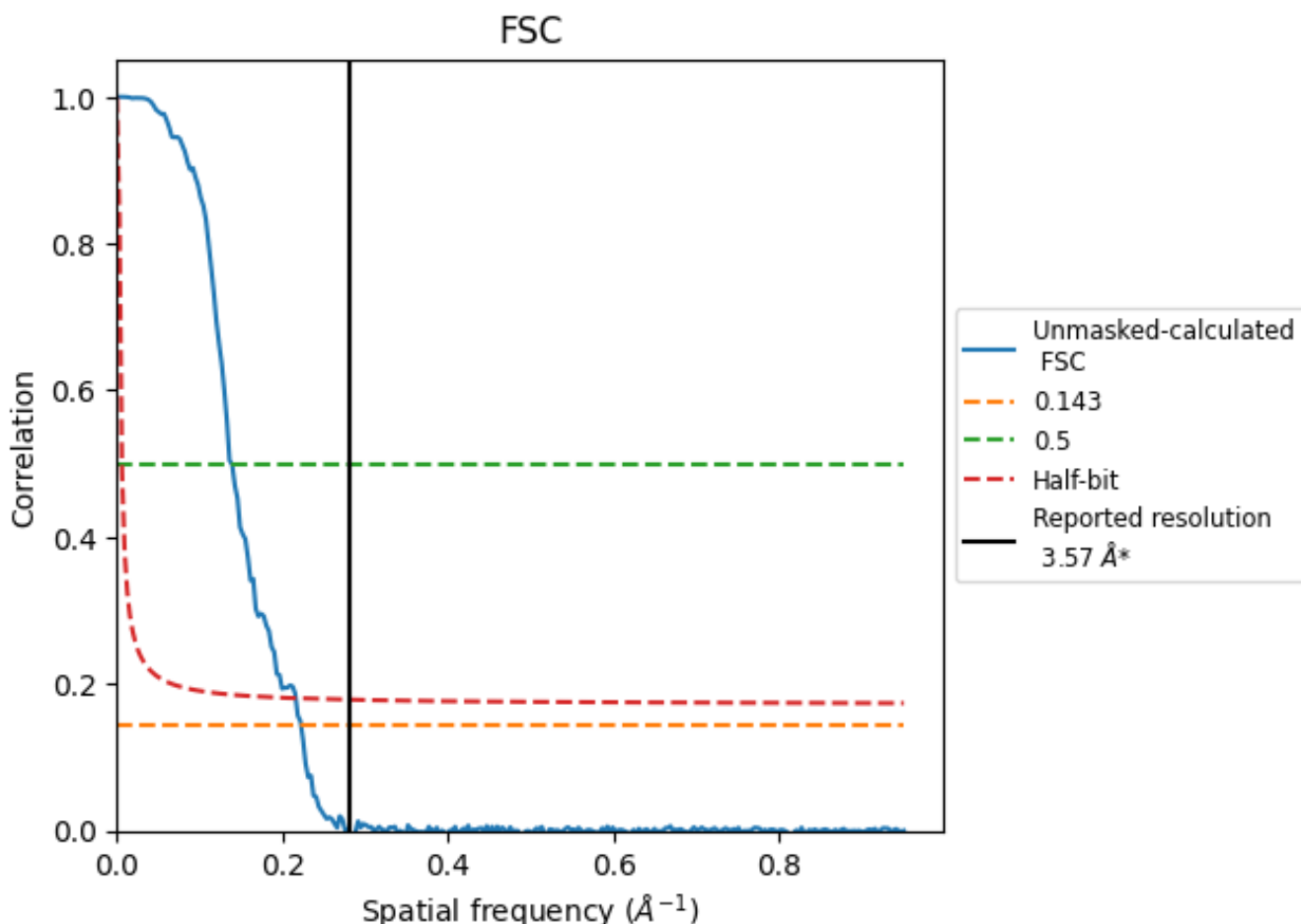


*Reported resolution corresponds to spatial frequency of 0.280 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.280 Å⁻¹

8.2 Resolution estimates [i](#)

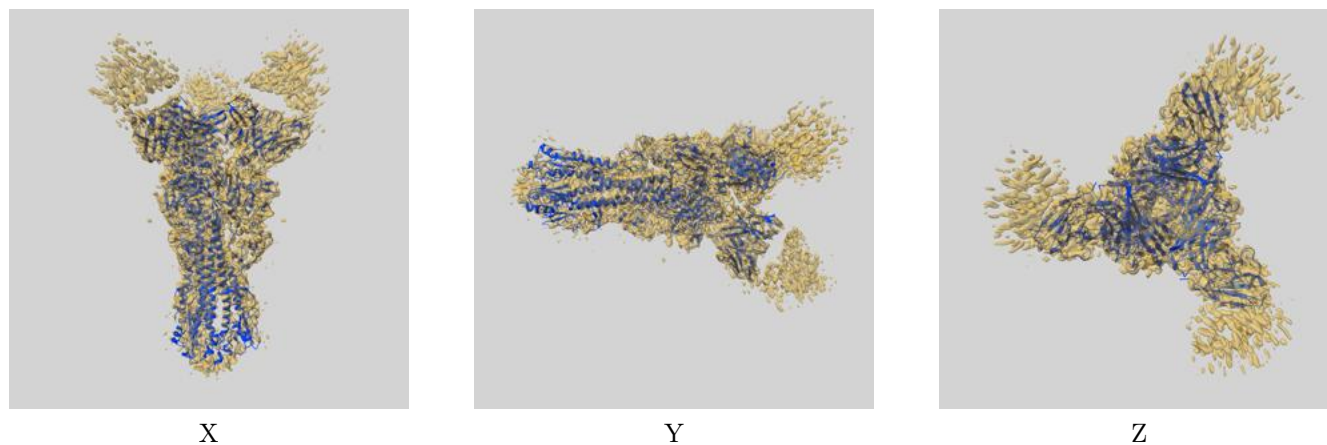
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.57	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.49	7.22	4.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.49 differs from the reported value 3.57 by more than 10 %

9 Map-model fit [i](#)

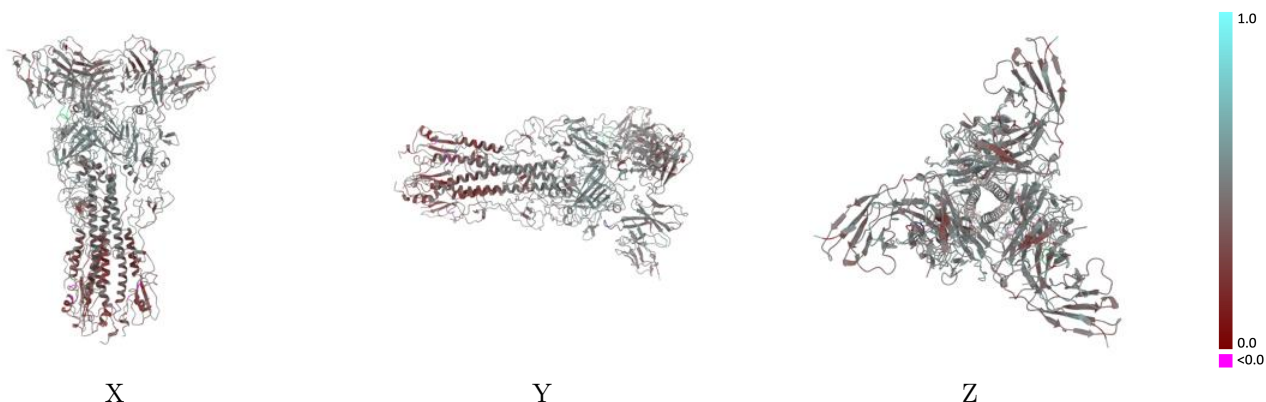
This section contains information regarding the fit between EMDB map EMD-43008 and PDB model 8V7O. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



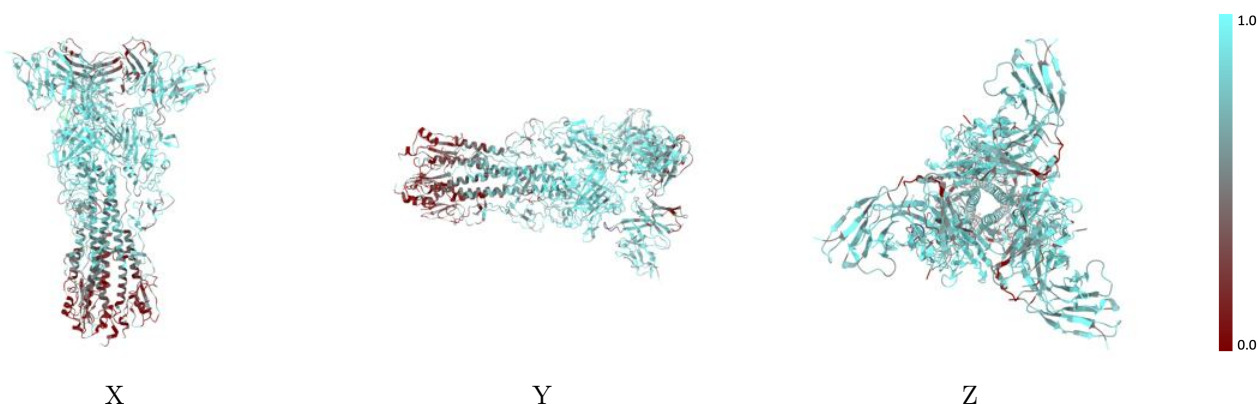
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



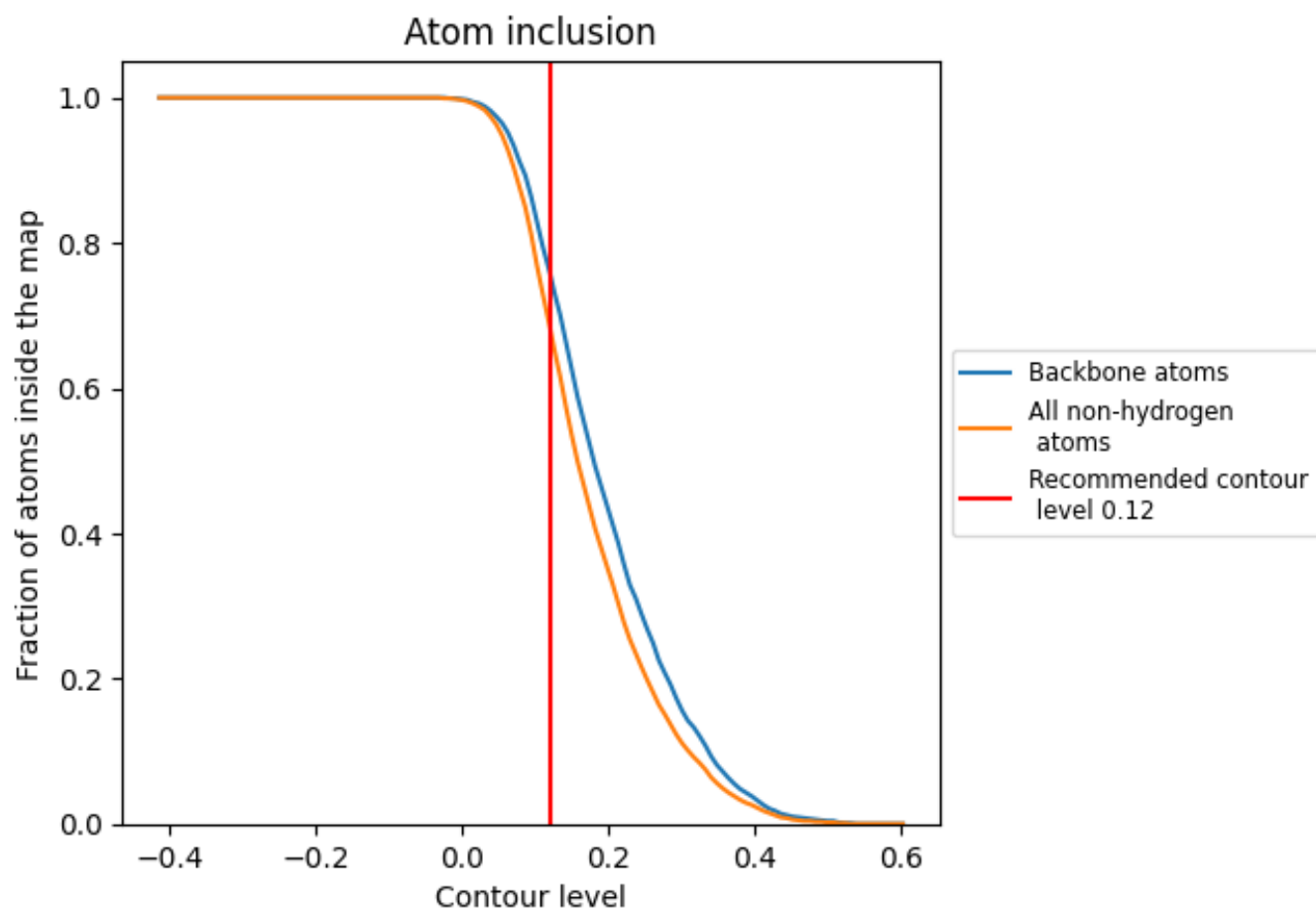
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6830	 0.4530
A	 0.6680	 0.4520
B	 0.6680	 0.4510
C	 0.6690	 0.4530
H	 0.6800	 0.4590
I	 0.6830	 0.4580
J	 0.6730	 0.4610
L	 0.7610	 0.4490
M	 0.7590	 0.4510
N	 0.7590	 0.4520

