



Full wwPDB EM Validation Report ⓘ

Sep 4, 2026 – 11:02 AM EDT

PDB ID : 12TF / pdb_000012tf
EMDB ID : EMD-76740
Title : GII.4 Syd T=4 (raised) VLP
Deposited on : 2026-04-17
Resolution : 3.89 Å (reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

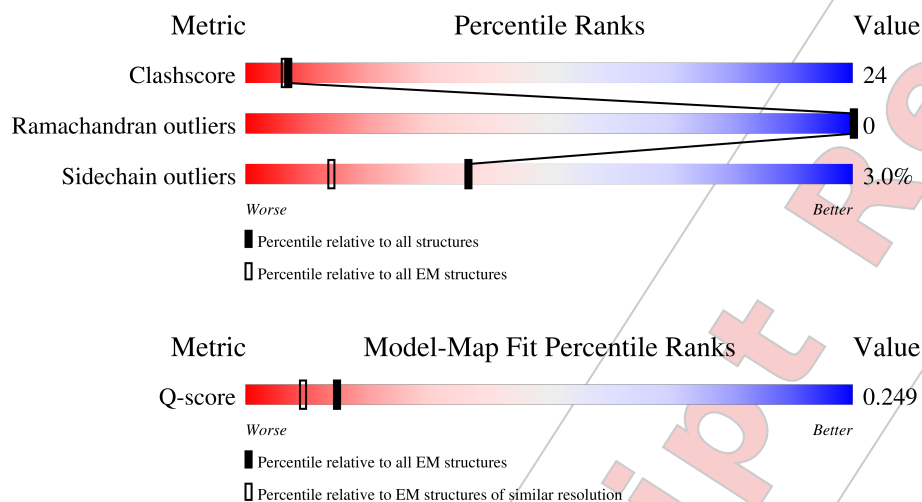
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.89 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	8712 (3.39 - 4.39)

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	540	50% 38% 10%
1	B	540	51% 38% 10%
1	C	540	48% 41% 10%
1	D	540	49% 40% 10%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 15053 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.

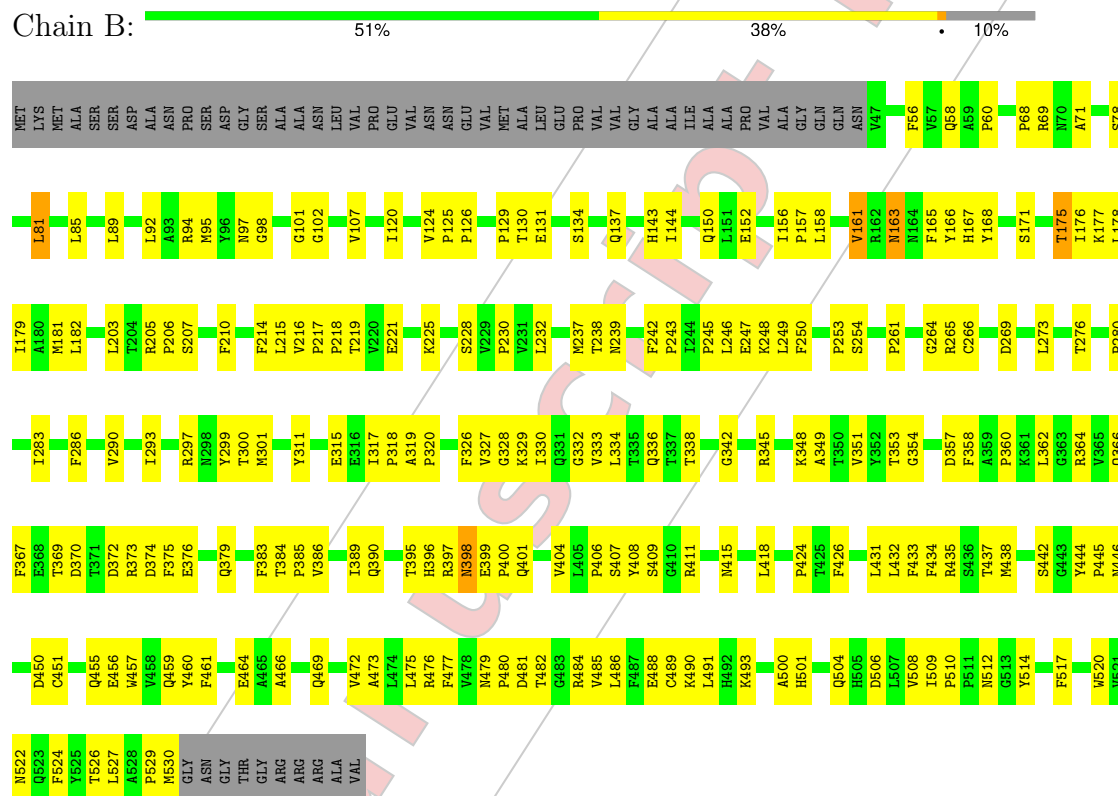
- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	484	Total	C	N	O	S	0	0
			3767	2413	638	702	14		
1	D	484	Total	C	N	O	S	0	0
			3767	2413	638	702	14		
1	C	484	Total	C	N	O	S	0	0
			3761	2410	635	702	14		
1	A	484	Total	C	N	O	S	0	0
			3758	2409	634	701	14		

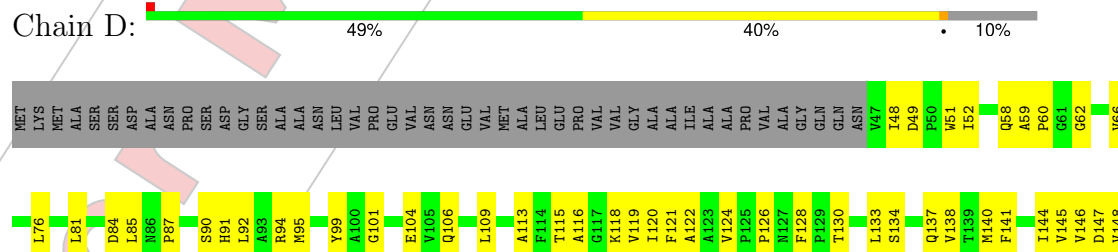
3 Residue-property plots

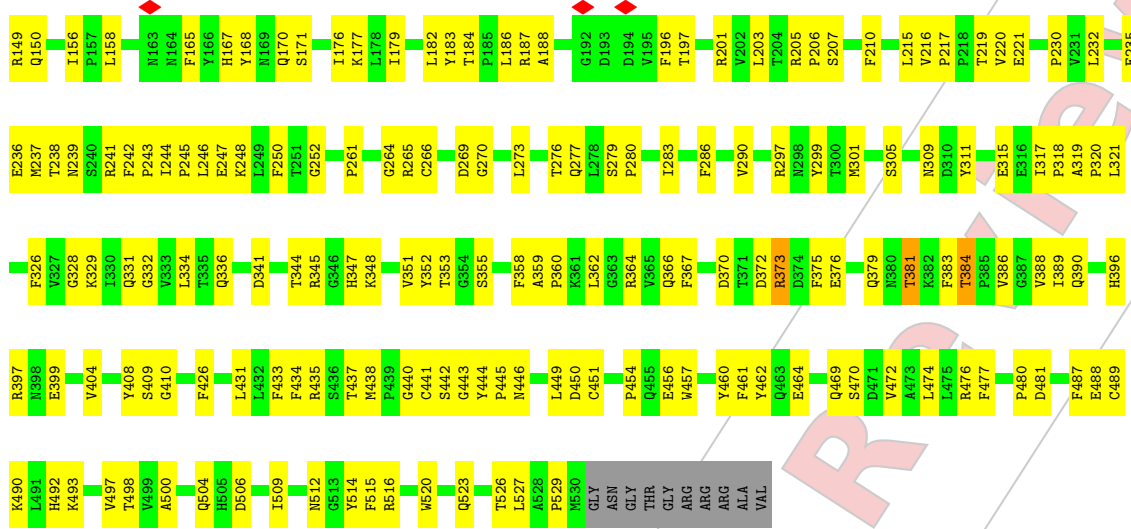
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: VP1



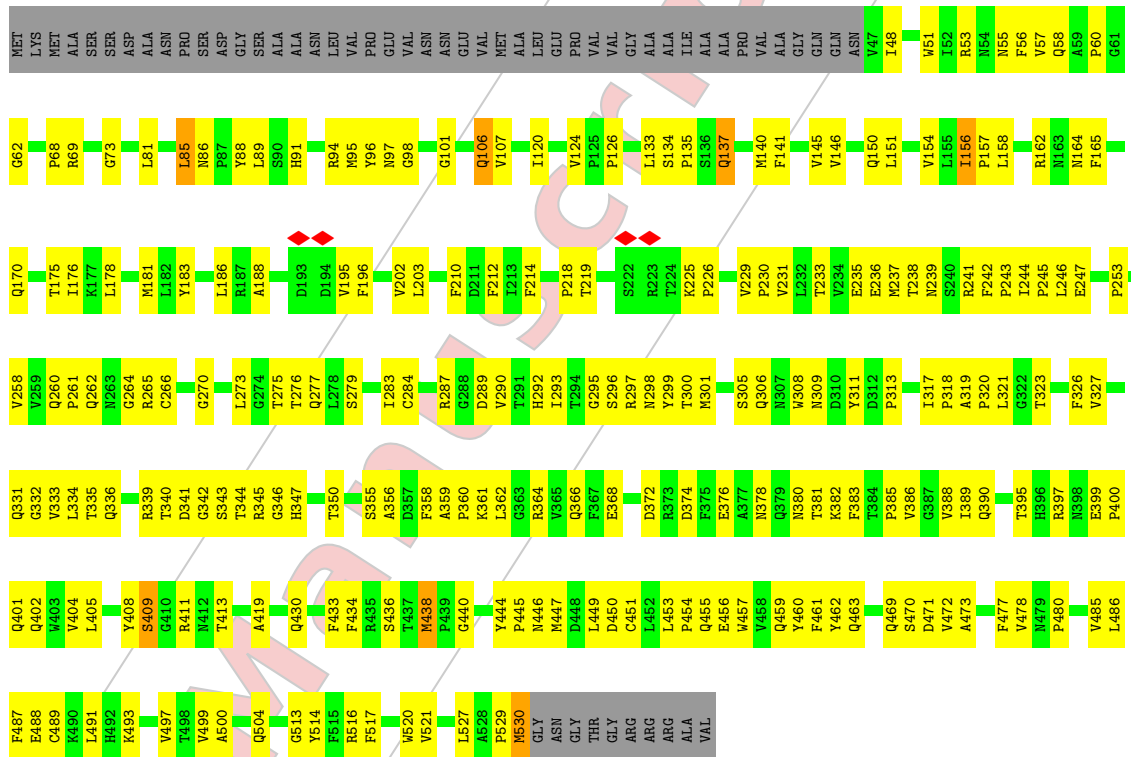
- Molecule 1: VP1





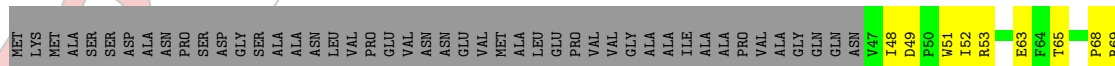
• Molecule 1: VP1

Chain C: 48% 41% 10%



• Molecule 1: VP1

Chain A: 50% 38% 10%



G73	M163	P261	F358	S442	R515
E74	M164	R265	A359	G443	R516
I75	F165	C266	K361	Y444	W520
L76	Y166	L273	L362	P445	N521
W77	H167	G274	G363	N446	N522
L81	Y168	T275	R364	M447	Q523
G82	N169	Q276	V365	D448	F524
P83	Q170	T277	Q366	L449	Y525
D84	T175	Q277	D370	D450	T526
S90	I179	P280	T371	P454	L527
H91	A180	I283	D372	Q455	A528
L92	M181	C284	R373	E456	P529
A93	L182	F375	D374	W457	N530
R94	Y183	T285	F376	V458	GLY
N97	T184	F286	Q379	Q459	ASN
G98	R187	R287	F383	Y460	GLY
Y99	A188	R297	V386	A465	THR
A100	S199	L303	G387	Q469	GLY
G101	C200	W308	V388	S470	ARG
Q106	R201	Y311	I389	D471	ARG
V107	V202	L321	Q390	V472	ALA
I108	F210	E315	T395	R476	VAL
L109	I213	E316	H396	F477	
N112	F214	I317	R397	V478	
A113	L215	P318	N398	N479	
F114	V216	A319	E399	P480	
T115	V220	P320	Q401	D481	
A116	R223	P324	V404	T482	
G117	K118	V327	S407	G483	
K119	V119	G328	Y408	R484	
I120	K225	K329	G410	V485	
F121	P226	G332	R411	L486	
L133	P230	V333	W415	F487	
S134	V234	Q336	L418	E488	
P135	M237	T337	P424	C489	
S136	T238	T338	T425	K490	
Q137	N239	G342	F426	L491	
V138	S240	R345	L431	H492	
T139	R241	G346	L432	K493	
H143	F242	H347	F433	V497	
I144	P243	T353	F434	T498	
V145	I244	G354	R435	V499	
V146	P245	S355	S436	A500	
D147	L246	A356	T437	Q504	
P153	E247	D357	M438	H505	
I156	K248			D506	
P157	L249			I509	
L158	F250			P510	
	P253			F511	
				N512	
				G513	
				Y514	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16898	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.550	Depositor
Minimum map value	-0.162	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.076	Depositor
Map size (Å)	1058.4, 1058.4, 1058.4	wwPDB
Map dimensions	980, 980, 980	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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	0.31	0/3874	0.45	0/5314
1	B	0.32	0/3883	0.42	0/5325
1	C	0.28	0/3877	0.42	0/5318
1	D	0.24	0/3883	0.39	0/5325
All	All	0.29	0/15517	0.42	0/21282

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3758	0	3619	178	0
1	B	3767	0	3634	180	0
1	C	3761	0	3623	205	0
1	D	3767	0	3634	175	0
All	All	15053	0	14510	710	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 (710) 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:165:PHE:HB3	1:B:167:HIS:CE1	1.75	1.20
1:A:135:PRO:HB3	1:A:183:TYR:CD1	2.00	0.97
1:B:165:PHE:CB	1:B:167:HIS:CE1	2.52	0.93
1:B:165:PHE:HB3	1:B:167:HIS:HE1	1.37	0.86
1:B:490:LYS:HG3	1:B:527:LEU:HD21	1.57	0.86
1:C:56:PHE:HB3	1:C:203:LEU:HD12	1.58	0.86
1:D:443:GLY:HA3	1:C:344:THR:HG23	1.59	0.85
1:A:360:PRO:HD2	1:A:408:TYR:HA	1.58	0.84
1:D:84:ASP:HA	1:D:90:SER:HB2	1.60	0.82
1:A:238:THR:HA	1:A:245:PRO:HA	1.61	0.82
1:A:253:PRO:HD2	1:A:504:GLN:HG2	1.61	0.82
1:A:120:ILE:HG21	1:A:183:TYR:CE1	2.15	0.82
1:B:120:ILE:HG23	1:B:181:MET:HB3	1.62	0.82
1:C:287:ARG:HH12	1:C:306:GLN:HA	1.46	0.80
1:C:480:PRO:HD3	1:C:513:GLY:HA2	1.62	0.80
1:A:115:THR:HG23	1:A:188:ALA:HB2	1.64	0.79
1:C:331:GLN:HB2	1:C:389:ILE:HG23	1.64	0.79
1:B:473:ALA:HB3	1:B:491:LEU:HD21	1.65	0.79
1:A:445:PRO:HG2	1:A:447:MET:HE3	1.66	0.78
1:C:120:ILE:HG23	1:C:181:MET:HB3	1.65	0.78
1:B:97:ASN:HB3	1:B:214:PHE:HB3	1.64	0.78
1:C:261:PRO:HG2	1:C:265:ARG:HD3	1.66	0.78
1:D:94:ARG:HH12	1:D:220:VAL:HA	1.48	0.77
1:B:286:PHE:HB2	1:B:383:PHE:HB3	1.64	0.77
1:A:490:LYS:HG3	1:A:527:LEU:HD21	1.67	0.77
1:B:358:PHE:HD2	1:B:411:ARG:HH22	1.32	0.77
1:D:433:PHE:HB3	1:D:450:ASP:HB3	1.67	0.77
1:C:181:MET:HE2	1:C:181:MET:HA	1.67	0.76
1:C:238:THR:HA	1:C:245:PRO:HA	1.68	0.76
1:D:106:GLN:HE21	1:D:203:LEU:HB2	1.52	0.75
1:C:253:PRO:HD2	1:C:504:GLN:HG2	1.67	0.75
1:A:433:PHE:HB3	1:A:450:ASP:HB3	1.67	0.75
1:A:181:MET:HE3	1:A:182:LEU:N	2.01	0.74
1:B:120:ILE:HD11	1:B:143:HIS:HB2	1.68	0.74
1:C:68:PRO:HA	1:C:186:LEU:HD21	1.68	0.74
1:D:359:ALA:HB3	1:D:364:ARG:HH21	1.50	0.73
1:A:249:LEU:HD11	1:A:432:LEU:HG	1.70	0.73
1:B:161:VAL:HB	1:B:165:PHE:HZ	1.51	0.73
1:A:318:PRO:HB2	1:A:408:TYR:HD2	1.54	0.72
1:B:247:GLU:HG2	1:B:248:LYS:HG2	1.71	0.72
1:B:161:VAL:HB	1:B:165:PHE:CZ	2.24	0.71
1:B:372:ASP:HB3	1:B:373:ARG:HD3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:ASP:H	1:D:493:LYS:HZ3	1.39	0.71
1:B:248:LYS:HZ1	1:B:506:ASP:HB3	1.56	0.71
1:D:523:GLN:HE22	1:A:524:PHE:HB3	1.55	0.71
1:C:453:LEU:HD12	1:C:454:PRO:HD2	1.72	0.70
1:D:118:LYS:HB2	1:D:184:THR:HG23	1.74	0.70
1:D:332:GLY:HA2	1:D:386:VAL:HG13	1.73	0.70
1:A:120:ILE:HG21	1:A:183:TYR:CZ	2.25	0.70
1:B:297:ARG:HH21	1:B:370:ASP:HA	1.57	0.69
1:D:476:ARG:HG2	1:D:488:GLU:HG3	1.74	0.69
1:A:224:THR:HG22	1:A:225:LYS:H	1.58	0.68
1:B:238:THR:HA	1:B:245:PRO:HA	1.76	0.68
1:D:168:TYR:HB2	1:D:171:SER:HB2	1.74	0.68
1:C:397:ARG:HG3	1:C:446:ASN:HA	1.75	0.68
1:C:107:VAL:HG22	1:C:202:VAL:HA	1.75	0.68
1:A:297:ARG:HH21	1:A:370:ASP:HA	1.57	0.68
1:C:292:HIS:CE1	1:C:295:GLY:H	2.12	0.68
1:D:290:VAL:HG13	1:D:381:THR:HG21	1.76	0.67
1:C:260:GLN:HE21	1:C:405:LEU:HG	1.59	0.67
1:C:290:VAL:HG11	1:C:334:LEU:HD21	1.74	0.67
1:A:400:PRO:HD3	1:A:445:PRO:HB2	1.76	0.67
1:C:478:VAL:HG11	1:C:516:ARG:HH21	1.60	0.67
1:B:486:LEU:HD22	1:B:509:ILE:HG22	1.77	0.67
1:B:469:GLN:HB2	1:B:520:TRP:CD1	2.30	0.67
1:C:318:PRO:HB2	1:C:408:TYR:HD2	1.60	0.66
1:C:491:LEU:HA	1:C:497:VAL:HG22	1.76	0.66
1:C:478:VAL:HG12	1:C:485:VAL:HG12	1.78	0.66
1:A:81:LEU:HD13	1:A:82:GLY:H	1.61	0.66
1:C:120:ILE:HB	1:C:145:VAL:HG22	1.78	0.66
1:A:469:GLN:HB2	1:A:520:TRP:CD1	2.31	0.66
1:D:247:GLU:HG2	1:D:248:LYS:HG2	1.78	0.65
1:D:445:PRO:HD2	1:C:342:GLY:HA3	1.78	0.65
1:D:469:GLN:HB2	1:D:520:TRP:CD1	2.30	0.65
1:C:433:PHE:HB3	1:C:450:ASP:HB3	1.78	0.65
1:B:389:ILE:HG22	1:B:442:SER:H	1.60	0.65
1:C:292:HIS:HE1	1:C:296:SER:H	1.44	0.65
1:A:120:ILE:HD11	1:A:143:HIS:HB2	1.78	0.65
1:A:476:ARG:HD2	1:A:485:VAL:HG11	1.79	0.65
1:A:120:ILE:HG23	1:A:181:MET:HB3	1.79	0.65
1:A:424:PRO:HD3	1:A:431:LEU:HG	1.79	0.65
1:B:476:ARG:HD2	1:B:485:VAL:HG11	1.78	0.65
1:D:242:PHE:HD2	1:D:244:ILE:HG12	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ILE:HD13	1:A:179:ILE:HG23	1.78	0.65
1:A:248:LYS:HZ1	1:A:506:ASP:HB3	1.63	0.64
1:D:140:MET:HE1	1:D:141:PHE:CE1	2.32	0.64
1:D:360:PRO:HD2	1:D:408:TYR:HA	1.79	0.64
1:A:73:GLY:H	1:A:181:MET:HE2	1.61	0.64
1:C:62:GLY:HA3	1:C:202:VAL:HB	1.79	0.64
1:C:297:ARG:HA	1:C:372:ASP:HB3	1.78	0.64
1:B:98:GLY:HA3	1:B:166:TYR:CE2	2.33	0.64
1:B:246:LEU:HD11	1:B:434:PHE:HB3	1.80	0.64
1:A:91:HIS:HA	1:A:94:ARG:HH22	1.63	0.64
1:B:248:LYS:HG3	1:B:435:ARG:HD3	1.80	0.64
1:B:95:MET:HG2	1:B:218:PRO:HB3	1.80	0.64
1:B:168:TYR:HB2	1:B:171:SER:HB2	1.79	0.64
1:C:339:ARG:HH22	1:C:376:GLU:HB2	1.61	0.63
1:A:318:PRO:HB2	1:A:408:TYR:CD2	2.33	0.63
1:A:372:ASP:HB3	1:A:373:ARG:HD3	1.79	0.63
1:A:135:PRO:HB3	1:A:183:TYR:CE1	2.33	0.63
1:D:331:GLN:HG2	1:D:348:LYS:HE3	1.80	0.62
1:D:205:ARG:HG2	1:D:206:PRO:HD2	1.80	0.62
1:C:477:PHE:HD2	1:C:486:LEU:HD12	1.65	0.62
1:D:372:ASP:HB3	1:D:373:ARG:HD3	1.81	0.62
1:A:68:PRO:HB2	1:A:69:ARG:HH22	1.63	0.62
1:B:98:GLY:HA3	1:B:166:TYR:HE2	1.65	0.61
1:C:350:THR:HB	1:C:368:GLU:HB2	1.82	0.61
1:D:397:ARG:HD3	1:D:446:ASN:HA	1.82	0.61
1:D:116:ALA:HB3	1:D:187:ARG:HE	1.64	0.61
1:D:119:VAL:HA	1:D:183:TYR:H	1.66	0.61
1:C:499:VAL:HG22	1:C:530:MET:HG3	1.83	0.61
1:B:249:LEU:HD11	1:B:432:LEU:HG	1.83	0.61
1:C:101:GLY:HA3	1:C:210:PHE:HA	1.82	0.61
1:B:134:SER:HB2	1:B:137:GLN:HE22	1.66	0.61
1:A:106:GLN:HE21	1:A:153:PRO:HB2	1.64	0.61
1:B:362:LEU:HG	1:B:409:SER:HA	1.82	0.60
1:D:113:ALA:HA	1:D:149:ARG:HG2	1.83	0.60
1:D:444:TYR:HD1	1:C:341:ASP:HB3	1.66	0.60
1:C:318:PRO:HB2	1:C:408:TYR:CD2	2.36	0.60
1:B:349:ALA:HA	1:B:369:THR:HA	1.82	0.60
1:C:470:SER:HB2	1:C:520:TRP:HB3	1.82	0.60
1:A:247:GLU:HG2	1:A:248:LYS:HG2	1.84	0.60
1:C:48:ILE:HG12	1:C:53:ARG:HH21	1.65	0.60
1:C:68:PRO:HB2	1:C:69:ARG:NH2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:PHE:HA	1:C:404:VAL:O	2.02	0.60
1:C:409:SER:HB2	1:C:413:THR:HB	1.83	0.60
1:B:243:PRO:HD3	1:B:283:ILE:HB	1.83	0.60
1:D:119:VAL:HG22	1:D:182:LEU:HD23	1.84	0.60
1:D:480:PRO:HB3	1:D:514:TYR:HE1	1.67	0.59
1:A:120:ILE:HG21	1:A:183:TYR:CD1	2.36	0.59
1:A:328:GLY:H	1:A:353:THR:HG23	1.66	0.59
1:B:390:GLN:HB2	1:B:445:PRO:HB3	1.85	0.59
1:D:134:SER:HB2	1:D:137:GLN:HG3	1.84	0.59
1:B:205:ARG:HG2	1:B:206:PRO:HD2	1.85	0.59
1:B:338:THR:HB	1:B:342:GLY:H	1.68	0.59
1:B:269:ASP:H	1:B:493:LYS:HZ1	1.50	0.59
1:C:247:GLU:OE1	1:C:436:SER:HA	2.03	0.59
1:C:287:ARG:NH1	1:C:306:GLN:HA	2.18	0.59
1:D:362:LEU:HG	1:D:409:SER:HA	1.84	0.59
1:B:280:PRO:HA	1:B:283:ILE:HD11	1.85	0.59
1:A:480:PRO:HB3	1:A:514:TYR:HE1	1.68	0.59
1:A:447:MET:HE2	1:A:447:MET:HA	1.84	0.58
1:C:241:ARG:HH22	1:C:402:GLN:HB2	1.67	0.58
1:C:292:HIS:HE2	1:C:372:ASP:HB2	1.65	0.58
1:A:286:PHE:HB2	1:A:383:PHE:HB3	1.85	0.58
1:D:165:PHE:HB3	1:A:163:ASN:ND2	2.19	0.58
1:D:470:SER:HB2	1:D:520:TRP:HB3	1.84	0.58
1:C:48:ILE:H	1:C:53:ARG:NH2	2.02	0.58
1:C:48:ILE:H	1:C:53:ARG:HH21	1.50	0.58
1:C:488:GLU:HB2	1:C:530:MET:HE1	1.86	0.58
1:A:478:VAL:HG12	1:A:485:VAL:HG12	1.86	0.58
1:B:315:GLU:HB2	1:B:317:ILE:HG12	1.86	0.57
1:C:81:LEU:HD22	1:C:158:LEU:HD21	1.85	0.57
1:D:477:PHE:HA	1:D:515:PHE:HA	1.86	0.57
1:A:389:ILE:HG22	1:A:442:SER:H	1.69	0.57
1:B:101:GLY:HA3	1:B:210:PHE:HA	1.85	0.57
1:B:157:PRO:C	1:B:158:LEU:HD22	2.29	0.57
1:D:297:ARG:HH21	1:D:370:ASP:HA	1.69	0.57
1:B:332:GLY:HA2	1:B:386:VAL:HG12	1.87	0.57
1:D:490:LYS:HG3	1:D:527:LEU:HD21	1.85	0.57
1:B:328:GLY:H	1:B:353:THR:HG23	1.69	0.57
1:C:359:ALA:HB1	1:C:362:LEU:HD12	1.87	0.57
1:B:397:ARG:HA	1:B:446:ASN:N	2.20	0.57
1:D:120:ILE:HB	1:D:145:VAL:HG22	1.87	0.56
1:C:96:TYR:CE1	1:C:212:PHE:HB3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:VAL:HG22	1:C:381:THR:HG21	1.85	0.56
1:B:253:PRO:HD2	1:B:504:GLN:HG2	1.86	0.56
1:B:476:ARG:HB3	1:B:485:VAL:HG11	1.87	0.56
1:D:99:TYR:CE2	1:D:167:HIS:HD2	2.23	0.56
1:C:339:ARG:HH21	1:C:378:ASN:HB3	1.70	0.56
1:A:338:THR:HB	1:A:342:GLY:H	1.71	0.56
1:B:426:PHE:HE2	1:B:526:THR:HG23	1.70	0.56
1:A:277:GLN:HB3	1:A:321:LEU:HB3	1.87	0.56
1:C:317:ILE:O	1:C:361:LYS:HE2	2.06	0.56
1:C:388:VAL:HG21	1:C:400:PRO:HG3	1.86	0.56
1:D:124:VAL:HB	1:D:128:PHE:CD2	2.40	0.56
1:D:243:PRO:HD3	1:D:283:ILE:HB	1.86	0.56
1:A:181:MET:HE3	1:A:182:LEU:H	1.71	0.56
1:B:354:GLY:HA2	1:B:406:PRO:HB3	1.88	0.56
1:C:246:LEU:HD13	1:C:434:PHE:HB3	1.87	0.56
1:B:68:PRO:HB2	1:B:69:ARG:HH22	1.70	0.56
1:B:472:VAL:HG11	1:B:490:LYS:HD2	1.88	0.56
1:C:91:HIS:HA	1:C:94:ARG:NE	2.20	0.56
1:C:275:THR:HA	1:C:321:LEU:HD22	1.87	0.56
1:C:244:ILE:HD12	1:C:436:SER:OG	2.06	0.55
1:B:424:PRO:HD3	1:B:431:LEU:HG	1.87	0.55
1:C:358:PHE:HD2	1:C:411:ARG:HH22	1.54	0.55
1:B:254:SER:HB3	1:B:433:PHE:HZ	1.71	0.55
1:C:68:PRO:HB2	1:C:69:ARG:HH22	1.70	0.55
1:B:332:GLY:HA2	1:B:386:VAL:H	1.71	0.55
1:A:240:SER:HA	1:A:455:GLN:HB2	1.89	0.55
1:B:320:PRO:HD2	1:B:360:PRO:HB2	1.88	0.55
1:C:57:VAL:C	1:C:203:LEU:HD13	2.32	0.55
1:B:376:GLU:HG3	1:B:379:GLN:HG3	1.89	0.55
1:D:442:SER:C	1:C:344:THR:H	2.15	0.55
1:C:237:MET:HB2	1:C:246:LEU:HB2	1.89	0.55
1:A:345:ARG:HD3	1:A:374:ASP:O	2.07	0.55
1:B:479:ASN:ND2	1:B:510:PRO:HG3	2.22	0.54
1:D:60:PRO:HG3	1:D:87:PRO:HG3	1.88	0.54
1:D:445:PRO:HD2	1:C:343:SER:H	1.72	0.54
1:C:265:ARG:H	1:C:276:THR:HG21	1.71	0.54
1:A:522:ASN:ND2	1:A:524:PHE:HB2	2.22	0.54
1:B:156:ILE:HD12	1:B:157:PRO:HD2	1.87	0.54
1:D:320:PRO:HD2	1:D:360:PRO:HB2	1.89	0.54
1:B:125:PRO:HG3	1:A:214:PHE:CZ	2.42	0.54
1:D:476:ARG:HB2	1:D:516:ARG:HH21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:PRO:HA	1:D:283:ILE:HD11	1.90	0.54
1:C:445:PRO:HG2	1:C:447:MET:HE3	1.88	0.54
1:B:237:MET:HB2	1:B:246:LEU:HD23	1.89	0.54
1:B:360:PRO:HD2	1:B:408:TYR:HA	1.90	0.54
1:D:301:MET:HB3	1:D:367:PHE:HE2	1.72	0.54
1:C:284:CYS:HB2	1:C:385:PRO:HG2	1.90	0.54
1:C:292:HIS:CE1	1:C:296:SER:H	2.25	0.54
1:C:133:LEU:HD12	1:C:134:SER:H	1.71	0.54
1:A:84:ASP:HA	1:A:90:SER:HB2	1.89	0.54
1:B:460:TYR:O	1:B:464:GLU:HG3	2.08	0.53
1:A:472:VAL:HG22	1:A:492:HIS:HA	1.90	0.53
1:C:456:GLU:HA	1:C:459:GLN:HE21	1.73	0.53
1:A:133:LEU:HD11	1:A:137:GLN:HB2	1.90	0.53
1:B:131:GLU:CD	1:B:131:GLU:H	2.15	0.53
1:D:277:GLN:HB3	1:D:321:LEU:HB3	1.90	0.53
1:C:186:LEU:H	1:C:186:LEU:HD23	1.73	0.53
1:D:59:ALA:HB3	1:D:62:GLY:HA3	1.89	0.53
1:D:101:GLY:HA3	1:D:210:PHE:HA	1.91	0.53
1:C:91:HIS:HA	1:C:94:ARG:CZ	2.38	0.53
1:D:384:THR:HG21	1:C:386:VAL:HG13	1.90	0.53
1:C:133:LEU:HD11	1:C:137:GLN:HB2	1.91	0.53
1:D:480:PRO:HG2	1:D:512:ASN:ND2	2.24	0.53
1:A:237:MET:HG3	1:A:246:LEU:HD12	1.91	0.53
1:B:390:GLN:HE22	1:B:396:HIS:HD2	1.57	0.53
1:D:188:ALA:HB1	1:D:196:PHE:HB3	1.90	0.53
1:D:237:MET:HB2	1:D:246:LEU:HD12	1.90	0.53
1:D:481:ASP:CG	1:D:512:ASN:HD21	2.16	0.52
1:C:469:GLN:HB2	1:C:520:TRP:CD1	2.44	0.52
1:D:328:GLY:H	1:D:353:THR:HG23	1.75	0.52
1:D:426:PHE:HE2	1:D:526:THR:HG23	1.74	0.52
1:A:280:PRO:HA	1:A:283:ILE:HD11	1.90	0.52
1:A:48:ILE:HG22	1:A:53:ARG:NH2	2.24	0.52
1:C:68:PRO:HD2	1:C:195:VAL:HG13	1.91	0.52
1:C:170:GLN:CD	1:C:170:GLN:H	2.17	0.52
1:C:270:GLY:HA3	1:C:462:TYR:HA	1.91	0.52
1:A:119:VAL:HG22	1:A:182:LEU:HA	1.92	0.52
1:A:478:VAL:HA	1:A:485:VAL:HA	1.92	0.52
1:B:479:ASN:HB3	1:B:482:THR:OG1	2.09	0.52
1:D:476:ARG:HH11	1:D:488:GLU:HG2	1.75	0.52
1:B:266:CYS:HA	1:B:273:LEU:HG	1.92	0.52
1:D:261:PRO:HG2	1:D:265:ARG:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PRO:HB2	1:A:69:ARG:NH2	2.25	0.52
1:C:356:ALA:HA	1:C:411:ARG:HG2	1.91	0.51
1:D:66:VAL:HG22	1:D:76:LEU:HD22	1.93	0.51
1:C:188:ALA:HB1	1:C:196:PHE:CD1	2.45	0.51
1:A:500:ALA:O	1:A:529:PRO:HA	2.09	0.51
1:D:51:TRP:HE3	1:D:52:ILE:HD13	1.75	0.51
1:D:376:GLU:CD	1:D:379:GLN:HG3	2.35	0.51
1:C:319:ALA:HB3	1:C:323:THR:HG21	1.91	0.51
1:A:246:LEU:HD22	1:A:434:PHE:HB3	1.93	0.51
1:B:126:PRO:HD3	1:B:176:ILE:HA	1.92	0.51
1:B:399:GLU:HB3	1:B:445:PRO:HB3	1.92	0.51
1:D:311:TYR:CE1	1:D:320:PRO:HG3	2.45	0.51
1:A:426:PHE:HE2	1:A:526:THR:HG23	1.75	0.51
1:D:396:HIS:HB3	1:C:341:ASP:OD2	2.10	0.51
1:C:91:HIS:HD2	1:C:94:ARG:NH1	2.08	0.51
1:A:332:GLY:HA2	1:A:386:VAL:H	1.74	0.51
1:A:477:PHE:CD2	1:A:486:LEU:HD13	2.45	0.51
1:C:487:PHE:HB2	1:C:530:MET:SD	2.51	0.51
1:D:115:THR:OG1	1:D:186:LEU:HD11	2.11	0.51
1:D:500:ALA:O	1:D:529:PRO:HA	2.09	0.51
1:C:230:PRO:HG2	1:C:457:TRP:CD1	2.46	0.51
1:C:233:THR:HG22	1:C:236:GLU:HG2	1.93	0.51
1:A:454:PRO:HB2	1:A:457:TRP:HB2	1.93	0.51
1:D:118:LYS:NZ	1:D:147:ASP:HB2	2.26	0.51
1:D:474:LEU:HD21	1:D:476:ARG:HH12	1.76	0.51
1:C:287:ARG:HG2	1:C:382:LYS:HB2	1.92	0.51
1:C:264:GLY:H	1:C:276:THR:HG22	1.76	0.50
1:B:480:PRO:HB3	1:B:514:TYR:HE1	1.77	0.50
1:D:91:HIS:HA	1:D:94:ARG:HD3	1.93	0.50
1:B:78:SER:HB3	1:B:179:ILE:HG22	1.94	0.50
1:B:490:LYS:HE2	1:B:527:LEU:HG	1.94	0.50
1:D:472:VAL:HG22	1:D:492:HIS:HA	1.93	0.50
1:A:500:ALA:HB2	1:A:527:LEU:HB2	1.93	0.50
1:B:68:PRO:HB2	1:B:69:ARG:NH2	2.26	0.50
1:D:431:LEU:HD23	1:D:498:THR:HB	1.93	0.50
1:C:477:PHE:CD2	1:C:486:LEU:HD12	2.45	0.50
1:A:303:LEU:HD11	1:A:365:VAL:HG23	1.92	0.50
1:B:230:PRO:HG2	1:B:457:TRP:CD1	2.47	0.50
1:B:332:GLY:HA3	1:B:385:PRO:HA	1.93	0.50
1:C:266:CYS:HA	1:C:273:LEU:HG	1.94	0.50
1:D:390:GLN:HB2	1:D:445:PRO:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ARG:HD2	1:C:372:ASP:HB3	1.92	0.50
1:C:311:TYR:OH	1:C:361:LYS:HD2	2.11	0.50
1:B:327:VAL:HG13	1:B:354:GLY:HA3	1.93	0.50
1:B:480:PRO:HG2	1:B:512:ASN:ND2	2.26	0.50
1:C:239:ASN:HD22	1:C:436:SER:HB3	1.77	0.50
1:C:242:PHE:HA	1:C:283:ILE:HG21	1.93	0.50
1:D:445:PRO:HD2	1:C:343:SER:N	2.27	0.50
1:C:319:ALA:HA	1:C:361:LYS:HD3	1.94	0.50
1:C:140:MET:HE2	1:C:140:MET:C	2.37	0.50
1:C:287:ARG:HH22	1:C:308:TRP:H	1.59	0.50
1:A:224:THR:HG22	1:A:225:LYS:N	2.26	0.50
1:C:253:PRO:HA	1:C:430:GLN:HG2	1.93	0.49
1:A:120:ILE:HB	1:A:145:VAL:HG23	1.93	0.49
1:A:318:PRO:HG3	1:A:418:LEU:HD23	1.94	0.49
1:B:250:PHE:HB2	1:B:435:ARG:HD2	1.93	0.49
1:B:406:PRO:HD2	1:B:408:TYR:OH	2.13	0.49
1:C:229:VAL:HG11	1:C:517:PHE:H	1.78	0.49
1:C:292:HIS:NE2	1:C:372:ASP:HB2	2.27	0.49
1:A:135:PRO:HB3	1:A:183:TYR:HD1	1.66	0.49
1:D:124:VAL:HG22	1:D:177:LYS:O	2.13	0.49
1:C:262:GLN:HE22	1:C:419:ALA:H	1.58	0.49
1:A:261:PRO:HG2	1:A:265:ARG:HD3	1.95	0.49
1:D:230:PRO:HD3	1:D:460:TYR:CD2	2.48	0.49
1:D:441:CYS:SG	1:C:335:THR:HA	2.53	0.49
1:A:118:LYS:N	1:A:184:THR:OG1	2.44	0.49
1:A:243:PRO:HD3	1:A:283:ILE:HB	1.94	0.49
1:B:261:PRO:HG2	1:B:265:ARG:HD3	1.94	0.49
1:D:126:PRO:HG3	1:D:176:ILE:N	2.28	0.49
1:B:130:THR:HG21	1:B:177:LYS:HE3	1.94	0.49
1:B:345:ARG:HD3	1:B:374:ASP:O	2.13	0.49
1:A:489:CYS:HB2	1:A:497:VAL:HG22	1.94	0.49
1:B:522:ASN:ND2	1:B:524:PHE:HB2	2.28	0.49
1:D:58:GLN:OE1	1:D:201:ARG:HG2	2.13	0.49
1:D:140:MET:HE1	1:D:141:PHE:CD1	2.48	0.49
1:C:308:TRP:CH2	1:C:380:ASN:HB2	2.47	0.49
1:C:480:PRO:HG3	1:C:514:TYR:CD2	2.47	0.49
1:A:156:ILE:HD12	1:A:157:PRO:HD2	1.94	0.49
1:D:290:VAL:HA	1:D:301:MET:HA	1.95	0.49
1:C:500:ALA:HB2	1:C:527:LEU:HB2	1.94	0.49
1:A:336:GLN:HB3	1:A:345:ARG:HD2	1.95	0.49
1:A:479:ASN:CG	1:A:510:PRO:HG3	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:MET:HE1	1:C:141:PHE:CD1	2.48	0.49
1:B:333:VAL:HG22	1:B:348:LYS:HD3	1.95	0.48
1:A:249:LEU:HD21	1:A:432:LEU:HD21	1.95	0.48
1:B:215:LEU:HD23	1:B:216:VAL:N	2.28	0.48
1:A:319:ALA:HB2	1:A:408:TYR:CG	2.48	0.48
1:B:397:ARG:HH12	1:B:444:TYR:HB3	1.77	0.48
1:C:246:LEU:HD11	1:C:454:PRO:HB3	1.95	0.48
1:B:319:ALA:HB2	1:B:408:TYR:CG	2.48	0.48
1:D:221:GLU:CD	1:D:221:GLU:H	2.22	0.48
1:A:170:GLN:OE1	1:A:170:GLN:N	2.40	0.48
1:D:232:LEU:HD22	1:D:236:GLU:HG3	1.95	0.48
1:C:98:GLY:HA3	1:C:214:PHE:HE2	1.77	0.48
1:A:357:ASP:OD2	1:A:366:GLN:HB2	2.13	0.48
1:B:479:ASN:HB2	1:B:486:LEU:HD11	1.96	0.48
1:C:58:GLN:H	1:A:139:THR:HG21	1.78	0.48
1:C:400:PRO:HD2	1:C:446:ASN:H	1.78	0.48
1:B:143:HIS:O	1:B:144:ILE:HD13	2.14	0.48
1:B:225:LYS:HG3	1:B:466:ALA:HA	1.94	0.48
1:D:355:SER:O	1:D:358:PHE:HB3	2.13	0.48
1:C:243:PRO:HD3	1:C:283:ILE:HB	1.95	0.48
1:A:225:LYS:HE3	1:A:465:ALA:H	1.77	0.48
1:D:336:GLN:HE21	1:D:345:ARG:HD2	1.78	0.48
1:D:389:ILE:O	1:D:399:GLU:HG2	2.13	0.48
1:C:313:PRO:HB3	1:C:361:LYS:O	2.13	0.48
1:C:459:GLN:O	1:C:463:GLN:HG2	2.14	0.48
1:C:472:VAL:HB	1:C:521:VAL:HG23	1.96	0.48
1:B:239:ASN:HB3	1:B:242:PHE:O	2.14	0.48
1:B:522:ASN:HD21	1:B:524:PHE:HB2	1.79	0.48
1:A:99:TYR:CE1	1:A:167:HIS:HB2	2.49	0.48
1:B:225:LYS:CE	1:B:464:GLU:HB2	2.44	0.47
1:B:330:ILE:HB	1:B:351:VAL:HG12	1.96	0.47
1:B:433:PHE:HB3	1:B:450:ASP:HB3	1.95	0.47
1:D:359:ALA:HB2	1:D:410:GLY:H	1.78	0.47
1:C:133:LEU:HD12	1:C:134:SER:N	2.28	0.47
1:C:332:GLY:HA3	1:C:383:PHE:CZ	2.49	0.47
1:A:230:PRO:HD3	1:A:460:TYR:CD2	2.49	0.47
1:C:230:PRO:HG3	1:C:460:TYR:CG	2.49	0.47
1:C:287:ARG:HH21	1:C:308:TRP:CG	2.32	0.47
1:C:473:ALA:HB3	1:C:491:LEU:HD23	1.96	0.47
1:A:248:LYS:HG3	1:A:435:ARG:HD3	1.97	0.47
1:A:311:TYR:CE1	1:A:320:PRO:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:GLN:HA	1:B:203:LEU:HG	1.95	0.47
1:B:318:PRO:CB	1:B:415:ASN:HB3	2.45	0.47
1:B:364:ARG:CZ	1:B:364:ARG:HB2	2.43	0.47
1:C:438:MET:HE1	1:C:449:LEU:HB2	1.94	0.47
1:A:118:LYS:HD3	1:A:147:ASP:HA	1.96	0.47
1:B:311:TYR:CE1	1:B:320:PRO:HG3	2.49	0.47
1:D:241:ARG:HB2	1:D:449:LEU:HD21	1.95	0.47
1:B:126:PRO:HB3	1:B:175:THR:O	2.14	0.47
1:B:254:SER:HB3	1:B:433:PHE:CZ	2.50	0.47
1:B:264:GLY:H	1:B:276:THR:HG23	1.80	0.47
1:A:48:ILE:HG12	1:A:49:ASP:H	1.80	0.47
1:A:397:ARG:HA	1:A:446:ASN:N	2.29	0.47
1:A:488:GLU:HG2	1:A:527:LEU:HD22	1.97	0.47
1:B:165:PHE:C	1:B:167:HIS:H	2.23	0.47
1:D:104:GLU:OE1	1:D:207:SER:HA	2.15	0.47
1:C:95:MET:HB2	1:C:218:PRO:HG3	1.97	0.47
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.61	0.47
1:B:456:GLU:HA	1:B:459:GLN:OE1	2.15	0.47
1:B:477:PHE:CD2	1:B:486:LEU:HD13	2.49	0.47
1:D:345:ARG:HG3	1:D:375:PHE:CD1	2.49	0.47
1:B:177:LYS:HG2	1:B:178:LEU:H	1.80	0.47
1:D:351:VAL:HG23	1:D:366:GLN:O	2.15	0.47
1:B:395:THR:HG23	1:B:398:ASN:HB3	1.96	0.46
1:C:472:VAL:HA	1:C:491:LEU:O	2.15	0.46
1:A:333:VAL:HG23	1:A:386:VAL:HG11	1.96	0.46
1:A:509:ILE:HD12	1:A:509:ILE:O	2.15	0.46
1:B:177:LYS:HG2	1:B:178:LEU:N	2.31	0.46
1:D:128:PHE:CD2	1:D:130:THR:HG22	2.50	0.46
1:D:364:ARG:CZ	1:D:364:ARG:HB2	2.45	0.46
1:C:241:ARG:NH2	1:C:402:GLN:HB2	2.28	0.46
1:C:438:MET:HE3	1:C:438:MET:HB3	1.81	0.46
1:A:401:GLN:O	1:A:404:VAL:HG22	2.15	0.46
1:A:476:ARG:HA	1:A:488:GLU:HA	1.97	0.46
1:B:129:PRO:HB2	1:B:131:GLU:OE2	2.15	0.46
1:C:60:PRO:HD3	1:C:85:LEU:O	2.15	0.46
1:C:62:GLY:O	1:C:202:VAL:N	2.47	0.46
1:A:470:SER:HB2	1:A:520:TRP:HB3	1.97	0.46
1:B:475:LEU:HB2	1:B:489:CYS:SG	2.55	0.46
1:D:286:PHE:HB2	1:D:383:PHE:HB3	1.96	0.46
1:D:457:TRP:HB3	1:D:461:PHE:CZ	2.50	0.46
1:C:262:GLN:NE2	1:C:419:ALA:H	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:TYR:O	1:C:366:GLN:HA	2.15	0.46
1:A:266:CYS:HA	1:A:273:LEU:HG	1.96	0.46
1:D:66:VAL:O	1:D:197:THR:HG23	2.16	0.46
1:D:264:GLY:H	1:D:276:THR:HG23	1.79	0.46
1:A:213:ILE:HG22	1:A:214:PHE:HB2	1.98	0.46
1:D:270:GLY:HA3	1:D:462:TYR:HA	1.96	0.46
1:C:258:VAL:HG22	1:C:260:GLN:OE1	2.16	0.46
1:A:109:LEU:HG	1:A:200:CYS:SG	2.55	0.46
1:D:435:ARG:HH12	1:D:437:THR:HG23	1.81	0.46
1:C:233:THR:HG23	1:C:235:GLU:H	1.80	0.46
1:A:242:PHE:HD2	1:A:244:ILE:HG12	1.79	0.46
1:B:400:PRO:HD3	1:B:445:PRO:HB2	1.97	0.46
1:B:486:LEU:HD21	1:B:510:PRO:HD2	1.98	0.46
1:C:489:CYS:HB2	1:C:497:VAL:HG11	1.98	0.46
1:A:362:LEU:HG	1:A:409:SER:HA	1.98	0.46
1:B:242:PHE:CG	1:B:243:PRO:HD2	2.51	0.46
1:D:109:LEU:HD21	1:D:150:GLN:O	2.16	0.46
1:A:332:GLY:HA2	1:A:386:VAL:HG22	1.97	0.46
1:C:98:GLY:N	1:C:214:PHE:HD2	2.14	0.46
1:A:345:ARG:HB2	1:A:347:HIS:CE1	2.51	0.46
1:B:400:PRO:HG3	1:B:446:ASN:HB3	1.97	0.45
1:D:329:LYS:HD3	1:D:352:TYR:CG	2.52	0.45
1:C:69:ARG:HH11	1:C:69:ARG:HG2	1.81	0.45
1:C:305:SER:HB3	1:C:309:ASN:HB2	1.97	0.45
1:C:400:PRO:HB2	1:C:446:ASN:HB3	1.98	0.45
1:A:51:TRP:CE3	1:A:52:ILE:HD13	2.51	0.45
1:D:170:GLN:CD	1:D:170:GLN:H	2.24	0.45
1:D:238:THR:HA	1:D:245:PRO:HA	1.98	0.45
1:C:358:PHE:HD2	1:C:411:ARG:NH2	2.13	0.45
1:C:434:PHE:O	1:C:450:ASP:HA	2.16	0.45
1:A:355:SER:O	1:A:358:PHE:HB3	2.16	0.45
1:D:286:PHE:HD2	1:D:383:PHE:HD2	1.65	0.45
1:C:162:ARG:HE	1:C:165:PHE:C	2.24	0.45
1:B:150:GLN:HG3	1:B:152:GLU:H	1.82	0.45
1:B:477:PHE:HD2	1:B:486:LEU:HD13	1.80	0.45
1:D:440:GLY:HA3	1:C:343:SER:O	2.16	0.45
1:A:490:LYS:HE2	1:A:527:LEU:HG	1.98	0.45
1:C:73:GLY:HA2	1:C:135:PRO:HG3	1.97	0.45
1:C:473:ALA:HB2	1:C:520:TRP:CZ3	2.52	0.45
1:A:81:LEU:HA	1:A:81:LEU:HD22	1.73	0.45
1:A:120:ILE:HG21	1:A:183:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:PHE:HB3	1:A:435:ARG:HB3	1.98	0.45
1:D:252:GLY:HA3	1:D:504:GLN:OE1	2.15	0.45
1:C:51:TRP:O	1:C:55:ASN:HB2	2.17	0.45
1:C:231:VAL:HG13	1:C:514:TYR:CD1	2.52	0.45
1:C:289:ASP:HA	1:C:381:THR:HG22	1.98	0.45
1:C:376:GLU:CD	1:C:376:GLU:H	2.25	0.45
1:B:71:ALA:C	1:B:182:LEU:HD23	2.41	0.45
1:B:473:ALA:HB1	1:B:517:PHE:CE1	2.52	0.45
1:D:246:LEU:HD13	1:D:434:PHE:CD2	2.52	0.45
1:D:441:CYS:C	1:C:343:SER:HB3	2.41	0.45
1:D:456:GLU:CD	1:D:456:GLU:H	2.24	0.45
1:C:345:ARG:NH1	1:C:347:HIS:CD2	2.85	0.45
1:A:170:GLN:H	1:A:170:GLN:CD	2.24	0.45
1:A:223:ARG:CZ	1:A:226:PRO:HA	2.47	0.45
1:A:315:GLU:HB2	1:A:317:ILE:HG12	1.99	0.45
1:A:320:PRO:HD2	1:A:360:PRO:HB2	1.99	0.45
1:A:376:GLU:CD	1:A:379:GLN:HG3	2.42	0.45
1:A:390:GLN:HB2	1:A:445:PRO:HB3	1.99	0.45
1:B:144:ILE:HG12	1:B:156:ILE:HD13	1.99	0.45
1:B:181:MET:HA	1:B:181:MET:HE2	1.98	0.45
1:D:215:LEU:HB3	1:C:88:TYR:OH	2.17	0.45
1:D:318:PRO:HB2	1:D:408:TYR:HD2	1.81	0.45
1:C:91:HIS:CD2	1:C:94:ARG:HD2	2.51	0.45
1:A:63:GLU:CD	1:A:201:ARG:HB3	2.42	0.45
1:A:432:LEU:HD13	1:A:499:VAL:HG11	1.98	0.45
1:B:60:PRO:HD3	1:B:85:LEU:O	2.17	0.45
1:B:482:THR:OG1	1:B:484:ARG:HG3	2.16	0.45
1:D:315:GLU:HB2	1:D:317:ILE:HG12	1.99	0.45
1:C:500:ALA:O	1:C:529:PRO:HA	2.17	0.45
1:A:101:GLY:HA3	1:A:210:PHE:HA	1.97	0.45
1:A:265:ARG:HB2	1:A:273:LEU:HB2	1.98	0.45
1:B:390:GLN:HB2	1:B:445:PRO:CB	2.46	0.44
1:D:148:VAL:HG11	1:D:186:LEU:HD13	1.97	0.44
1:A:241:ARG:HB2	1:A:449:LEU:HD21	1.99	0.44
1:B:334:LEU:HB3	1:B:375:PHE:CZ	2.52	0.44
1:C:293:ILE:HG13	1:C:296:SER:HB3	1.98	0.44
1:C:355:SER:O	1:C:358:PHE:HB3	2.17	0.44
1:B:336:GLN:HB3	1:B:345:ARG:HD2	1.99	0.44
1:D:215:LEU:HD13	1:C:88:TYR:HE2	1.82	0.44
1:A:157:PRO:C	1:A:158:LEU:HD22	2.42	0.44
1:A:280:PRO:HB3	1:A:455:GLN:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:489:CYS:HB2	1:D:497:VAL:HG12	2.00	0.44
1:A:107:VAL:HG11	1:A:121:PHE:CE2	2.53	0.44
1:A:336:GLN:NE2	1:A:379:GLN:HB2	2.32	0.44
1:A:455:GLN:HE21	1:A:459:GLN:HE21	1.65	0.44
1:B:457:TRP:HB3	1:B:461:PHE:CZ	2.53	0.44
1:D:386:VAL:HG11	1:C:333:VAL:HG21	1.99	0.44
1:D:523:GLN:NE2	1:A:524:PHE:HB3	2.28	0.44
1:C:244:ILE:HD11	1:C:449:LEU:HD23	1.98	0.44
1:C:400:PRO:CD	1:C:446:ASN:H	2.30	0.44
1:A:329:LYS:HA	1:A:329:LYS:HD2	1.78	0.44
1:A:400:PRO:HG3	1:A:446:ASN:O	2.18	0.44
1:B:329:LYS:HB2	1:B:389:ILE:O	2.18	0.44
1:C:225:LYS:HD2	1:C:226:PRO:HD2	2.00	0.44
1:A:230:PRO:HD2	1:A:457:TRP:CE2	2.53	0.44
1:A:490:LYS:HB2	1:A:527:LEU:HD11	1.99	0.44
1:A:492:HIS:HE1	1:A:498:THR:HB	1.83	0.44
1:C:96:TYR:CD1	1:C:212:PHE:HB3	2.52	0.44
1:C:97:ASN:HB3	1:C:214:PHE:CD2	2.53	0.44
1:C:126:PRO:HG3	1:C:175:THR:C	2.43	0.44
1:A:477:PHE:HB2	1:A:515:PHE:CE1	2.52	0.44
1:B:239:ASN:OD1	1:B:451:CYS:HB3	2.18	0.44
1:B:488:GLU:OE2	1:B:527:LEU:HB3	2.18	0.44
1:A:115:THR:HG23	1:A:188:ALA:CB	2.43	0.44
1:A:284:CYS:SG	1:A:324:PRO:HG3	2.58	0.44
1:A:332:GLY:HA2	1:A:386:VAL:HG13	2.00	0.44
1:B:81:LEU:HD22	1:B:81:LEU:HA	1.77	0.43
1:B:500:ALA:O	1:B:529:PRO:HA	2.17	0.43
1:D:348:LYS:HD2	1:D:348:LYS:HA	1.77	0.43
1:C:98:GLY:HA3	1:C:214:PHE:CE2	2.52	0.43
1:C:239:ASN:OD1	1:C:451:CYS:HB3	2.16	0.43
1:B:457:TRP:HB3	1:B:461:PHE:CE2	2.52	0.43
1:D:121:PHE:HB2	1:D:144:ILE:HG13	2.00	0.43
1:C:68:PRO:CA	1:C:186:LEU:HD21	2.45	0.43
1:C:390:GLN:HA	1:C:399:GLU:OE1	2.18	0.43
1:A:477:PHE:HA	1:A:515:PHE:HA	1.98	0.43
1:D:266:CYS:HA	1:D:273:LEU:HG	1.99	0.43
1:D:434:PHE:CZ	1:D:454:PRO:HD3	2.54	0.43
1:C:265:ARG:H	1:C:276:THR:CG2	2.31	0.43
1:C:311:TYR:CE1	1:C:320:PRO:HG3	2.53	0.43
1:A:179:ILE:HD13	1:A:179:ILE:HA	1.85	0.43
1:A:275:THR:HA	1:A:321:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:THR:HG23	1:A:484:ARG:HG3	1.99	0.43
1:B:290:VAL:HB	1:B:299:TYR:HB3	2.00	0.43
1:D:441:CYS:HA	1:C:336:GLN:O	2.18	0.43
1:C:124:VAL:O	1:C:176:ILE:HG13	2.18	0.43
1:C:290:VAL:HG13	1:C:381:THR:HG21	2.00	0.43
1:A:364:ARG:CZ	1:A:364:ARG:HB2	2.46	0.43
1:A:480:PRO:HG2	1:A:512:ASN:ND2	2.33	0.43
1:A:481:ASP:CG	1:A:512:ASN:HD21	2.26	0.43
1:B:56:PHE:HB3	1:B:203:LEU:HB3	1.99	0.43
1:B:481:ASP:CG	1:B:512:ASN:HD21	2.27	0.43
1:D:58:GLN:CD	1:D:201:ARG:HG2	2.43	0.43
1:D:319:ALA:HB2	1:D:408:TYR:CG	2.54	0.43
1:A:327:VAL:HG13	1:A:353:THR:O	2.18	0.43
1:B:248:LYS:HZ1	1:B:506:ASP:CB	2.27	0.43
1:D:347:HIS:HB3	1:D:370:ASP:OD1	2.18	0.43
1:C:301:MET:HE1	1:C:381:THR:HG23	2.00	0.43
1:C:470:SER:CB	1:C:520:TRP:HB3	2.47	0.43
1:D:186:LEU:HG	1:D:187:ARG:N	2.27	0.43
1:D:239:ASN:HB3	1:D:242:PHE:O	2.18	0.43
1:D:441:CYS:HB2	1:C:345:ARG:O	2.18	0.43
1:C:277:GLN:H	1:C:277:GLN:HG3	1.71	0.43
1:A:493:LYS:HA	1:A:493:LYS:HD2	1.79	0.43
1:B:94:ARG:HH22	1:B:221:GLU:N	2.16	0.43
1:B:290:VAL:HA	1:B:301:MET:HA	2.01	0.43
1:B:357:ASP:OD2	1:B:366:GLN:HB2	2.18	0.43
1:A:63:GLU:OE2	1:A:201:ARG:HB3	2.18	0.43
1:A:479:ASN:HB2	1:A:486:LEU:HD11	2.00	0.43
1:B:389:ILE:O	1:B:389:ILE:HD12	2.19	0.43
1:D:188:ALA:O	1:D:196:PHE:HB3	2.19	0.43
1:D:441:CYS:SG	1:C:346:GLY:HA2	2.59	0.43
1:A:476:ARG:HB2	1:A:516:ARG:HH21	1.84	0.43
1:D:290:VAL:HB	1:D:299:TYR:HB3	1.99	0.43
1:D:487:PHE:HE1	1:D:509:ILE:HD11	1.84	0.43
1:A:407:SER:CB	1:A:411:ARG:HA	2.49	0.43
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.79	0.42
1:B:225:LYS:HD3	1:B:225:LYS:HA	1.71	0.42
1:D:345:ARG:HB2	1:D:347:HIS:CE1	2.55	0.42
1:A:287:ARG:HE	1:A:308:TRP:HE3	1.67	0.42
1:A:336:GLN:O	1:A:345:ARG:HG2	2.19	0.42
1:B:293:ILE:HD11	1:B:300:THR:OG1	2.19	0.42
1:B:336:GLN:O	1:B:345:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:LYS:HD3	1:B:348:LYS:HA	1.96	0.42
1:C:287:ARG:HA	1:C:382:LYS:HA	2.01	0.42
1:A:115:THR:HA	1:A:188:ALA:HB2	2.01	0.42
1:B:476:ARG:HB3	1:B:485:VAL:CG1	2.49	0.42
1:C:106:GLN:HA	1:C:154:VAL:O	2.19	0.42
1:C:460:TYR:HD2	1:C:461:PHE:CD1	2.37	0.42
1:A:99:TYR:HD1	1:A:169:ASN:OD1	2.03	0.42
1:A:230:PRO:HG2	1:A:457:TRP:CD1	2.55	0.42
1:B:163:ASN:H	1:B:165:PHE:HZ	1.66	0.42
1:B:318:PRO:HB3	1:B:415:ASN:HB3	2.02	0.42
1:C:120:ILE:HG22	1:C:183:TYR:HB2	2.01	0.42
1:A:77:TRP:CH2	1:A:202:VAL:HG21	2.54	0.42
1:A:97:ASN:HB3	1:A:214:PHE:HB3	2.02	0.42
1:D:235:GLU:O	1:D:237:MET:HG2	2.19	0.42
1:A:242:PHE:CG	1:A:243:PRO:HD2	2.54	0.42
1:B:165:PHE:HB2	1:B:167:HIS:CE1	2.49	0.42
1:B:488:GLU:CG	1:B:527:LEU:HD22	2.50	0.42
1:D:48:ILE:HG22	1:D:49:ASP:H	1.83	0.42
1:D:165:PHE:HB3	1:A:163:ASN:CG	2.44	0.42
1:D:336:GLN:O	1:D:345:ARG:HG2	2.20	0.42
1:D:390:GLN:HE22	1:D:444:TYR:HB2	1.85	0.42
1:C:469:GLN:HB2	1:C:520:TRP:CG	2.55	0.42
1:A:390:GLN:NE2	1:A:396:HIS:HA	2.34	0.42
1:B:176:ILE:H	1:B:176:ILE:HD12	1.84	0.42
1:A:225:LYS:HE3	1:A:465:ALA:N	2.35	0.42
1:A:407:SER:HA	1:A:415:ASN:HD21	1.85	0.42
1:D:58:GLN:HA	1:D:203:LEU:HG	2.00	0.42
1:D:217:PRO:O	1:D:219:THR:HG23	2.20	0.42
1:D:334:LEU:HD12	1:D:334:LEU:HA	1.81	0.42
1:D:353:THR:HA	1:D:358:PHE:CD1	2.54	0.42
1:D:443:GLY:N	1:C:343:SER:HA	2.34	0.42
1:C:409:SER:HB2	1:C:413:THR:CB	2.50	0.42
1:C:471:ASP:O	1:C:493:LYS:HG3	2.19	0.42
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.79	0.42
1:B:390:GLN:NE2	1:B:396:HIS:HA	2.35	0.42
1:B:407:SER:HA	1:B:415:ASN:OD1	2.20	0.42
1:B:501:HIS:HB2	1:B:530:MET:SD	2.59	0.42
1:D:133:LEU:HD23	1:D:138:VAL:HG22	2.02	0.42
1:B:318:PRO:HG3	1:B:418:LEU:HD23	2.02	0.42
1:B:411:ARG:HD3	1:B:411:ARG:HA	1.76	0.42
1:B:469:GLN:HB2	1:B:520:TRP:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:ALA:HB2	1:D:187:ARG:HH21	1.85	0.42
1:B:435:ARG:HH22	1:B:437:THR:HG23	1.85	0.41
1:D:122:ALA:HB3	1:D:179:ILE:HD11	2.02	0.41
1:D:435:ARG:HA	1:D:449:LEU:O	2.20	0.41
1:C:360:PRO:HG2	1:C:408:TYR:HB3	2.02	0.41
1:A:435:ARG:HH12	1:A:437:THR:HG23	1.85	0.41
1:B:205:ARG:HD2	1:B:206:PRO:O	2.20	0.41
1:D:92:LEU:HD23	1:D:92:LEU:HA	1.75	0.41
1:D:438:MET:SD	1:D:438:MET:N	2.94	0.41
1:C:156:ILE:HD12	1:C:157:PRO:HD2	2.02	0.41
1:C:266:CYS:SG	1:C:270:GLY:HA2	2.60	0.41
1:C:292:HIS:HE1	1:C:295:GLY:H	1.66	0.41
1:C:434:PHE:CE1	1:C:454:PRO:HD3	2.55	0.41
1:D:81:LEU:HD12	1:D:85:LEU:HD12	2.01	0.41
1:D:182:LEU:HD22	1:D:184:THR:O	2.19	0.41
1:D:230:PRO:HG2	1:D:457:TRP:CD1	2.54	0.41
1:D:318:PRO:HB2	1:D:408:TYR:CD2	2.55	0.41
1:D:500:ALA:HB2	1:D:527:LEU:HB2	2.01	0.41
1:C:229:VAL:CG1	1:C:517:PHE:H	2.33	0.41
1:C:287:ARG:HB3	1:C:308:TRP:CH2	2.55	0.41
1:A:398:ASN:O	1:A:401:GLN:HG3	2.20	0.41
1:B:125:PRO:HG3	1:A:214:PHE:CE2	2.56	0.41
1:B:230:PRO:HD3	1:B:460:TYR:CD2	2.55	0.41
1:B:290:VAL:HB	1:B:299:TYR:CD2	2.55	0.41
1:D:124:VAL:HB	1:D:128:PHE:HD2	1.83	0.41
1:D:344:THR:HG21	1:C:440:GLY:HA3	2.03	0.41
1:A:116:ALA:N	1:A:187:ARG:O	2.54	0.41
1:A:388:VAL:HG21	1:A:438:MET:HE2	2.03	0.41
1:A:470:SER:HB3	1:A:520:TRP:HE3	1.84	0.41
1:D:124:VAL:HG21	1:D:130:THR:HG21	2.02	0.41
1:B:216:VAL:HG12	1:B:217:PRO:O	2.21	0.41
1:B:358:PHE:HD2	1:B:411:ARG:NH2	2.08	0.41
1:B:396:HIS:CE1	1:B:444:TYR:HB2	2.55	0.41
1:B:461:PHE:HA	1:B:464:GLU:OE2	2.21	0.41
1:D:248:LYS:HD3	1:D:435:ARG:HD3	2.02	0.41
1:D:493:LYS:HA	1:D:493:LYS:HD2	1.85	0.41
1:A:108:ILE:HG12	1:A:153:PRO:HA	2.02	0.41
1:A:239:ASN:HB3	1:A:242:PHE:O	2.20	0.41
1:B:144:ILE:HG12	1:B:156:ILE:CD1	2.50	0.41
1:B:336:GLN:NE2	1:B:379:GLN:HB2	2.35	0.41
1:B:500:ALA:HB2	1:B:527:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:ARG:HB2	1:D:273:LEU:HB2	2.02	0.41
1:D:326:PHE:HA	1:D:404:VAL:O	2.20	0.41
1:D:390:GLN:HG3	1:D:399:GLU:HB2	2.02	0.41
1:D:144:ILE:HG12	1:D:156:ILE:HD12	2.03	0.41
1:D:158:LEU:HD12	1:D:158:LEU:HA	1.74	0.41
1:D:341:ASP:HB3	1:C:444:TYR:HE2	1.85	0.41
1:D:444:TYR:CD1	1:C:341:ASP:HB3	2.52	0.41
1:C:300:THR:HG23	1:C:364:ARG:HG2	2.03	0.41
1:C:455:GLN:C	1:C:457:TRP:H	2.28	0.41
1:A:138:VAL:HB	1:A:183:TYR:OH	2.20	0.41
1:A:477:PHE:HD2	1:A:486:LEU:HD13	1.86	0.41
1:B:326:PHE:HA	1:B:404:VAL:O	2.21	0.41
1:D:246:LEU:HD22	1:D:434:PHE:HB3	2.01	0.41
1:C:94:ARG:O	1:C:218:PRO:HB3	2.21	0.41
1:C:262:GLN:HE22	1:C:419:ALA:N	2.18	0.41
1:C:400:PRO:HG2	1:C:446:ASN:H	1.85	0.41
1:A:469:GLN:HB2	1:A:520:TRP:NE1	2.35	0.41
1:B:102:GLY:C	1:B:207:SER:HB3	2.46	0.41
1:B:407:SER:OG	1:B:411:ARG:HA	2.21	0.41
1:B:438:MET:HE1	1:B:446:ASN:O	2.20	0.41
1:C:260:GLN:NE2	1:C:405:LEU:HG	2.32	0.41
1:C:327:VAL:HG23	1:C:401:GLN:HG3	2.03	0.41
1:A:112:ASN:ND2	1:A:114:PHE:HB2	2.36	0.41
1:A:432:LEU:HD12	1:A:432:LEU:HA	1.94	0.41
1:B:351:VAL:HG23	1:B:366:GLN:O	2.21	0.40
1:D:242:PHE:CG	1:D:243:PRO:HD2	2.56	0.40
1:D:250:PHE:HD1	1:D:506:ASP:OD1	2.04	0.40
1:C:298:ASN:ND2	1:C:366:GLN:HB3	2.36	0.40
1:A:65:THR:HA	1:A:199:SER:HA	2.03	0.40
1:A:225:LYS:N	1:A:226:PRO:HD3	2.36	0.40
1:A:396:HIS:CE1	1:A:444:TYR:HB2	2.57	0.40
1:B:232:LEU:CD1	1:B:237:MET:HE1	2.51	0.40
1:B:490:LYS:HB2	1:B:527:LEU:HD11	2.04	0.40
1:D:182:LEU:HD21	1:D:186:LEU:HB2	2.03	0.40
1:D:297:ARG:HG2	1:D:372:ASP:HB2	2.02	0.40
1:C:86:ASN:HB3	1:C:89:LEU:HB2	2.02	0.40
1:B:351:VAL:HB	1:B:367:PHE:CD1	2.56	0.40
1:B:353:THR:HA	1:B:358:PHE:CD1	2.57	0.40
1:B:488:GLU:HG3	1:B:527:LEU:HD22	2.03	0.40
1:D:116:ALA:CB	1:D:187:ARG:HE	2.30	0.40
1:D:305:SER:HB3	1:D:309:ASN:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:ALA:O	1:C:491:LEU:HB3	2.20	0.40
1:B:455:GLN:HG3	1:B:459:GLN:NE2	2.37	0.40
1:C:97:ASN:HB3	1:C:214:PHE:HB2	2.03	0.40
1:C:345:ARG:HE	1:C:374:ASP:CG	2.28	0.40
1:C:462:TYR:HD2	1:C:463:GLN:NE2	2.19	0.40
1:A:390:GLN:HB2	1:A:445:PRO:CB	2.51	0.40
1:B:249:LEU:HD12	1:B:433:PHE:O	2.21	0.40
1:B:327:VAL:O	1:B:401:GLN:HB2	2.21	0.40
1:D:51:TRP:CE3	1:D:52:ILE:HD13	2.56	0.40
1:D:94:ARG:HH22	1:D:220:VAL:HB	1.87	0.40
1:D:434:PHE:HB2	1:D:451:CYS:SG	2.61	0.40
1:A:399:GLU:HB3	1:A:445:PRO:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	482/540 (89%)	436 (90%)	46 (10%)	0	100	100
1	B	482/540 (89%)	438 (91%)	44 (9%)	0	100	100
1	C	482/540 (89%)	445 (92%)	37 (8%)	0	100	100
1	D	482/540 (89%)	445 (92%)	37 (8%)	0	100	100
All	All	1928/2160 (89%)	1764 (92%)	164 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	413/459 (90%)	399 (97%)	14 (3%)	32	55
1	B	415/459 (90%)	404 (97%)	11 (3%)	39	60
1	C	414/459 (90%)	398 (96%)	16 (4%)	28	52
1	D	415/459 (90%)	406 (98%)	9 (2%)	45	64
All	All	1657/1836 (90%)	1607 (97%)	50 (3%)	37	57

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	81	LEU
1	B	107	VAL
1	B	124	VAL
1	B	161	VAL
1	B	163	ASN
1	B	175	THR
1	B	219	THR
1	B	228	SER
1	B	384	THR
1	B	398	ASN
1	B	508	VAL
1	D	95	MET
1	D	146	VAL
1	D	216	VAL
1	D	279	SER
1	D	373	ARG
1	D	381	THR
1	D	384	THR
1	D	388	VAL
1	D	464	GLU
1	C	85	LEU
1	C	106	GLN
1	C	137	GLN
1	C	146	VAL
1	C	150	GLN
1	C	151	LEU
1	C	156	ILE
1	C	164	ASN

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Mol	Chain	Res	Type
1	C	178	LEU
1	C	219	THR
1	C	279	SER
1	C	340	THR
1	C	395	THR
1	C	409	SER
1	C	438	MET
1	C	530	MET
1	A	75	ILE
1	A	81	LEU
1	A	156	ILE
1	A	165	PHE
1	A	175	THR
1	A	182	LEU
1	A	183	TYR
1	A	216	VAL
1	A	220	VAL
1	A	234	VAL
1	A	353	THR
1	A	376	GLU
1	A	395	THR
1	A	411	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	163	ASN
1	B	167	HIS
1	B	396	HIS
1	B	504	GLN
1	D	91	HIS
1	D	106	GLN
1	D	260	GLN
1	D	336	GLN
1	D	396	HIS
1	D	469	GLN
1	D	523	GLN
1	C	55	ASN
1	C	91	HIS
1	C	282	ASN
1	C	302	ASN
1	C	309	ASN

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Mol	Chain	Res	Type
1	C	336	GLN
1	C	347	HIS
1	C	396	HIS
1	C	459	GLN
1	A	91	HIS
1	A	143	HIS
1	A	167	HIS
1	A	347	HIS
1	A	366	GLN
1	A	380	ASN
1	A	415	ASN
1	A	417	HIS
1	A	459	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

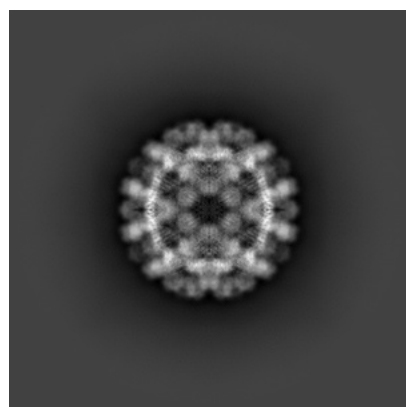
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-76740. These allow visual inspection of the internal detail of the map and identification of artifacts.

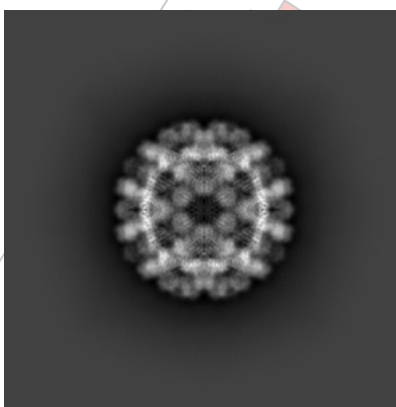
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

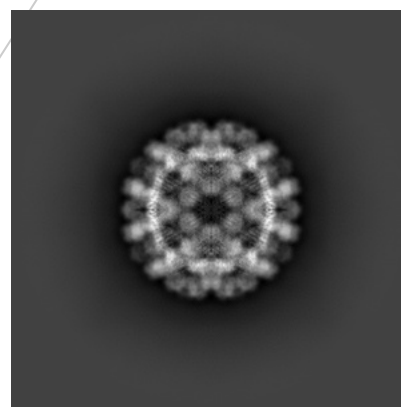
6.1.1 Primary map



X

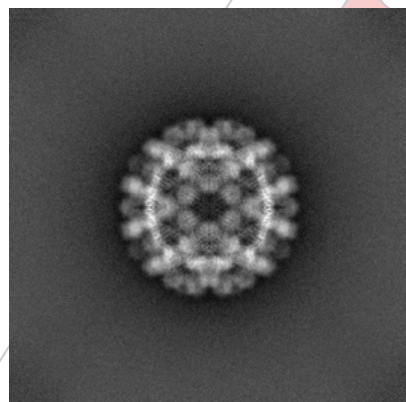


Y

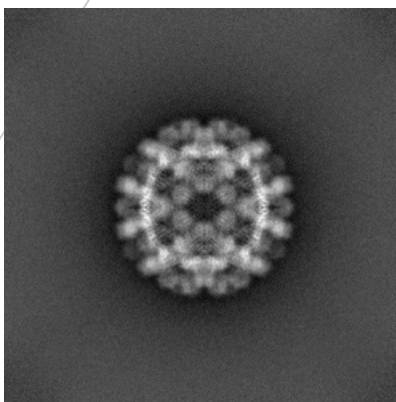


Z

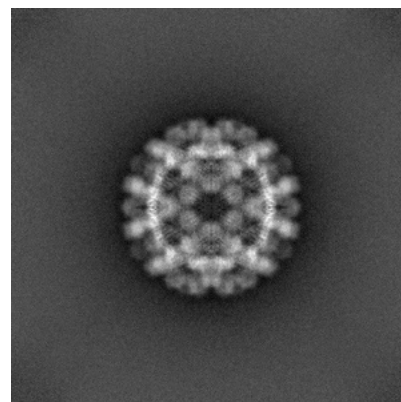
6.1.2 Raw map



X



Y

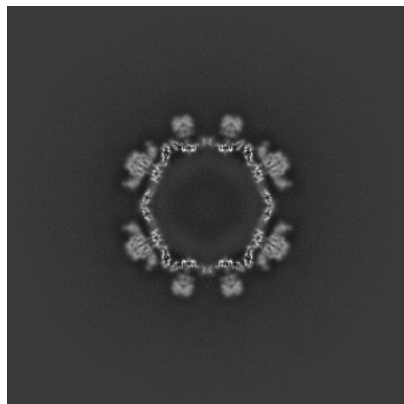


Z

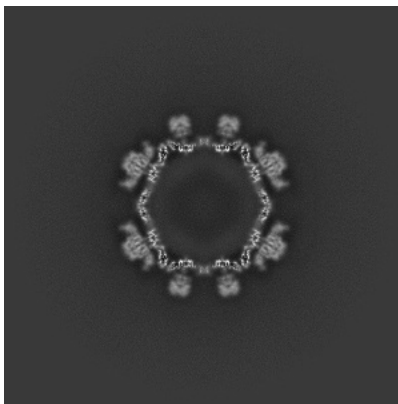
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

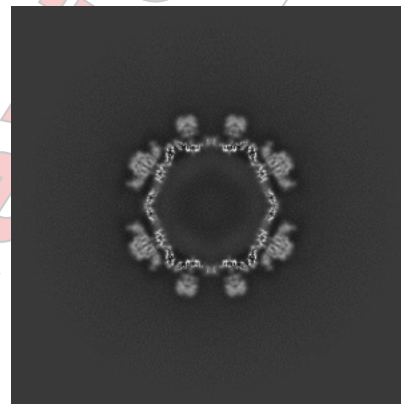
6.2.1 Primary map



X Index: 490

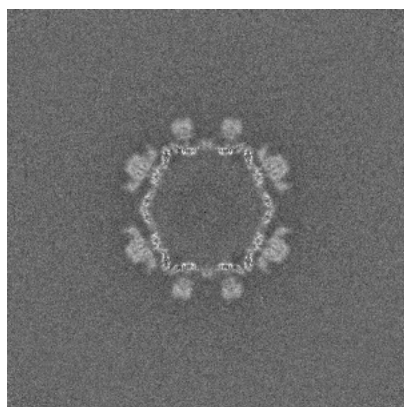


Y Index: 490

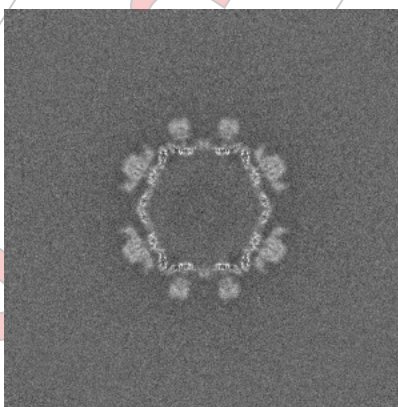


Z Index: 490

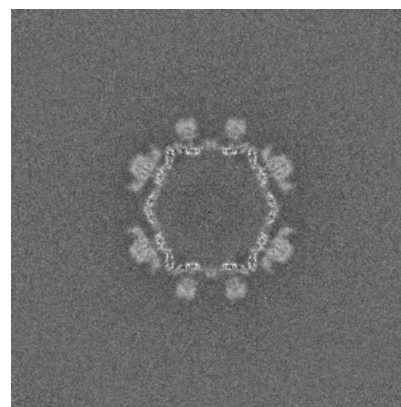
6.2.2 Raw map



X Index: 490



Y Index: 490

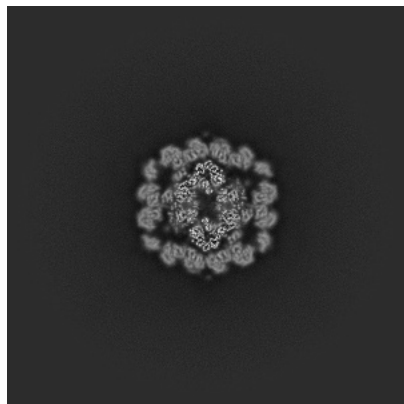


Z Index: 490

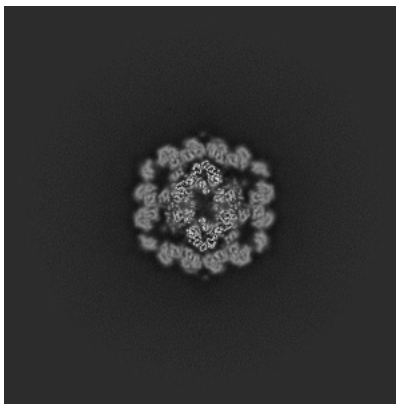
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

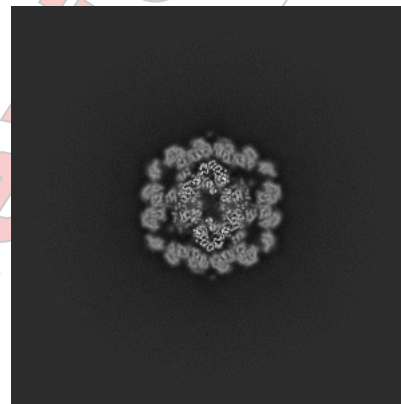
6.3.1 Primary map



X Index: 355

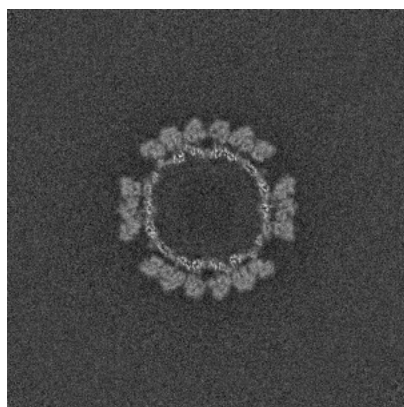


Y Index: 355

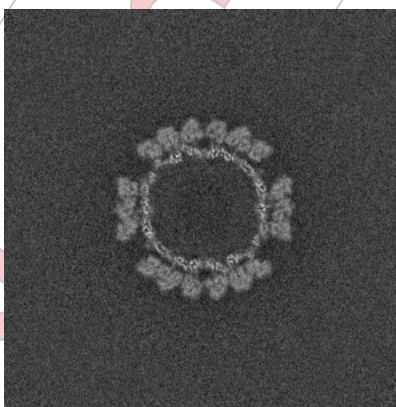


Z Index: 355

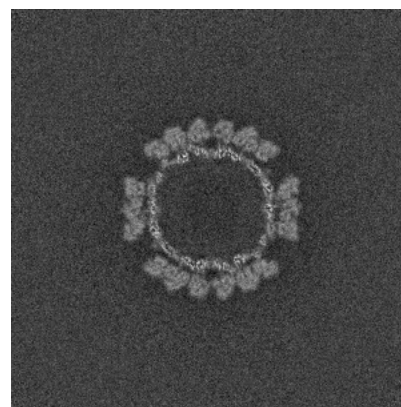
6.3.2 Raw map



X Index: 533



Y Index: 533

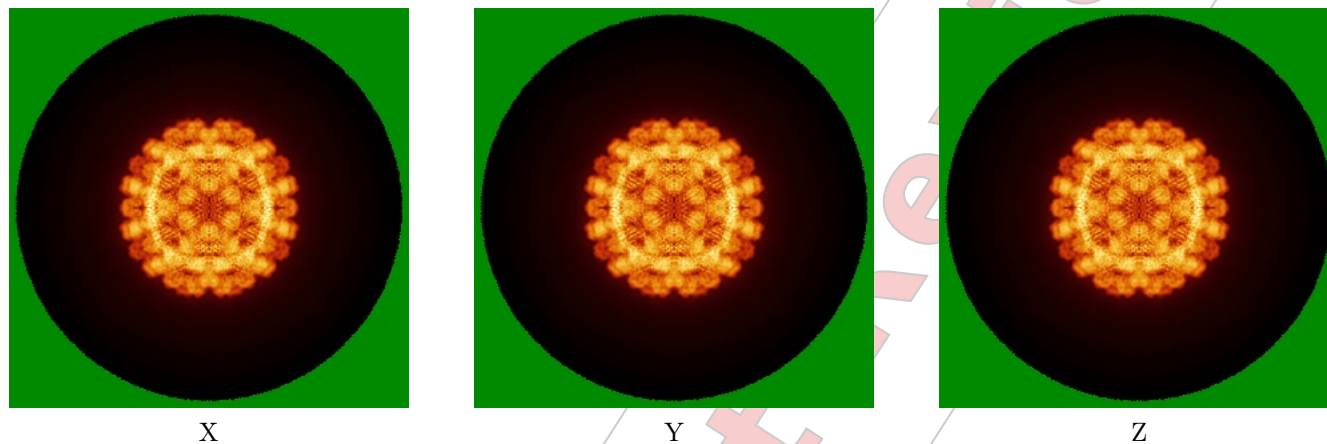


Z Index: 533

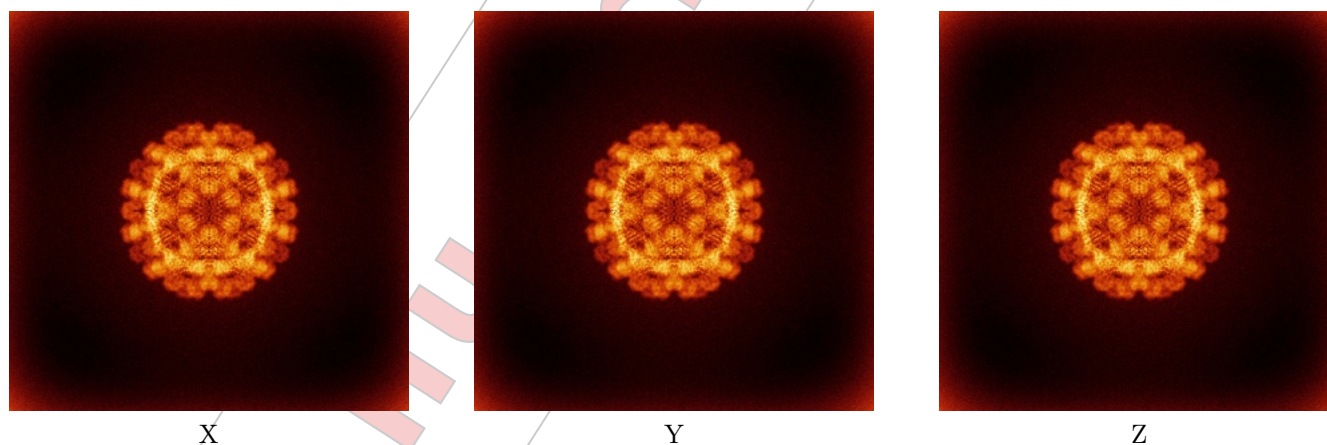
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



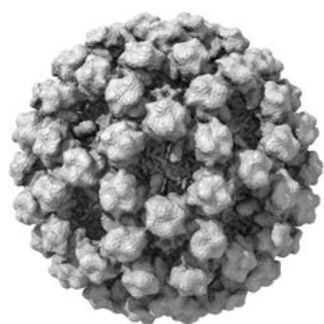
6.4.2 Raw map



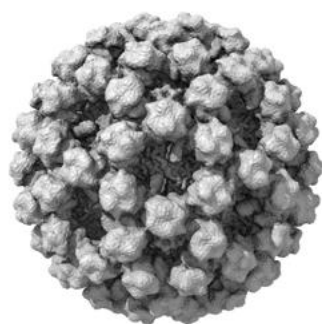
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

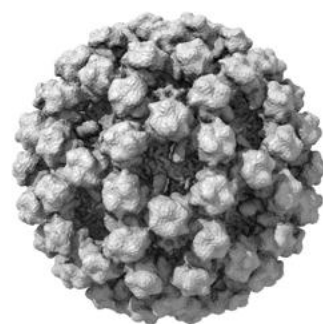
6.5.1 Primary map



X



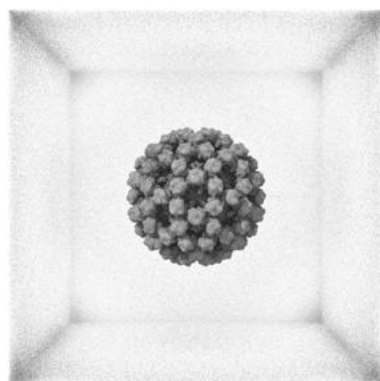
Y



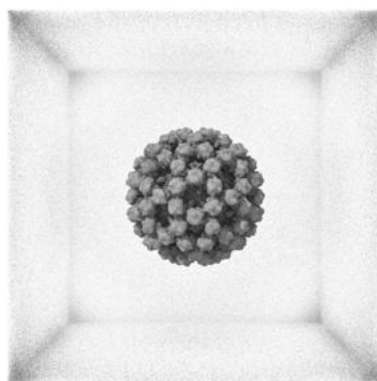
Z

The images above show the 3D surface view of the map at the recommended contour level 0.076. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

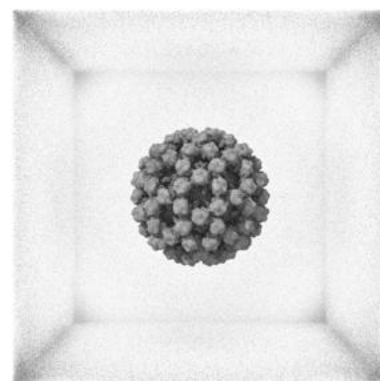
6.5.2 Raw map



X



Y



Z

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.

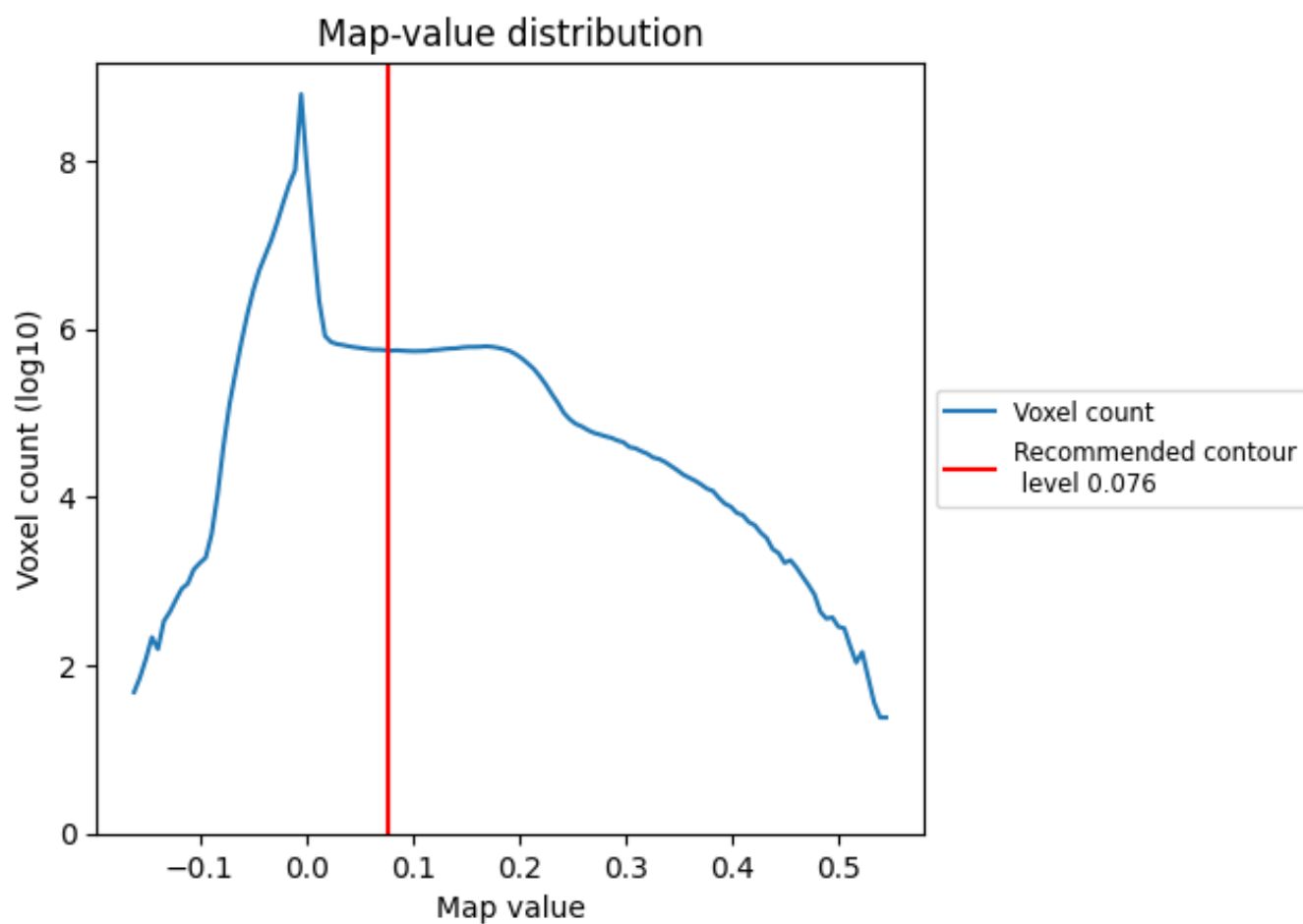
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

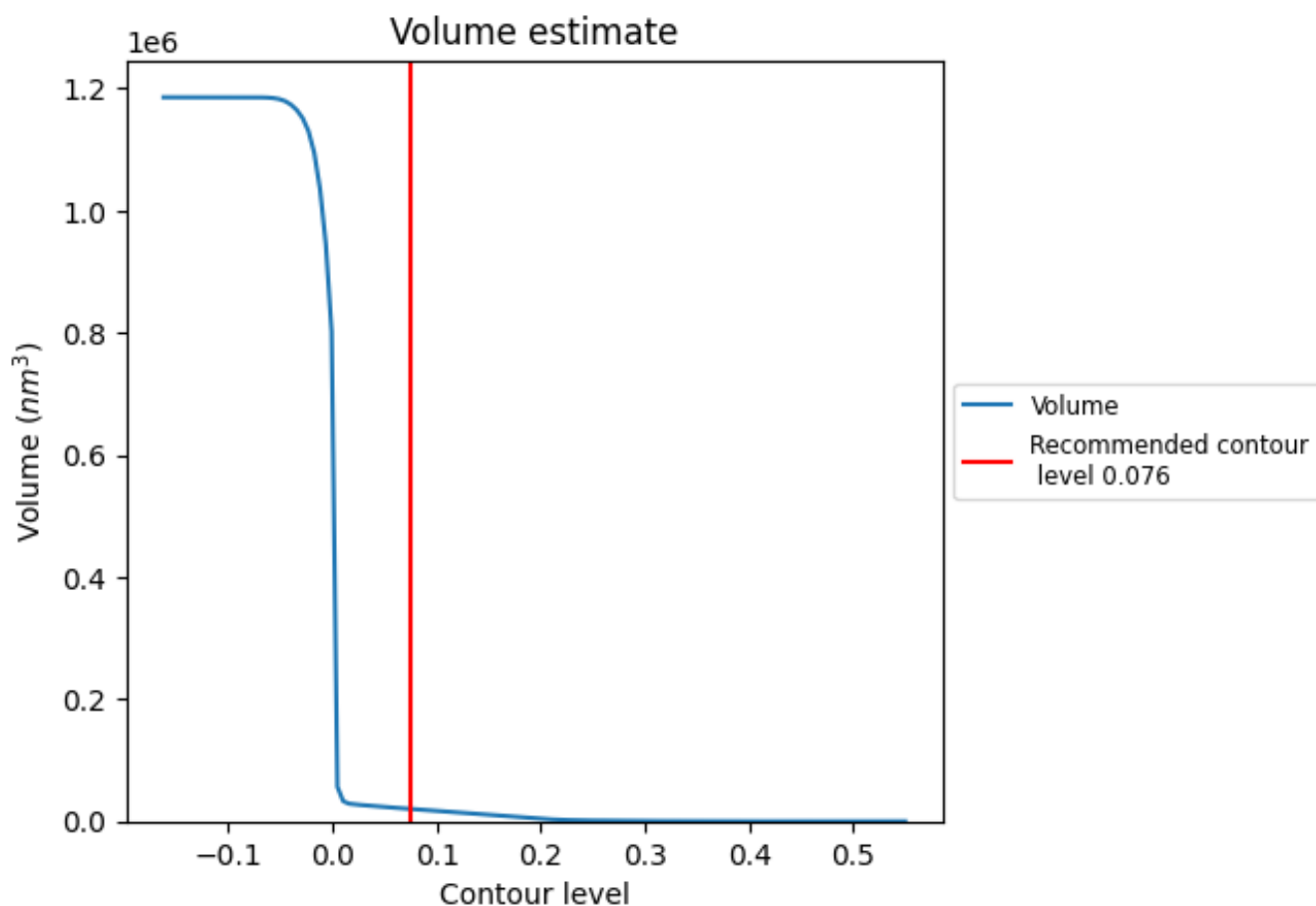
This section contains the results of statistical analysis of the map.

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.

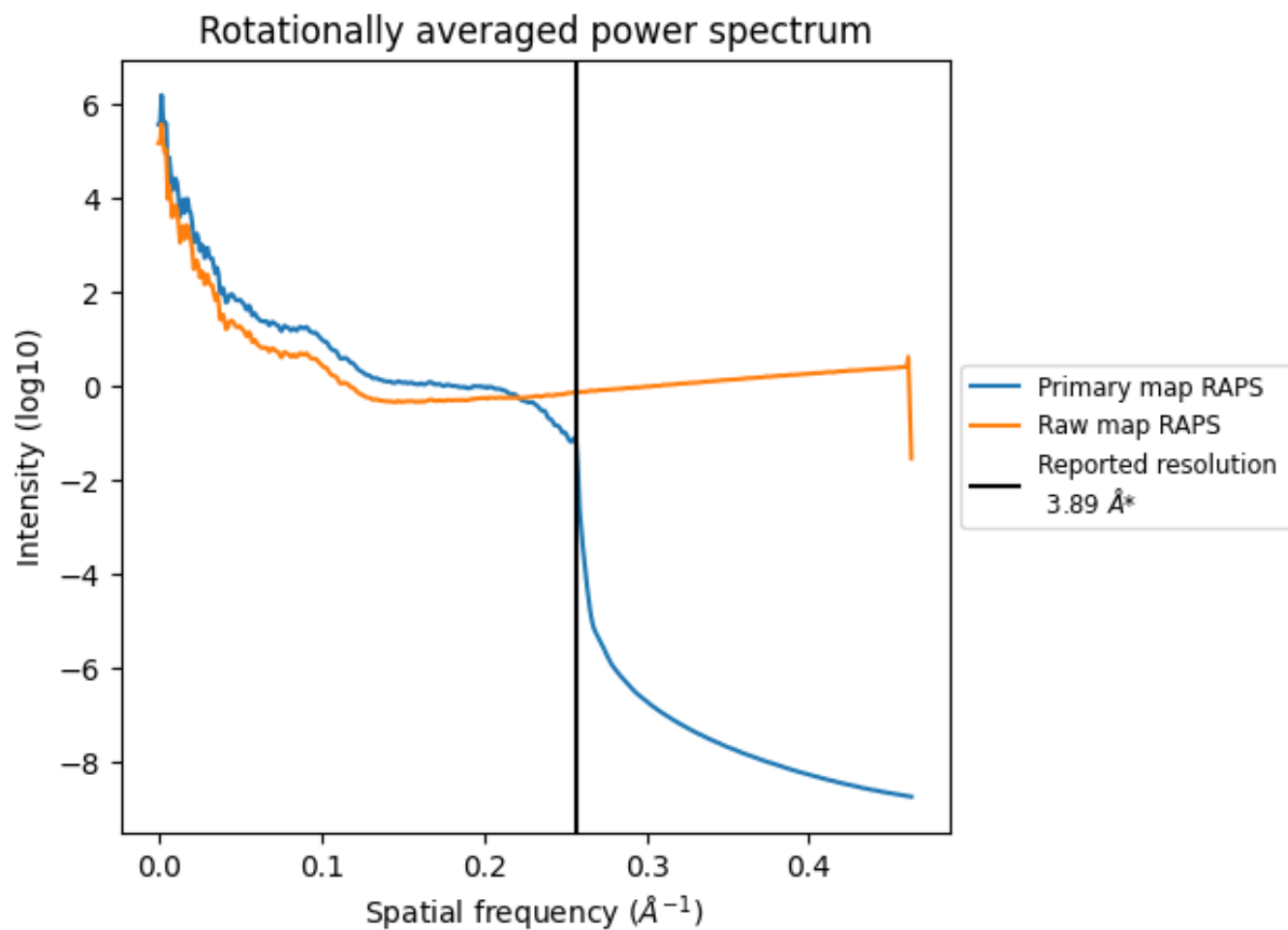
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 20172 nm³; this corresponds to an approximate mass of 18222 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 ⓘ

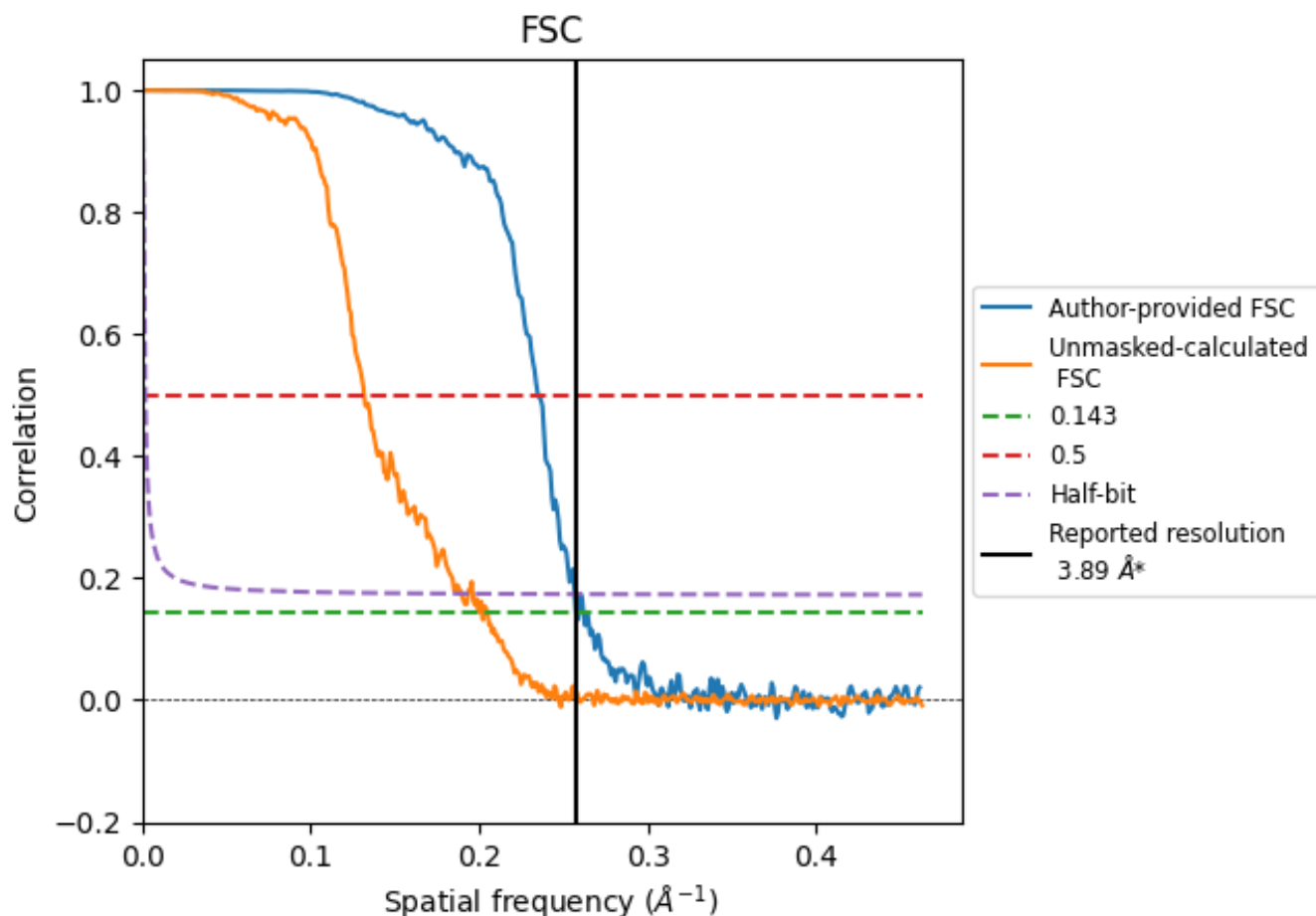


*Reported resolution corresponds to spatial frequency of 0.257 Å⁻¹

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 $0.257 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.89	-	-
Author-provided FSC curve	3.88	4.25	3.89
Unmasked-calculated*	4.96	7.59	5.28

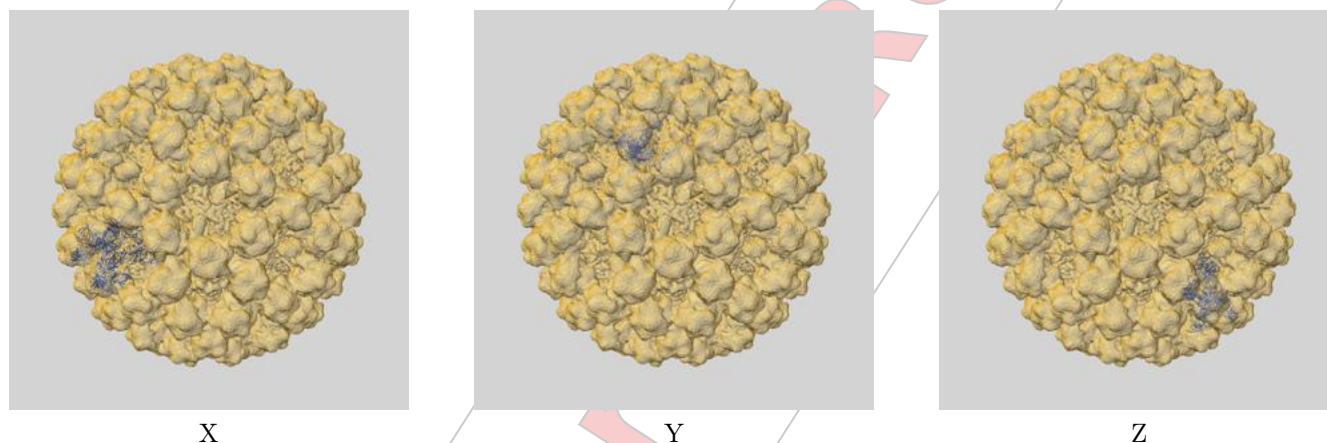
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.96 differs from the reported value 3.89 by more than 10 %

9 Map-model fit ⓘ

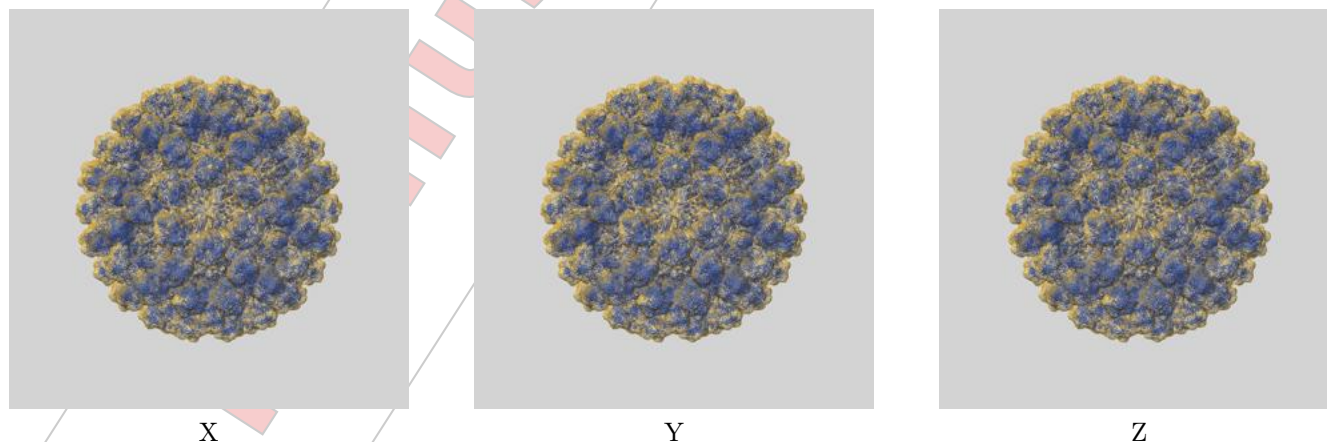
This section contains information regarding the fit between EMDB map EMD-76740 and PDB model 12TF. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

9.1.1 Map-model overlay ⓘ



9.1.2 Map-model assembly overlay ⓘ



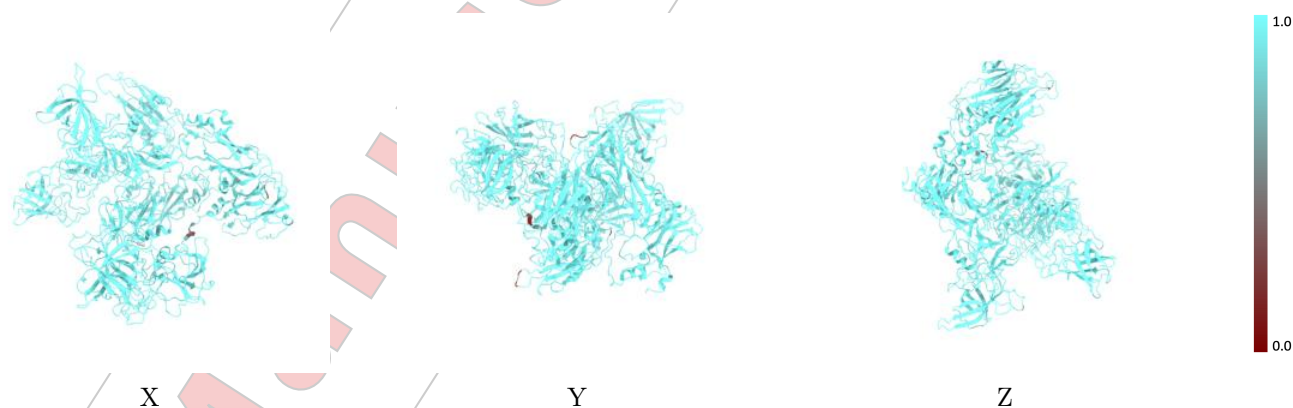
The images above show the 3D surface view of the map at the recommended contour level 0.076 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



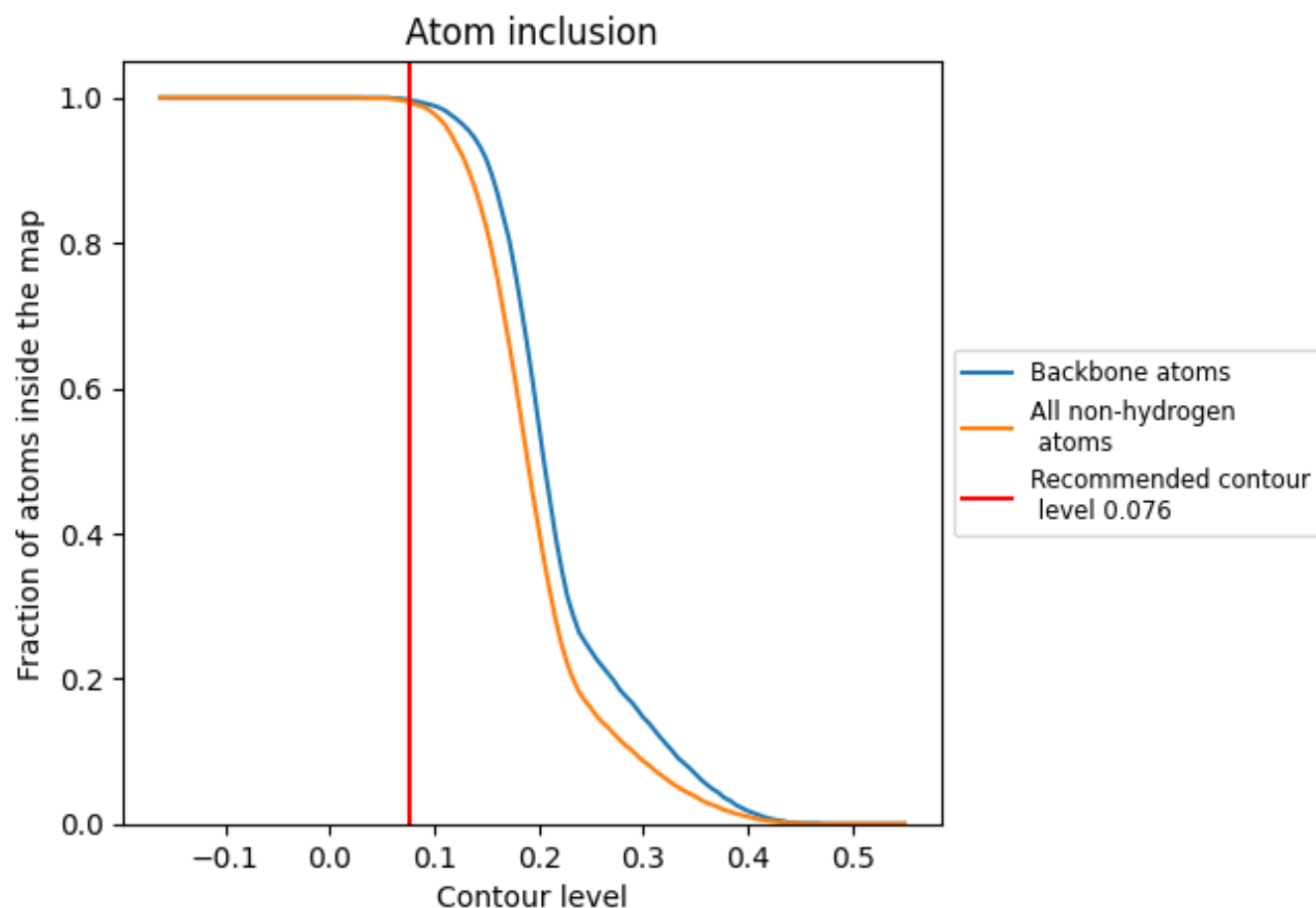
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.076).

9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.076) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9940	 0.2490
A	 0.9950	 0.2470
B	 0.9970	 0.2680
C	 0.9910	 0.2470
D	 0.9910	 0.2340

