



Full wwPDB EM Validation Report ⓘ

Jun 25, 2025 – 10:02 PM JST

PDB ID : 8WFZ / pdb_00008wfz
EMDB ID : EMD-37500
Title : AtGORK Full length 2
Authors : Chen, Y.H.; Li, Q.Y.; Qin, L.; Tang, L.H.; zhang, C.R.
Deposited on : 2023-09-20
Resolution : 4.30 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

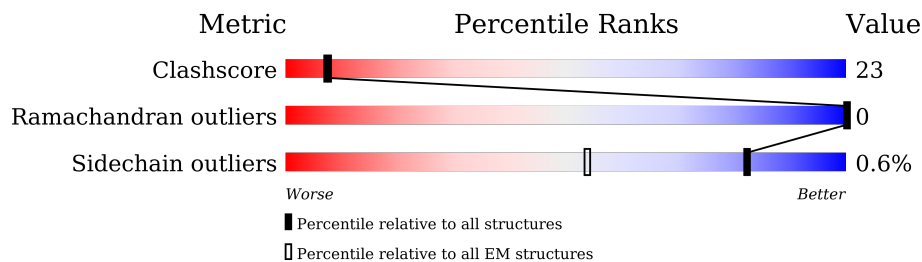
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	820	<div> <div>14%</div> <div>45%</div> <div>35%</div> <div>20%</div> </div>
1	B	820	<div> <div>15%</div> <div>45%</div> <div>35%</div> <div>20%</div> </div>
1	C	820	<div> <div>16%</div> <div>44%</div> <div>36%</div> <div>20%</div> </div>
1	D	820	<div> <div>13%</div> <div>48%</div> <div>32%</div> <div>20%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21266 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.

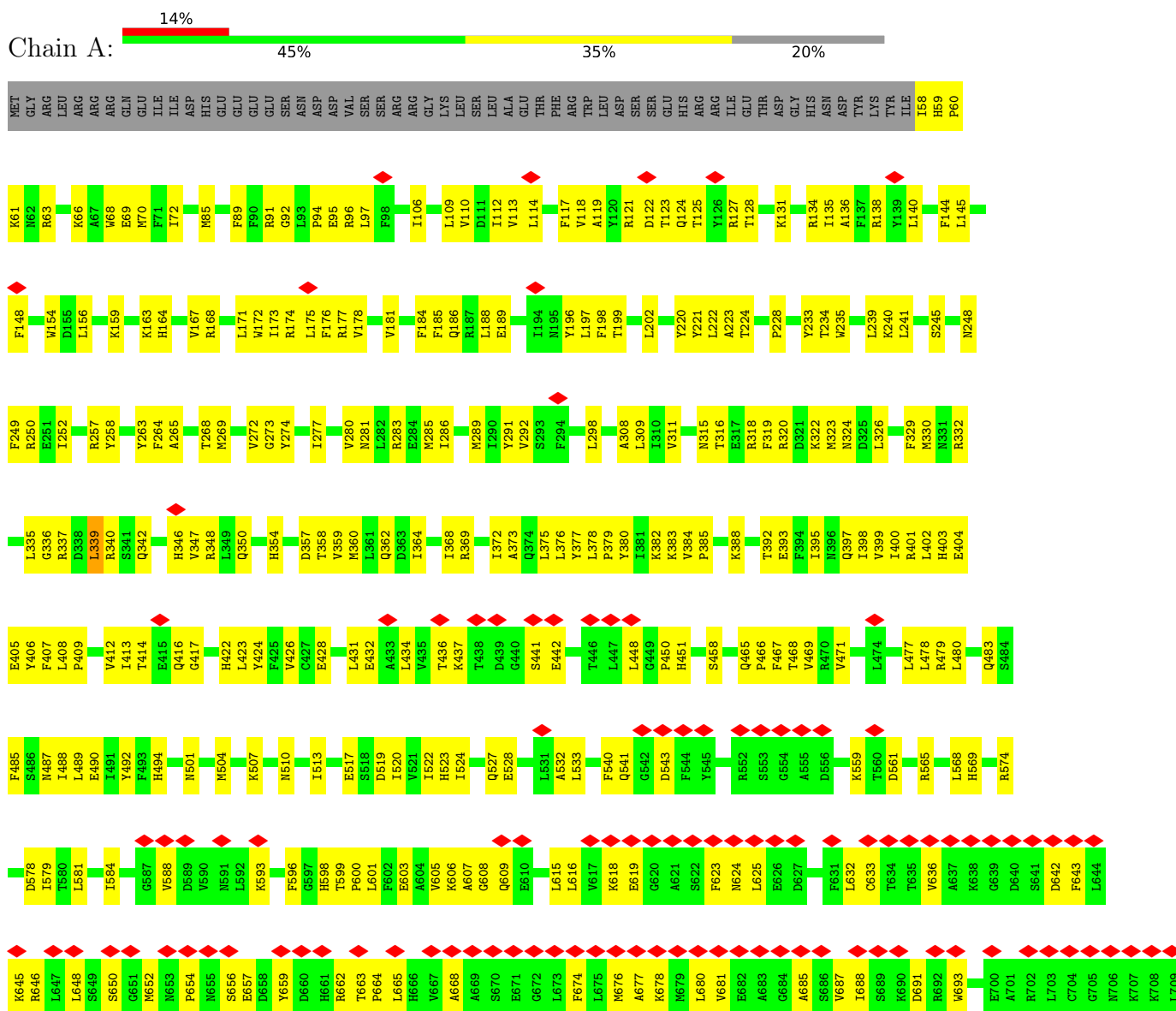
- Molecule 1 is a protein called Potassium channel GORK.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	656	Total	C	N	O	S	0	0
			5315	3452	885	953	25		
1	B	656	Total	C	N	O	S	0	0
			5315	3452	885	953	25		
1	C	656	Total	C	N	O	S	0	0
			5321	3455	887	954	25		
1	D	656	Total	C	N	O	S	0	0
			5315	3452	885	953	25		

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: Potassium channel GORK



Chain C: 16% 44% 36% 20%

0.01

Legend:

- Red: 16%
- Green: 44%
- Yellow: 36%
- Grey: 20%

Chain D:

Amino Acid	Percentage
Met	13%
Gly	48%
Arg	32%
Leu	20%
Val	
Ala	
Thr	
Phe	
Arg	
Trp	
Leu	
Asp	
Ser	
Ser	
Glu	
His	
Arg	
Arg	
Ile	
Glu	
Thr	
Asp	
Gly	
His	
Asn	
Asp	
Tyr	

ALA	GLU	D658	L592	S509	L431	I343	L252	L140	R63
GLN	K593	R510	K594	R511	L434	V347	D253	K141	R64
SER	D594	R512	K595	R513	V435	R348	R257	S142	Y65
LEU	K596	I513	F596	I514	T436	L349	Y258	H143	K66
ASP	G597	K514	K437	K514	T438	Q350	T259	I149	A67
PRO	H598	D519	T438	D519	D439	T356	L262	W154	W68
SER	T599	Q527	D439	Q527	G440	D357	Y263	D155	E69
SER	P600	E530	G440	E530	S441	F264	A265	I72	W70
LEU	L601	L533	S441	L533	E442	Y266	I266	Y158	I73
ARG	F602	K534	E442	K534	V445	Y267	Y267	K159	L77
GLU	E603	V535	V445	V535	T446	T268	T268	K163	Y78
LEU	A607	F544	T446	F544	L447	M269	M269	L81	L81
GLN	G608	Y545	L447	Y545	L448	D272	D272	V167	F92
GLU	Q609	Q548	L448	Q548	L448	G273	G273	R168	T83
ARG	Q610	S549	L448	S549	A366	Y274	Y274	Y169	P84
ILE	G611	L550	S453	L550	A366	G275	G275	L170	P84
GLU	G611	L550	S453	L550	A366	D276	D276	L171	H85
ARG	V612	Q548	S453	Q548	A366	I277	I277	R174	E86
ARG	L615	Y545	S458	Y545	R369	R177	R177	F87	G88
LYS	L615	Y545	I459	Y545	Q374	N281	N281	G88	G88
THR	K618	Q546	I459	Q546	Q374	L282	L282	F89	F89
VAL	E619	L547	I460	L547	L378	V177	V177	F90	F90
PHE	M679	K548	N462	K548	L378	R179	R179	R91	R91
PRO	G620	S549	N462	S549	K382	K180	K180	G92	G92
PHE	L680	L550	I463	L550	K382	V181	V181	L93	L93
HIS	V681	I551	I463	I551	F387	V182	V182	P94	P94
GLN	E682	R552	F467	R552	K388	E183	E183	E95	E95
GLU	A683	S553	T468	S553	G389	F184	F184	F98	F98
GLU	G684	G554	V469	G554	E393	F185	F185	Q104	Q104
ALA	A685	A555	R470	A555	F394	Q186	Q186	Q105	Q105
LYS	S686	D556	V471	D556	Q397	R187	R187	I106	I106
GLU	V687	P557	G472	P557	L309	E189	E189	A107	A107
ARG	I688	N558	L474	N558	I310	D191	D191	F108	F108
SER	S689	G559	H476	G559	V311	T192	T192	L109	L109
ARG	K690	T560	L477	T560	F319	E208	E208	I112	I112
LYS	D691	D561	L478	D561	K401	Y220	Y220	V113	V113
GLY	R692	Y562	K482	Y562	L402	L226	L226	L114	L114
VAL	W693	G564	F485	G564	H403	E231	E231	Q115	Q115
VAL	G694	R565	S486	R565	E404	L239	L239	K131	K131
VAL	N695	H569	S486	H569	E405	K240	K240	R134	R134
TRP	A637	L570	N487	L570	Y406	Y246	Y246	I135	I135
ILE	K638	A571	I488	A571	F407	A136	A136	F137	F137
PRO	G639	G572	L489	G572	L408	R250	R250	Y139	Y139
SER	D640	A572	E490	A572	P409	E247	E247		
ASN	S641	G575	E490	G575	G410				
LEU	D642	G575	D495	G575	E411				
GLU	F643	I579	G496	I579	V420				
LYS	L644	I579	R497	I579	D421				
ILE	K645	I584	L500	I584	Y424				
VAL	R646	Q585	I503	Q585	F425				
THR	G704	E586	M504	E586	V426				
GLY	G705	G587	E505	G587	C427				
ALA	N706	V588	E506	V588	G428				
ALA	K707	S650	K507	S650	G429				
LYS	K708	G651	E508	G651	L430				
	L709	N591		N591					
	I710								
	K711								
	L712								
	L713								
	GLU								
	ASP								
	VAL								
	LYS								
	ASN								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39551	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.363	Depositor
Minimum map value	-0.173	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.085	Depositor
Map size (Å)	305.27997, 305.27997, 305.27997	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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	0.27	0/5438	0.52	3/7356 (0.0%)
1	B	0.35	0/5438	0.62	5/7356 (0.1%)
1	C	0.30	0/5445	0.56	5/7365 (0.1%)
1	D	0.37	0/5438	0.63	8/7356 (0.1%)
All	All	0.33	0/21759	0.59	21/29433 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	GLU	N-CA-C	-9.32	101.10	111.07
1	D	186	GLN	N-CA-C	-7.88	102.69	111.28
1	B	359	VAL	N-CA-C	7.12	117.89	110.62
1	D	95	GLU	N-CA-C	-7.01	103.68	111.82
1	C	326	LEU	N-CA-C	-6.92	103.73	111.28
1	C	267	VAL	N-CA-C	-6.83	103.56	111.00
1	B	184	PHE	N-CA-C	6.11	118.44	111.11
1	D	436	THR	N-CA-C	-5.93	101.64	110.23
1	B	512	ARG	N-CA-C	-5.92	105.71	113.12
1	A	339	LEU	N-CA-C	5.81	117.30	110.97
1	D	267	VAL	N-CA-C	-5.80	104.85	110.42
1	B	516	LEU	N-CA-C	-5.79	103.92	111.74
1	C	186	GLN	N-CA-C	5.76	117.56	111.28
1	C	328	SER	N-CA-C	-5.76	104.91	111.07
1	D	98	PHE	N-CA-C	-5.57	105.21	111.28
1	A	154	TRP	N-CA-C	-5.52	107.55	114.56
1	B	513	ILE	N-CA-C	-5.43	106.53	113.22
1	C	574	ARG	N-CA-C	5.43	118.12	111.82
1	D	250	ARG	N-CA-C	5.20	116.63	111.07
1	D	283	ARG	N-CA-C	-5.11	105.61	111.07
1	D	435	VAL	N-CA-C	-5.05	107.42	111.91

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5315	0	5344	257	0
1	B	5315	0	5344	271	0
1	C	5321	0	5352	268	0
1	D	5315	0	5344	251	0
All	All	21266	0	21384	977	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 23.

All (977) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LEU:CD1	1:A:340:ARG:HG2	1.52	1.36
1:C:271:THR:HA	1:D:272:VAL:CG2	1.63	1.25
1:C:356:THR:HG22	1:C:360:MET:CE	1.68	1.23
1:C:271:THR:CA	1:D:272:VAL:HG22	1.73	1.18
1:A:265:ALA:O	1:A:268:THR:HG22	1.41	1.17
1:B:568:LEU:CD1	1:B:583:LEU:HD21	1.76	1.15
1:A:339:LEU:HD12	1:A:340:ARG:HG2	1.21	1.15
1:B:448:LEU:HD11	1:B:452:THR:HG21	1.30	1.08
1:B:448:LEU:CD1	1:B:452:THR:HG21	1.85	1.07
1:A:339:LEU:HD13	1:A:340:ARG:HG2	1.33	1.06
1:C:356:THR:CG2	1:C:360:MET:HE1	1.90	1.01
1:A:339:LEU:CD1	1:A:340:ARG:CG	2.41	0.99
1:B:568:LEU:HD12	1:B:583:LEU:HD21	1.41	0.99
1:C:356:THR:HG22	1:C:360:MET:HE1	1.01	0.98
1:D:333:LYS:O	1:D:334:LYS:HG2	1.62	0.98
1:A:520:ILE:HD12	1:A:523:HIS:HE1	1.30	0.96
1:C:271:THR:HA	1:D:272:VAL:HG22	0.96	0.95
1:B:568:LEU:HD13	1:B:583:LEU:CD2	1.97	0.95
1:A:339:LEU:HD12	1:A:340:ARG:CG	1.98	0.93
1:D:104:GLY:O	1:D:108:PHE:CD2	2.22	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:LYS:HD3	1:C:245:SER:HB3	1.50	0.91
1:B:568:LEU:CD1	1:B:583:LEU:CD2	2.48	0.90
1:A:339:LEU:HD12	1:A:340:ARG:N	1.86	0.89
1:B:357:ASP:O	1:B:361:LEU:HG	1.73	0.89
1:D:73:LEU:HB3	1:D:180:LYS:HZ2	1.37	0.88
1:A:265:ALA:O	1:A:268:THR:CG2	2.22	0.87
1:B:568:LEU:HD13	1:B:583:LEU:HD21	1.55	0.87
1:D:266:ILE:HA	1:D:269:MET:HG2	1.56	0.87
1:B:448:LEU:CG	1:B:452:THR:HG21	2.05	0.86
1:B:568:LEU:HD13	1:B:583:LEU:CD1	2.06	0.85
1:C:376:LEU:HD21	1:D:333:LYS:HD2	1.58	0.85
1:C:356:THR:HG22	1:C:360:MET:SD	2.16	0.84
1:C:289:MET:HE1	1:D:262:LEU:HD23	1.58	0.84
1:C:350:GLN:HG3	1:C:354:HIS:HB2	1.61	0.82
1:A:274:TYR:O	1:D:275:GLY:HA2	1.77	0.82
1:B:373:ALA:HB1	1:B:399:VAL:HG22	1.59	0.82
1:B:448:LEU:HD11	1:B:452:THR:CG2	2.07	0.81
1:A:407:PHE:HE2	1:A:477:LEU:HB2	1.46	0.81
1:B:364:ILE:HG21	1:B:369:ARG:HB2	1.62	0.81
1:D:430:LEU:HD11	1:D:447:LEU:HD13	1.62	0.81
1:B:188:LEU:HD12	1:B:188:LEU:O	1.81	0.81
1:B:514:LYS:NZ	1:B:520:ILE:HG21	1.95	0.81
1:D:281:ASN:HB3	1:D:284:GLU:HG2	1.63	0.79
1:D:333:LYS:O	1:D:334:LYS:CG	2.31	0.79
1:D:104:GLY:O	1:D:108:PHE:HD2	1.62	0.79
1:A:69:GLU:HA	1:A:72:ILE:HG12	1.65	0.78
1:B:289:MET:CE	1:C:266:ILE:HD11	2.13	0.78
1:A:417:GLY:H	1:A:466:PRO:HA	1.49	0.78
1:A:605:VAL:HG11	1:A:650:SER:HB3	1.67	0.77
1:D:266:ILE:O	1:D:269:MET:HG2	1.85	0.77
1:B:568:LEU:HD13	1:B:583:LEU:HD11	1.67	0.77
1:D:272:VAL:O	1:D:274:TYR:CD2	2.37	0.77
1:D:593:LYS:HB3	1:D:597:GLY:HA2	1.67	0.76
1:B:301:TYR:HD1	1:C:306:ILE:HD11	1.48	0.76
1:B:289:MET:HE3	1:C:266:ILE:HD11	1.68	0.76
1:C:289:MET:HE1	1:D:262:LEU:CD2	2.14	0.76
1:A:402:LEU:HD11	1:A:478:LEU:HB3	1.67	0.76
1:A:268:THR:CG2	1:A:291:TYR:HE2	1.99	0.75
1:A:323:MET:HG2	1:A:348:ARG:HD3	1.68	0.75
1:A:369:ARG:NH1	1:A:400:ILE:O	2.20	0.75
1:A:264:PHE:HB2	1:A:277:ILE:HD13	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:MET:HG3	1:A:335:LEU:HD12	1.69	0.74
1:C:304:GLY:HA2	1:D:307:THR:HG22	1.69	0.74
1:D:266:ILE:HG13	1:D:269:MET:SD	2.28	0.74
1:A:520:ILE:HD12	1:A:523:HIS:CE1	2.21	0.73
1:B:448:LEU:HD21	1:B:452:THR:HG22	1.68	0.73
1:B:416:GLN:NE2	1:B:466:PRO:O	2.22	0.73
1:D:435:VAL:HG12	1:D:435:VAL:O	1.86	0.73
1:A:528:GLU:OE1	1:A:559:LYS:NZ	2.21	0.73
1:D:330:MET:HG2	1:D:340:ARG:HG2	1.71	0.73
1:D:543:ASP:HB3	1:D:546:GLN:HB2	1.70	0.73
1:D:264:PHE:CE2	1:D:277:ILE:HG22	2.24	0.72
1:A:145:LEU:HA	1:A:148:PHE:CE1	2.23	0.72
1:B:558:ASN:OD1	1:B:558:ASN:O	2.06	0.72
1:B:92:GLY:H	1:B:168:ARG:HH12	1.35	0.72
1:C:470:ARG:NH1	1:C:471:VAL:O	2.22	0.72
1:A:95:GLU:HG2	1:A:96:ARG:HD3	1.72	0.72
1:C:518:SER:CB	1:C:523:HIS:HE1	2.02	0.72
1:C:356:THR:CG2	1:C:360:MET:SD	2.76	0.72
1:A:186:GLN:O	1:A:189:GLU:HG2	1.89	0.72
1:C:518:SER:HB2	1:C:523:HIS:HE1	1.54	0.72
1:C:519:ASP:HB2	1:C:522:ILE:HG12	1.72	0.72
1:D:131:LYS:HE3	1:D:134:ARG:HH12	1.56	0.71
1:B:430:LEU:HB3	1:B:447:LEU:HD12	1.71	0.71
1:C:699:ASP:OD1	1:C:702:ARG:NH2	2.23	0.71
1:D:143:HIS:NE2	1:D:179:ARG:HD3	2.04	0.71
1:B:424:TYR:HB3	1:B:477:LEU:HD12	1.71	0.71
1:D:402:LEU:HD22	1:D:478:LEU:HD12	1.73	0.71
1:A:131:LYS:HG3	1:A:134:ARG:HG2	1.73	0.70
1:D:208:GLU:OE2	1:D:269:MET:HE3	1.90	0.70
1:A:678:LYS:HB2	1:A:712:LEU:HD13	1.73	0.70
1:A:426:VAL:O	1:A:451:HIS:N	2.24	0.70
1:D:266:ILE:CA	1:D:269:MET:HG2	2.21	0.70
1:D:378:LEU:HG	1:D:382:LYS:HE2	1.72	0.70
1:C:404:GLU:HG2	1:C:476:HIS:HE1	1.57	0.70
1:A:265:ALA:C	1:A:268:THR:HG22	2.17	0.69
1:A:263:TYR:CD1	1:D:285:MET:SD	2.85	0.69
1:D:115:GLN:HG2	1:D:139:TYR:CE2	2.26	0.69
1:A:385:PRO:O	1:A:388:LYS:NZ	2.25	0.69
1:C:383:LYS:HD2	1:C:451:HIS:CD2	2.26	0.69
1:A:431:LEU:HB2	1:A:448:LEU:HB2	1.76	0.68
1:C:271:THR:C	1:D:272:VAL:HG22	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:LYS:C	1:D:334:LYS:HG2	2.19	0.68
1:A:402:LEU:HG	1:A:478:LEU:HD12	1.76	0.67
1:C:374:GLN:HA	1:C:399:VAL:HG11	1.76	0.67
1:A:414:THR:HG22	1:A:469:VAL:HG22	1.77	0.67
1:C:518:SER:HB2	1:C:523:HIS:CE1	2.30	0.67
1:A:663:THR:HG22	1:A:665:LEU:H	1.59	0.67
1:C:569:HIS:O	1:C:573:CYS:SG	2.53	0.67
1:C:289:MET:HE1	1:D:262:LEU:CG	2.25	0.67
1:A:268:THR:HG21	1:A:291:TYR:CE2	2.30	0.67
1:C:91:ARG:HD2	1:C:168:ARG:HH11	1.59	0.66
1:B:312:LYS:NZ	1:C:311:VAL:HG23	2.11	0.66
1:D:239:LEU:HD11	1:D:246:TYR:CD2	2.30	0.66
1:D:266:ILE:HA	1:D:269:MET:CG	2.25	0.66
1:B:329:PHE:HA	1:B:332:ARG:HE	1.60	0.66
1:D:281:ASN:HB3	1:D:284:GLU:CG	2.25	0.66
1:A:109:LEU:O	1:A:112:ILE:HG22	1.95	0.66
1:A:510:ASN:HB3	1:A:513:ILE:HG22	1.76	0.66
1:A:642:ASP:HA	1:A:645:LYS:HE3	1.78	0.66
1:C:93:LEU:HD12	1:C:94:PRO:HD2	1.78	0.66
1:D:336:GLY:HA2	1:D:340:ARG:HE	1.61	0.66
1:A:645:LYS:HA	1:A:648:LEU:HD12	1.79	0.65
1:C:404:GLU:HG2	1:C:476:HIS:CE1	2.30	0.65
1:D:220:TYR:CE1	1:D:236:ILE:HD13	2.31	0.65
1:B:593:LYS:HG3	1:B:599:THR:HG22	1.77	0.65
1:B:208:GLU:O	1:B:212:THR:HG23	1.96	0.65
1:B:140:LEU:HA	1:B:144:PHE:HB3	1.79	0.65
1:D:364:ILE:O	1:D:369:ARG:NH2	2.29	0.65
1:A:319:PHE:O	1:A:323:MET:HG3	1.96	0.65
1:A:681:VAL:HA	1:A:685:ALA:HB3	1.77	0.65
1:C:601:LEU:HD13	1:C:616:LEU:HD22	1.77	0.65
1:D:630:ASN:HD22	1:D:659:TYR:HB3	1.61	0.65
1:A:119:ALA:O	1:A:138:ARG:NH2	2.30	0.65
1:C:356:THR:HG21	1:D:329:PHE:CD1	2.32	0.65
1:B:448:LEU:HG	1:B:452:THR:HG21	1.78	0.64
1:B:663:THR:HB	1:B:666:HIS:CG	2.32	0.64
1:D:220:TYR:HE1	1:D:236:ILE:HD13	1.59	0.64
1:D:330:MET:HE1	1:D:339:LEU:HD23	1.79	0.64
1:B:172:TRP:HZ2	1:B:218:ILE:HD11	1.61	0.64
1:B:312:LYS:HZ2	1:C:311:VAL:HG23	1.62	0.64
1:B:345:GLY:HA2	1:B:348:ARG:HE	1.62	0.64
1:B:511:ASP:HA	1:B:514:LYS:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LYS:O	1:C:66:LYS:NZ	2.31	0.64
1:C:568:LEU:HD21	1:C:590:VAL:HG22	1.79	0.64
1:C:356:THR:CG2	1:C:360:MET:CE	2.61	0.64
1:A:173:ILE:HD12	1:A:176:PHE:HD2	1.62	0.64
1:A:268:THR:CG2	1:A:291:TYR:CE2	2.79	0.64
1:C:573:CYS:SG	1:C:603:GLU:OE1	2.55	0.64
1:D:347:VAL:O	1:D:350:GLN:HG3	1.97	0.64
1:C:408:LEU:HA	1:C:474:LEU:HG	1.80	0.64
1:D:431:LEU:HD22	1:D:448:LEU:HD12	1.80	0.64
1:C:678:LYS:HB2	1:C:712:LEU:HD13	1.80	0.64
1:A:268:THR:HG21	1:A:291:TYR:HE2	1.61	0.64
1:A:156:LEU:HD12	1:A:159:LYS:HE2	1.80	0.63
1:D:208:GLU:OE2	1:D:269:MET:CE	2.46	0.63
1:D:337:ARG:HD2	1:D:339:LEU:H	1.62	0.63
1:B:197:LEU:HB2	1:B:309:LEU:HD13	1.80	0.63
1:D:565:ARG:HD3	1:D:569:HIS:HB3	1.78	0.63
1:B:336:GLY:O	1:B:337:ARG:HG2	1.98	0.63
1:B:507:LYS:HE3	1:B:514:LYS:HE2	1.80	0.63
1:C:599:THR:HB	1:C:624:ASN:HB2	1.80	0.63
1:D:424:TYR:HB3	1:D:477:LEU:HD11	1.79	0.63
1:A:517:GLU:O	1:A:520:ILE:HG22	1.99	0.63
1:B:94:PRO:HG2	1:B:97:LEU:HD13	1.81	0.63
1:C:266:ILE:HA	1:C:269:MET:HB2	1.80	0.63
1:C:535:VAL:HG22	1:C:550:LEU:HD21	1.81	0.63
1:B:568:LEU:HD12	1:B:583:LEU:CD2	2.19	0.62
1:B:329:PHE:O	1:B:332:ARG:HG2	1.99	0.62
1:D:690:LYS:HD2	1:D:694:GLY:HA2	1.81	0.62
1:C:428:GLU:O	1:C:475:CYS:HA	1.99	0.62
1:C:573:CYS:SG	1:C:603:GLU:HB3	2.39	0.62
1:A:140:LEU:HA	1:A:144:PHE:HB3	1.81	0.62
1:B:122:ASP:O	1:B:126:TYR:N	2.28	0.62
1:B:337:ARG:HG3	1:B:338:ASP:H	1.64	0.62
1:C:497:ARG:HA	1:C:500:LEU:HD12	1.82	0.62
1:A:324:ASN:ND2	1:D:192:THR:O	2.33	0.62
1:C:428:GLU:HG3	1:C:476:HIS:HB3	1.82	0.62
1:D:108:PHE:CE1	1:D:177:ARG:HD3	2.35	0.61
1:D:561:ASP:OD1	1:D:565:ARG:N	2.32	0.61
1:A:578:ASP:OD1	1:A:579:ILE:HD12	1.99	0.61
1:B:285:MET:O	1:B:289:MET:HG2	2.00	0.61
1:B:574:ARG:NH2	1:B:576:TYR:OH	2.34	0.61
1:B:632:LEU:HD13	1:B:654:PRO:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:LEU:HD22	1:B:524:ILE:HD13	1.81	0.61
1:C:289:MET:HE1	1:D:262:LEU:HG	1.83	0.61
1:A:163:LYS:HG3	1:A:164:HIS:H	1.65	0.61
1:D:401:ARG:HH21	1:D:488:ILE:HD11	1.66	0.61
1:B:693:TRP:HE1	1:C:662:ARG:HH22	1.49	0.61
1:C:268:THR:HG23	1:D:274:TYR:OH	2.01	0.61
1:A:434:LEU:HD22	1:A:442:GLU:HB2	1.82	0.60
1:B:105:GLN:OE1	1:B:174:ARG:NH2	2.34	0.60
1:B:544:PHE:HA	1:B:547:LEU:HD12	1.83	0.60
1:B:252:ILE:O	1:B:257:ARG:NH2	2.34	0.60
1:C:266:ILE:HB	1:C:269:MET:HE3	1.81	0.60
1:D:266:ILE:C	1:D:269:MET:HG2	2.25	0.60
1:D:458:SER:HA	1:D:463:ILE:HG23	1.83	0.60
1:A:364:ILE:HD11	1:A:368:ILE:HB	1.83	0.60
1:D:185:PHE:CD1	1:D:188:LEU:HD12	2.37	0.60
1:A:286:ILE:O	1:A:289:MET:HB2	2.00	0.60
1:A:593:LYS:NZ	1:A:624:ASN:HB2	2.16	0.60
1:C:269:MET:HG2	1:C:295:ASP:OD2	2.01	0.59
1:D:272:VAL:HB	1:D:274:TYR:CE2	2.37	0.59
1:B:360:MET:SD	1:B:403:HIS:HD2	2.25	0.59
1:A:280:VAL:HG12	1:B:241:LEU:HG	1.85	0.59
1:D:115:GLN:HG2	1:D:139:TYR:HE2	1.66	0.59
1:A:196:TYR:O	1:A:199:THR:OG1	2.20	0.59
1:B:514:LYS:CE	1:B:520:ILE:HG21	2.32	0.59
1:D:660:ASP:HB3	1:D:662:ARG:HG3	1.84	0.59
1:C:356:THR:HG21	1:D:329:PHE:CE1	2.37	0.59
1:A:561:ASP:OD1	1:A:565:ARG:N	2.35	0.59
1:B:593:LYS:HB3	1:B:599:THR:HA	1.83	0.59
1:B:417:GLY:N	1:B:465:GLN:O	2.36	0.59
1:D:272:VAL:O	1:D:274:TYR:HD2	1.86	0.59
1:A:323:MET:HE3	1:A:348:ARG:HH11	1.67	0.59
1:B:431:LEU:HB2	1:B:448:LEU:HB3	1.84	0.59
1:D:121:ARG:HD3	1:D:126:TYR:HA	1.85	0.59
1:A:178:VAL:O	1:A:181:VAL:HG12	2.03	0.59
1:D:264:PHE:HE2	1:D:277:ILE:HG22	1.67	0.58
1:A:431:LEU:O	1:A:448:LEU:N	2.36	0.58
1:A:360:MET:HE1	1:B:329:PHE:CE2	2.38	0.58
1:C:394:PHE:HD1	1:C:492:TYR:HD2	1.50	0.58
1:A:66:LYS:O	1:A:70:MET:HG2	2.04	0.58
1:A:369:ARG:HA	1:A:372:ILE:HG12	1.84	0.58
1:D:240:LYS:HG2	1:D:240:LYS:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:MET:SD	1:B:263:TYR:CD1	2.97	0.58
1:A:339:LEU:HD12	1:A:340:ARG:CB	2.32	0.58
1:A:504:MET:O	1:A:507:LYS:HG2	2.03	0.58
1:B:223:ALA:HB2	1:B:235:TRP:HE1	1.68	0.58
1:B:190:LYS:HD3	1:C:344:THR:HG21	1.85	0.58
1:B:151:CYS:HA	1:B:174:ARG:HH22	1.69	0.58
1:C:266:ILE:HA	1:C:269:MET:CB	2.33	0.58
1:C:385:PRO:HA	1:C:388:LYS:HG3	1.86	0.57
1:A:533:LEU:HD21	1:D:533:LEU:HB3	1.85	0.57
1:B:448:LEU:HD21	1:B:452:THR:CG2	2.34	0.57
1:C:518:SER:CB	1:C:523:HIS:CE1	2.86	0.57
1:D:548:LYS:O	1:D:552:ARG:HG2	2.04	0.57
1:A:409:PRO:HD3	1:D:127:ARG:CZ	2.34	0.57
1:B:448:LEU:CG	1:B:452:THR:CG2	2.81	0.57
1:C:180:LYS:O	1:C:183:GLU:HG3	2.03	0.57
1:C:409:PRO:HD3	1:C:474:LEU:HG	1.87	0.57
1:C:601:LEU:HD23	1:C:623:PHE:HB3	1.86	0.57
1:C:642:ASP:O	1:C:646:ARG:HG2	2.04	0.57
1:D:669:ALA:HA	1:D:709:LEU:HD21	1.86	0.57
1:B:189:GLU:HG2	1:B:192:THR:HG23	1.86	0.57
1:B:356:THR:HG22	1:C:329:PHE:CE1	2.39	0.57
1:B:301:TYR:O	1:B:305:ASN:OD1	2.23	0.57
1:D:366:ALA:HA	1:D:369:ARG:HG2	1.85	0.57
1:A:339:LEU:HD13	1:A:340:ARG:CG	2.19	0.57
1:A:347:VAL:O	1:A:350:GLN:HG2	2.04	0.57
1:B:248:ASN:HB3	1:B:251:GLU:CD	2.30	0.57
1:A:600:PRO:HB2	1:A:616:LEU:HD21	1.87	0.57
1:B:240:LYS:O	1:B:240:LYS:HD3	2.05	0.57
1:C:381:ILE:HG21	1:C:395:ILE:HG23	1.87	0.57
1:C:493:PHE:HB2	1:C:497:ARG:HH12	1.70	0.57
1:A:431:LEU:HD13	1:A:471:VAL:HA	1.84	0.57
1:A:532:ALA:HB2	1:A:559:LYS:HE3	1.87	0.56
1:B:580:THR:O	1:B:583:LEU:HG	2.05	0.56
1:D:264:PHE:CD2	1:D:277:ILE:HG22	2.40	0.56
1:C:518:SER:OG	1:C:523:HIS:CE1	2.59	0.56
1:C:599:THR:HG23	1:C:602:PHE:H	1.69	0.56
1:B:233:TYR:CE2	1:B:281:ASN:HA	2.40	0.56
1:C:662:ARG:NH1	1:C:691:ASP:OD2	2.38	0.56
1:A:134:ARG:HH12	1:A:138:ARG:HE	1.52	0.56
1:C:493:PHE:HB2	1:C:497:ARG:NH1	2.20	0.56
1:D:425:PHE:CD1	1:D:453:SER:HB2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:GLY:N	1:A:466:PRO:HA	2.19	0.56
1:B:153:PRO:HB2	1:B:156:LEU:HD13	1.87	0.56
1:C:374:GLN:O	1:C:378:LEU:HG	2.05	0.56
1:A:329:PHE:CZ	1:D:356:THR:HG22	2.40	0.56
1:A:398:ILE:HD11	1:A:488:ILE:HG21	1.86	0.56
1:A:606:LYS:HG2	1:A:643:PHE:HE1	1.70	0.56
1:C:330:MET:HE2	1:C:343:ILE:HD11	1.88	0.56
1:D:155:ASP:OD1	1:D:159:LYS:NZ	2.37	0.56
1:D:459:ILE:HG12	1:D:482:LYS:HZ2	1.71	0.56
1:B:644:LEU:HD23	1:B:648:LEU:HD23	1.87	0.56
1:B:122:ASP:HB3	1:B:124:GLN:CD	2.31	0.56
1:B:170:LEU:O	1:B:173:ILE:HG12	2.06	0.56
1:C:72:ILE:HD12	1:C:180:LYS:NZ	2.21	0.56
1:D:397:GLN:HB3	1:D:401:ARG:HH22	1.71	0.56
1:A:106:ILE:O	1:A:110:VAL:HG23	2.06	0.55
1:C:466:PRO:HB3	1:C:517:GLU:HG2	1.89	0.55
1:C:507:LYS:HA	1:C:514:LYS:HD2	1.88	0.55
1:A:263:TYR:CG	1:D:285:MET:SD	2.99	0.55
1:D:500:LEU:HA	1:D:503:ILE:HD12	1.88	0.55
1:D:591:ASN:HD21	1:D:624:ASN:HB2	1.71	0.55
1:A:234:THR:HG22	1:A:235:TRP:N	2.21	0.55
1:A:593:LYS:HZ1	1:A:624:ASN:HB2	1.71	0.55
1:B:364:ILE:HG22	1:B:366:ALA:H	1.72	0.55
1:B:692:ARG:HH22	1:C:666:HIS:HB3	1.71	0.55
1:A:407:PHE:CE2	1:A:477:LEU:HB2	2.34	0.55
1:B:337:ARG:HG3	1:B:338:ASP:N	2.21	0.55
1:C:296:MET:HE1	1:D:269:MET:HE2	1.87	0.55
1:D:407:PHE:O	1:D:474:LEU:HA	2.06	0.55
1:B:409:PRO:HD3	1:B:474:LEU:HB3	1.87	0.55
1:B:673:LEU:HD23	1:B:676:MET:HG3	1.87	0.55
1:A:377:TYR:HB2	1:A:399:VAL:HG13	1.89	0.55
1:B:368:ILE:O	1:B:372:ILE:HG12	2.07	0.55
1:A:228:PRO:HG3	1:A:250:ARG:HH12	1.71	0.55
1:A:618:LYS:NZ	1:A:619:GLU:OE2	2.40	0.55
1:D:431:LEU:HD21	1:D:469:VAL:HG23	1.89	0.55
1:A:519:ASP:HA	1:A:522:ILE:HG12	1.89	0.55
1:C:281:ASN:HB3	1:C:284:GLU:OE2	2.07	0.55
1:C:567:PRO:HA	1:C:570:LEU:HD13	1.89	0.55
1:D:330:MET:HE3	1:D:336:GLY:H	1.73	0.55
1:D:572:ALA:HA	1:D:612:VAL:HG11	1.87	0.55
1:A:329:PHE:O	1:A:332:ARG:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:THR:HG22	1:B:566:SER:HA	1.89	0.54
1:C:416:GLN:HG3	1:C:436:THR:HB	1.87	0.54
1:C:514:LYS:HB2	1:C:520:ILE:HD11	1.89	0.54
1:A:319:PHE:CZ	1:A:348:ARG:HG2	2.42	0.54
1:B:188:LEU:HD12	1:B:188:LEU:C	2.31	0.54
1:B:380:TYR:CZ	1:B:427:CYS:HA	2.43	0.54
1:B:507:LYS:HB2	1:B:514:LYS:HG2	1.89	0.54
1:C:413:ILE:HB	1:C:469:VAL:HB	1.88	0.54
1:D:446:THR:HG23	1:D:511:ASP:HB2	1.90	0.54
1:A:487:ASN:O	1:A:490:GLU:HG3	2.07	0.54
1:A:523:HIS:O	1:A:527:GLN:N	2.23	0.54
1:B:220:TYR:CZ	1:B:257:ARG:HD3	2.43	0.54
1:B:435:VAL:O	1:B:443:GLU:HG3	2.07	0.54
1:B:109:LEU:O	1:B:112:ILE:HG22	2.06	0.54
1:C:519:ASP:CB	1:C:522:ILE:HG12	2.38	0.54
1:C:355:TYR:O	1:C:358:THR:OG1	2.26	0.54
1:B:79:SER:O	1:B:83:THR:HG23	2.08	0.54
1:C:286:ILE:O	1:C:289:MET:HB2	2.08	0.54
1:D:630:ASN:ND2	1:D:659:TYR:HB3	2.22	0.54
1:B:514:LYS:HZ2	1:B:520:ILE:HG21	1.71	0.54
1:C:657:GLU:HA	1:C:664:PRO:HD3	1.90	0.54
1:D:445:VAL:HG12	1:D:446:THR:N	2.23	0.54
1:A:330:MET:HG2	1:A:337:ARG:HH22	1.73	0.54
1:B:329:PHE:CE2	1:B:333:LYS:HG3	2.43	0.54
1:D:337:ARG:HD2	1:D:338:ASP:N	2.23	0.54
1:B:335:LEU:HD12	1:B:339:LEU:HD22	1.89	0.53
1:C:178:VAL:O	1:C:181:VAL:HG22	2.09	0.53
1:C:394:PHE:CE1	1:C:488:ILE:HG12	2.43	0.53
1:D:691:ASP:OD1	1:D:692:ARG:N	2.38	0.53
1:B:421:ASP:OD1	1:B:482:LYS:HB3	2.08	0.53
1:C:574:ARG:NH2	1:C:576:TYR:OH	2.41	0.53
1:D:86:GLU:HG3	1:D:171:LEU:HD21	1.89	0.53
1:C:409:PRO:HG3	1:C:473:GLU:HA	1.90	0.53
1:C:410:GLY:H	1:C:470:ARG:NH1	2.05	0.53
1:C:669:ALA:HA	1:C:709:LEU:HD21	1.91	0.53
1:B:603:GLU:HA	1:B:606:LYS:HG2	1.91	0.53
1:A:272:VAL:O	1:D:273:GLY:HA3	2.08	0.53
1:A:520:ILE:O	1:A:524:ILE:HG12	2.09	0.53
1:A:593:LYS:NZ	1:A:599:THR:HB	2.24	0.53
1:B:565:ARG:HG3	1:B:594:ASP:OD1	2.08	0.53
1:C:275:GLY:O	1:C:278:HIS:NE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:PHE:HB2	1:B:652:MET:SD	2.48	0.53
1:D:179:ARG:HA	1:D:182:VAL:HG12	1.91	0.53
1:B:180:LYS:HA	1:B:183:GLU:OE1	2.08	0.53
1:A:357:ASP:HA	1:A:360:MET:HE3	1.90	0.53
1:C:413:ILE:HD13	1:C:469:VAL:HG12	1.91	0.53
1:D:69:GLU:O	1:D:180:LYS:NZ	2.41	0.53
1:C:284:GLU:OE2	1:C:284:GLU:N	2.34	0.53
1:D:347:VAL:HG22	1:D:351:TYR:CE2	2.44	0.53
1:C:706:ASN:HB3	1:C:709:LEU:HB3	1.90	0.52
1:D:435:VAL:O	1:D:435:VAL:CG1	2.56	0.52
1:D:615:LEU:HA	1:D:618:LYS:HG2	1.91	0.52
1:B:308:ALA:HA	1:B:312:LYS:HZ3	1.74	0.52
1:A:606:LYS:HE2	1:D:596:PHE:HE1	1.74	0.52
1:B:500:LEU:HA	1:B:503:ILE:HG12	1.90	0.52
1:C:91:ARG:HD2	1:C:168:ARG:NH1	2.24	0.52
1:C:363:ASP:OD1	1:C:364:ILE:N	2.43	0.52
1:D:92:GLY:H	1:D:168:ARG:HH12	1.55	0.52
1:A:607:ALA:HB1	1:A:609:GLN:HE22	1.74	0.52
1:B:249:PHE:O	1:B:257:ARG:NH2	2.23	0.52
1:C:59:HIS:CG	1:C:60:PRO:HD2	2.45	0.52
1:A:189:GLU:HA	1:A:199:THR:HG21	1.91	0.52
1:B:666:HIS:CE1	1:B:691:ASP:HB2	2.43	0.52
1:A:168:ARG:O	1:A:171:LEU:HD23	2.09	0.52
1:A:272:VAL:O	1:D:273:GLY:CA	2.57	0.52
1:A:492:TYR:HD1	1:A:494:HIS:CE1	2.28	0.52
1:A:603:GLU:HA	1:A:606:LYS:HB2	1.92	0.52
1:B:311:VAL:HG12	1:B:312:LYS:HD3	1.92	0.52
1:B:328:SER:HA	1:B:331:ASN:HD21	1.75	0.52
1:B:329:PHE:HA	1:B:332:ARG:NE	2.25	0.52
1:C:369:ARG:NH1	1:C:372:ILE:HD11	2.24	0.52
1:C:393:GLU:HA	1:C:396:ASN:HD21	1.73	0.52
1:C:518:SER:OG	1:C:523:HIS:HE1	1.92	0.52
1:C:543:ASP:OD1	1:C:543:ASP:N	2.43	0.52
1:C:605:VAL:HG11	1:C:652:MET:HE1	1.91	0.52
1:A:128:THR:HB	1:A:135:ILE:HD11	1.91	0.52
1:C:349:LEU:HD21	1:C:406:TYR:HB3	1.92	0.52
1:C:410:GLY:H	1:C:470:ARG:CZ	2.22	0.52
1:D:272:VAL:O	1:D:274:TYR:CE2	2.61	0.52
1:D:336:GLY:HA2	1:D:340:ARG:NE	2.23	0.52
1:A:69:GLU:HG3	1:A:70:MET:HE3	1.92	0.52
1:A:402:LEU:HD21	1:A:478:LEU:HG	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:ASP:HA	1:B:702:ARG:NH1	2.26	0.51
1:C:121:ARG:HB2	1:C:128:THR:HG22	1.92	0.51
1:D:329:PHE:CE1	1:D:333:LYS:HE2	2.45	0.51
1:D:445:VAL:HG12	1:D:446:THR:H	1.75	0.51
1:D:540:PHE:HA	1:D:570:LEU:HD21	1.92	0.51
1:B:565:ARG:HG3	1:B:594:ASP:CG	2.35	0.51
1:C:540:PHE:HA	1:C:574:ARG:HG3	1.92	0.51
1:B:205:LEU:O	1:B:208:GLU:HB2	2.10	0.51
1:C:152:PHE:O	1:C:174:ARG:NH2	2.43	0.51
1:C:547:LEU:O	1:C:551:ILE:HG12	2.10	0.51
1:C:319:PHE:CD2	1:C:351:TYR:CD1	2.98	0.51
1:C:415:GLU:HG2	1:C:416:GLN:H	1.76	0.51
1:D:530:GLU:O	1:D:534:LYS:HG2	2.11	0.51
1:A:131:LYS:HZ2	1:A:134:ARG:HB3	1.75	0.51
1:A:174:ARG:HB3	1:A:177:ARG:NH2	2.26	0.51
1:D:70:MET:O	1:D:73:LEU:HG	2.10	0.51
1:A:533:LEU:HD11	1:D:533:LEU:HB3	1.93	0.51
1:D:266:ILE:HA	1:D:269:MET:SD	2.51	0.51
1:C:432:GLU:HG2	1:C:470:ARG:HB3	1.92	0.51
1:B:521:VAL:O	1:B:524:ILE:HG22	2.11	0.51
1:D:109:LEU:O	1:D:112:ILE:HG22	2.11	0.51
1:B:190:LYS:NZ	1:C:337:ARG:HH22	2.08	0.51
1:C:394:PHE:HD1	1:C:492:TYR:CD2	2.29	0.51
1:C:110:VAL:HA	1:C:113:VAL:HG12	1.93	0.51
1:C:281:ASN:OD1	1:C:282:LEU:N	2.44	0.51
1:D:65:TYR:HE1	1:D:114:LEU:HD21	1.76	0.51
1:B:358:THR:HA	1:B:361:LEU:HD12	1.92	0.50
1:C:282:LEU:HD11	1:D:259:THR:HG21	1.92	0.50
1:C:459:ILE:HG12	1:C:482:LYS:HE2	1.92	0.50
1:D:231:GLU:O	1:D:234:THR:OG1	2.27	0.50
1:B:221:TYR:O	1:B:224:THR:OG1	2.20	0.50
1:B:120:TYR:HB3	1:B:135:ILE:HG12	1.93	0.50
1:B:507:LYS:HE3	1:B:514:LYS:CE	2.41	0.50
1:C:531:LEU:O	1:C:535:VAL:HG23	2.11	0.50
1:A:350:GLN:NE2	1:A:405:GLU:OE2	2.44	0.50
1:A:378:LEU:O	1:A:382:LYS:HG2	2.12	0.50
1:D:236:ILE:HA	1:D:239:LEU:HD23	1.92	0.50
1:A:543:ASP:OD1	1:A:543:ASP:N	2.45	0.50
1:B:417:GLY:H	1:B:466:PRO:HA	1.77	0.50
1:D:337:ARG:HH11	1:D:338:ASP:HB3	1.77	0.50
1:A:615:LEU:O	1:A:618:LYS:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:701:ALA:HB2	1:C:713:LEU:HD23	1.94	0.50
1:A:112:ILE:HG13	1:A:144:PHE:CE1	2.47	0.50
1:A:197:LEU:HB3	1:A:309:LEU:HD12	1.94	0.50
1:A:625:LEU:HD21	1:A:652:MET:SD	2.52	0.50
1:B:190:LYS:HZ1	1:C:337:ARG:HH22	1.58	0.50
1:C:212:THR:HG21	1:C:269:MET:HE2	1.93	0.50
1:C:346:HIS:HD2	1:C:349:LEU:HD23	1.77	0.50
1:D:329:PHE:HE1	1:D:333:LYS:HE2	1.77	0.50
1:A:85:MET:O	1:A:89:PHE:N	2.40	0.49
1:A:329:PHE:CD1	1:A:332:ARG:HD3	2.47	0.49
1:A:354:HIS:O	1:A:358:THR:HG23	2.12	0.49
1:B:548:LYS:HZ3	1:B:582:PHE:HD2	1.60	0.49
1:C:87:PHE:HA	1:C:168:ARG:NH2	2.27	0.49
1:A:385:PRO:O	1:A:388:LYS:HG3	2.11	0.49
1:B:138:ARG:O	1:B:141:LYS:HG2	2.12	0.49
1:B:401:ARG:CZ	1:B:481:ASP:HB2	2.42	0.49
1:D:394:PHE:CE2	1:D:488:ILE:HG22	2.47	0.49
1:D:592:LEU:O	1:D:599:THR:HA	2.12	0.49
1:A:319:PHE:CE1	1:A:348:ARG:HG2	2.47	0.49
1:A:404:GLU:O	1:A:479:ARG:NE	2.44	0.49
1:C:289:MET:CE	1:D:262:LEU:HG	2.42	0.49
1:C:575:GLY:HA2	1:C:612:VAL:HG11	1.94	0.49
1:A:424:TYR:HB3	1:A:477:LEU:HD12	1.93	0.49
1:B:422:HIS:HA	1:B:480:LEU:O	2.12	0.49
1:C:272:VAL:HG23	1:C:273:GLY:H	1.76	0.49
1:C:610:GLU:OE2	1:C:646:ARG:NH1	2.46	0.49
1:C:209:VAL:O	1:C:212:THR:OG1	2.24	0.49
1:A:185:PHE:HA	1:A:188:LEU:HD12	1.95	0.49
1:A:601:LEU:HD23	1:A:623:PHE:HD2	1.78	0.49
1:D:154:TRP:CZ3	1:D:170:LEU:HB3	2.48	0.49
1:D:226:LEU:HD21	1:D:281:ASN:HD21	1.78	0.49
1:A:268:THR:HG23	1:A:269:MET:N	2.27	0.49
1:A:569:HIS:HD2	1:A:600:PRO:HG3	1.77	0.49
1:B:522:ILE:O	1:B:526:LYS:HG3	2.12	0.49
1:B:568:LEU:HD13	1:B:583:LEU:CG	2.42	0.49
1:A:66:LYS:O	1:A:69:GLU:HG2	2.13	0.49
1:A:400:ILE:HG13	1:A:401:ARG:HD3	1.95	0.49
1:A:596:PHE:HB2	1:A:598:HIS:CD2	2.48	0.49
1:B:353:SER:O	1:B:356:THR:OG1	2.25	0.49
1:B:386:LEU:HD22	1:B:453:SER:HB2	1.94	0.49
1:C:375:LEU:HD11	1:D:335:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:PHE:HD1	1:A:646:ARG:HH21	1.60	0.49
1:B:401:ARG:NH2	1:B:481:ASP:HB2	2.28	0.49
1:B:551:ILE:HA	1:B:555:ALA:HB3	1.93	0.49
1:D:387:PHE:HE1	1:D:394:PHE:HE1	1.61	0.49
1:D:154:TRP:HZ3	1:D:170:LEU:HB3	1.78	0.49
1:A:240:LYS:HD2	1:A:245:SER:HB2	1.94	0.48
1:B:504:MET:O	1:B:507:LYS:HG2	2.12	0.48
1:C:356:THR:CG2	1:D:329:PHE:CD1	2.96	0.48
1:B:189:GLU:CG	1:B:192:THR:HG23	2.43	0.48
1:C:247:GLU:OE1	1:C:247:GLU:N	2.40	0.48
1:A:426:VAL:HG22	1:A:477:LEU:HD11	1.94	0.48
1:B:328:SER:HA	1:B:331:ASN:ND2	2.27	0.48
1:C:414:THR:HG21	1:C:465:GLN:HG2	1.95	0.48
1:A:346:HIS:HB3	1:A:408:LEU:HG	1.95	0.48
1:A:380:TYR:O	1:A:384:VAL:HG23	2.14	0.48
1:B:565:ARG:HD3	1:C:596:PHE:HZ	1.77	0.48
1:B:612:VAL:O	1:B:615:LEU:HG	2.13	0.48
1:A:136:ALA:O	1:A:140:LEU:HB2	2.13	0.48
1:A:541:GLN:NE2	1:D:562:TYR:OH	2.42	0.48
1:B:368:ILE:HD13	1:C:343:ILE:HG22	1.96	0.48
1:B:448:LEU:HG	1:B:452:THR:CG2	2.43	0.48
1:B:500:LEU:HD23	1:B:503:ILE:HD11	1.95	0.48
1:C:59:HIS:CD2	1:C:60:PRO:HD2	2.49	0.48
1:C:252:ILE:O	1:C:257:ARG:NH1	2.46	0.48
1:C:375:LEU:CD1	1:D:335:LEU:HD12	2.44	0.48
1:A:360:MET:HE1	1:B:329:PHE:CZ	2.49	0.48
1:C:240:LYS:HG3	1:C:240:LYS:O	2.14	0.48
1:C:409:PRO:HA	1:C:471:VAL:HG23	1.96	0.48
1:C:535:VAL:HG22	1:C:550:LEU:HD11	1.96	0.48
1:C:665:LEU:HD22	1:C:713:LEU:HD13	1.95	0.48
1:A:483:GLN:OE1	1:A:487:ASN:ND2	2.46	0.48
1:A:517:GLU:HA	1:A:520:ILE:HG22	1.96	0.48
1:B:63:ARG:HD2	1:B:66:LYS:HZ1	1.78	0.48
1:B:158:TYR:CE2	1:B:163:LYS:HG3	2.49	0.48
1:B:484:SER:O	1:B:488:ILE:HG12	2.14	0.48
1:C:132:PRO:HA	1:C:135:ILE:HD12	1.95	0.48
1:D:86:GLU:O	1:D:168:ARG:NH2	2.47	0.48
1:D:358:THR:HB	1:D:362:GLN:HE22	1.78	0.48
1:A:408:LEU:O	1:A:471:VAL:HG21	2.13	0.48
1:B:323:MET:O	1:B:327:ILE:HG12	2.14	0.48
1:B:565:ARG:NH2	1:C:563:ASP:OD2	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ILE:HD13	1:A:369:ARG:HB3	1.96	0.48
1:A:416:GLN:CD	1:A:436:THR:HB	2.38	0.48
1:D:143:HIS:CD2	1:D:179:ARG:HD3	2.49	0.48
1:D:331:ASN:OD1	1:D:340:ARG:NH2	2.44	0.48
1:A:268:THR:HG23	1:A:291:TYR:CE2	2.48	0.48
1:A:401:ARG:HH22	1:A:488:ILE:HD13	1.79	0.48
1:A:507:LYS:HA	1:A:513:ILE:HG12	1.96	0.48
1:A:674:PHE:HB2	1:A:712:LEU:HD12	1.95	0.48
1:C:83:THR:OG1	1:C:84:PRO:HD3	2.14	0.48
1:C:385:PRO:HA	1:C:388:LYS:HE2	1.96	0.48
1:C:460:ILE:HD11	1:C:500:LEU:HD23	1.96	0.48
1:A:581:LEU:HA	1:A:584:ILE:HD12	1.95	0.47
1:B:501:ASN:HA	1:B:504:MET:HE3	1.96	0.47
1:C:103:VAL:O	1:C:106:ILE:HG22	2.13	0.47
1:A:59:HIS:CD2	1:A:61:LYS:H	2.32	0.47
1:A:501:ASN:O	1:A:504:MET:HG3	2.14	0.47
1:A:520:ILE:HA	1:A:523:HIS:CE1	2.49	0.47
1:A:615:LEU:O	1:A:618:LYS:N	2.47	0.47
1:B:113:VAL:HA	1:B:116:PHE:HD2	1.78	0.47
1:C:145:LEU:O	1:C:149:ILE:HG13	2.14	0.47
1:C:352:ASP:OD1	1:C:353:SER:N	2.47	0.47
1:D:411:GLU:O	1:D:471:VAL:HG12	2.13	0.47
1:A:323:MET:HG2	1:A:348:ARG:CD	2.42	0.47
1:B:239:LEU:HD23	1:B:246:TYR:CE2	2.49	0.47
1:B:558:ASN:OD1	1:B:558:ASN:C	2.58	0.47
1:B:637:ALA:HB1	1:C:659:TYR:CG	2.49	0.47
1:D:89:PHE:CZ	1:D:258:TYR:HA	2.50	0.47
1:C:356:THR:O	1:C:359:VAL:HG22	2.15	0.47
1:D:108:PHE:CE1	1:D:177:ARG:CD	2.97	0.47
1:A:198:PHE:O	1:A:202:LEU:HD23	2.14	0.47
1:B:150:GLY:O	1:B:174:ARG:NH2	2.47	0.47
1:B:239:LEU:HD23	1:B:246:TYR:HE2	1.80	0.47
1:B:364:ILE:CG2	1:B:369:ARG:HB2	2.38	0.47
1:B:504:MET:HG2	1:B:507:LYS:HZ3	1.79	0.47
1:D:565:ARG:NH2	1:D:594:ASP:OD2	2.47	0.47
1:A:376:LEU:O	1:A:379:PRO:HD2	2.14	0.47
1:A:569:HIS:CD2	1:A:600:PRO:HG3	2.50	0.47
1:D:323:MET:O	1:D:327:ILE:HG12	2.14	0.47
1:D:335:LEU:HD22	1:D:339:LEU:CB	2.45	0.47
1:A:339:LEU:HD12	1:A:340:ARG:H	1.71	0.47
1:A:662:ARG:HH12	1:A:693:TRP:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:PHE:HB2	1:B:277:ILE:HD12	1.96	0.47
1:B:425:PHE:HD1	1:B:453:SER:HG	1.62	0.47
1:B:655:ASN:HB3	1:B:685:ALA:HA	1.97	0.47
1:B:662:ARG:HG3	1:B:663:THR:N	2.30	0.47
1:B:690:LYS:HD2	1:B:690:LYS:HA	1.41	0.47
1:C:431:LEU:HB2	1:C:448:LEU:HB2	1.96	0.47
1:C:550:LEU:HG	1:C:555:ALA:HB3	1.97	0.47
1:D:86:GLU:HG2	1:D:87:PHE:N	2.28	0.47
1:D:319:PHE:O	1:D:323:MET:HG2	2.14	0.47
1:D:640:ASP:OD1	1:D:640:ASP:N	2.48	0.47
1:A:59:HIS:CD2	1:A:61:LYS:HB2	2.50	0.47
1:A:68:TRP:O	1:A:72:ILE:HG23	2.15	0.47
1:B:255:TRP:O	1:B:259:THR:HG23	2.15	0.47
1:B:407:PHE:CD2	1:B:471:VAL:HG21	2.49	0.47
1:B:693:TRP:HE1	1:C:662:ARG:NH2	2.13	0.47
1:C:599:THR:HG21	1:C:624:ASN:H	1.80	0.47
1:D:323:MET:HE1	1:D:347:VAL:HG11	1.95	0.47
1:B:194:ILE:HD12	1:B:199:THR:HG22	1.96	0.47
1:B:416:GLN:NE2	1:B:435:VAL:HG23	2.30	0.47
1:D:235:TRP:CZ3	1:D:277:ILE:HG21	2.50	0.47
1:D:335:LEU:HD22	1:D:339:LEU:HB3	1.97	0.47
1:D:404:GLU:OE1	1:D:476:HIS:NE2	2.48	0.47
1:D:428:GLU:HB3	1:D:476:HIS:HB3	1.97	0.47
1:C:434:LEU:HB3	1:C:442:GLU:OE1	2.15	0.47
1:A:315:ASN:OD1	1:A:316:THR:N	2.48	0.46
1:B:418:ASN:O	1:B:465:GLN:HG2	2.15	0.46
1:D:263:TYR:O	1:D:266:ILE:HG22	2.15	0.46
1:D:264:PHE:CD2	1:D:277:ILE:CG2	2.97	0.46
1:D:357:ASP:O	1:D:361:LEU:HG	2.15	0.46
1:D:461:CYS:HB3	1:D:519:ASP:CG	2.40	0.46
1:D:503:ILE:HA	1:D:506:GLU:OE2	2.16	0.46
1:A:636:VAL:HG21	1:A:664:PRO:HB3	1.97	0.46
1:B:349:LEU:HD23	1:B:408:LEU:HG	1.97	0.46
1:B:431:LEU:HD13	1:B:471:VAL:HG22	1.97	0.46
1:C:112:ILE:HG21	1:C:148:PHE:CE2	2.50	0.46
1:D:181:VAL:HG12	1:D:185:PHE:HE2	1.80	0.46
1:D:556:ASP:O	1:D:559:LYS:HG2	2.16	0.46
1:A:368:ILE:O	1:A:372:ILE:HG23	2.15	0.46
1:A:465:GLN:HE21	1:A:467:PHE:HB2	1.81	0.46
1:B:167:VAL:HA	1:B:170:LEU:HD12	1.98	0.46
1:B:220:TYR:O	1:B:224:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:GLN:O	1:B:530:GLU:HG3	2.15	0.46
1:C:71:PHE:O	1:C:75:TRP:HD1	1.98	0.46
1:D:158:TYR:HE2	1:D:163:LYS:HZ2	1.63	0.46
1:B:102:ILE:O	1:B:106:ILE:HG12	2.15	0.46
1:C:272:VAL:HG23	1:C:273:GLY:N	2.31	0.46
1:C:397:GLN:O	1:C:400:ILE:HG12	2.15	0.46
1:A:606:LYS:HG2	1:A:643:PHE:CE1	2.49	0.46
1:B:642:ASP:O	1:B:645:LYS:HG2	2.15	0.46
1:C:149:ILE:HG23	1:C:154:TRP:HZ2	1.80	0.46
1:C:315:ASN:HA	1:C:318:ARG:CZ	2.45	0.46
1:C:522:ILE:HG13	1:C:523:HIS:CD2	2.51	0.46
1:A:326:LEU:HD11	1:A:348:ARG:NH2	2.30	0.46
1:B:330:MET:HE1	1:B:340:ARG:N	2.30	0.46
1:B:540:PHE:HA	1:B:570:LEU:HD21	1.97	0.46
1:C:189:GLU:HB2	1:C:199:THR:HG21	1.96	0.46
1:C:402:LEU:HD22	1:C:478:LEU:HB3	1.98	0.46
1:C:481:ASP:OD2	1:C:483:GLN:HB3	2.16	0.46
1:C:506:GLU:HA	1:C:509:SER:OG	2.16	0.46
1:A:249:PHE:HA	1:A:252:ILE:HD13	1.97	0.46
1:B:90:PHE:O	1:B:168:ARG:NH2	2.47	0.46
1:B:281:ASN:OD1	1:B:283:ARG:N	2.39	0.46
1:B:336:GLY:C	1:B:337:ARG:HG2	2.41	0.46
1:B:402:LEU:HB3	1:B:478:LEU:HD12	1.98	0.46
1:C:393:GLU:HA	1:C:396:ASN:ND2	2.31	0.46
1:D:420:VAL:O	1:D:482:LYS:HD2	2.15	0.46
1:D:434:LEU:O	1:D:467:PHE:HB2	2.15	0.46
1:D:625:LEU:HD23	1:D:625:LEU:HA	1.77	0.46
1:B:666:HIS:HE1	1:B:691:ASP:HB2	1.81	0.46
1:C:426:VAL:O	1:C:451:HIS:N	2.48	0.46
1:C:636:VAL:HG11	1:C:667:VAL:HG23	1.98	0.46
1:D:73:LEU:HB3	1:D:180:LYS:NZ	2.21	0.46
1:D:83:THR:HA	1:D:86:GLU:CD	2.41	0.46
1:D:671:GLU:HG3	1:D:673:LEU:HG	1.97	0.46
1:A:357:ASP:HA	1:A:360:MET:CE	2.46	0.46
1:B:82:PHE:O	1:B:85:MET:HG2	2.15	0.46
1:C:398:ILE:HG13	1:C:399:VAL:N	2.30	0.46
1:D:129:VAL:HG13	1:D:135:ILE:HD11	1.97	0.46
1:A:668:ALA:HB1	1:A:677:ALA:HB2	1.97	0.46
1:B:523:HIS:HA	1:B:526:LYS:HE2	1.97	0.46
1:C:380:TYR:CE1	1:C:427:CYS:HB3	2.51	0.46
1:C:394:PHE:HA	1:C:488:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:561:ASP:OD2	1:C:565:ARG:NH2	2.46	0.46
1:A:164:HIS:O	1:A:167:VAL:HG12	2.15	0.45
1:A:403:HIS:HB2	1:A:479:ARG:HG3	1.97	0.45
1:A:422:HIS:HA	1:A:480:LEU:O	2.17	0.45
1:B:565:ARG:NH2	1:C:565:ARG:NH1	2.64	0.45
1:C:344:THR:O	1:C:348:ARG:HG2	2.17	0.45
1:A:423:LEU:HB2	1:A:480:LEU:HB3	1.97	0.45
1:B:319:PHE:HA	1:B:322:LYS:HE2	1.98	0.45
1:C:271:THR:HA	1:D:272:VAL:HG21	1.81	0.45
1:C:663:THR:HG22	1:C:665:LEU:H	1.82	0.45
1:D:504:MET:O	1:D:507:LYS:HB2	2.16	0.45
1:A:398:ILE:O	1:A:402:LEU:HB2	2.16	0.45
1:B:307:THR:O	1:B:311:VAL:HG23	2.15	0.45
1:B:514:LYS:O	1:B:514:LYS:HG3	2.17	0.45
1:B:603:GLU:HA	1:B:606:LYS:HE3	1.98	0.45
1:C:384:VAL:HG12	1:C:387:PHE:H	1.81	0.45
1:C:465:GLN:CD	1:C:465:GLN:H	2.24	0.45
1:C:525:GLY:O	1:C:528:GLU:HG2	2.16	0.45
1:D:431:LEU:HD21	1:D:469:VAL:CG2	2.46	0.45
1:A:135:ILE:HG12	1:A:138:ARG:NH2	2.31	0.45
1:C:512:ARG:HA	1:C:516:LEU:HD12	1.98	0.45
1:D:565:ARG:HH12	1:D:603:GLU:CD	2.24	0.45
1:A:128:THR:HG21	1:A:134:ARG:HD3	1.98	0.45
1:B:301:TYR:CD1	1:C:306:ILE:HD11	2.39	0.45
1:C:174:ARG:HG3	1:C:177:ARG:NH2	2.30	0.45
1:C:237:GLY:HA2	1:C:247:GLU:HA	1.97	0.45
1:D:628:SER:HB2	1:D:652:MET:SD	2.56	0.45
1:A:397:GLN:HB3	1:A:401:ARG:HH12	1.82	0.45
1:A:485:PHE:CE2	1:A:489:LEU:HD11	2.52	0.45
1:B:226:LEU:HD21	1:B:283:ARG:CZ	2.46	0.45
1:C:115:GLN:O	1:C:118:VAL:HG12	2.17	0.45
1:C:130:TYR:CG	1:C:130:TYR:O	2.68	0.45
1:D:445:VAL:CG1	1:D:446:THR:H	2.30	0.45
1:A:60:PRO:HD3	1:A:118:VAL:HG13	1.98	0.45
1:A:330:MET:HE3	1:A:337:ARG:HH22	1.82	0.45
1:B:514:LYS:HE3	1:B:520:ILE:HG21	1.98	0.45
1:D:623:PHE:CD2	1:D:625:LEU:HB2	2.52	0.45
1:A:94:PRO:HD2	1:A:97:LEU:HD12	1.97	0.45
1:A:184:PHE:O	1:A:188:LEU:HG	2.17	0.45
1:A:380:TYR:HA	1:A:383:LYS:HD2	1.99	0.45
1:B:415:GLU:O	1:B:465:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:GLU:HG2	1:D:394:PHE:N	2.31	0.45
1:A:163:LYS:HG3	1:A:164:HIS:N	2.32	0.45
1:B:120:TYR:CE2	1:B:138:ARG:HG3	2.51	0.45
1:B:402:LEU:HD23	1:B:402:LEU:HA	1.82	0.45
1:B:428:GLU:O	1:B:475:CYS:HB2	2.16	0.45
1:B:433:ALA:HB1	1:B:467:PHE:CE2	2.51	0.45
1:B:662:ARG:NH2	1:C:692:ARG:HH21	2.14	0.45
1:C:223:ALA:HB2	1:C:235:TRP:NE1	2.32	0.45
1:D:394:PHE:O	1:D:398:ILE:HG12	2.16	0.45
1:D:409:PRO:HB3	1:D:473:GLU:HA	1.99	0.45
1:A:298:LEU:HD23	1:A:298:LEU:HA	1.85	0.45
1:A:616:LEU:HD12	1:A:616:LEU:HA	1.85	0.45
1:B:372:ILE:O	1:B:375:LEU:HG	2.17	0.45
1:B:514:LYS:HZ1	1:B:520:ILE:HG21	1.80	0.45
1:C:173:ILE:HD12	1:C:173:ILE:H	1.82	0.45
1:D:174:ARG:HG2	1:D:177:ARG:HH12	1.82	0.45
1:A:221:TYR:O	1:A:224:THR:OG1	2.26	0.44
1:C:239:LEU:HD12	1:C:246:TYR:OH	2.16	0.44
1:D:303:ILE:O	1:D:307:THR:HG23	2.17	0.44
1:C:540:PHE:CD1	1:C:574:ARG:HD3	2.51	0.44
1:D:81:LEU:O	1:D:84:PRO:HD2	2.17	0.44
1:A:222:LEU:HD22	1:A:283:ARG:HB3	1.99	0.44
1:A:372:ILE:HG13	1:A:373:ALA:N	2.32	0.44
1:A:636:VAL:HG13	1:A:676:MET:HE1	1.98	0.44
1:A:654:PRO:HB3	1:A:680:LEU:HD23	2.00	0.44
1:B:539:ALA:HA	1:B:547:LEU:HD11	1.99	0.44
1:C:285:MET:O	1:C:288:VAL:HG12	2.18	0.44
1:D:93:LEU:H	1:D:159:LYS:NZ	2.15	0.44
1:D:547:LEU:HD22	1:D:579:ILE:HD12	1.99	0.44
1:D:547:LEU:O	1:D:551:ILE:HG12	2.16	0.44
1:D:678:LYS:HA	1:D:681:VAL:HG22	2.00	0.44
1:A:110:VAL:O	1:A:114:LEU:HD23	2.18	0.44
1:C:304:GLY:C	1:D:310:ILE:HD11	2.43	0.44
1:D:374:GLN:HA	1:D:399:VAL:HG11	1.99	0.44
1:A:124:GLN:HG2	1:A:125:THR:N	2.32	0.44
1:B:188:LEU:O	1:B:188:LEU:CD1	2.60	0.44
1:B:265:ALA:O	1:B:268:THR:OG1	2.31	0.44
1:B:378:LEU:HB3	1:B:379:PRO:HD3	2.00	0.44
1:C:418:ASN:C	1:C:465:GLN:HE22	2.25	0.44
1:C:538:ALA:HA	1:C:541:GLN:HG2	2.00	0.44
1:C:569:HIS:NE2	1:C:600:PRO:HD3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:ILE:H	1:D:149:ILE:HD12	1.83	0.44
1:D:235:TRP:HZ3	1:D:277:ILE:HG21	1.81	0.44
1:A:140:LEU:HG	1:A:144:PHE:CD2	2.53	0.44
1:A:308:ALA:HA	1:A:311:VAL:HG12	2.00	0.44
1:A:326:LEU:HD11	1:A:348:ARG:HH21	1.82	0.44
1:B:356:THR:HG22	1:C:329:PHE:HE1	1.83	0.44
1:B:568:LEU:CD1	1:B:583:LEU:HD11	2.42	0.44
1:C:121:ARG:HA	1:C:128:THR:HA	2.00	0.44
1:C:418:ASN:O	1:C:465:GLN:NE2	2.50	0.44
1:C:647:LEU:HG	1:C:652:MET:HB2	1.99	0.44
1:D:339:LEU:O	1:D:343:ILE:HD12	2.17	0.44
1:A:122:ASP:OD2	1:A:124:GLN:NE2	2.39	0.44
1:A:659:TYR:CG	1:D:637:ALA:HB1	2.52	0.44
1:B:407:PHE:HD2	1:B:471:VAL:HG21	1.82	0.44
1:B:596:PHE:HB2	1:B:598:HIS:ND1	2.33	0.44
1:C:86:GLU:HG3	1:C:90:PHE:CE1	2.53	0.44
1:C:487:ASN:O	1:C:490:GLU:HG3	2.18	0.44
1:D:251:GLU:C	1:D:251:GLU:CD	2.85	0.44
1:A:239:LEU:CD2	1:A:241:LEU:HB2	2.48	0.44
1:A:432:GLU:OE2	1:A:434:LEU:HB3	2.18	0.44
1:A:593:LYS:HZ3	1:A:599:THR:HB	1.82	0.44
1:A:687:VAL:HG23	1:A:688:ILE:HG23	1.99	0.44
1:B:355:TYR:O	1:B:359:VAL:HG13	2.18	0.44
1:B:564:GLY:N	1:B:595:LYS:HB3	2.32	0.44
1:C:358:THR:O	1:C:362:GLN:OE1	2.35	0.44
1:C:488:ILE:HA	1:C:491:ILE:HG22	1.99	0.44
1:D:115:GLN:HE22	1:D:140:LEU:HA	1.81	0.44
1:A:479:ARG:H	1:A:479:ARG:HG2	1.66	0.44
1:A:608:GLY:HA2	1:A:646:ARG:HD2	2.00	0.44
1:B:437:LYS:HB3	1:B:441:SER:HB3	2.00	0.44
1:B:659:TYR:HB2	1:C:637:ALA:HB2	2.00	0.44
1:C:149:ILE:HG23	1:C:154:TRP:CZ2	2.53	0.44
1:A:124:GLN:HG2	1:A:125:THR:HG23	2.00	0.43
1:A:281:ASN:O	1:A:285:MET:N	2.51	0.43
1:A:330:MET:HE3	1:A:337:ARG:NH2	2.32	0.43
1:B:196:TYR:HB2	1:C:320:ARG:HE	1.83	0.43
1:B:525:GLY:O	1:B:528:GLU:HG3	2.17	0.43
1:B:642:ASP:OD1	1:B:642:ASP:N	2.50	0.43
1:D:137:PHE:O	1:D:141:LYS:HG3	2.17	0.43
1:D:514:LYS:HB3	1:D:514:LYS:HE2	1.71	0.43
1:D:575:GLY:HA2	1:D:612:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:LEU:HD21	1:B:337:ARG:HH22	1.83	0.43
1:A:382:LYS:HZ3	1:A:392:THR:HA	1.83	0.43
1:C:343:ILE:HG13	1:C:344:THR:N	2.33	0.43
1:C:383:LYS:HD2	1:C:451:HIS:CG	2.53	0.43
1:D:131:LYS:CE	1:D:134:ARG:HH12	2.27	0.43
1:A:172:TRP:O	1:A:175:LEU:HB3	2.19	0.43
1:A:485:PHE:O	1:A:488:ILE:HG22	2.18	0.43
1:C:308:ALA:HA	1:C:311:VAL:HG12	2.01	0.43
1:C:583:LEU:O	1:C:586:GLU:HB2	2.19	0.43
1:D:394:PHE:HB2	1:D:495:ASP:OD2	2.19	0.43
1:D:527:GLN:O	1:D:530:GLU:HG3	2.18	0.43
1:A:59:HIS:ND1	1:A:60:PRO:HD2	2.33	0.43
1:A:91:ARG:HA	1:A:168:ARG:NH1	2.33	0.43
1:A:289:MET:O	1:A:292:VAL:HG22	2.18	0.43
1:D:68:TRP:CZ2	1:D:72:ILE:HD11	2.53	0.43
1:D:393:GLU:O	1:D:397:GLN:HG2	2.18	0.43
1:D:487:ASN:O	1:D:490:GLU:HG3	2.18	0.43
1:D:497:ARG:NH1	1:D:553:SER:O	2.51	0.43
1:A:60:PRO:HG3	1:A:117:PHE:HE2	1.83	0.43
1:A:397:GLN:O	1:A:400:ILE:HG12	2.19	0.43
1:A:485:PHE:CZ	1:A:489:LEU:HD11	2.54	0.43
1:B:527:GLN:O	1:B:531:LEU:HG	2.18	0.43
1:D:106:ILE:HD12	1:D:109:LEU:HD12	1.99	0.43
1:D:507:LYS:C	1:D:509:SER:H	2.26	0.43
1:D:535:VAL:HG12	1:D:550:LEU:HD22	2.00	0.43
1:D:601:LEU:HD11	1:D:621:ALA:HB3	2.01	0.43
1:B:194:ILE:CD1	1:B:199:THR:HG22	2.49	0.43
1:D:269:MET:HA	1:D:295:ASP:OD2	2.18	0.43
1:D:425:PHE:HD1	1:D:453:SER:HB2	1.82	0.43
1:D:547:LEU:O	1:D:550:LEU:HG	2.19	0.43
1:B:384:VAL:HA	1:B:451:HIS:HB3	2.00	0.43
1:B:433:ALA:HB3	1:B:446:THR:OG1	2.19	0.43
1:C:511:ASP:HB2	1:C:515:LYS:HB3	2.01	0.43
1:A:273:GLY:HA3	1:B:272:VAL:O	2.19	0.43
1:B:378:LEU:HA	1:B:381:ILE:HG22	2.00	0.43
1:C:383:LYS:O	1:C:383:LYS:HG2	2.18	0.43
1:C:435:VAL:HG22	1:C:467:PHE:CD1	2.54	0.43
1:C:576:TYR:O	1:C:580:THR:HG23	2.18	0.43
1:A:326:LEU:HD12	1:A:326:LEU:C	2.44	0.43
1:B:507:LYS:CB	1:B:514:LYS:HG2	2.49	0.43
1:C:402:LEU:HD23	1:C:402:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:LEU:HD11	1:D:246:TYR:CE2	2.54	0.43
1:D:589:ASP:OD1	1:D:589:ASP:N	2.51	0.43
1:A:223:ALA:HB2	1:A:235:TRP:HE1	1.83	0.43
1:B:424:TYR:HA	1:B:478:LEU:O	2.18	0.43
1:B:594:ASP:OD1	1:B:595:LYS:N	2.49	0.43
1:C:408:LEU:HD23	1:C:409:PRO:O	2.19	0.43
1:A:412:VAL:HG23	1:A:468:THR:HG23	2.00	0.42
1:A:507:LYS:HA	1:A:513:ILE:HG23	2.01	0.42
1:B:129:VAL:HB	1:B:135:ILE:HD11	2.01	0.42
1:B:345:GLY:HA2	1:B:348:ARG:HG2	2.00	0.42
1:B:410:GLY:N	1:B:471:VAL:O	2.50	0.42
1:C:399:VAL:O	1:C:402:LEU:HB2	2.19	0.42
1:C:582:PHE:HA	1:C:585:GLN:NE2	2.33	0.42
1:C:593:LYS:HD3	1:C:624:ASN:HB3	1.99	0.42
1:D:131:LYS:HE3	1:D:134:ARG:NH1	2.30	0.42
1:D:333:LYS:C	1:D:334:LYS:CG	2.87	0.42
1:A:223:ALA:HB2	1:A:235:TRP:NE1	2.34	0.42
1:B:74:VAL:HA	1:B:77:ILE:HG12	2.01	0.42
1:B:448:LEU:CD2	1:B:452:THR:CG2	2.97	0.42
1:D:561:ASP:OD2	1:D:565:ARG:HB3	2.18	0.42
1:D:645:LYS:HG2	1:D:679:MET:HG2	2.00	0.42
1:A:89:PHE:CZ	1:A:258:TYR:HA	2.54	0.42
1:B:168:ARG:HA	1:B:171:LEU:HD13	2.01	0.42
1:C:549:SER:HA	1:C:552:ARG:HG2	2.01	0.42
1:D:251:GLU:CD	1:D:251:GLU:O	2.63	0.42
1:D:308:ALA:O	1:D:311:VAL:HG12	2.18	0.42
1:D:497:ARG:NH2	1:D:553:SER:HB2	2.34	0.42
1:A:63:ARG:HA	1:A:66:LYS:HG2	2.02	0.42
1:B:280:VAL:HG11	1:C:242:GLY:HA3	2.02	0.42
1:B:336:GLY:O	1:B:337:ARG:CG	2.66	0.42
1:B:374:GLN:HA	1:B:378:LEU:HB2	2.02	0.42
1:B:615:LEU:HA	1:B:618:LYS:HG2	2.00	0.42
1:C:190:LYS:HD3	1:C:190:LYS:HA	1.64	0.42
1:C:349:LEU:HD22	1:C:474:LEU:HD23	1.99	0.42
1:C:396:ASN:O	1:C:400:ILE:HG23	2.19	0.42
1:D:445:VAL:CG1	1:D:446:THR:N	2.83	0.42
1:A:220:TYR:OH	1:A:257:ARG:HD2	2.20	0.42
1:B:72:ILE:HG12	1:B:111:ASP:OD1	2.19	0.42
1:B:83:THR:O	1:B:86:GLU:HG3	2.19	0.42
1:B:115:GLN:HB3	1:B:139:TYR:CZ	2.55	0.42
1:B:194:ILE:O	1:C:320:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:LEU:HD22	1:B:284:GLU:OE1	2.20	0.42
1:C:270:ALA:O	1:C:272:VAL:HG13	2.19	0.42
1:D:424:TYR:HA	1:D:478:LEU:O	2.19	0.42
1:A:413:ILE:HB	1:A:469:VAL:HG23	2.01	0.42
1:A:691:ASP:OD1	1:A:691:ASP:N	2.52	0.42
1:B:72:ILE:HD12	1:B:72:ILE:HA	1.92	0.42
1:B:393:GLU:H	1:B:393:GLU:CD	2.25	0.42
1:C:339:LEU:HA	1:C:339:LEU:HD23	1.76	0.42
1:C:456:ASP:OD2	1:C:457:ILE:N	2.52	0.42
1:D:185:PHE:HA	1:D:188:LEU:HD12	2.02	0.42
1:D:322:LYS:O	1:D:326:LEU:HB2	2.20	0.42
1:A:122:ASP:O	1:A:123:THR:OG1	2.28	0.42
1:C:579:ILE:HD12	1:C:579:ILE:H	1.85	0.42
1:D:226:LEU:CD2	1:D:281:ASN:HD21	2.32	0.42
1:D:666:HIS:CD2	1:D:700:GLU:HB2	2.54	0.42
1:A:359:VAL:O	1:A:362:GLN:HG2	2.20	0.42
1:B:65:TYR:O	1:B:69:GLU:HG3	2.19	0.42
1:B:172:TRP:O	1:B:175:LEU:HG	2.20	0.42
1:B:700:GLU:H	1:B:700:GLU:HG2	1.63	0.42
1:C:89:PHE:HA	1:C:220:TYR:CD1	2.55	0.42
1:C:507:LYS:HE2	1:C:515:LYS:HD3	2.02	0.42
1:C:533:LEU:HD11	1:C:562:TYR:CE1	2.55	0.42
1:C:673:LEU:HD21	1:C:676:MET:HE3	2.02	0.42
1:D:181:VAL:CG1	1:D:185:PHE:HE2	2.33	0.42
1:A:234:THR:CG2	1:A:235:TRP:N	2.83	0.42
1:B:154:TRP:HE1	1:B:173:ILE:HD11	1.85	0.42
1:B:281:ASN:HD21	1:B:283:ARG:NH2	2.17	0.42
1:B:396:ASN:O	1:B:400:ILE:HG23	2.19	0.42
1:B:433:ALA:HB1	1:B:467:PHE:HE2	1.85	0.42
1:B:504:MET:O	1:B:508:GLU:OE1	2.37	0.42
1:C:584:ILE:HD13	1:C:619:GLU:OE2	2.19	0.42
1:A:248:ASN:O	1:A:252:ILE:HD12	2.20	0.42
1:B:208:GLU:OE1	1:B:298:LEU:HG	2.19	0.42
1:B:310:ILE:HD13	1:B:310:ILE:HA	1.83	0.42
1:B:330:MET:HE2	1:B:336:GLY:HA2	2.02	0.42
1:C:519:ASP:HB2	1:C:522:ILE:CG1	2.45	0.42
1:C:136:ALA:O	1:C:140:LEU:HD23	2.20	0.41
1:A:437:LYS:HD2	1:A:441:SER:OG	2.20	0.41
1:B:90:PHE:CZ	1:B:254:LEU:HD13	2.55	0.41
1:B:239:LEU:CD1	1:B:277:ILE:HG22	2.50	0.41
1:B:418:ASN:O	1:B:465:GLN:N	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:PHE:CZ	1:C:258:TYR:HA	2.55	0.41
1:C:540:PHE:HD1	1:C:574:ARG:CG	2.33	0.41
1:C:543:ASP:HB2	1:C:545:TYR:CE2	2.55	0.41
1:D:158:TYR:HD1	1:D:167:VAL:HB	1.85	0.41
1:D:183:GLU:O	1:D:187:ARG:NE	2.50	0.41
1:A:233:TYR:HB3	1:B:243:ASP:HB2	2.01	0.41
1:B:219:PHE:HD1	1:B:284:GLU:OE2	2.04	0.41
1:C:231:GLU:OE2	1:C:248:ASN:HA	2.21	0.41
1:C:360:MET:HG3	1:C:369:ARG:NH2	2.35	0.41
1:D:62:ASN:OD1	1:D:63:ARG:N	2.54	0.41
1:D:264:PHE:HD2	1:D:277:ILE:CG2	2.33	0.41
1:D:548:LYS:HG3	1:D:552:ARG:HH21	1.86	0.41
1:A:632:LEU:HD23	1:A:656:SER:O	2.20	0.41
1:B:352:ASP:O	1:B:356:THR:HG23	2.20	0.41
1:B:642:ASP:O	1:B:646:ARG:HG2	2.20	0.41
1:C:101:ASP:O	1:C:105:GLN:HG2	2.20	0.41
1:C:456:ASP:O	1:C:460:ILE:HG22	2.21	0.41
1:C:493:PHE:HD2	1:C:497:ARG:HH22	1.67	0.41
1:C:578:ASP:OD1	1:C:578:ASP:N	2.48	0.41
1:D:109:LEU:O	1:D:113:VAL:HG23	2.21	0.41
1:D:426:VAL:HG13	1:D:426:VAL:O	2.21	0.41
1:A:95:GLU:HG2	1:A:96:ARG:N	2.35	0.41
1:A:58:ILE:O	1:A:118:VAL:HG12	2.19	0.41
1:C:423:LEU:HD12	1:C:454:PHE:O	2.21	0.41
1:D:281:ASN:O	1:D:284:GLU:HB2	2.20	0.41
1:D:347:VAL:HG22	1:D:351:TYR:HE2	1.83	0.41
1:D:397:GLN:HB3	1:D:401:ARG:NH2	2.33	0.41
1:D:425:PHE:O	1:D:477:LEU:HD12	2.20	0.41
1:A:174:ARG:HG2	1:A:177:ARG:HH12	1.85	0.41
1:A:329:PHE:HZ	1:D:356:THR:HG22	1.82	0.41
1:B:393:GLU:OE2	1:B:393:GLU:N	2.40	0.41
1:C:255:TRP:O	1:C:259:THR:HG23	2.21	0.41
1:A:428:GLU:HA	1:A:450:PRO:HB3	2.02	0.41
1:A:501:ASN:HA	1:A:504:MET:HG3	2.02	0.41
1:B:220:TYR:CE1	1:B:257:ARG:HD3	2.55	0.41
1:C:616:LEU:O	1:C:620:GLY:N	2.52	0.41
1:D:77:ILE:HG13	1:D:78:TYR:N	2.36	0.41
1:D:485:PHE:CE2	1:D:489:LEU:HD11	2.56	0.41
1:A:121:ARG:NH1	1:A:127:ARG:HB2	2.36	0.41
1:A:134:ARG:HG3	1:A:135:ILE:N	2.35	0.41
1:A:336:GLY:O	1:A:339:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLN:HB2	1:A:406:TYR:HB2	2.02	0.41
1:A:375:LEU:HD22	1:B:335:LEU:HD11	2.01	0.41
1:A:540:PHE:CE2	1:D:562:TYR:HB3	2.55	0.41
1:B:375:LEU:HD12	1:B:376:LEU:HB2	2.02	0.41
1:B:599:THR:HG21	1:B:623:PHE:O	2.20	0.41
1:B:666:HIS:CG	1:B:700:GLU:HG3	2.55	0.41
1:C:270:ALA:HB3	1:C:272:VAL:HG22	2.02	0.41
1:C:273:GLY:N	1:D:272:VAL:HG13	2.35	0.41
1:C:397:GLN:HB3	1:C:488:ILE:HD12	2.03	0.41
1:C:420:VAL:O	1:C:482:LYS:NZ	2.51	0.41
1:C:486:SER:O	1:C:489:LEU:HG	2.21	0.41
1:D:58:ILE:HD11	1:D:62:ASN:HD22	1.86	0.41
1:D:239:LEU:C	1:D:239:LEU:HD12	2.45	0.41
1:D:257:ARG:H	1:D:257:ARG:HG3	1.73	0.41
1:D:267:VAL:HG22	1:D:274:TYR:CD2	2.56	0.41
1:A:320:ARG:O	1:A:323:MET:HB2	2.20	0.41
1:A:458:SER:OG	1:A:465:GLN:HB2	2.22	0.41
1:B:496:GLY:O	1:B:499:ILE:HG22	2.20	0.41
1:B:524:ILE:HD12	1:B:524:ILE:HA	1.92	0.41
1:D:66:LYS:HB3	1:D:66:LYS:HE3	1.85	0.41
1:D:91:ARG:NH2	1:D:168:ARG:HD2	2.36	0.41
1:B:504:MET:HG2	1:B:507:LYS:NZ	2.35	0.40
1:C:200:ARG:O	1:C:204:LEU:HD23	2.21	0.40
1:D:335:LEU:HD22	1:D:339:LEU:CD2	2.51	0.40
1:D:590:VAL:HB	1:D:619:GLU:HG2	2.03	0.40
1:A:568:LEU:HD22	1:A:588:VAL:HG13	2.03	0.40
1:A:633:CYS:HB3	1:A:657:GLU:O	2.22	0.40
1:B:347:VAL:O	1:B:350:GLN:HG2	2.21	0.40
1:C:361:LEU:HD23	1:C:369:ARG:HD2	2.03	0.40
1:C:582:PHE:HA	1:C:585:GLN:CD	2.46	0.40
1:A:92:GLY:H	1:A:168:ARG:HH12	1.69	0.40
1:A:110:VAL:O	1:A:113:VAL:HG22	2.22	0.40
1:B:89:PHE:HA	1:B:220:TYR:CE2	2.56	0.40
1:B:190:LYS:NZ	1:C:337:ARG:NH2	2.69	0.40
1:B:544:PHE:O	1:B:548:LYS:HD3	2.21	0.40
1:C:205:LEU:HA	1:C:205:LEU:HD12	1.80	0.40
1:C:266:ILE:CG2	1:C:269:MET:HE3	2.52	0.40
1:C:377:TYR:HB2	1:C:399:VAL:HG13	2.04	0.40
1:D:266:ILE:O	1:D:269:MET:CG	2.62	0.40
1:A:318:ARG:C	1:A:322:LYS:HZ2	2.30	0.40
1:A:574:ARG:HA	1:A:574:ARG:HD2	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:PHE:HA	1:B:153:PRO:HD3	1.97	0.40
1:B:181:VAL:CG1	1:B:185:PHE:HE2	2.33	0.40
1:B:661:HIS:O	1:B:661:HIS:CG	2.75	0.40
1:D:349:LEU:HD21	1:D:406:TYR:HB2	2.04	0.40
1:D:563:ASP:HA	1:D:595:LYS:HG3	2.02	0.40
1:B:84:PRO:HB2	1:B:217:CYS:SG	2.61	0.40
1:B:98:PHE:CE2	1:B:102:ILE:HD11	2.56	0.40
1:B:172:TRP:CZ2	1:B:218:ILE:HD11	2.49	0.40
1:C:220:TYR:O	1:C:224:THR:HG23	2.22	0.40
1:C:356:THR:HG23	1:C:360:MET:SD	2.59	0.40
1:C:572:ALA:HB1	1:C:604:ALA:HB2	2.04	0.40
1:D:190:LYS:HD3	1:D:190:LYS:HA	1.90	0.40
1:D:591:ASN:ND2	1:D:624:ASN:OD1	2.55	0.40
1:D:676:MET:SD	1:D:677:ALA:N	2.95	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	654/820 (80%)	634 (97%)	20 (3%)	0	100	100
1	B	654/820 (80%)	637 (97%)	17 (3%)	0	100	100
1	C	654/820 (80%)	640 (98%)	14 (2%)	0	100	100
1	D	654/820 (80%)	642 (98%)	12 (2%)	0	100	100
All	All	2616/3280 (80%)	2553 (98%)	63 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	577/729 (79%)	575 (100%)	2 (0%)	91	92
1	B	577/729 (79%)	572 (99%)	5 (1%)	75	83
1	C	579/729 (79%)	576 (100%)	3 (0%)	86	90
1	D	577/729 (79%)	574 (100%)	3 (0%)	86	90
All	All	2310/2916 (79%)	2297 (99%)	13 (1%)	82	88

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	GLN
1	A	395	ILE
1	B	359	VAL
1	B	513	ILE
1	B	566	SER
1	B	688	ILE
1	B	690	LYS
1	C	267	VAL
1	C	326	LEU
1	C	327	ILE
1	D	247	GLU
1	D	253	ASP
1	D	267	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	465	GLN
1	A	487	ASN
1	A	501	ASN
1	A	527	GLN
1	A	666	HIS
1	B	248	ASN

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Mol	Chain	Res	Type
1	B	346	HIS
1	B	350	GLN
1	B	403	HIS
1	B	465	GLN
1	B	558	ASN
1	B	591	ASN
1	B	666	HIS
1	C	186	GLN
1	C	350	GLN
1	C	397	GLN
1	C	487	ASN
1	C	523	HIS
1	C	630	ASN
1	C	653	ASN
1	D	59	HIS
1	D	124	GLN
1	D	502	ASN
1	D	558	ASN
1	D	655	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

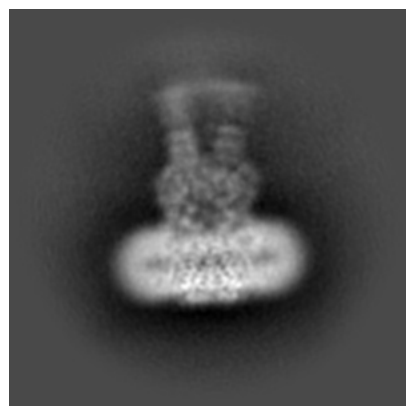
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37500. These allow visual inspection of the internal detail of the map and identification of artifacts.

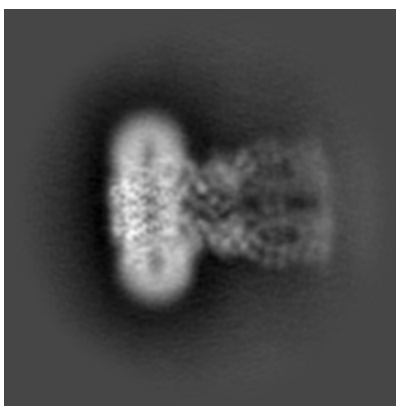
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

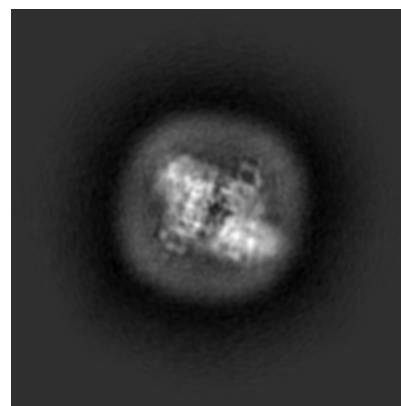
6.1.1 Primary map



X

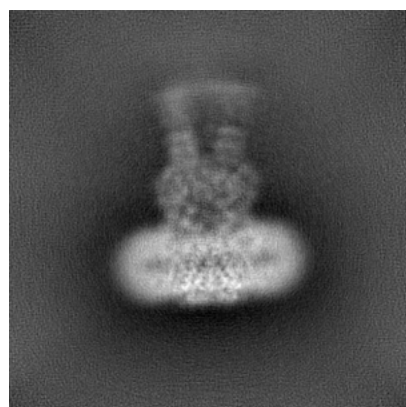


Y

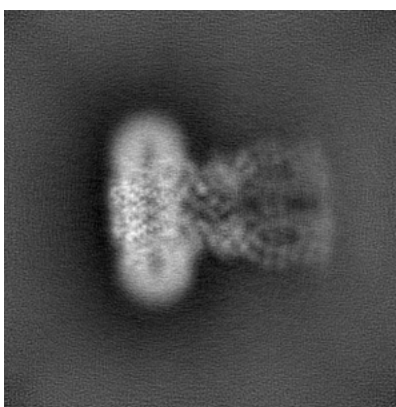


Z

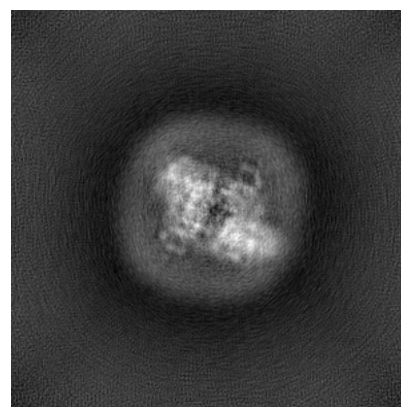
6.1.2 Raw map



X



Y

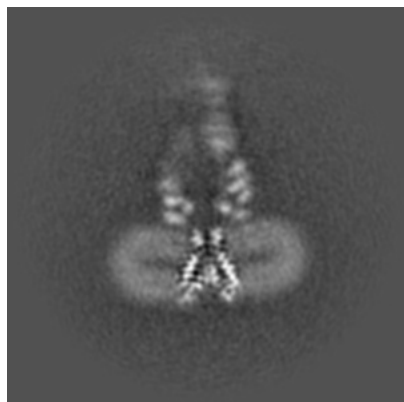


Z

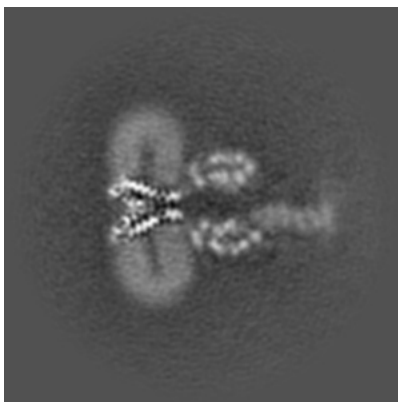
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

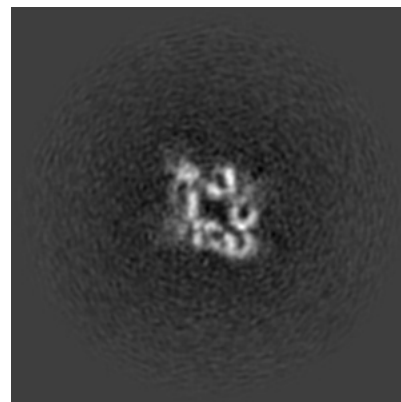
6.2.1 Primary map



X Index: 144

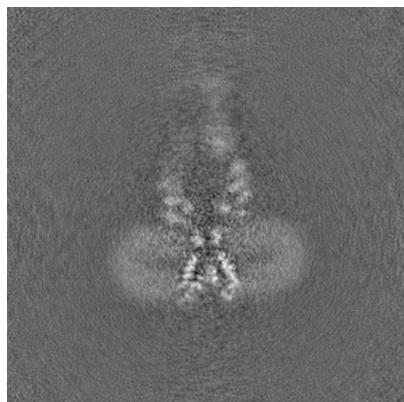


Y Index: 144

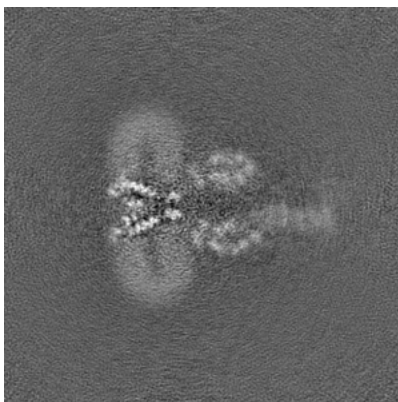


Z Index: 144

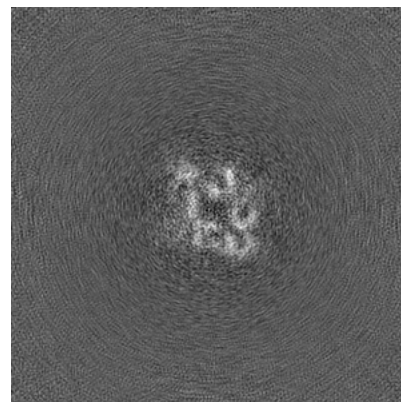
6.2.2 Raw map



X Index: 144



Y Index: 144

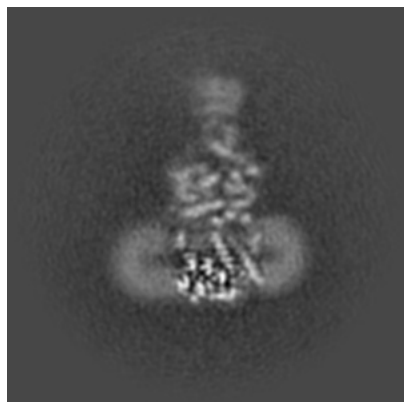


Z Index: 144

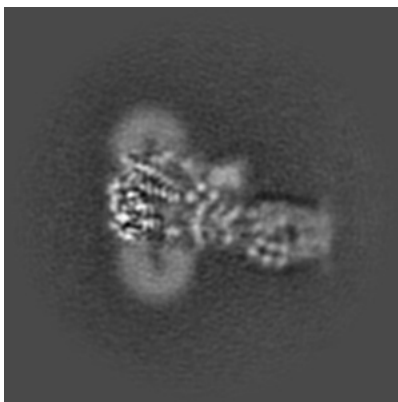
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

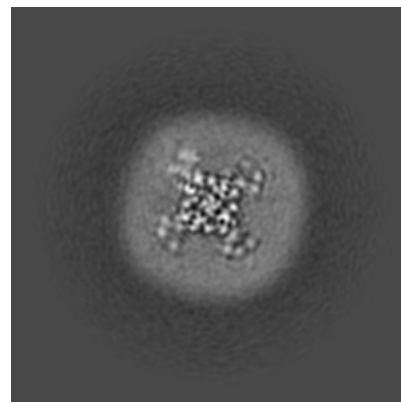
6.3.1 Primary map



X Index: 130

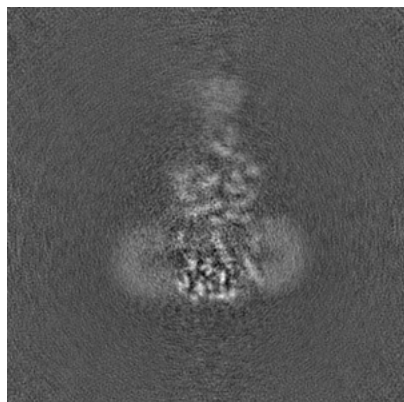


Y Index: 159

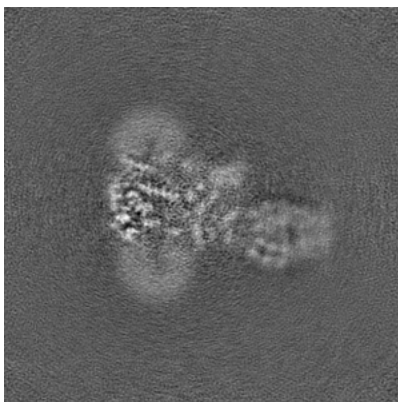


Z Index: 92

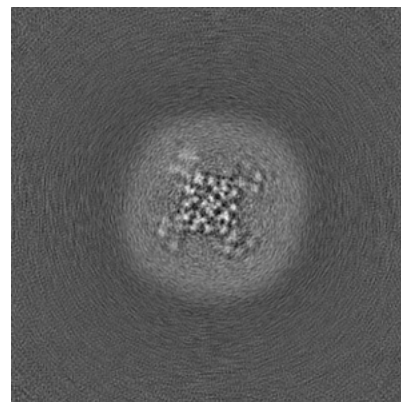
6.3.2 Raw map



X Index: 130



Y Index: 158

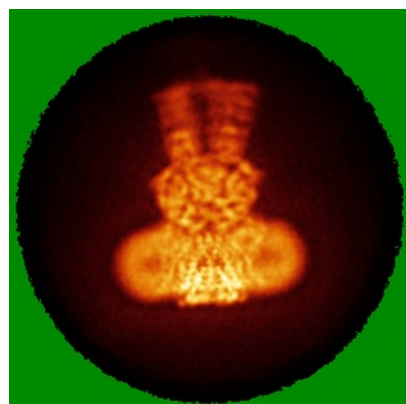


Z Index: 92

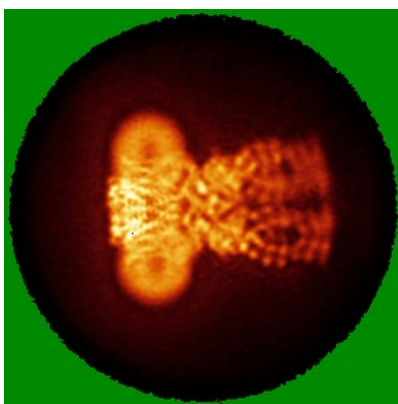
The images above show the largest variance slices of the map in three orthogonal directions.

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

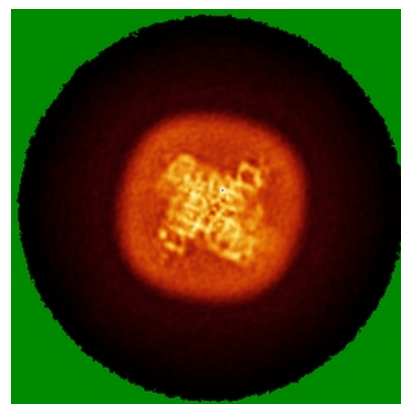
6.4.1 Primary map



X

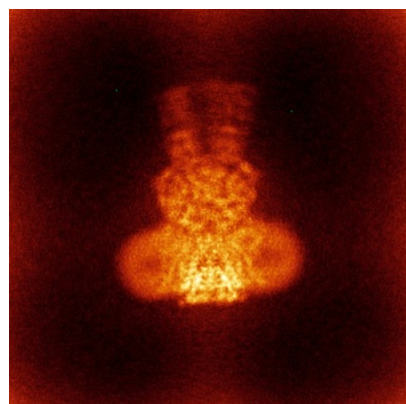


Y

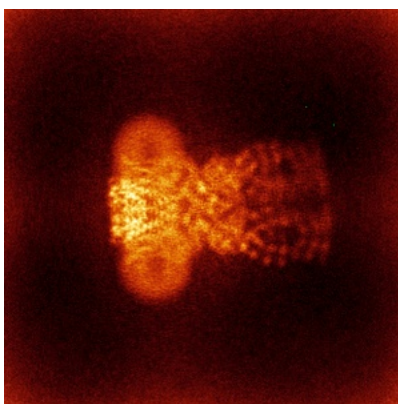


Z

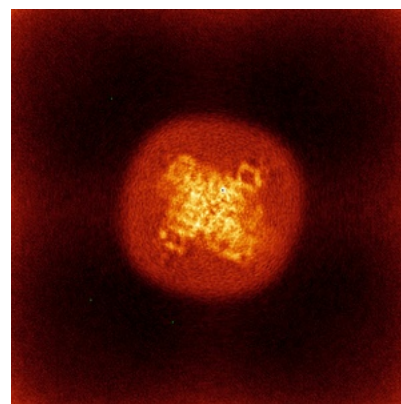
6.4.2 Raw map



X



Y

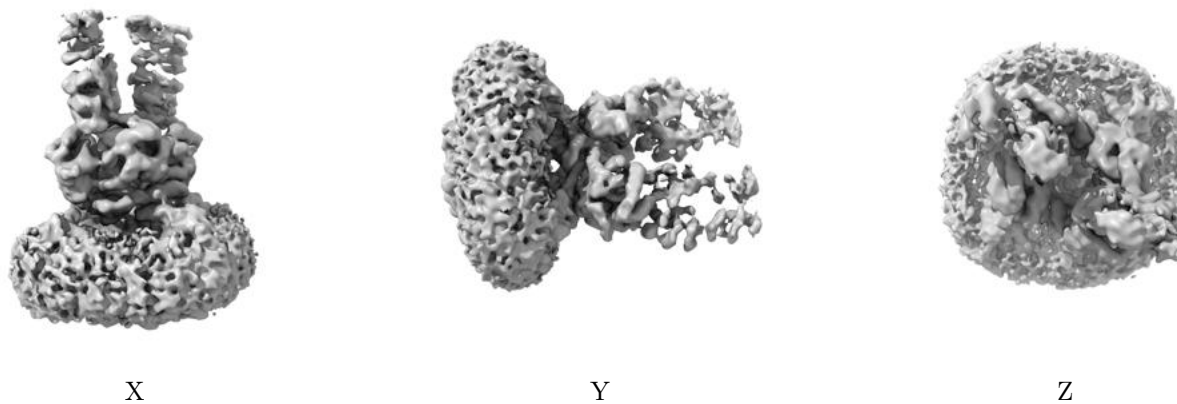


Z

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.

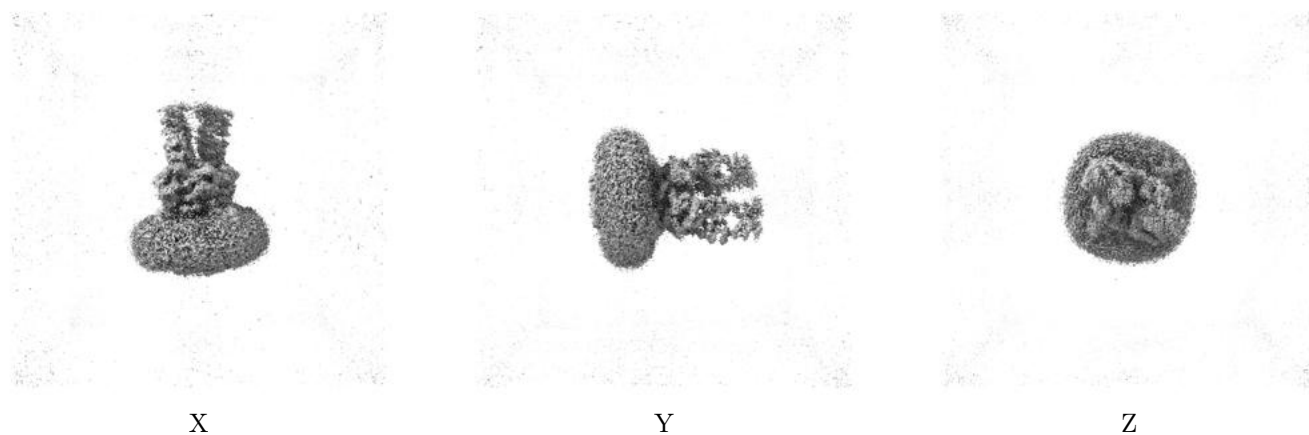
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.085. 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.

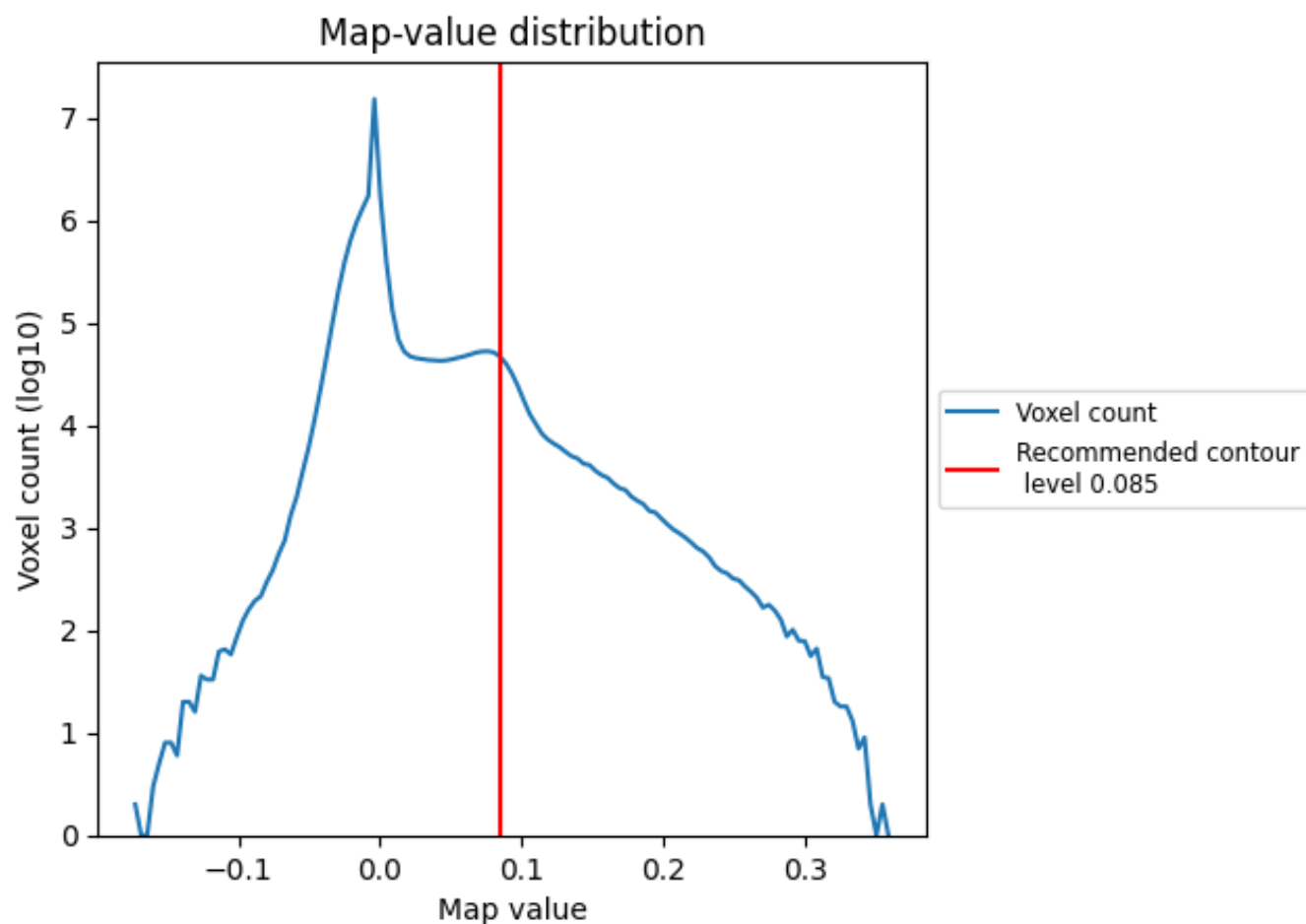
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

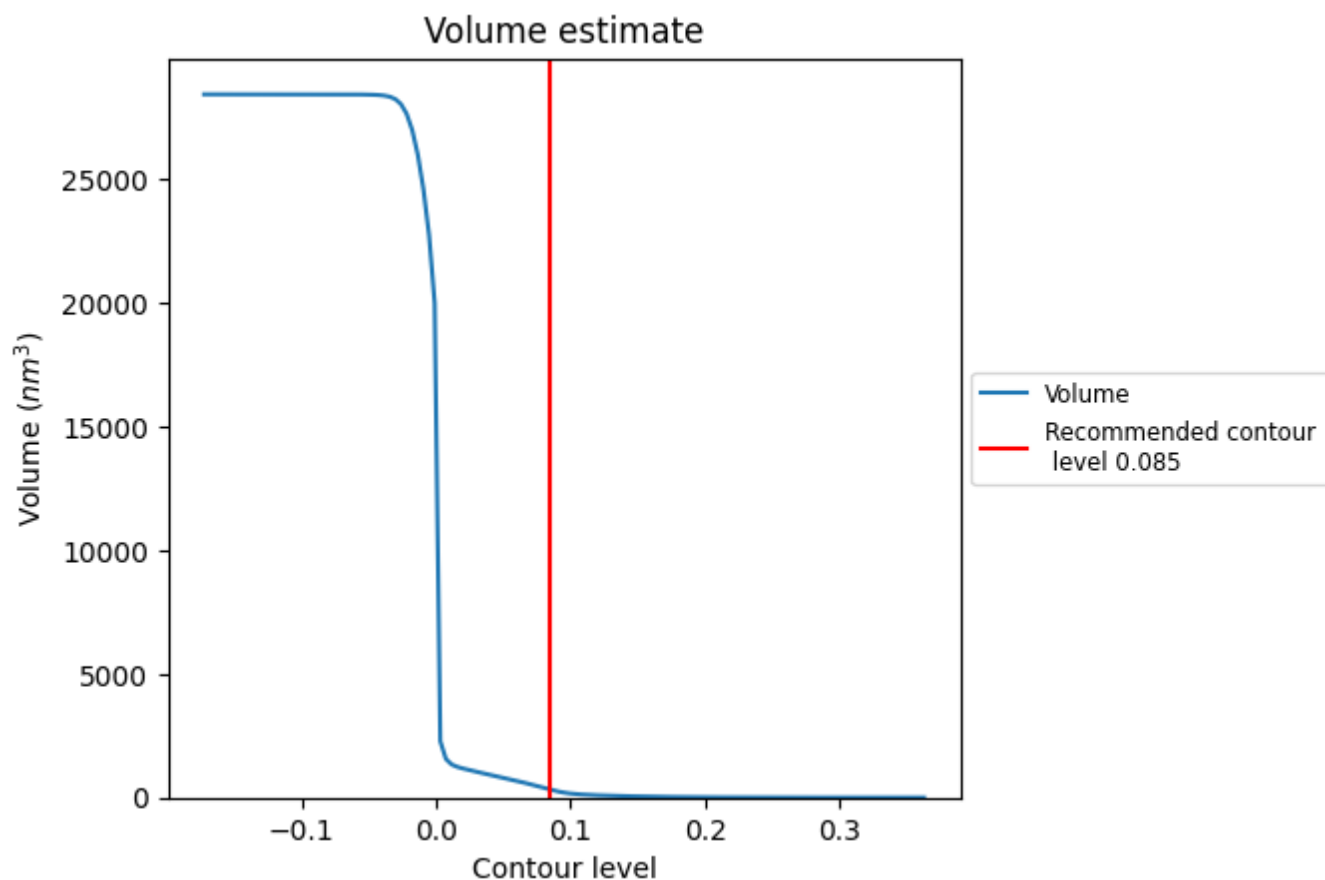
This section contains the results of statistical analysis of the map.

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.

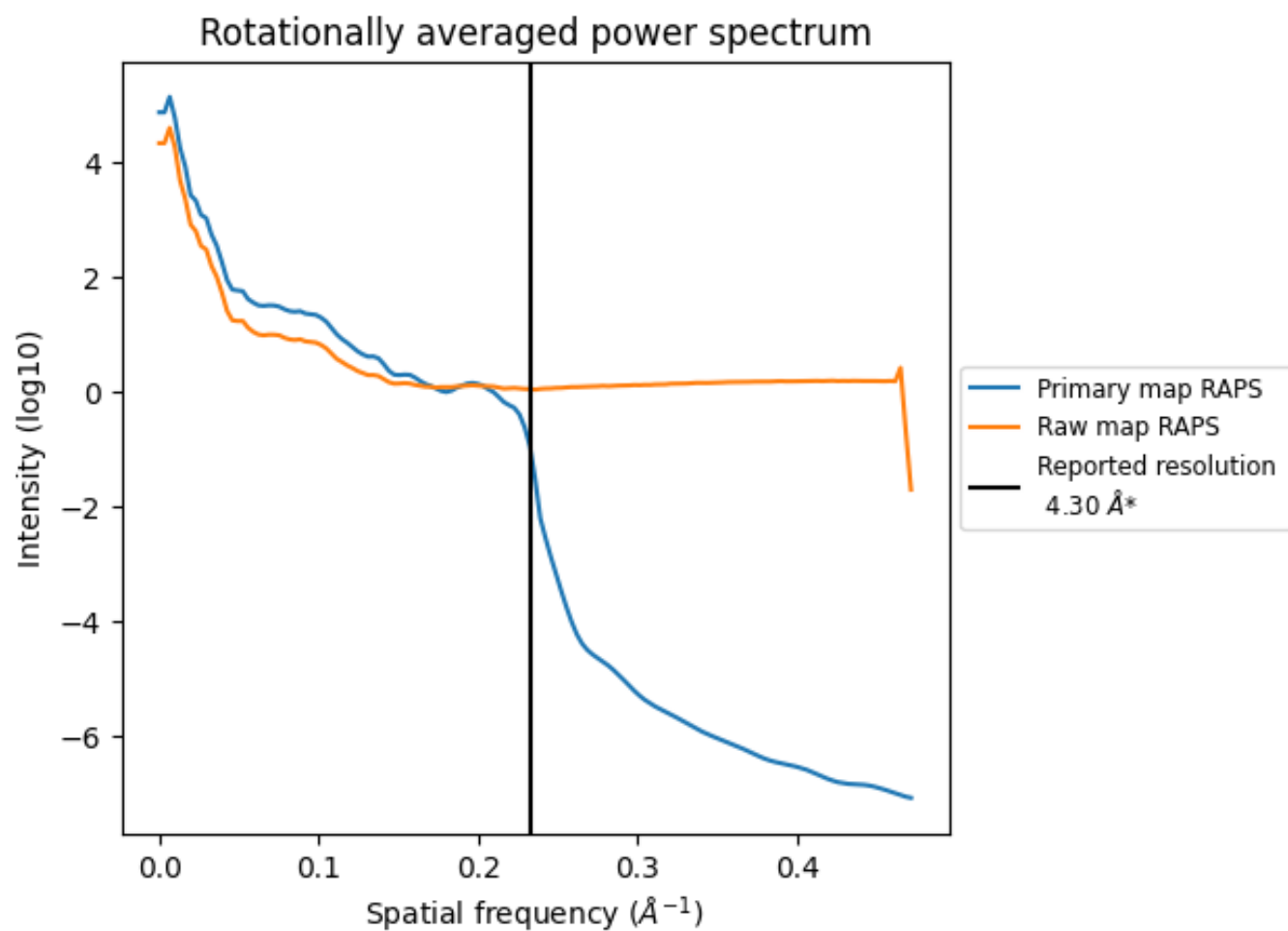
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 321 nm³; this corresponds to an approximate mass of 290 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 ⓘ

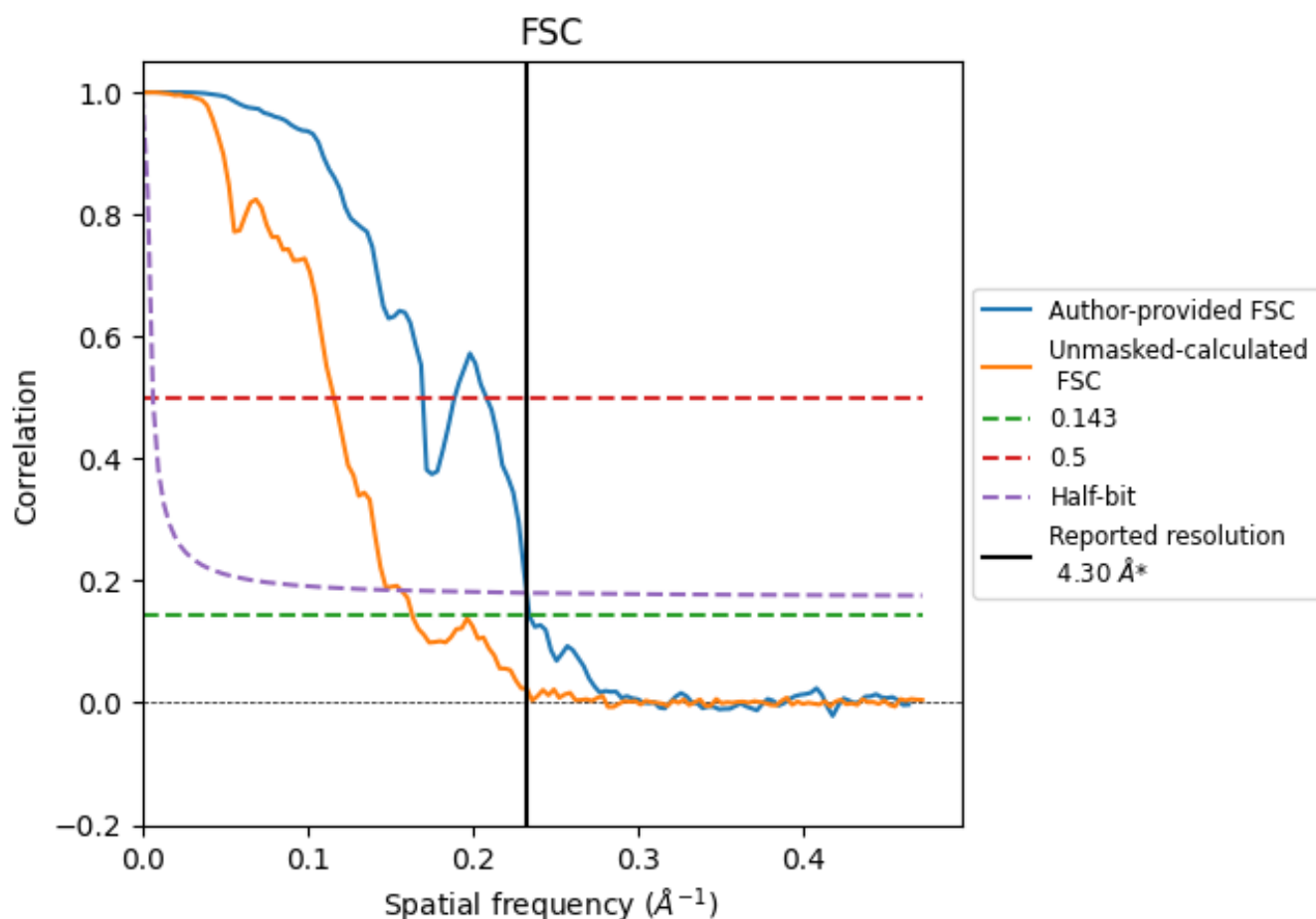


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 \AA^{-1}

8.2 Resolution estimates [i](#)

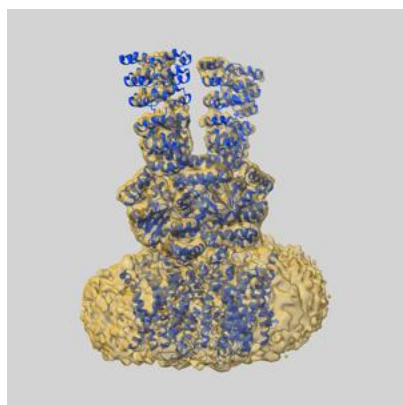
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.27	5.89	4.30
Unmasked-calculated*	6.12	8.62	6.38

*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 6.12 differs from the reported value 4.3 by more than 10 %

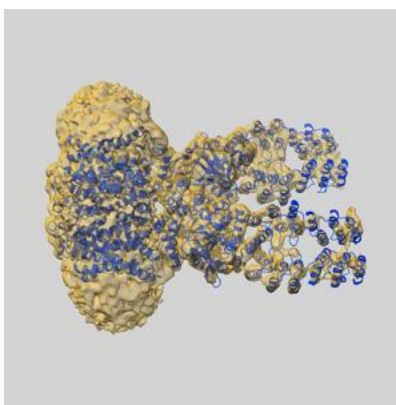
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37500 and PDB model 8WFZ. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

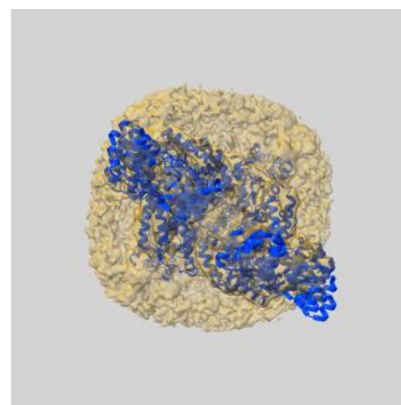
9.1 Map-model overlay [i](#)



X



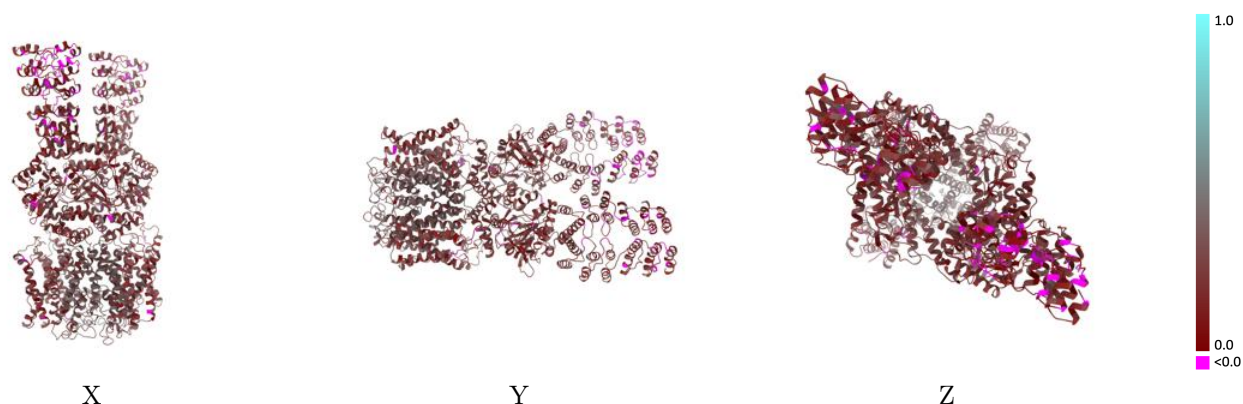
Y



Z

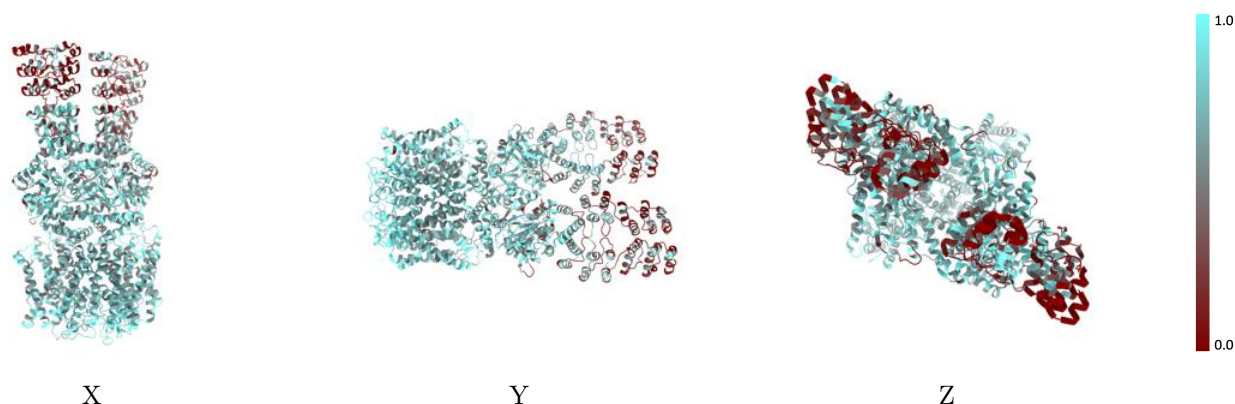
The images above show the 3D surface view of the map at the recommended contour level 0.085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



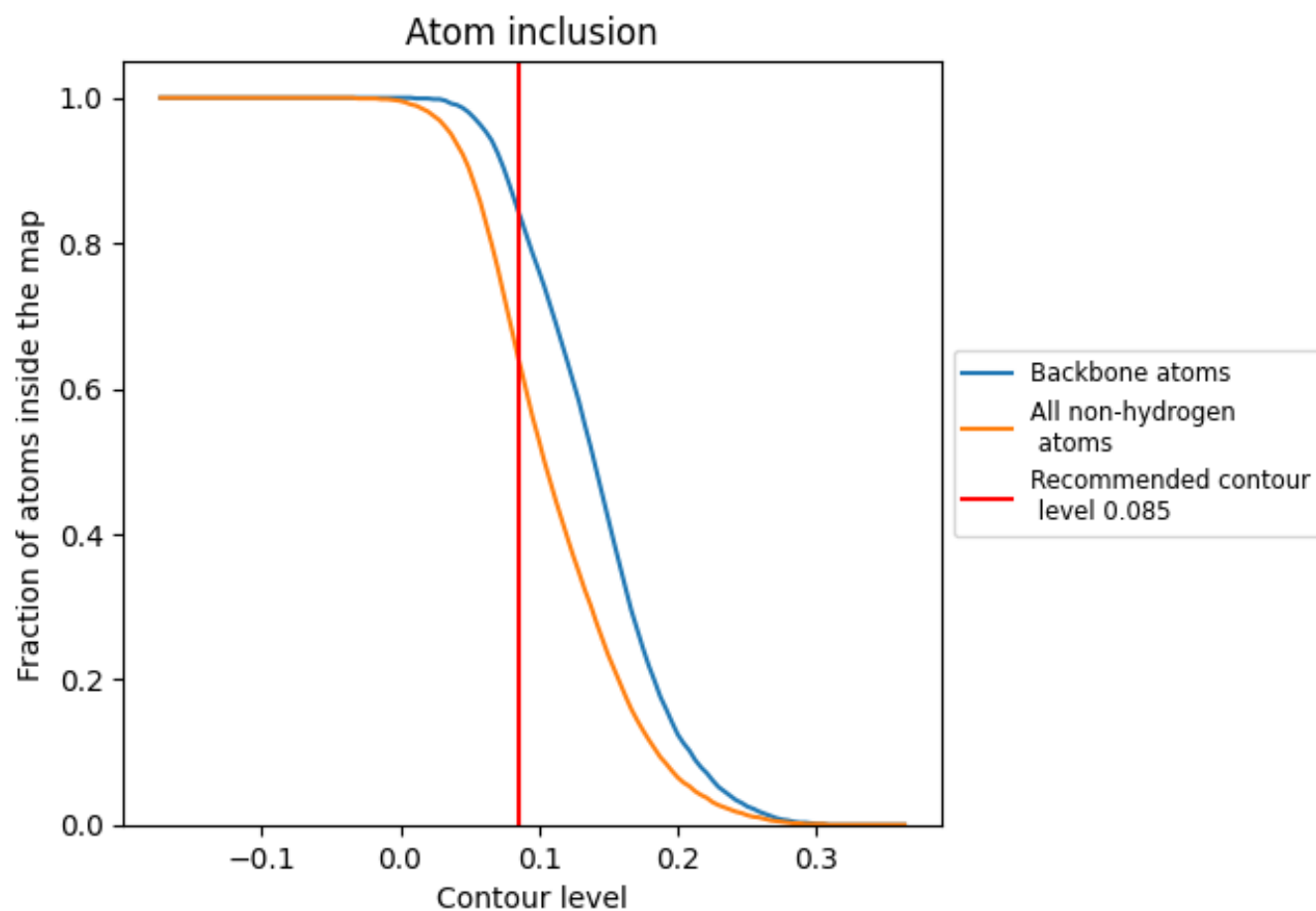
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.085).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 64% 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 (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6420	<div></div> 0.2330
A	<div></div> 0.6580	<div></div> 0.2300
B	<div></div> 0.6370	<div></div> 0.2330
C	<div></div> 0.6230	<div></div> 0.2430
D	<div></div> 0.6480	<div></div> 0.2280

