



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 06:07 PM UTC

PDB ID : 7UHZ / pdb_00007uhz
EMDB ID : EMD-26520
Title : Post-fusion ectodomain of HSV-1 gB in complex with BMPC-23 Fab
Authors : Windsor, I.W.; Kong, S.L.; Garforth, S.J.; Almo, S.C.; Harrison, S.C.
Deposited on : 2022-03-28
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

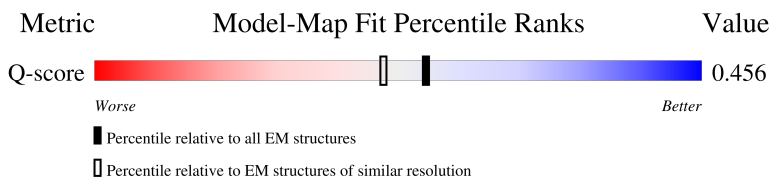
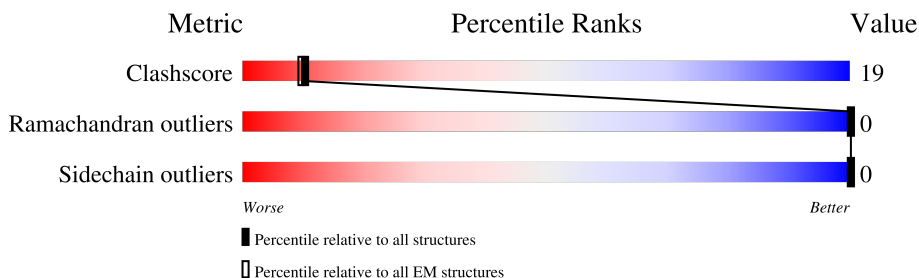
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	H	121	17% 57% 42% .
1	I	121	15% 54% 45% .
1	J	121	17% 55% 44% .
2	L	112	22% 56% 43% .

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Mol	Chain	Length	Quality of chain
2	M	112	21% 55% 44%
2	N	112	22% 55% 44%
3	A	628	7% 55% 37% 8%
3	B	628	8% 58% 34% 8%
3	C	628	8% 56% 35% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19299 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 BMPC-23 Fab Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	120	Total	C	N	O	S	0	0
			940	593	153	190	4		
1	I	120	Total	C	N	O	S	0	0
			940	593	153	190	4		
1	J	120	Total	C	N	O	S	0	0
			940	593	153	190	4		

- Molecule 2 is a protein called BMPC-23 Fab Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	111	Total	C	N	O	S	0	0
			835	526	139	165	5		
2	M	111	Total	C	N	O	S	0	0
			835	526	139	165	5		
2	N	111	Total	C	N	O	S	0	0
			835	526	139	165	5		

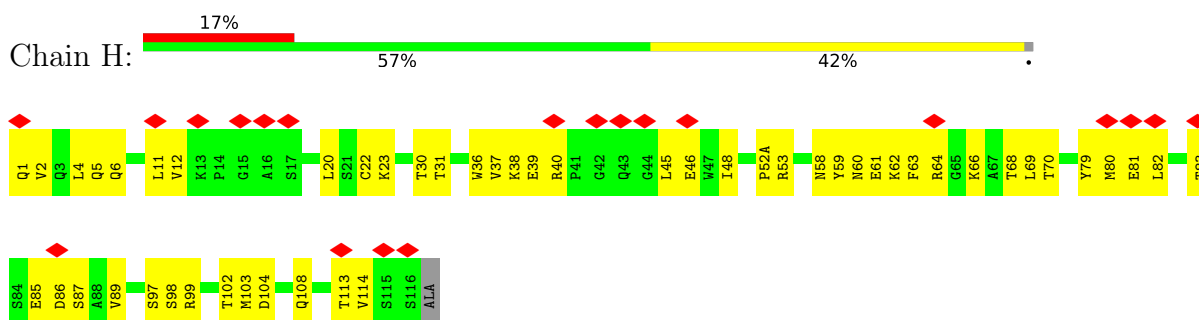
- Molecule 3 is a protein called Envelope glycoprotein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	576	Total	C	N	O	S	0	0
			4658	2941	819	876	22		
3	B	576	Total	C	N	O	S	0	0
			4658	2941	819	876	22		
3	C	576	Total	C	N	O	S	0	0
			4658	2941	819	876	22		

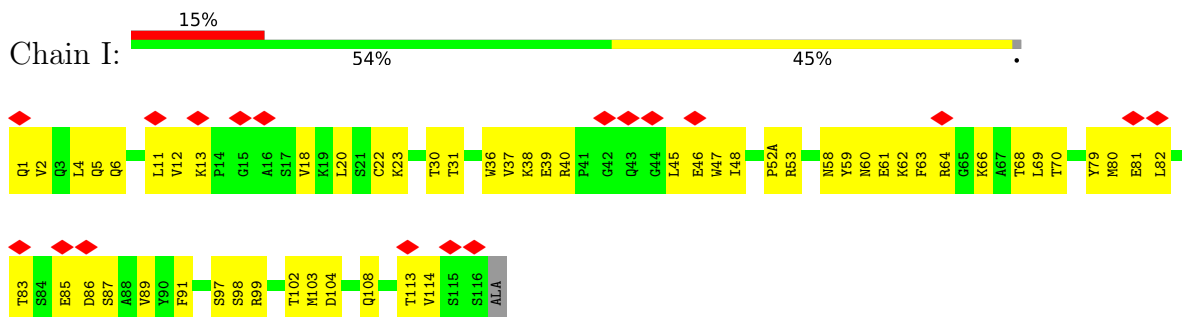
3 Residue-property plots [i](#)

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.

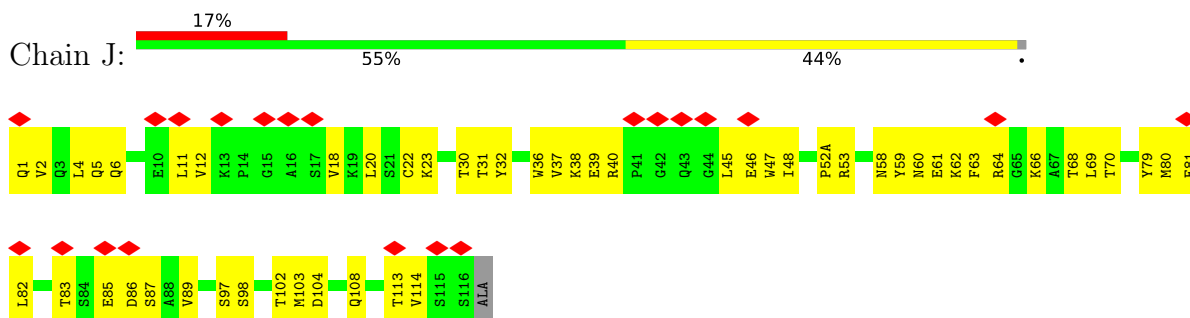
- Molecule 1: BMPC-23 Fab Heavy chain



- Molecule 1: BMPC-23 Fab Heavy chain

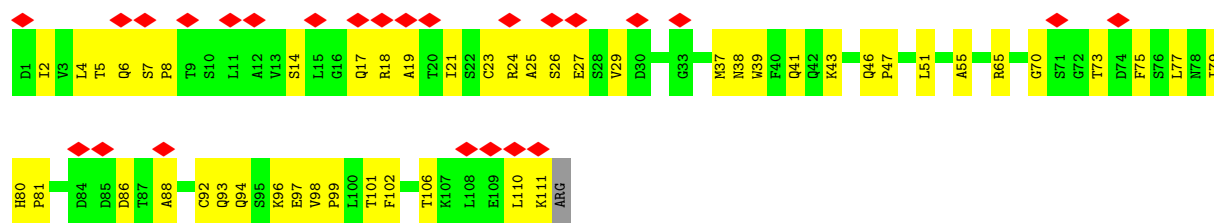


- Molecule 1: BMPC-23 Fab Heavy chain

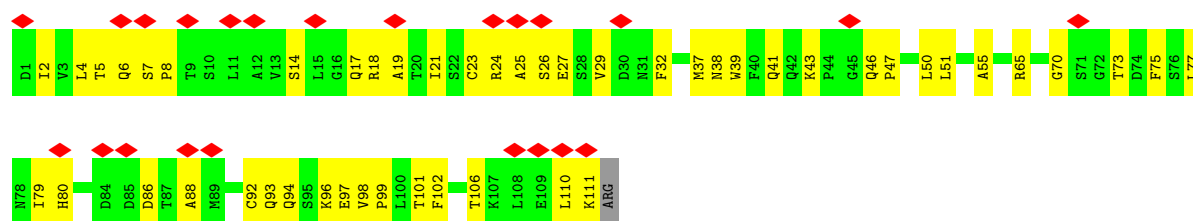


- Molecule 2: BMPC-23 Fab Light chain

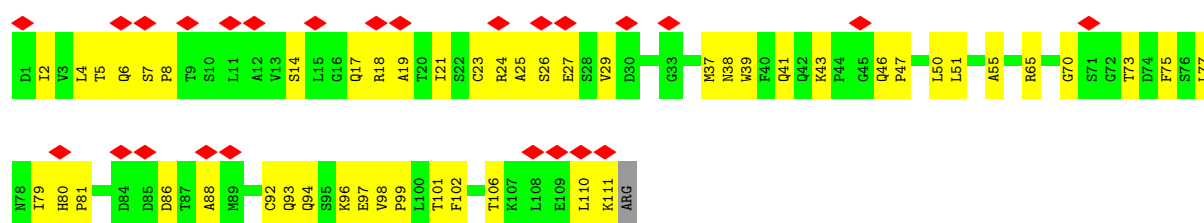




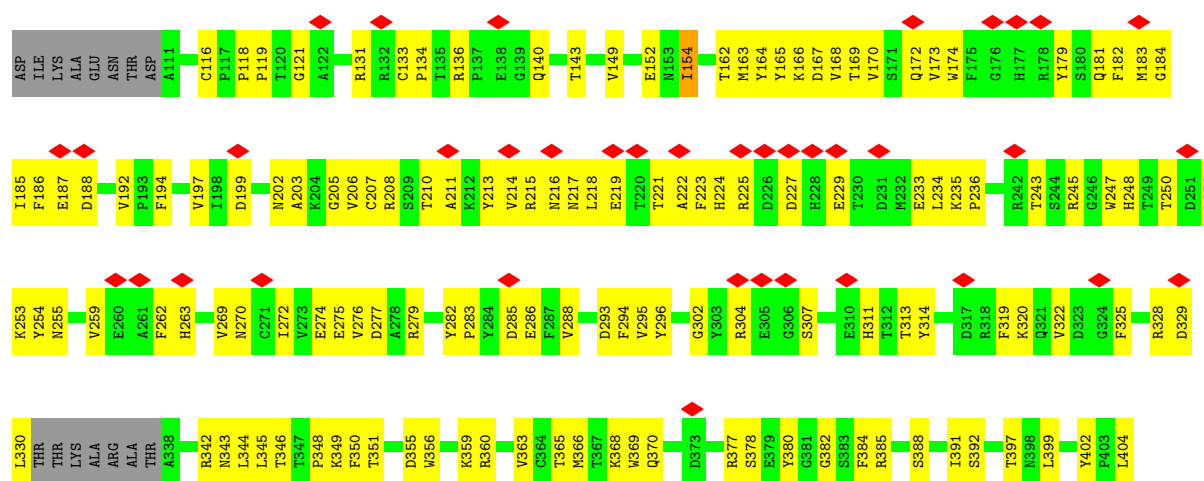
• Molecule 2: BMPC-23 Fab Light chain



• Molecule 2: BMPC-23 Fab Light chain



• Molecule 3: Envelope glycoprotein B



ASP	V192	N255	L330	D408	ALA	P600	E704
ILE	P193	P256	THR	D411	ASN	R605	V705
LYS	F194	S257	THR	C412	ALA		Q706
ALA		R258	LYS	I413	SER		R707
GLU	V197	V259	ALA	I414	V492	G609	Q710
ASN	I198	E260	ARG	G414	E493	G610	L711
THR	D199	A261	ALA	K415	R494	P611	H712
ASP		F262	THR	D416		L612	D713
A111	N202	H263	A338	A417	I501	V613	
C116	A203	R264	P339		E502	E614	D718
	A204	Y265	R342	M421	F503	G618	
A122	G205		N343	D422	A504	E619	L719
T123	V206	V269	L344		R505	N620	D720
T124	C207	N270	L345	Y429	L506	N621	T721
V125	R208	C371	T346	N430	Q507	E622	V722
Q126	S209	I272	T347	A431		L623	L725
	T210		F348	T432	Y510	R624	H724
R132	A211	E275	F349	H433	N511		A725
C133	K212	V276	F350	I434	H512	R627	ASP
P134	Y213	D277	T351	K435	I513	D628	ALA
T135	V214	A278	D355	Y441	O514	T634	ASN
R136	R215	R279	W356	Y442	H515	V635	ALA
P137	N216	S280	K359	Q443	H516		
E138	N217	Y281	R360	A444	D519	R638	
Q139	L218	Y282		L449	G522	R639	
Q140	E219	P283	V363	I450	W528	G644	
	T220	Y284	C364	A451	C529	F650	
T143	T221	D285	T367	Y452	E530	Y653	
V149	A222	V288	K368	T459	L531		
I154	F223	F294		LEU	H534	R661	
T162	H224	V295	R377	ALA	E535		
M163	R225	Y296	S378	GLU	L536	F670	
Y164	D226		E379	LEU	T537	L673	
Y165	D227	R304	Y380	TYR	L538	N674	
K166	H228	E305	G381	VAL	W539	L675	
D167	E229	G306	G382	GLU	T554	T676	
V168	T230	S307	S383	HIS	V555	R677	
T169	D231		F384	LEU	R558	L678	
V170	M232	H311	R385	ARG	V559	H681	
S171	E233	T312		GLN	S560	E682	
Q172	L234	Y313	S388	SER			
V173	K235	Y314	I391	ARG	T572	L686	
	P236	A315	S392	LYS		E687	
G176	A237	A316	T397	PRO	M587	V688	
H177	N238	D317	N398	ASN	T583	Y689	
A178	A239	R318	L399	PRO	S590		
Y179	T241	F319		THR	S591	D696	
	R242	Q321	Y402	PRO	R592		
F182		V322	P403	PRO	P593	L699	
M183	R245	D323	L404	PRO		L700	
G184	G246	G324	GLY	ALA	Y597	D701	
I185	V247	F325	R406		S598	T703	
F186	H248	Y326	V407	SER	R599		
E187	T249	R328					
D188	T250	D329					
	D251						
	L252						
	K253						
	Y254						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	218056	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.8	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.040	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	369.6, 369.6, 369.6	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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	H	0.18	0/965	0.45	0/1311
1	I	0.19	0/965	0.45	0/1311
1	J	0.19	0/965	0.45	0/1311
2	L	0.21	0/853	0.52	0/1155
2	M	0.21	0/853	0.52	0/1155
2	N	0.21	0/853	0.52	0/1155
3	A	0.26	0/4775	0.47	3/6488 (0.0%)
3	B	0.26	0/4775	0.47	3/6488 (0.0%)
3	C	0.26	0/4775	0.47	3/6488 (0.0%)
All	All	0.24	0/19779	0.47	9/26862 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	154	ILE	N-CA-C	-5.34	107.77	112.90
3	A	154	ILE	N-CA-C	-5.33	107.78	112.90
3	C	154	ILE	N-CA-C	-5.28	107.83	112.90
3	A	705	VAL	CA-C-N	-5.25	112.29	122.06
3	A	705	VAL	C-N-CA	-5.25	112.29	122.06
3	B	705	VAL	CA-C-N	-5.22	112.34	122.06
3	B	705	VAL	C-N-CA	-5.22	112.34	122.06
3	C	705	VAL	CA-C-N	-5.21	112.36	122.06
3	C	705	VAL	C-N-CA	-5.21	112.36	122.06

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	H	940	0	884	33	0
1	I	940	0	884	40	0
1	J	940	0	884	41	0
2	L	835	0	815	39	0
2	M	835	0	815	43	0
2	N	835	0	815	44	0
3	A	4658	0	4467	223	0
3	B	4658	0	4467	190	0
3	C	4658	0	4467	207	0
All	All	19299	0	18498	722	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 (722) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:97:GLU:HG3	2:N:99:PRO:HD2	1.52	0.92
2:M:97:GLU:HG3	2:M:99:PRO:HD2	1.52	0.92
1:H:58:ASN:ND2	3:A:590:SER:O	2.03	0.91
3:A:179:TYR:HE2	3:C:221:THR:H	1.17	0.91
2:L:97:GLU:HG3	2:L:99:PRO:HD2	1.52	0.90
3:A:179:TYR:CD2	3:C:221:THR:HG22	2.08	0.89
2:L:18:ARG:HE	2:L:80:HIS:HB2	1.40	0.86
2:M:18:ARG:HE	2:M:80:HIS:HB2	1.40	0.85
3:B:116:CYS:HB3	3:B:560:SER:HB2	1.59	0.84
2:N:18:ARG:HE	2:N:80:HIS:HB2	1.40	0.84
3:C:116:CYS:HB3	3:C:560:SER:HB2	1.59	0.84
3:A:296:TYR:CZ	3:C:711:LEU:HD22	2.12	0.84
3:C:253:LYS:NZ	3:C:255:ASN:OD1	2.11	0.84
3:A:253:LYS:NZ	3:A:255:ASN:OD1	2.11	0.83
3:B:253:LYS:NZ	3:B:255:ASN:OD1	2.11	0.82
1:I:5:GLN:HB2	1:I:23:LYS:HB3	1.60	0.82
1:J:5:GLN:HB2	1:J:23:LYS:HB3	1.60	0.82
1:H:5:GLN:HB2	1:H:23:LYS:HB3	1.60	0.81
3:A:116:CYS:HB3	3:A:560:SER:HB2	1.59	0.81
3:B:224:HIS:HB2	3:B:269:VAL:HB	1.62	0.81
3:A:678:LEU:HB2	3:C:516:HIS:CE1	2.16	0.80
3:A:224:HIS:HB2	3:A:269:VAL:HB	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:417:ALA:HB1	3:C:421:MET:HE1	1.63	0.80
3:B:417:ALA:HB1	3:B:421:MET:HE1	1.63	0.80
3:C:224:HIS:HB2	3:C:269:VAL:HB	1.62	0.79
3:A:417:ALA:HB1	3:A:421:MET:HE1	1.63	0.78
3:A:179:TYR:HE2	3:C:221:THR:N	1.81	0.78
3:A:703:THR:HG22	3:C:699:LEU:HB2	1.66	0.77
3:A:707:ARG:HH22	3:C:241:THR:HG23	1.49	0.76
3:B:166:LYS:NZ	3:B:210:THR:O	2.19	0.75
2:M:29:VAL:HA	2:M:96:LYS:HD2	1.69	0.74
3:A:520:MET:HE1	3:B:676:THR:HG22	1.69	0.74
2:L:29:VAL:HA	2:L:96:LYS:HD2	1.69	0.74
3:C:166:LYS:NZ	3:C:210:THR:O	2.19	0.74
2:N:29:VAL:HA	2:N:96:LYS:HD2	1.69	0.73
3:A:179:TYR:CE2	3:C:221:THR:HG22	2.23	0.72
3:B:342:ARG:NH1	3:B:355:ASP:OD1	2.22	0.72
3:A:707:ARG:HD2	3:C:242:ARG:HH12	1.54	0.72
1:H:40:ARG:NH1	1:H:85:GLU:O	2.23	0.72
1:J:40:ARG:NH1	1:J:85:GLU:O	2.23	0.72
3:A:166:LYS:NZ	3:A:210:THR:O	2.19	0.72
3:B:722:VAL:HG22	3:C:214:VAL:HG11	1.70	0.72
3:B:699:LEU:HB2	3:C:703:THR:HG22	1.72	0.72
3:C:342:ARG:NH1	3:C:355:ASP:OD1	2.22	0.72
3:A:342:ARG:NH1	3:A:355:ASP:OD1	2.22	0.71
1:I:58:ASN:ND2	3:B:590:SER:O	2.23	0.71
1:I:40:ARG:NH1	1:I:85:GLU:O	2.23	0.71
3:A:279:ARG:NH2	3:B:696:ASP:O	2.24	0.70
3:C:311:HIS:NE2	3:C:313:THR:OG1	2.24	0.70
3:C:143:THR:O	3:C:452:TYR:OH	2.10	0.70
1:J:68:THR:HB	1:J:81:GLU:HB2	1.74	0.70
3:B:311:HIS:NE2	3:B:313:THR:OG1	2.24	0.70
1:H:68:THR:HB	1:H:81:GLU:HB2	1.74	0.70
3:A:707:ARG:NH2	3:C:241:THR:HG23	2.06	0.70
3:B:143:THR:O	3:B:452:TYR:OH	2.10	0.69
3:A:143:THR:O	3:A:452:TYR:OH	2.10	0.69
3:B:248:HIS:ND1	3:B:250:THR:O	2.26	0.69
3:A:392:SER:HB3	3:A:505:ARG:HH21	1.58	0.69
3:B:702:TYR:HA	3:C:702:TYR:HE1	1.56	0.69
1:I:68:THR:HB	1:I:81:GLU:HB2	1.74	0.69
3:A:167:ASP:OD2	3:B:712:HIS:NE2	2.26	0.68
3:B:392:SER:HB3	3:B:505:ARG:HH21	1.58	0.68
3:B:680:ASP:OD1	3:C:514:GLN:NE2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:248:HIS:ND1	3:A:250:THR:O	2.26	0.68
3:C:392:SER:HB3	3:C:505:ARG:HH21	1.58	0.68
3:C:706:GLN:OE1	3:C:710:GLN:NE2	2.28	0.67
3:C:248:HIS:ND1	3:C:250:THR:O	2.26	0.67
3:B:706:GLN:OE1	3:B:710:GLN:NE2	2.28	0.67
3:A:599:ARG:HH12	3:A:619:GLU:HG2	1.60	0.67
1:J:47:TRP:CZ3	2:N:99:PRO:HA	2.30	0.66
1:J:47:TRP:HZ3	2:N:99:PRO:HA	1.59	0.66
3:A:182:PHE:HE2	3:C:215:ARG:HB3	1.61	0.66
3:A:706:GLN:OE1	3:A:710:GLN:NE2	2.28	0.66
3:C:599:ARG:HH12	3:C:619:GLU:HG2	1.60	0.66
3:B:599:ARG:HH12	3:B:619:GLU:HG2	1.60	0.66
3:A:523:ARG:NH1	3:B:674:ASN:O	2.29	0.65
3:A:311:HIS:NE2	3:A:313:THR:OG1	2.24	0.65
3:A:714:LEU:HD21	3:B:313:THR:HG21	1.79	0.65
1:I:99:ARG:HA	3:B:635:VAL:HG12	1.78	0.65
3:A:181:GLN:HA	3:C:220:THR:OG1	1.97	0.64
3:B:166:LYS:HD2	3:B:211:ALA:HB2	1.79	0.64
2:M:23:CYS:N	2:M:75:PHE:O	2.31	0.64
3:A:166:LYS:HD2	3:A:211:ALA:HB2	1.79	0.64
3:A:214:VAL:HA	3:A:219:GLU:HA	1.80	0.64
3:B:154:ILE:HG12	3:C:689:TYR:CE1	2.33	0.64
3:B:235:LYS:NZ	3:B:236:PRO:O	2.31	0.64
3:B:703:THR:O	3:B:707:ARG:HB2	1.98	0.64
3:C:703:THR:O	3:C:707:ARG:HB2	1.98	0.64
3:A:186:PHE:CE2	3:A:188:ASP:HB2	2.34	0.63
3:A:534:HIS:CD2	3:C:539:TRP:CZ2	2.86	0.63
3:C:214:VAL:HA	3:C:219:GLU:HA	1.80	0.63
3:A:295:VAL:HG13	3:A:345:LEU:HD23	1.81	0.63
3:C:235:LYS:NZ	3:C:236:PRO:O	2.31	0.63
1:J:103:MET:HE1	2:N:102:PHE:HZ	1.64	0.63
3:C:166:LYS:HD2	3:C:211:ALA:HB2	1.79	0.63
3:A:243:THR:HG22	3:B:707:ARG:HH12	1.64	0.63
3:B:295:VAL:HG13	3:B:345:LEU:HD23	1.80	0.63
3:B:186:PHE:CE2	3:B:188:ASP:HB2	2.33	0.63
3:A:703:THR:O	3:A:707:ARG:HB2	1.98	0.62
3:B:214:VAL:HA	3:B:219:GLU:HA	1.80	0.62
3:A:235:LYS:NZ	3:A:236:PRO:O	2.31	0.62
3:C:186:PHE:CE2	3:C:188:ASP:HB2	2.34	0.62
2:N:21:ILE:HG12	2:N:77:LEU:HB3	1.82	0.62
3:B:304:ARG:O	3:B:307:SER:OG	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:23:CYS:N	2:L:75:PHE:O	2.31	0.62
2:N:23:CYS:N	2:N:75:PHE:O	2.31	0.62
3:C:295:VAL:HG13	3:C:345:LEU:HD23	1.81	0.62
3:A:152:GLU:O	3:B:689:TYR:OH	2.13	0.62
3:C:194:PHE:HE2	3:C:344:LEU:HB2	1.66	0.61
3:A:211:ALA:O	3:A:221:THR:HA	2.00	0.61
3:B:194:PHE:HE2	3:B:344:LEU:HB2	1.65	0.61
3:B:703:THR:OG1	3:B:704:GLU:OE1	2.19	0.61
3:A:194:PHE:HE2	3:A:344:LEU:HB2	1.66	0.61
2:M:21:ILE:HG12	2:M:77:LEU:HB3	1.82	0.61
3:A:661:ARG:NE	3:B:126:GLN:OE1	2.32	0.61
3:A:715:ARG:HG2	3:C:240:ALA:HB2	1.82	0.61
3:B:211:ALA:O	3:B:221:THR:HA	2.00	0.61
3:C:211:ALA:O	3:C:221:THR:HA	2.00	0.61
2:L:21:ILE:HG12	2:L:77:LEU:HB3	1.82	0.60
3:A:304:ARG:O	3:A:307:SER:OG	2.17	0.60
3:A:532:GLN:HB3	3:C:670:PHE:CD1	2.36	0.60
3:C:304:ARG:O	3:C:307:SER:OG	2.17	0.60
3:A:215:ARG:NH1	3:A:348:PRO:O	2.34	0.60
3:A:545:LEU:HD11	3:B:545:LEU:HD11	1.84	0.60
3:B:169:THR:HA	3:B:187:GLU:HA	1.83	0.60
3:C:213:TYR:CE1	3:C:215:ARG:HB2	2.37	0.60
3:C:215:ARG:NH1	3:C:348:PRO:O	2.34	0.60
3:C:559:VAL:HG12	3:C:572:THR:HA	1.84	0.60
2:N:38:ASN:HB2	2:N:93:GLN:HE21	1.66	0.60
3:B:215:ARG:NH1	3:B:348:PRO:O	2.34	0.60
1:H:20:LEU:HB2	1:H:80:MET:HB3	1.84	0.60
1:J:47:TRP:HB2	2:N:102:PHE:HE2	1.67	0.59
2:L:38:ASN:HB2	2:L:93:GLN:HE21	1.66	0.59
2:M:41:GLN:HB3	2:M:51:LEU:HD21	1.83	0.59
3:A:169:THR:HA	3:A:187:GLU:HA	1.83	0.59
3:A:213:TYR:CE1	3:A:215:ARG:HB2	2.37	0.59
3:A:703:THR:OG1	3:A:704:GLU:OE1	2.19	0.59
3:C:703:THR:OG1	3:C:704:GLU:OE1	2.19	0.59
2:L:41:GLN:HB3	2:L:51:LEU:HD21	1.84	0.59
3:B:213:TYR:CE1	3:B:215:ARG:HB2	2.37	0.59
1:J:6:GLN:H	1:J:108:GLN:HE22	1.50	0.59
2:M:38:ASN:HB2	2:M:93:GLN:HE21	1.67	0.59
2:M:38:ASN:HB2	2:M:93:GLN:NE2	2.18	0.59
3:A:605:ARG:NH1	3:A:610:GLY:O	2.36	0.59
2:L:38:ASN:HB2	2:L:93:GLN:NE2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:559:VAL:HG12	3:A:572:THR:HA	1.84	0.59
2:N:41:GLN:HB3	2:N:51:LEU:HD21	1.84	0.59
3:C:283:PRO:HG2	3:C:285:ASP:HB2	1.85	0.59
1:I:83:THR:N	1:I:86:ASP:OD2	2.35	0.58
1:I:20:LEU:HB2	1:I:80:MET:HB3	1.84	0.58
1:J:83:THR:N	1:J:86:ASP:OD2	2.35	0.58
1:J:30:THR:HA	1:J:52(A):PRO:HB2	1.85	0.58
3:B:559:VAL:HG12	3:B:572:THR:HA	1.84	0.58
3:A:194:PHE:CE2	3:A:344:LEU:HB2	2.38	0.58
3:B:605:ARG:NH1	3:B:610:GLY:O	2.36	0.58
3:C:169:THR:HA	3:C:187:GLU:HA	1.83	0.58
1:H:6:GLN:H	1:H:108:GLN:HE22	1.50	0.58
1:I:47:TRP:HB2	2:M:102:PHE:HE2	1.67	0.58
1:J:20:LEU:HB2	1:J:80:MET:HB3	1.84	0.58
3:A:179:TYR:CE2	3:C:221:THR:N	2.68	0.58
1:I:6:GLN:H	1:I:108:GLN:HE22	1.50	0.58
3:C:605:ARG:NH1	3:C:610:GLY:O	2.36	0.58
2:N:38:ASN:HB2	2:N:93:GLN:NE2	2.18	0.58
3:B:194:PHE:CE2	3:B:344:LEU:HB2	2.38	0.58
2:N:98:VAL:HG13	2:N:99:PRO:HD3	1.85	0.58
1:J:12:VAL:HB	1:J:114:VAL:HG12	1.86	0.58
2:M:98:VAL:HG13	2:M:99:PRO:HD3	1.85	0.57
3:B:210:THR:HG1	3:B:221:THR:HG1	1.35	0.57
1:I:12:VAL:HB	1:I:114:VAL:HG12	1.86	0.57
2:L:98:VAL:HG13	2:L:99:PRO:HD3	1.85	0.57
1:H:12:VAL:HB	1:H:114:VAL:HG12	1.86	0.57
1:H:98:SER:OG	1:H:102:THR:OG1	2.22	0.57
3:B:520:MET:HE1	3:C:676:THR:HG22	1.86	0.57
2:M:19:ALA:HB3	2:M:79:ILE:HB	1.87	0.57
1:I:30:THR:HA	1:I:52(A):PRO:HB2	1.85	0.57
3:A:283:PRO:HG2	3:A:285:ASP:HB2	1.85	0.57
3:B:699:LEU:HB2	3:C:703:THR:CG2	2.34	0.57
3:C:194:PHE:CE2	3:C:344:LEU:HB2	2.38	0.57
3:B:661:ARG:NE	3:C:126:GLN:OE1	2.35	0.57
3:A:707:ARG:HD2	3:C:242:ARG:NH1	2.20	0.57
3:B:283:PRO:HG2	3:B:285:ASP:HB2	1.85	0.57
3:A:276:VAL:HG12	3:B:708:ARG:NH2	2.20	0.57
1:H:30:THR:HA	1:H:52(A):PRO:HB2	1.85	0.56
3:A:296:TYR:CE2	3:C:711:LEU:HD22	2.40	0.56
2:L:14:SER:HB2	2:L:17:GLN:HE22	1.70	0.56
2:N:19:ALA:HB3	2:N:79:ILE:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:710:GLN:CD	3:B:294:PHE:HD2	2.13	0.56
3:B:234:LEU:HD22	3:B:330:LEU:HD11	1.87	0.56
2:M:14:SER:HB2	2:M:17:GLN:HE22	1.71	0.56
3:A:234:LEU:HD22	3:A:330:LEU:HD11	1.88	0.56
2:N:14:SER:HB2	2:N:17:GLN:HE22	1.71	0.56
3:A:272:ILE:HD13	3:B:716:PHE:CD2	2.40	0.56
3:A:121:GLY:HA3	3:C:638:ARG:HD2	1.87	0.56
3:C:234:LEU:HD22	3:C:330:LEU:HD11	1.87	0.56
2:N:70:GLY:HA3	2:N:75:PHE:HA	1.88	0.56
3:A:587:MET:HE2	3:A:650:PHE:CD2	2.41	0.56
2:L:19:ALA:HB3	2:L:79:ILE:HB	1.87	0.56
2:M:70:GLY:HA3	2:M:75:PHE:HA	1.88	0.56
3:B:702:TYR:HA	3:C:702:TYR:CE1	2.40	0.56
3:C:587:MET:HE2	3:C:650:PHE:CD2	2.41	0.56
3:A:286:GLU:OE2	3:C:707:ARG:NE	2.39	0.55
1:I:47:TRP:HZ3	2:M:99:PRO:HA	1.69	0.55
3:C:259:VAL:HG13	3:C:262:PHE:HB2	1.88	0.55
1:I:98:SER:OG	1:I:102:THR:OG1	2.22	0.55
3:A:154:ILE:HG12	3:B:689:TYR:CE1	2.40	0.55
3:A:402:TYR:OH	3:A:493:GLU:OE2	2.24	0.55
3:A:210:THR:HG1	3:A:221:THR:HG1	1.33	0.55
3:A:377:ARG:HD3	3:A:384:PHE:CD1	2.41	0.55
3:A:136:ARG:NH2	3:A:519:ASP:OD1	2.40	0.55
3:B:136:ARG:NH2	3:B:519:ASP:OD1	2.40	0.55
3:B:587:MET:HE2	3:B:650:PHE:CD2	2.41	0.55
3:A:697:SER:CB	3:C:154:ILE:HD12	2.36	0.55
3:B:377:ARG:HD3	3:B:384:PHE:CD1	2.41	0.55
3:A:259:VAL:HG13	3:A:262:PHE:HB2	1.88	0.55
3:B:634:THR:N	3:B:653:TYR:OH	2.40	0.55
3:B:402:TYR:OH	3:B:493:GLU:OE2	2.24	0.55
3:B:499:SER:HA	3:C:688:VAL:HG11	1.88	0.55
3:A:634:THR:N	3:A:653:TYR:OH	2.40	0.55
3:B:215:ARG:N	3:B:218:LEU:O	2.40	0.55
2:N:65:ARG:HH12	2:N:86:ASP:CG	2.15	0.54
3:A:172:GLN:HG2	3:A:183:MET:HE3	1.89	0.54
3:B:703:THR:O	3:B:707:ARG:CB	2.56	0.54
3:C:402:TYR:OH	3:C:493:GLU:OE2	2.24	0.54
2:L:70:GLY:HA3	2:L:75:PHE:HA	1.88	0.54
2:M:4:LEU:HD12	2:M:23:CYS:SG	2.48	0.54
3:B:245:ARG:HG3	3:B:245:ARG:HH11	1.73	0.54
1:H:4:LEU:HD12	1:H:22:CYS:SG	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:65:ARG:HH12	2:L:86:ASP:CG	2.15	0.54
3:A:532:GLN:HB3	3:C:670:PHE:HD1	1.72	0.54
3:A:671:ILE:HD11	3:C:534:HIS:CG	2.42	0.54
1:J:4:LEU:HD12	1:J:22:CYS:SG	2.48	0.54
3:A:253:LYS:HD3	3:C:216:ASN:ND2	2.23	0.54
3:A:703:THR:O	3:A:707:ARG:CB	2.56	0.54
3:C:377:ARG:HD3	3:C:384:PHE:CD1	2.41	0.54
1:I:103:MET:HE1	2:M:102:PHE:HZ	1.71	0.54
3:C:215:ARG:N	3:C:218:LEU:O	2.40	0.54
3:C:703:THR:O	3:C:707:ARG:CB	2.56	0.54
3:A:527:ALA:HB1	3:C:528:TRP:CZ2	2.42	0.54
3:B:259:VAL:HG13	3:B:262:PHE:HB2	1.88	0.54
1:I:47:TRP:CZ3	2:M:99:PRO:HA	2.43	0.54
2:L:4:LEU:HD12	2:L:23:CYS:SG	2.48	0.54
3:B:677:MET:HE1	3:C:522:GLY:HA2	1.89	0.54
3:C:136:ARG:NH2	3:C:519:ASP:OD1	2.40	0.54
3:C:245:ARG:HG3	3:C:245:ARG:HH11	1.73	0.54
1:H:38:LYS:N	1:H:46:GLU:O	2.36	0.54
3:C:558:ARG:HH22	3:C:622:GLU:HB2	1.73	0.54
3:B:172:GLN:HG2	3:B:183:MET:HE3	1.89	0.53
1:H:83:THR:N	1:H:86:ASP:OD2	2.35	0.53
1:I:4:LEU:HD12	1:I:22:CYS:SG	2.48	0.53
3:A:558:ARG:HH22	3:A:622:GLU:HB2	1.73	0.53
3:A:245:ARG:HG3	3:A:245:ARG:HH11	1.72	0.53
2:M:43:LYS:HD3	2:M:88:ALA:HB2	1.91	0.53
2:N:43:LYS:HD3	2:N:88:ALA:HB2	1.91	0.53
3:A:215:ARG:N	3:A:218:LEU:O	2.40	0.53
3:B:366:MET:HG3	3:B:413:ILE:HD11	1.91	0.53
2:N:4:LEU:HD12	2:N:23:CYS:SG	2.48	0.53
3:A:366:MET:HG3	3:A:413:ILE:HD11	1.91	0.53
3:A:507:GLN:HE22	3:C:682:GLU:HA	1.74	0.53
3:C:172:GLN:HG2	3:C:183:MET:HE3	1.89	0.53
3:A:513:ILE:HD13	3:C:513:ILE:HG21	1.91	0.52
3:B:558:ARG:HH22	3:B:622:GLU:HB2	1.73	0.52
3:A:699:LEU:HD21	3:C:281:VAL:HB	1.89	0.52
3:A:700:LEU:HB3	3:A:705:VAL:HG21	1.91	0.52
3:C:673:LEU:HG	3:C:675:ILE:HG12	1.91	0.52
3:A:501:ILE:HG21	3:B:686:LEU:HD23	1.90	0.52
3:B:700:LEU:HB3	3:B:705:VAL:HG21	1.91	0.52
3:C:700:LEU:HB3	3:C:705:VAL:HG21	1.91	0.52
1:J:98:SER:HG	1:J:102:THR:HG1	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:43:LYS:HD3	2:L:88:ALA:HB2	1.91	0.52
3:C:366:MET:HG3	3:C:413:ILE:HD11	1.91	0.52
3:A:253:LYS:CE	3:C:216:ASN:HB3	2.39	0.52
3:A:673:LEU:HG	3:A:675:ILE:HG12	1.91	0.52
3:C:634:THR:N	3:C:653:TYR:OH	2.40	0.52
3:B:168:VAL:O	3:B:188:ASP:N	2.40	0.52
3:B:665:THR:OG1	3:C:124:VAL:O	2.27	0.52
3:A:539:TRP:CD2	3:B:538:LEU:HD21	2.44	0.52
3:A:553:VAL:HG21	3:B:537:THR:OG1	2.10	0.52
3:C:194:PHE:CE2	3:C:320:LYS:HB2	2.45	0.52
3:C:397:THR:HG22	3:C:444:ALA:HA	1.92	0.52
3:A:205:GLY:N	3:A:328:ARG:HH12	2.08	0.52
3:A:564:LEU:C	3:C:639:ARG:HD3	2.35	0.52
3:C:149:VAL:HG12	3:C:450:ILE:HG12	1.92	0.52
1:H:99:ARG:HA	3:A:635:VAL:HG12	1.92	0.51
3:A:680:ASP:OD1	3:B:514:GLN:NE2	2.41	0.51
3:B:205:GLY:N	3:B:328:ARG:HH12	2.08	0.51
3:A:149:VAL:HG12	3:A:450:ILE:HG12	1.92	0.51
3:A:380:TYR:O	3:A:385:ARG:NH1	2.44	0.51
3:A:506:LEU:HD21	3:B:506:LEU:HD23	1.93	0.51
3:B:673:LEU:HG	3:B:675:ILE:HG12	1.91	0.51
3:A:194:PHE:CE2	3:A:320:LYS:HB2	2.45	0.51
3:A:714:LEU:HD21	3:B:313:THR:CG2	2.40	0.51
1:H:66:LYS:HE2	1:H:82:LEU:HD22	1.92	0.51
3:A:131:ARG:HG3	3:C:670:PHE:CE2	2.46	0.51
3:A:243:THR:HG22	3:B:707:ARG:NH1	2.26	0.51
3:B:194:PHE:CE2	3:B:320:LYS:HB2	2.45	0.51
3:C:380:TYR:O	3:C:385:ARG:NH1	2.43	0.51
3:A:530:GLU:O	3:A:534:HIS:HB2	2.11	0.51
3:B:365:THR:OG1	3:B:408:ASP:O	2.27	0.51
3:B:397:THR:HG22	3:B:444:ALA:HA	1.92	0.51
3:C:168:VAL:O	3:C:188:ASP:N	2.40	0.51
3:C:205:GLY:N	3:C:328:ARG:HH12	2.08	0.51
3:C:530:GLU:O	3:C:534:HIS:HB2	2.11	0.51
3:A:243:THR:CG2	3:B:707:ARG:HH12	2.24	0.51
3:B:380:TYR:O	3:B:385:ARG:NH1	2.44	0.51
1:I:66:LYS:HE2	1:I:82:LEU:HD22	1.92	0.51
3:C:279:ARG:O	3:C:288:VAL:HG22	2.11	0.51
3:C:501:ILE:HG22	3:C:505:ARG:HG3	1.93	0.51
3:A:279:ARG:O	3:A:288:VAL:HG22	2.11	0.51
3:B:279:ARG:NH2	3:C:696:ASP:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:702:TYR:HE2	3:C:706:GLN:HE21	1.59	0.50
1:J:32:TYR:OH	3:C:635:VAL:HG23	2.11	0.50
3:A:397:THR:HG22	3:A:444:ALA:HA	1.92	0.50
1:J:66:LYS:HE2	1:J:82:LEU:HD22	1.92	0.50
2:M:25:ALA:O	2:M:26:SER:OG	2.29	0.50
3:B:279:ARG:O	3:B:288:VAL:HG22	2.11	0.50
3:A:688:VAL:HB	3:C:501:ILE:HD11	1.93	0.50
2:N:26:SER:N	2:N:73:THR:OG1	2.45	0.50
3:C:349:LYS:HB2	3:C:350:PHE:CD2	2.47	0.50
3:A:184:GLY:HA2	3:C:186:PHE:CB	2.41	0.50
3:A:349:LYS:HB2	3:A:350:PHE:CD2	2.47	0.50
2:M:65:ARG:HH12	2:M:86:ASP:CG	2.15	0.50
3:B:530:GLU:O	3:B:534:HIS:HB2	2.11	0.50
1:I:1:GLN:NE2	1:I:2:VAL:HG23	2.27	0.50
2:L:25:ALA:O	2:L:26:SER:OG	2.29	0.50
3:A:162:THR:OG1	3:A:342:ARG:NH2	2.45	0.50
3:C:365:THR:OG1	3:C:408:ASP:O	2.27	0.50
1:J:1:GLN:NE2	1:J:2:VAL:HG23	2.27	0.49
2:L:26:SER:N	2:L:73:THR:OG1	2.45	0.49
3:A:665:THR:OG1	3:B:124:VAL:O	2.30	0.49
3:C:199:ASP:O	3:C:203:ALA:HB3	2.12	0.49
3:A:505:ARG:NH1	3:B:684:VAL:O	2.44	0.49
3:B:349:LYS:HB2	3:B:350:PHE:CD2	2.47	0.49
3:C:404:LEU:HD21	3:C:441:TYR:CG	2.47	0.49
3:A:199:ASP:O	3:A:203:ALA:HB3	2.12	0.49
3:A:599:ARG:NH1	3:A:618:GLY:O	2.45	0.49
3:B:199:ASP:O	3:B:203:ALA:HB3	2.12	0.49
1:H:1:GLN:NE2	1:H:2:VAL:HG23	2.27	0.49
3:A:168:VAL:O	3:A:188:ASP:N	2.40	0.49
3:A:499:SER:HA	3:B:688:VAL:HG11	1.94	0.49
3:B:501:ILE:HG22	3:B:505:ARG:HG3	1.93	0.49
2:L:43:LYS:HB2	2:L:46:GLN:HE21	1.78	0.49
2:N:43:LYS:HB2	2:N:46:GLN:HE21	1.77	0.49
3:A:404:LEU:HD21	3:A:441:TYR:CG	2.47	0.49
3:A:501:ILE:HG22	3:A:505:ARG:HG3	1.93	0.49
3:B:149:VAL:HG12	3:B:450:ILE:HG12	1.92	0.49
3:B:162:THR:OG1	3:B:342:ARG:NH2	2.45	0.49
3:B:535:GLU:OE1	3:B:538:LEU:HD12	2.12	0.49
3:C:599:ARG:NH1	3:C:618:GLY:O	2.45	0.49
2:M:26:SER:N	2:M:73:THR:OG1	2.45	0.49
3:B:680:ASP:HA	3:C:514:GLN:HE22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:38:LYS:N	1:J:46:GLU:O	2.36	0.49
1:J:98:SER:OG	1:J:102:THR:OG1	2.22	0.49
3:C:162:THR:OG1	3:C:342:ARG:NH2	2.45	0.49
3:B:714:LEU:HD22	3:C:296:TYR:HD2	1.78	0.49
2:M:43:LYS:HB2	2:M:46:GLN:HE21	1.78	0.48
3:A:274:GLU:OE2	3:B:708:ARG:NE	2.29	0.48
3:A:535:GLU:OE1	3:A:538:LEU:HD12	2.12	0.48
3:A:688:VAL:HB	3:C:501:ILE:HG12	1.95	0.48
3:B:368:LYS:NZ	3:B:416:ASP:HB3	2.28	0.48
3:B:599:ARG:NH1	3:B:618:GLY:O	2.45	0.48
3:A:253:LYS:HD3	3:C:216:ASN:CG	2.38	0.48
3:A:710:GLN:OE1	3:B:294:PHE:HD2	1.96	0.48
3:C:368:LYS:NZ	3:C:416:ASP:HB3	2.28	0.48
3:C:535:GLU:OE1	3:C:538:LEU:HD12	2.12	0.48
1:H:46:GLU:OE2	1:H:62:LYS:HD2	2.13	0.48
2:L:6:GLN:NE2	2:L:106:THR:OG1	2.46	0.48
3:A:252:LEU:HD22	3:C:217:ASN:ND2	2.28	0.48
3:B:422:ASP:OD1	3:B:435:LYS:NZ	2.47	0.48
3:B:605:ARG:HH21	3:B:612:LEU:HD13	1.79	0.48
3:B:702:TYR:HE2	3:B:706:GLN:HE21	1.59	0.48
3:B:702:TYR:CA	3:C:702:TYR:HE1	2.26	0.48
3:C:422:ASP:OD1	3:C:435:LYS:NZ	2.47	0.48
2:L:65:ARG:NH1	2:L:86:ASP:OD2	2.31	0.48
2:N:6:GLN:NE2	2:N:106:THR:OG1	2.46	0.48
3:A:368:LYS:NZ	3:A:416:ASP:HB3	2.28	0.48
3:A:605:ARG:HH21	3:A:612:LEU:HD13	1.79	0.48
2:M:37:MET:HB2	2:M:55:ALA:HB2	1.96	0.48
3:B:404:LEU:HD21	3:B:441:TYR:CG	2.47	0.48
1:J:58:ASN:ND2	3:C:590:SER:O	2.40	0.48
2:L:98:VAL:HA	3:A:593:PRO:HD3	1.95	0.48
3:C:328:ARG:HD2	3:C:329:ASP:H	1.79	0.48
3:C:605:ARG:HH21	3:C:612:LEU:HD13	1.79	0.48
3:A:181:GLN:HB2	3:C:221:THR:O	2.13	0.48
3:A:702:TYR:HE2	3:A:706:GLN:HE21	1.59	0.48
1:I:46:GLU:OE2	1:I:62:LYS:HD2	2.13	0.48
2:L:37:MET:HB2	2:L:55:ALA:HB2	1.96	0.48
2:N:25:ALA:O	2:N:26:SER:OG	2.29	0.48
3:A:422:ASP:OD1	3:A:435:LYS:NZ	2.47	0.48
3:B:328:ARG:HD2	3:B:329:ASP:H	1.79	0.48
3:B:681:HIS:HB3	3:C:510:TYR:CE2	2.48	0.48
1:J:104:ASP:HB3	2:N:50:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:166:LYS:HE2	3:B:207:CYS:SG	2.54	0.47
2:M:6:GLN:NE2	2:M:106:THR:OG1	2.46	0.47
1:J:46:GLU:OE2	1:J:62:LYS:HD2	2.13	0.47
3:A:167:ASP:OD2	3:B:712:HIS:CE1	2.66	0.47
3:A:370:GLN:HE21	3:B:686:LEU:HD11	1.80	0.47
3:C:164:TYR:HB2	3:C:351:THR:OG1	2.15	0.47
2:N:37:MET:HB2	2:N:55:ALA:HB2	1.96	0.47
3:A:697:SER:HB3	3:C:154:ILE:HD12	1.95	0.47
3:A:365:THR:OG1	3:A:408:ASP:O	2.27	0.47
3:A:621:ASN:OD1	3:A:644:GLY:N	2.48	0.47
3:B:429:TYR:HD2	3:B:433:HIS:CD2	2.33	0.47
1:I:104:ASP:HB3	2:M:50:LEU:HD22	1.96	0.47
3:A:164:TYR:HB2	3:A:351:THR:OG1	2.15	0.47
3:A:166:LYS:HE2	3:A:207:CYS:SG	2.54	0.47
3:A:166:LYS:HE3	3:A:192:VAL:HG12	1.96	0.47
3:A:294:PHE:HE2	3:C:706:GLN:HG3	1.80	0.47
3:A:429:TYR:HD2	3:A:433:HIS:CD2	2.33	0.47
3:B:599:ARG:HD3	3:B:600:PRO:HD2	1.97	0.47
3:C:166:LYS:HE3	3:C:192:VAL:HG12	1.96	0.47
3:C:328:ARG:HD2	3:C:329:ASP:N	2.30	0.47
3:A:514:GLN:NE2	3:C:678:LEU:O	2.33	0.47
3:A:516:HIS:CE1	3:B:678:LEU:HB2	2.50	0.47
3:B:164:TYR:HB2	3:B:351:THR:OG1	2.15	0.47
3:B:166:LYS:HE3	3:B:192:VAL:HG12	1.96	0.47
1:I:61:GLU:HA	1:I:64:ARG:HH21	1.79	0.47
1:J:103:MET:HE1	2:N:102:PHE:CZ	2.48	0.47
2:L:38:ASN:HD22	2:L:93:GLN:HE22	1.63	0.47
3:B:667:VAL:HB	3:C:554:THR:HG22	1.96	0.47
3:C:163:MET:HG2	3:C:165:TYR:CD2	2.50	0.47
3:A:328:ARG:HD2	3:A:329:ASP:N	2.30	0.47
3:A:539:TRP:CE2	3:B:538:LEU:HD21	2.49	0.47
3:C:429:TYR:HD2	3:C:433:HIS:CD2	2.33	0.47
3:C:599:ARG:HD3	3:C:600:PRO:HD2	1.97	0.47
3:B:621:ASN:OD1	3:B:644:GLY:N	2.48	0.46
3:B:714:LEU:HD22	3:C:296:TYR:CD2	2.50	0.46
3:C:166:LYS:HE2	3:C:207:CYS:SG	2.54	0.46
3:A:599:ARG:HD3	3:A:600:PRO:HD2	1.97	0.46
1:H:61:GLU:HA	1:H:64:ARG:HH21	1.79	0.46
3:B:163:MET:HG2	3:B:165:TYR:CD2	2.50	0.46
1:J:61:GLU:HA	1:J:64:ARG:HH21	1.79	0.46
3:A:328:ARG:HD2	3:A:329:ASP:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:621:ASN:OD1	3:C:644:GLY:N	2.48	0.46
3:A:163:MET:HG2	3:A:165:TYR:CD2	2.50	0.46
3:B:313:THR:HG22	3:B:313:THR:O	2.16	0.46
3:C:313:THR:HG22	3:C:313:THR:O	2.16	0.46
1:H:60:ASN:HB3	1:H:63:PHE:HD2	1.81	0.46
1:I:91:PHE:CE1	2:M:47:PRO:HB3	2.51	0.46
2:L:38:ASN:HD22	2:L:93:GLN:NE2	2.14	0.46
3:A:217:ASN:HD21	3:C:718:ASP:HB3	1.81	0.46
3:A:253:LYS:HE3	3:C:216:ASN:O	2.15	0.46
1:I:31:THR:HG22	1:I:53:ARG:HH21	1.81	0.46
3:C:430:ASN:OD1	3:C:431:ALA:N	2.49	0.46
3:A:702:TYR:HE1	3:C:702:TYR:N	2.14	0.46
3:B:133:CYS:HB2	3:B:134:PRO:HD2	1.97	0.46
3:B:328:ARG:HD2	3:B:329:ASP:N	2.30	0.46
3:B:430:ASN:OD1	3:B:431:ALA:N	2.49	0.46
3:C:359:LYS:O	3:C:363:VAL:HG12	2.16	0.46
3:A:359:LYS:O	3:A:363:VAL:HG12	2.16	0.46
1:J:60:ASN:HB3	1:J:63:PHE:HD2	1.81	0.46
2:N:93:GLN:HB2	2:N:101:THR:O	2.16	0.46
3:A:430:ASN:OD1	3:A:431:ALA:N	2.49	0.46
3:A:313:THR:O	3:A:313:THR:HG22	2.16	0.45
1:I:60:ASN:HB3	1:I:63:PHE:HD2	1.81	0.45
3:A:279:ARG:NH2	3:B:696:ASP:OD1	2.49	0.45
3:A:325:PHE:CG	3:A:342:ARG:HB2	2.51	0.45
3:B:325:PHE:CG	3:B:342:ARG:HB2	2.51	0.45
3:B:359:LYS:O	3:B:363:VAL:HG12	2.16	0.45
3:C:589:ILE:HG12	3:C:597:TYR:CE2	2.51	0.45
1:I:5:GLN:OE1	1:I:5:GLN:HA	2.17	0.45
2:M:38:ASN:HD22	2:M:93:GLN:HE22	1.63	0.45
3:B:589:ILE:HG12	3:B:597:TYR:CE2	2.51	0.45
1:H:31:THR:HG22	1:H:53:ARG:HH21	1.81	0.45
1:J:11:LEU:HD13	1:J:113:THR:OG1	2.17	0.45
2:L:93:GLN:HB2	2:L:101:THR:O	2.16	0.45
3:A:140:GLN:HG3	3:A:378:SER:HB2	1.98	0.45
3:C:133:CYS:HB2	3:C:134:PRO:HD2	1.97	0.45
3:C:194:PHE:CD2	3:C:320:LYS:HB2	2.52	0.45
2:L:39:TRP:CZ3	2:L:92:CYS:HB3	2.52	0.45
3:A:133:CYS:HB2	3:A:134:PRO:HD2	1.97	0.45
3:C:325:PHE:CG	3:C:342:ARG:HB2	2.51	0.45
1:H:37:VAL:HG11	1:H:45:LEU:HD13	1.98	0.45
1:J:31:THR:HG22	1:J:53:ARG:HH21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:59:TYR:CE1	1:J:69:LEU:HG	2.52	0.45
2:M:7:SER:OG	2:M:8:PRO:HD3	2.17	0.45
2:M:39:TRP:CZ3	2:M:92:CYS:HB3	2.52	0.45
2:N:38:ASN:HD22	2:N:93:GLN:HE22	1.63	0.45
3:A:589:ILE:HG12	3:A:597:TYR:CE2	2.51	0.45
1:I:11:LEU:HD13	1:I:113:THR:OG1	2.17	0.45
3:B:366:MET:HE3	3:B:366:MET:HB3	1.81	0.45
3:C:140:GLN:HG3	3:C:378:SER:HB2	1.98	0.45
1:H:11:LEU:HD13	1:H:113:THR:OG1	2.17	0.45
2:L:46:GLN:HB2	2:L:47:PRO:HD2	1.99	0.45
3:A:173:VAL:HA	3:A:182:PHE:HA	1.99	0.45
3:A:216:ASN:O	3:B:253:LYS:HE3	2.17	0.45
3:C:406:ARG:HG2	3:C:493:GLU:HG2	1.98	0.45
1:H:59:TYR:CE1	1:H:69:LEU:HG	2.52	0.45
2:N:39:TRP:CZ3	2:N:92:CYS:HB3	2.52	0.45
3:A:163:MET:HG2	3:A:165:TYR:CE2	2.52	0.45
3:A:688:VAL:HB	3:C:501:ILE:CD1	2.47	0.45
3:A:688:VAL:HB	3:C:501:ILE:CG1	2.47	0.45
3:B:163:MET:HG2	3:B:165:TYR:CE2	2.52	0.45
1:H:48:ILE:HG22	1:H:63:PHE:CE2	2.53	0.44
1:I:59:TYR:CE1	1:I:69:LEU:HG	2.52	0.44
1:J:37:VAL:HG11	1:J:45:LEU:HD13	1.98	0.44
3:B:140:GLN:HG3	3:B:378:SER:HB2	1.98	0.44
3:C:173:VAL:HA	3:C:182:PHE:HA	1.99	0.44
1:I:38:LYS:N	1:I:46:GLU:O	2.36	0.44
3:A:194:PHE:CD2	3:A:320:LYS:HB2	2.52	0.44
3:A:697:SER:HB2	3:C:154:ILE:HD12	1.99	0.44
3:B:406:ARG:HG2	3:B:493:GLU:HG2	1.98	0.44
3:C:388:SER:OG	3:C:391:ILE:HG12	2.17	0.44
2:M:46:GLN:HB2	2:M:47:PRO:HD2	2.00	0.44
2:N:38:ASN:HD22	2:N:93:GLN:NE2	2.14	0.44
3:A:296:TYR:OH	3:C:711:LEU:HD22	2.17	0.44
3:B:194:PHE:CD2	3:B:320:LYS:HB2	2.52	0.44
3:C:711:LEU:O	3:C:712:HIS:C	2.61	0.44
1:I:48:ILE:HG22	1:I:63:PHE:CE2	2.53	0.44
2:M:93:GLN:HB2	2:M:101:THR:O	2.16	0.44
3:A:215:ARG:HH12	3:A:349:LYS:HD3	1.83	0.44
3:B:173:VAL:HA	3:B:182:PHE:HA	1.99	0.44
3:C:215:ARG:HH12	3:C:349:LYS:HD3	1.83	0.44
1:H:5:GLN:OE1	1:H:5:GLN:HA	2.17	0.44
2:M:14:SER:H	2:M:111:LYS:NZ	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:38:ASN:HD22	2:M:93:GLN:NE2	2.14	0.44
2:N:46:GLN:HB2	2:N:47:PRO:HD2	1.99	0.44
3:A:388:SER:OG	3:A:391:ILE:HG12	2.17	0.44
1:J:48:ILE:HG22	1:J:63:PHE:CE2	2.53	0.44
2:M:21:ILE:HG21	2:M:106:THR:HG21	2.00	0.44
2:L:21:ILE:HG21	2:L:106:THR:HG21	2.00	0.44
3:A:185:ILE:HB	3:C:186:PHE:CE1	2.52	0.44
3:A:406:ARG:HG2	3:A:493:GLU:HG2	1.98	0.44
3:B:215:ARG:HH12	3:B:349:LYS:HD3	1.83	0.44
3:C:197:VAL:HG11	3:C:344:LEU:HD21	2.00	0.44
1:I:37:VAL:HG11	1:I:45:LEU:HD13	1.99	0.44
1:J:45:LEU:HD11	2:N:102:PHE:CD1	2.53	0.44
2:L:7:SER:OG	2:L:8:PRO:HD3	2.17	0.44
2:L:14:SER:H	2:L:111:LYS:NZ	2.15	0.44
2:M:18:ARG:HD3	2:M:19:ALA:H	1.83	0.44
2:N:7:SER:OG	2:N:8:PRO:HD3	2.17	0.44
3:B:219:GLU:C	3:C:179:TYR:HH	2.25	0.44
3:B:388:SER:OG	3:B:391:ILE:HG12	2.17	0.44
3:A:170:VAL:N	3:A:186:PHE:O	2.51	0.44
3:A:270:ASN:O	3:A:272:ILE:HG13	2.18	0.44
3:A:279:ARG:HH22	3:B:696:ASP:CG	2.26	0.44
3:A:319:PHE:O	3:A:320:LYS:HE2	2.18	0.44
3:A:715:ARG:HA	3:C:238:ASN:OD1	2.18	0.44
3:B:197:VAL:HG11	3:B:344:LEU:HD21	1.99	0.44
3:C:163:MET:HG2	3:C:165:TYR:CE2	2.52	0.44
1:I:99:ARG:HA	3:B:635:VAL:CG1	2.47	0.43
1:J:5:GLN:OE1	1:J:5:GLN:HA	2.17	0.43
2:L:18:ARG:HD3	2:L:19:ALA:H	1.83	0.43
2:N:18:ARG:HD3	2:N:19:ALA:H	1.83	0.43
2:N:21:ILE:HG21	2:N:106:THR:HG21	2.00	0.43
3:A:678:LEU:HD13	3:C:516:HIS:CG	2.53	0.43
3:A:711:LEU:O	3:A:712:HIS:C	2.61	0.43
3:C:170:VAL:N	3:C:186:PHE:O	2.51	0.43
3:C:225:ARG:NH2	3:C:254:TYR:HD1	2.16	0.43
3:C:707:ARG:O	3:C:711:LEU:HD23	2.18	0.43
1:I:13:LYS:HA	1:I:13:LYS:HD3	1.75	0.43
3:A:225:ARG:NH2	3:A:254:TYR:HD1	2.16	0.43
3:A:382:GLY:HA2	3:A:399:LEU:HD11	2.01	0.43
3:A:614:GLU:OE2	3:A:627:ARG:NH1	2.52	0.43
3:C:282:TYR:HB3	3:C:494:ARG:HH12	1.84	0.43
1:J:87:SER:OG	1:J:114:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:194:PHE:HZ	3:B:322:VAL:HG23	1.83	0.43
3:B:270:ASN:O	3:B:272:ILE:HG13	2.18	0.43
3:B:282:TYR:HB3	3:B:494:ARG:HH12	1.83	0.43
3:B:503:PHE:CG	3:B:504:ALA:N	2.87	0.43
3:B:614:GLU:OE2	3:B:627:ARG:NH1	2.52	0.43
3:B:670:PHE:CZ	3:C:536:LEU:HD12	2.53	0.43
1:H:87:SER:OG	1:H:114:VAL:HG22	2.18	0.43
3:A:293:ASP:HA	3:C:710:GLN:HE22	1.83	0.43
3:B:382:GLY:HA2	3:B:399:LEU:HD11	2.00	0.43
3:C:194:PHE:HZ	3:C:322:VAL:HG23	1.84	0.43
3:C:349:LYS:HB2	3:C:350:PHE:HD2	1.83	0.43
3:B:118:PRO:HA	3:B:119:PRO:HD3	1.87	0.43
3:B:170:VAL:N	3:B:186:PHE:O	2.51	0.43
1:I:87:SER:OG	1:I:114:VAL:HG22	2.18	0.43
2:N:98:VAL:CG1	2:N:99:PRO:HD3	2.49	0.43
2:N:65:ARG:NH1	2:N:86:ASP:OD2	2.31	0.43
3:A:197:VAL:HG11	3:A:344:LEU:HD21	1.99	0.43
3:A:346:THR:HG22	3:A:351:THR:HG22	2.01	0.43
3:B:319:PHE:O	3:B:320:LYS:HE2	2.18	0.43
3:B:558:ARG:NH2	3:B:622:GLU:HB2	2.34	0.43
3:C:270:ASN:O	3:C:272:ILE:HG13	2.18	0.43
3:C:614:GLU:OE2	3:C:627:ARG:NH1	2.51	0.43
2:M:32:PHE:CD1	3:B:632:PRO:HG3	2.53	0.43
3:A:282:TYR:HB3	3:A:494:ARG:HH12	1.84	0.43
2:M:65:ARG:NH1	2:M:86:ASP:OD2	2.31	0.43
2:N:14:SER:H	2:N:111:LYS:NZ	2.15	0.43
3:A:133:CYS:HB2	3:A:134:PRO:CD	2.49	0.43
3:B:225:ARG:NH2	3:B:254:TYR:HD1	2.16	0.43
3:C:503:PHE:CG	3:C:504:ALA:N	2.86	0.43
3:A:223:PHE:HB3	3:A:227:ASP:O	2.19	0.42
3:A:558:ARG:NH2	3:A:622:GLU:HB2	2.34	0.42
3:B:223:PHE:HB3	3:B:227:ASP:O	2.19	0.42
3:B:707:ARG:O	3:B:711:LEU:HD23	2.18	0.42
3:C:223:PHE:HB3	3:C:227:ASP:O	2.19	0.42
3:A:343:ASN:HB2	3:A:356:TRP:HB2	2.01	0.42
3:A:349:LYS:HB2	3:A:350:PHE:HD2	1.83	0.42
3:A:707:ARG:O	3:A:711:LEU:HD23	2.18	0.42
3:C:558:ARG:NH2	3:C:622:GLU:HB2	2.34	0.42
3:A:194:PHE:HZ	3:A:322:VAL:HG23	1.83	0.42
3:A:503:PHE:CG	3:A:504:ALA:N	2.87	0.42
3:B:670:PHE:CE1	3:C:536:LEU:HD12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:319:PHE:O	3:C:320:LYS:HE2	2.18	0.42
3:A:366:MET:HE3	3:A:366:MET:HB3	1.81	0.42
3:B:133:CYS:HB2	3:B:134:PRO:CD	2.49	0.42
3:B:343:ASN:HB2	3:B:356:TRP:HB2	2.01	0.42
3:C:133:CYS:HB2	3:C:134:PRO:CD	2.49	0.42
3:C:206:VAL:HG12	3:C:233:GLU:HA	2.01	0.42
1:H:39:GLU:N	1:H:89:VAL:O	2.50	0.42
1:I:39:GLU:N	1:I:89:VAL:O	2.50	0.42
3:B:661:ARG:HA	3:B:661:ARG:HD2	1.73	0.42
3:B:667:VAL:HG11	3:C:555:VAL:HG22	2.01	0.42
3:C:442:TYR:O	3:C:449:LEU:HD12	2.20	0.42
1:H:70:THR:OG1	1:H:79:TYR:HB2	2.20	0.42
2:L:29:VAL:HG21	2:L:94:GLN:HB2	2.01	0.42
2:N:2:ILE:HG13	2:N:97:GLU:OE1	2.20	0.42
3:B:206:VAL:HG12	3:B:233:GLU:HA	2.01	0.42
3:B:711:LEU:O	3:B:712:HIS:C	2.61	0.42
1:H:12:VAL:O	1:H:114:VAL:HA	2.20	0.42
1:I:12:VAL:O	1:I:114:VAL:HA	2.19	0.42
2:L:80:HIS:HA	2:L:81:PRO:HA	1.84	0.42
3:A:677:MET:HE1	3:B:522:GLY:HA2	2.02	0.42
3:C:382:GLY:HA2	3:C:399:LEU:HD11	2.01	0.42
1:J:12:VAL:O	1:J:114:VAL:HA	2.19	0.42
1:J:36:TRP:O	1:J:48:ILE:HG12	2.20	0.42
2:L:14:SER:HA	2:L:110:LEU:HD12	2.01	0.42
3:A:368:LYS:HZ1	3:A:416:ASP:HB3	1.85	0.42
3:A:531:LEU:O	3:A:535:GLU:HG2	2.20	0.42
3:B:531:LEU:O	3:B:535:GLU:HG2	2.20	0.42
3:C:346:THR:HG22	3:C:351:THR:HG22	2.01	0.42
1:I:70:THR:OG1	1:I:79:TYR:HB2	2.20	0.42
2:M:14:SER:HA	2:M:110:LEU:HD12	2.01	0.42
2:N:5:THR:OG1	2:N:24:ARG:HB2	2.20	0.42
2:M:5:THR:OG1	2:M:24:ARG:HB2	2.20	0.42
3:A:206:VAL:HG12	3:A:233:GLU:HA	2.01	0.42
3:B:392:SER:HB2	3:C:681:HIS:NE2	2.34	0.42
3:C:360:ARG:HB3	3:C:411:ASP:OD2	2.20	0.42
3:A:270:ASN:ND2	3:B:716:PHE:O	2.52	0.41
3:C:686:LEU:HD12	3:C:686:LEU:HA	1.83	0.41
1:H:36:TRP:O	1:H:48:ILE:HG12	2.20	0.41
1:H:39:GLU:HB3	1:H:89:VAL:HB	2.02	0.41
1:J:97:SER:HB3	1:J:104:ASP:OD2	2.20	0.41
3:A:277:ASP:OD2	3:A:277:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:442:TYR:O	3:A:449:LEU:HD12	2.20	0.41
3:B:194:PHE:CZ	3:B:322:VAL:HG23	2.56	0.41
3:B:368:LYS:HZ1	3:B:416:ASP:HB3	1.85	0.41
3:B:442:TYR:O	3:B:449:LEU:HD12	2.20	0.41
1:H:97:SER:HB3	1:H:104:ASP:OD2	2.20	0.41
2:N:14:SER:HA	2:N:110:LEU:HD12	2.01	0.41
3:A:294:PHE:CE2	3:C:706:GLN:HG3	2.55	0.41
3:A:360:ARG:HB3	3:A:411:ASP:OD2	2.20	0.41
3:B:686:LEU:HD12	3:B:686:LEU:HA	1.82	0.41
3:C:343:ASN:HB2	3:C:356:TRP:HB2	2.01	0.41
3:C:531:LEU:O	3:C:535:GLU:HG2	2.20	0.41
2:L:2:ILE:HG12	2:L:27:GLU:OE2	2.20	0.41
2:N:2:ILE:HG12	2:N:27:GLU:OE2	2.20	0.41
3:A:194:PHE:CZ	3:A:322:VAL:HG23	2.56	0.41
3:A:208:ARG:HB3	3:A:229:GLU:CD	2.45	0.41
3:B:624:ARG:HH22	3:B:628:ASP:CG	2.28	0.41
3:C:173:VAL:HG22	3:C:182:PHE:CD1	2.55	0.41
3:C:592:ARG:HA	3:C:593:PRO:HD3	1.94	0.41
3:C:661:ARG:HD2	3:C:661:ARG:HA	1.73	0.41
2:M:2:ILE:HG12	2:M:27:GLU:OE2	2.20	0.41
3:A:173:VAL:HG22	3:A:182:PHE:CD1	2.55	0.41
3:B:173:VAL:HG22	3:B:182:PHE:CD1	2.55	0.41
3:B:441:TYR:HA	3:B:450:ILE:O	2.21	0.41
3:C:208:ARG:HB3	3:C:229:GLU:CD	2.45	0.41
1:I:36:TRP:O	1:I:48:ILE:HG12	2.20	0.41
1:I:97:SER:HB3	1:I:104:ASP:OD2	2.20	0.41
1:J:70:THR:OG1	1:J:79:TYR:HB2	2.20	0.41
3:B:211:ALA:O	3:B:213:TYR:HD2	2.03	0.41
3:B:277:ASP:OD2	3:B:277:ASP:N	2.53	0.41
3:B:346:THR:HG22	3:B:351:THR:HG22	2.01	0.41
2:L:5:THR:OG1	2:L:24:ARG:HB2	2.20	0.41
2:N:29:VAL:HG21	2:N:94:GLN:HB2	2.02	0.41
3:B:174:TRP:CD1	3:B:263:HIS:HD1	2.39	0.41
3:B:186:PHE:HE2	3:B:188:ASP:HB2	1.84	0.41
3:C:202:ASN:O	3:C:328:ARG:HD3	2.21	0.41
1:I:48:ILE:HD11	1:I:80:MET:HE1	2.03	0.41
1:J:12:VAL:HG21	1:J:18:VAL:HG11	2.02	0.41
2:L:2:ILE:HG13	2:L:97:GLU:OE1	2.20	0.41
2:M:98:VAL:CG1	2:M:99:PRO:HD3	2.49	0.41
2:N:80:HIS:HA	2:N:81:PRO:HA	1.84	0.41
3:A:186:PHE:HE2	3:A:188:ASP:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:202:ASN:O	3:A:328:ARG:HD3	2.21	0.41
3:A:599:ARG:HD3	3:A:600:PRO:CD	2.51	0.41
3:A:661:ARG:HD2	3:A:661:ARG:HA	1.73	0.41
3:B:314:TYR:CE2	3:B:345:LEU:HD21	2.56	0.41
3:C:211:ALA:O	3:C:213:TYR:HD2	2.03	0.41
3:C:288:VAL:HG12	3:C:294:PHE:CE1	2.56	0.41
1:I:12:VAL:HG21	1:I:18:VAL:HG11	2.02	0.41
2:M:2:ILE:HG13	2:M:97:GLU:OE1	2.20	0.41
2:M:29:VAL:HG21	2:M:94:GLN:HB2	2.01	0.41
3:A:174:TRP:CD1	3:A:263:HIS:HD1	2.39	0.41
3:A:314:TYR:CE2	3:A:345:LEU:HD21	2.56	0.41
3:B:208:ARG:HB3	3:B:229:GLU:CD	2.45	0.41
3:C:215:ARG:NH1	3:C:349:LYS:HD3	2.36	0.41
3:C:441:TYR:HA	3:C:450:ILE:O	2.21	0.41
3:C:507:GLN:HE21	3:C:511:ASN:CG	2.29	0.41
1:J:39:GLU:HB3	1:J:89:VAL:HB	2.02	0.41
3:A:118:PRO:HA	3:A:119:PRO:HD3	1.87	0.41
3:A:253:LYS:HE2	3:C:216:ASN:HB3	2.03	0.41
3:A:686:LEU:HA	3:A:686:LEU:HD12	1.82	0.41
3:C:624:ARG:HH22	3:C:628:ASP:CG	2.28	0.41
1:J:48:ILE:HD11	1:J:80:MET:HE1	2.03	0.40
2:L:98:VAL:CG1	2:L:99:PRO:HD3	2.49	0.40
3:A:288:VAL:HG12	3:A:294:PHE:CE1	2.56	0.40
3:C:182:PHE:CE1	3:C:185:ILE:HD11	2.56	0.40
3:C:194:PHE:CZ	3:C:322:VAL:HG23	2.56	0.40
1:J:39:GLU:N	1:J:89:VAL:O	2.50	0.40
3:A:211:ALA:O	3:A:213:TYR:HD2	2.03	0.40
3:B:360:ARG:HB3	3:B:411:ASP:OD2	2.20	0.40
3:C:162:THR:HG23	3:C:275:GLU:HG2	2.03	0.40
1:H:48:ILE:HD11	1:H:80:MET:HE1	2.03	0.40
3:A:214:VAL:HG21	3:C:722:VAL:HG22	2.04	0.40
3:A:369:TRP:HZ2	3:B:686:LEU:HG	1.86	0.40
3:B:215:ARG:NH1	3:B:349:LYS:HD3	2.36	0.40
3:C:214:VAL:HG22	3:C:219:GLU:HB3	2.03	0.40
1:H:103:MET:HE1	2:L:102:PHE:HZ	1.87	0.40
3:A:162:THR:HG23	3:A:275:GLU:HG2	2.03	0.40
3:A:210:THR:HA	3:A:222:ALA:O	2.22	0.40
3:B:288:VAL:HG12	3:B:294:PHE:CE1	2.56	0.40
3:C:277:ASP:OD2	3:C:277:ASP:N	2.53	0.40
3:A:234:LEU:HD21	3:A:247:TRP:CD1	2.56	0.40
3:A:302:GLY:HA2	3:A:319:PHE:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:680:ASP:HA	3:B:514:GLN:HE22	1.86	0.40
3:C:234:LEU:HD21	3:C:247:TRP:CD1	2.56	0.40
3:C:599:ARG:HD3	3:C:600:PRO:CD	2.51	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	H	118/121 (98%)	111 (94%)	7 (6%)	0	100	100
1	I	118/121 (98%)	111 (94%)	7 (6%)	0	100	100
1	J	118/121 (98%)	111 (94%)	7 (6%)	0	100	100
2	L	109/112 (97%)	102 (94%)	7 (6%)	0	100	100
2	M	109/112 (97%)	102 (94%)	7 (6%)	0	100	100
2	N	109/112 (97%)	102 (94%)	7 (6%)	0	100	100
3	A	570/628 (91%)	544 (95%)	26 (5%)	0	100	100
3	B	570/628 (91%)	544 (95%)	26 (5%)	0	100	100
3	C	570/628 (91%)	544 (95%)	26 (5%)	0	100	100
All	All	2391/2583 (93%)	2271 (95%)	120 (5%)	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	H	102/102 (100%)	102 (100%)	0	100	100
1	I	102/102 (100%)	102 (100%)	0	100	100
1	J	102/102 (100%)	102 (100%)	0	100	100
2	L	93/94 (99%)	93 (100%)	0	100	100
2	M	93/94 (99%)	93 (100%)	0	100	100
2	N	93/94 (99%)	93 (100%)	0	100	100
3	A	502/543 (92%)	502 (100%)	0	100	100
3	B	502/543 (92%)	502 (100%)	0	100	100
3	C	502/543 (92%)	502 (100%)	0	100	100
All	All	2091/2217 (94%)	2091 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	1	GLN
2	L	93	GLN
2	M	93	GLN
2	N	93	GLN
3	A	112	ASN
3	A	507	GLN
3	B	112	ASN
3	B	534	HIS
3	C	112	ASN
3	C	507	GLN
3	C	710	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

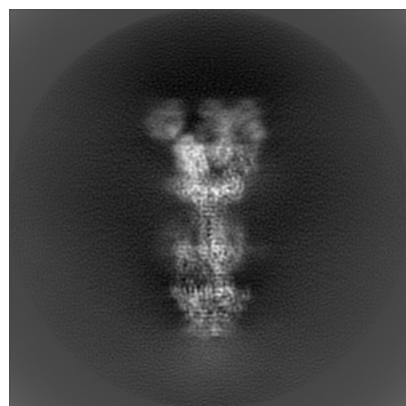
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26520. These allow visual inspection of the internal detail of the map and identification of artifacts.

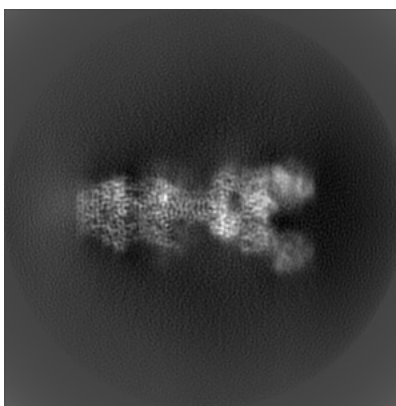
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

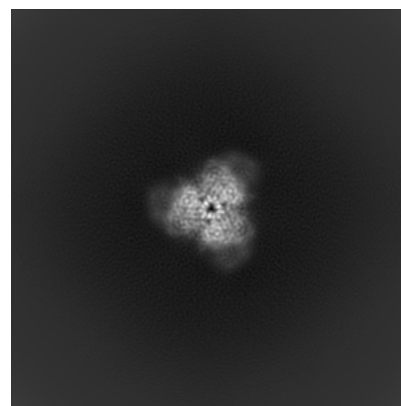
6.1.1 Primary map



X

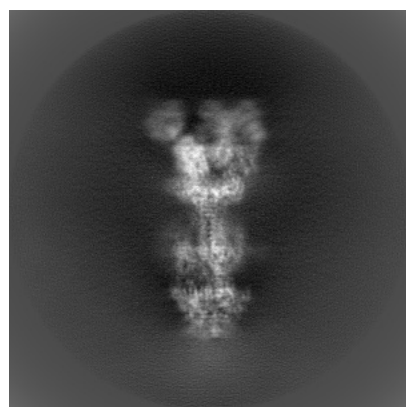


Y

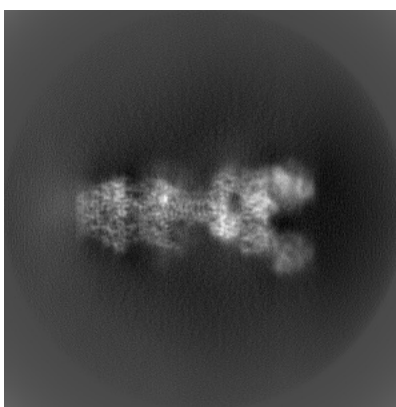


Z

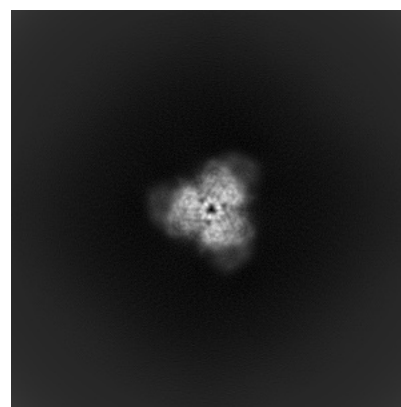
6.1.2 Raw map



X



Y

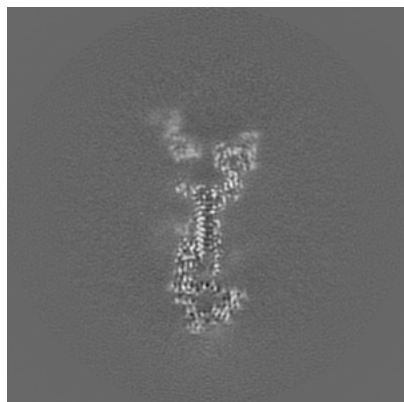


Z

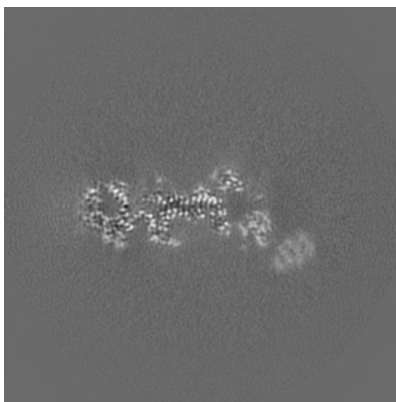
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

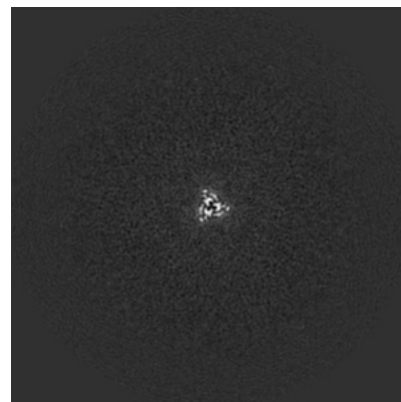
6.2.1 Primary map



X Index: 224

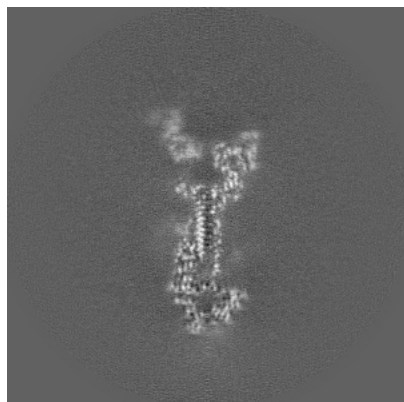


Y Index: 224

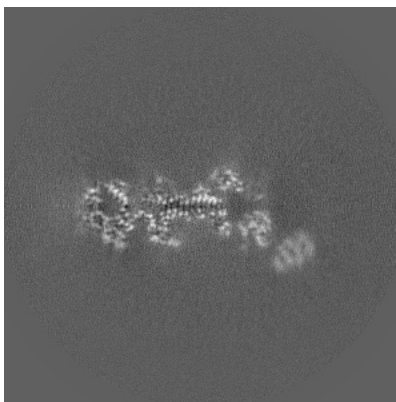


Z Index: 224

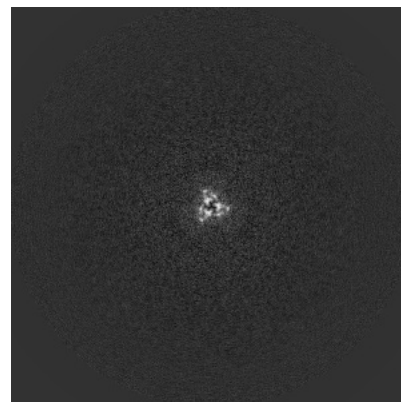
6.2.2 Raw map



X Index: 224



Y Index: 224

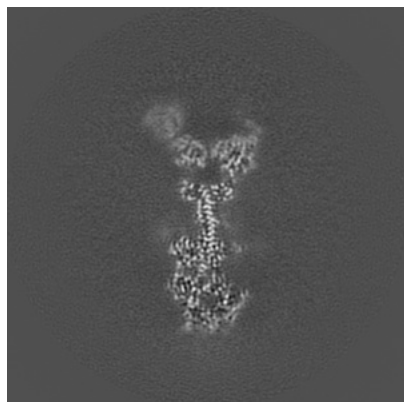


Z Index: 224

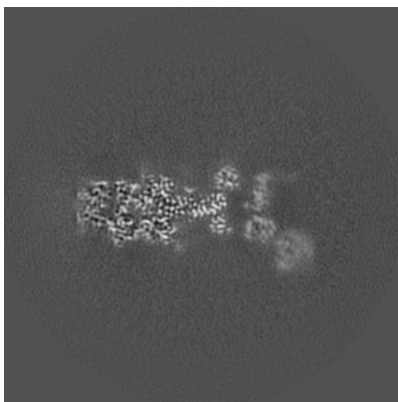
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

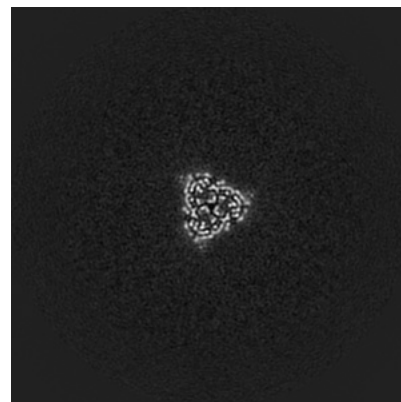
6.3.1 Primary map



X Index: 232

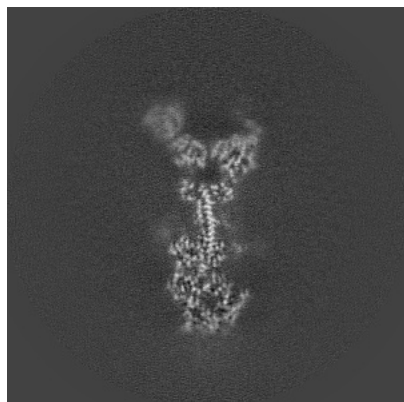


Y Index: 232

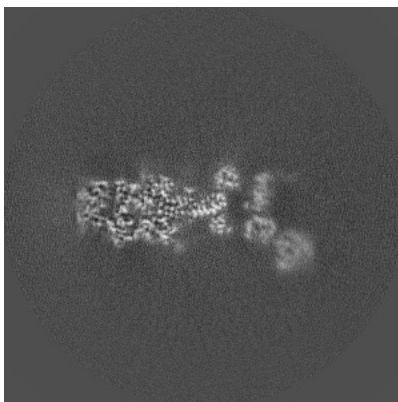


Z Index: 243

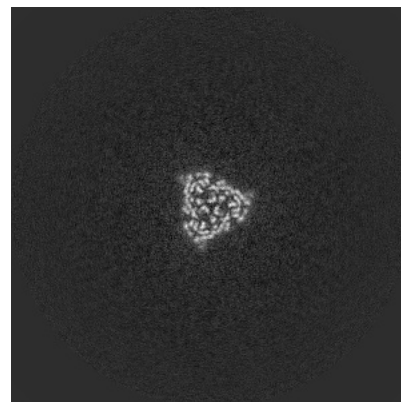
6.3.2 Raw map



X Index: 232



Y Index: 232

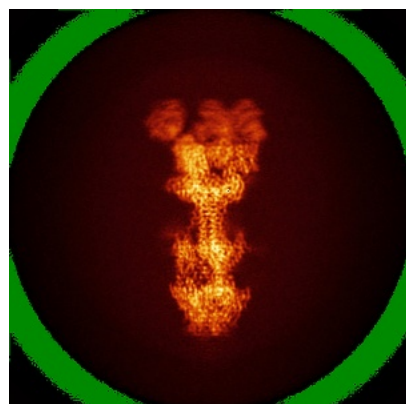


Z Index: 243

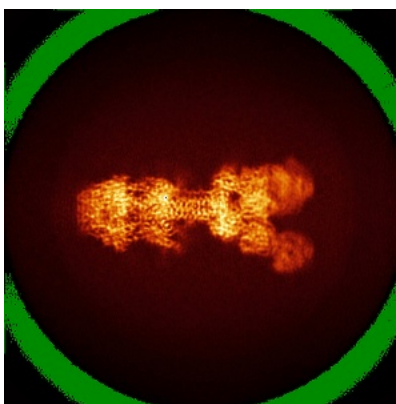
The images above show the largest variance slices of the map in three orthogonal directions.

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

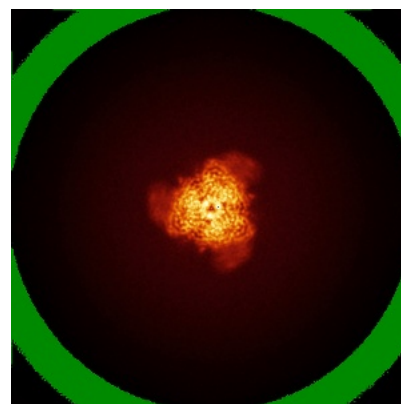
6.4.1 Primary map



X

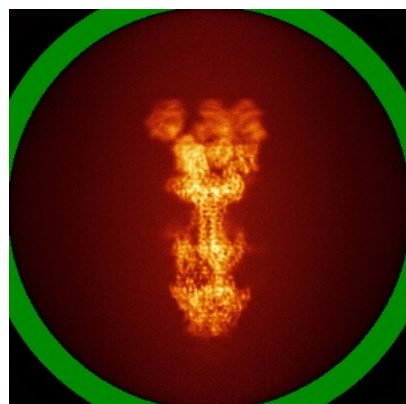


Y

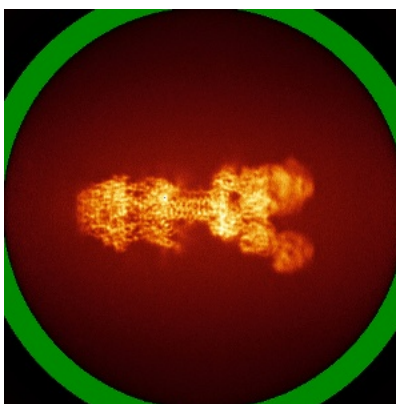


Z

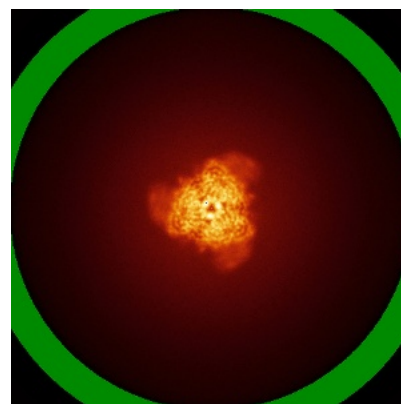
6.4.2 Raw map



X



Y

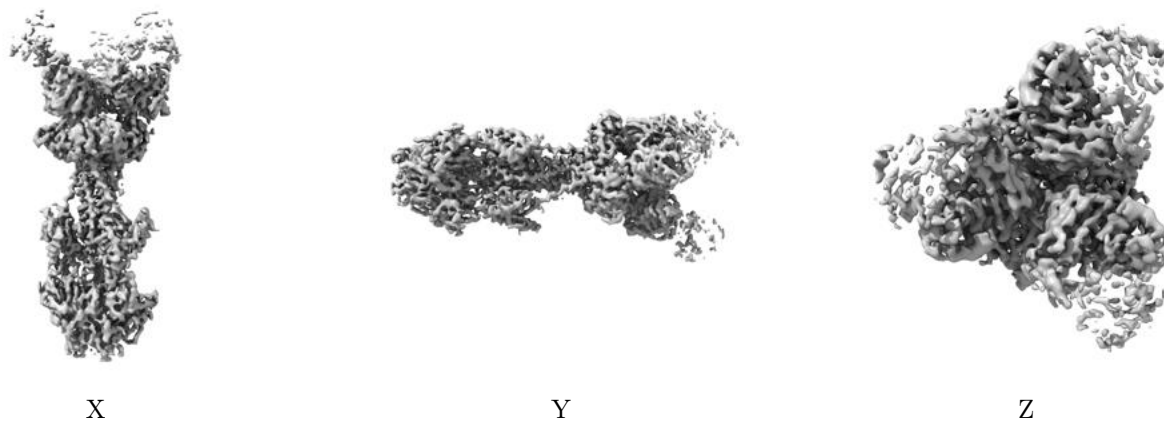


Z

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.

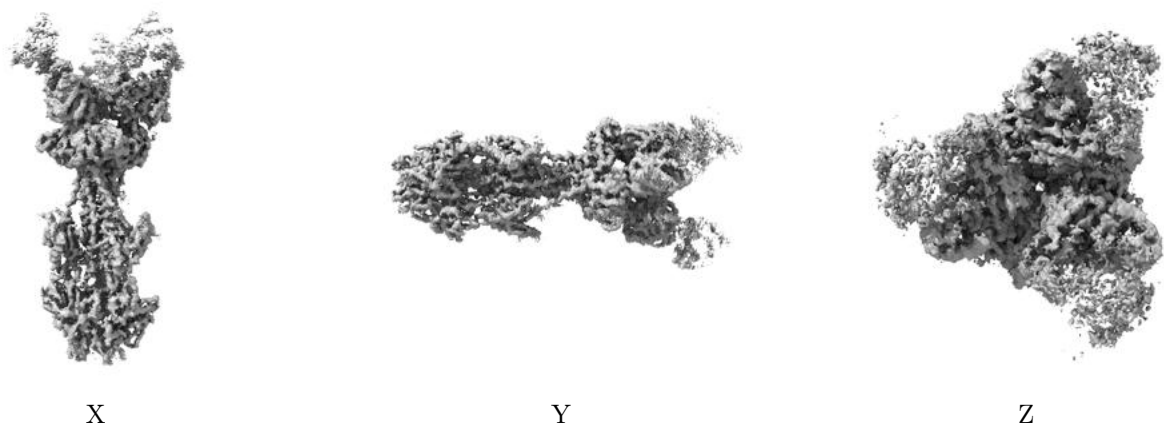
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

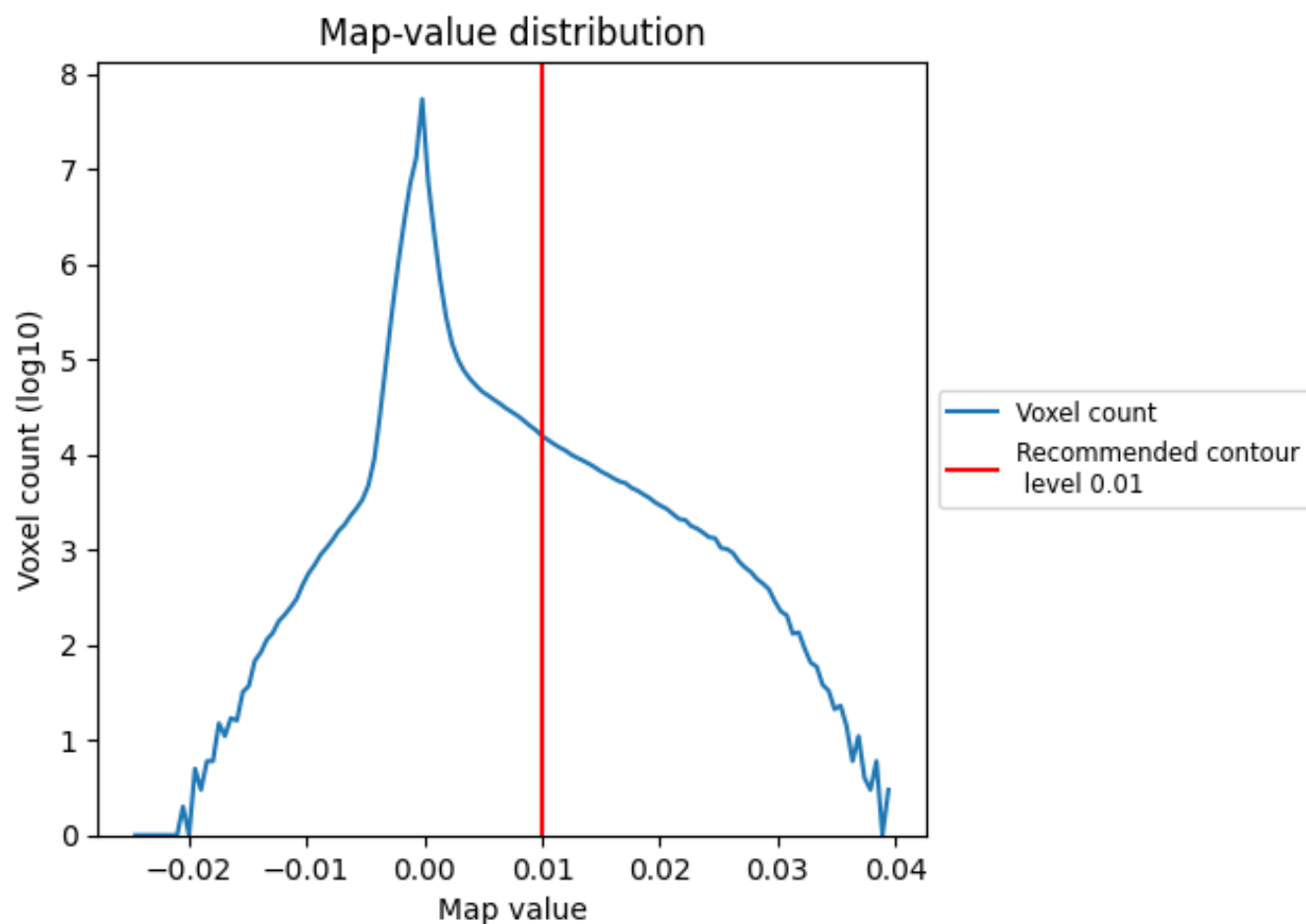
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

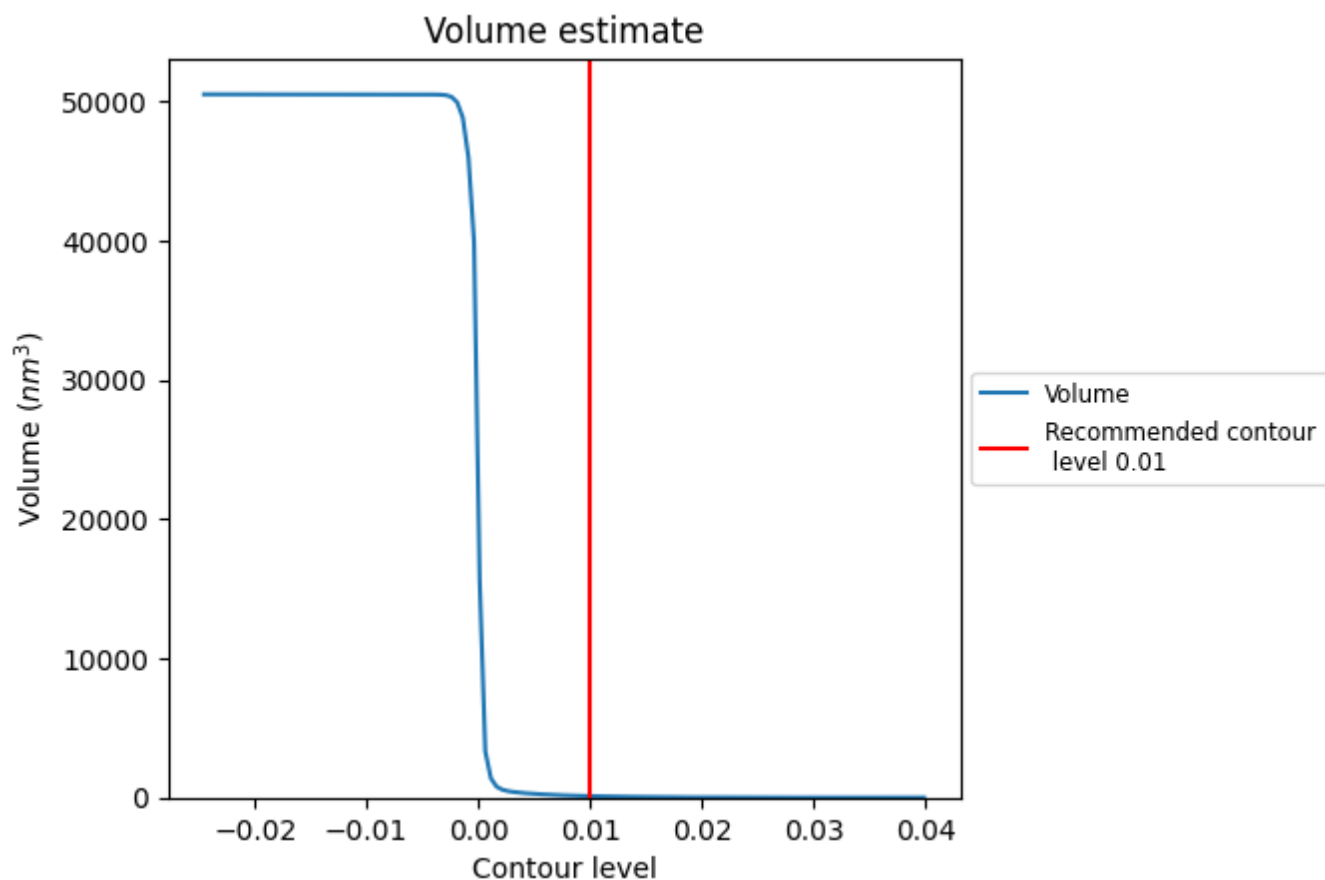
This section contains the results of statistical analysis of the map.

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.

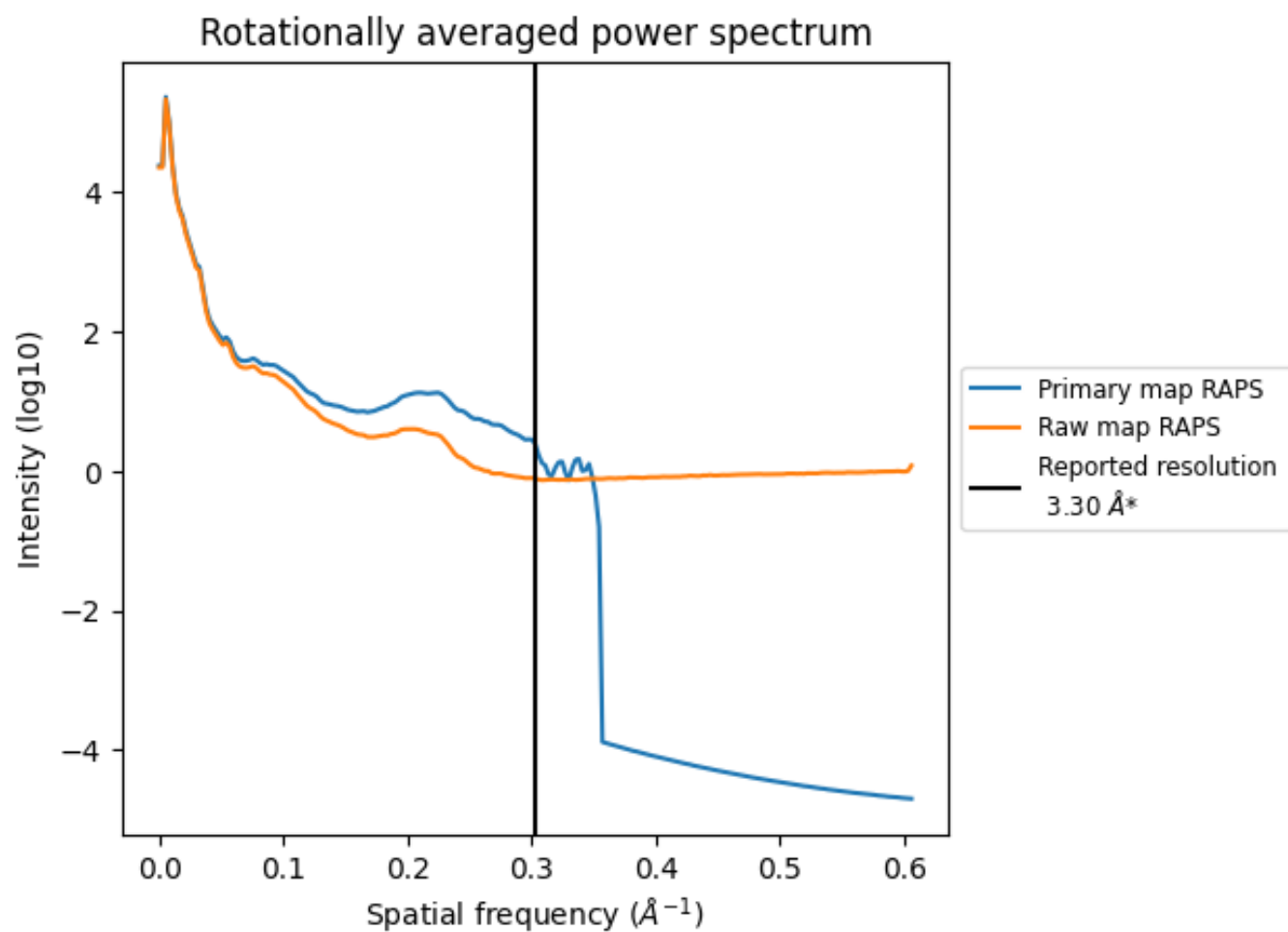
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm³; this corresponds to an approximate mass of 93 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 ⓘ

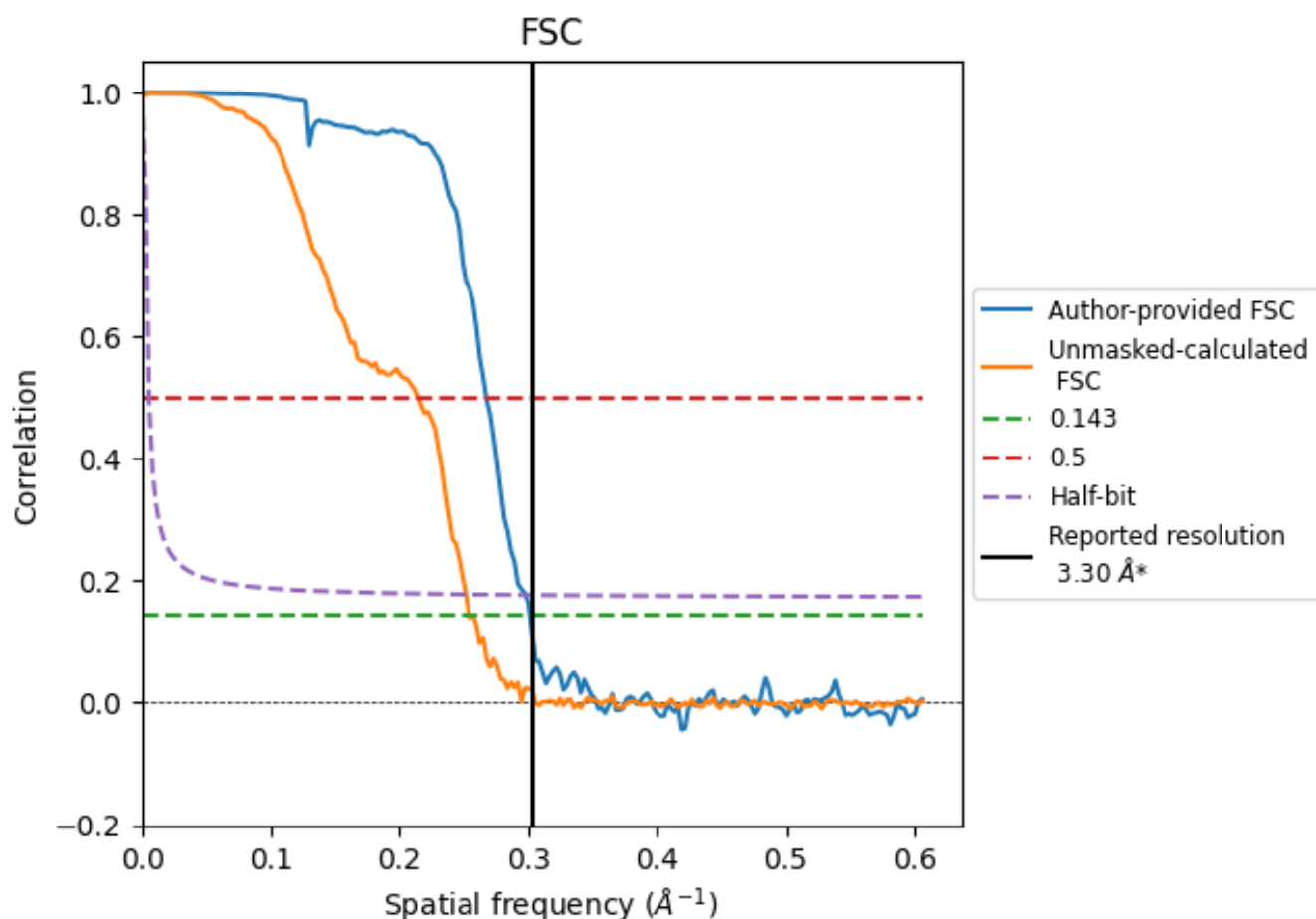


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

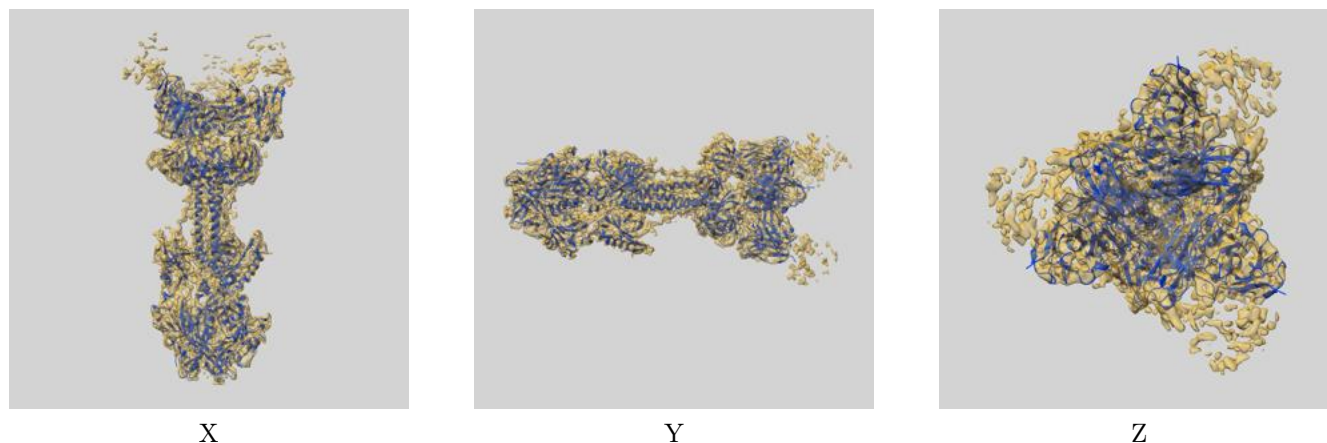
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.74	3.35
Unmasked-calculated*	3.94	4.66	3.97

*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 3.94 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

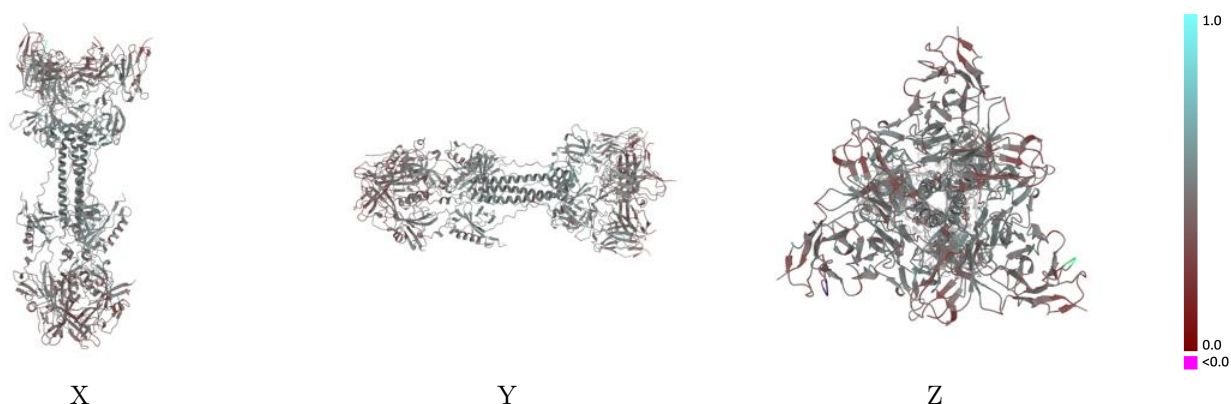
This section contains information regarding the fit between EMDB map EMD-26520 and PDB model 7UHZ. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



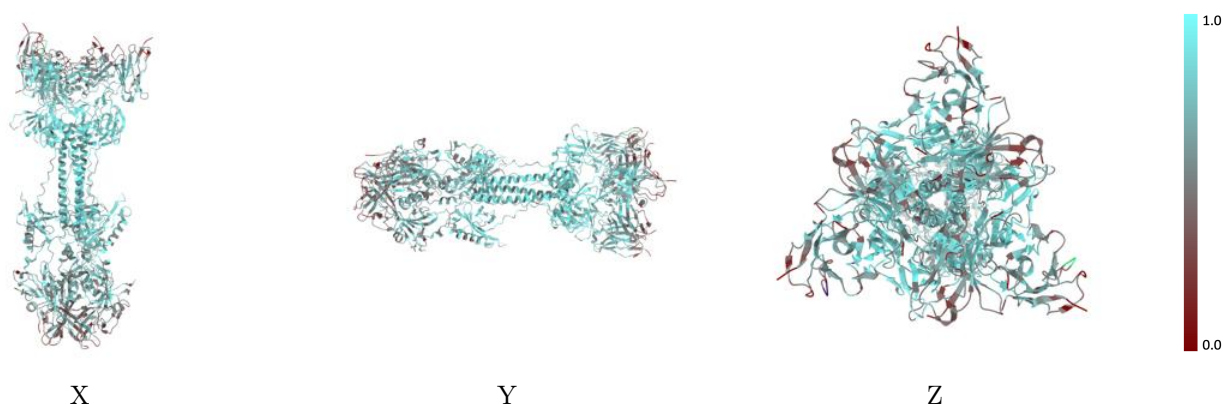
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



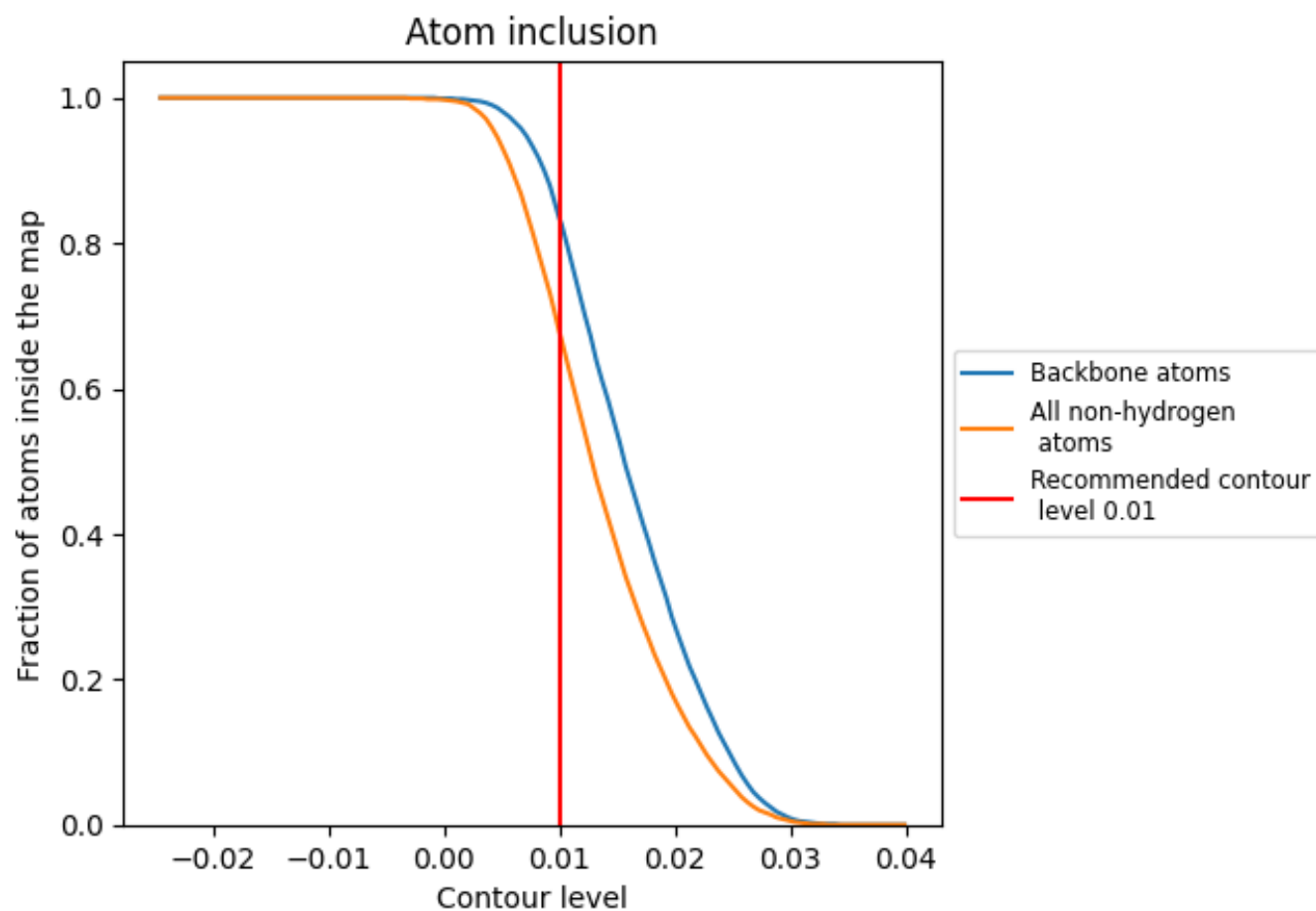
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6780	0.4560
A	0.7040	0.4680
B	0.7110	0.4730
C	0.7040	0.4610
H	0.6140	0.4350
I	0.6230	0.4350
J	0.6300	0.4410
L	0.5810	0.4030
M	0.5870	0.4240
N	0.5920	0.4130

1.0

0.0

<0.0