



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:26 PM UTC

PDB ID : 9LA0 / pdb_00009la0
EMDB ID : EMD-62915
Title : Arabidopsis GORK WT5
Authors : Yamanashi, T.; Kume, T.; Sekido, N.; Muraoka, Y.; Yokoyama, T.; Tanaka, Y.; Uozumi, N.
Deposited on : 2025-01-01
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

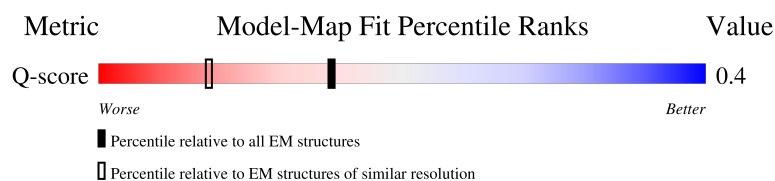
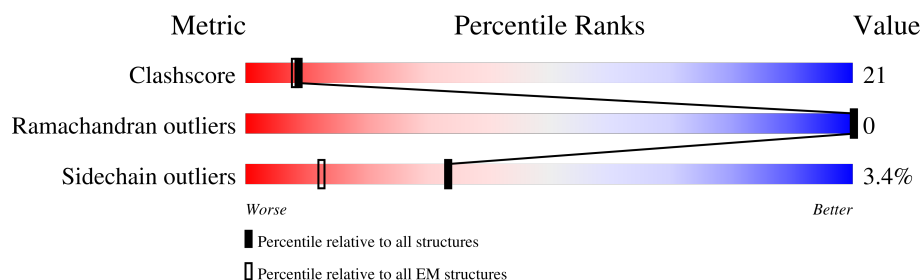
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	834	6% 47% 32% • 19%
1	B	834	8% 44% 35% • 19%
1	C	834	7% 46% 33% • 19%
1	D	834	6% 46% 34% • 19%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21944 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	676	Total	C	N	O	S	0	0
			5486	3559	914	988	25		
1	B	676	Total	C	N	O	S	0	0
			5486	3559	914	988	25		
1	C	676	Total	C	N	O	S	0	0
			5486	3559	914	988	25		
1	D	676	Total	C	N	O	S	0	0
			5486	3559	914	988	25		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP Q94A76
A	-6	ASP	-	expression tag	UNP Q94A76
A	-5	TYR	-	expression tag	UNP Q94A76
A	-4	LYS	-	expression tag	UNP Q94A76
A	-3	ASP	-	expression tag	UNP Q94A76
A	-2	ASP	-	expression tag	UNP Q94A76
A	-1	ASP	-	expression tag	UNP Q94A76
A	0	ASP	-	expression tag	UNP Q94A76
A	1	LYS	-	expression tag	UNP Q94A76
A	821	HIS	-	expression tag	UNP Q94A76
A	822	HIS	-	expression tag	UNP Q94A76
A	823	HIS	-	expression tag	UNP Q94A76
A	824	HIS	-	expression tag	UNP Q94A76
A	825	HIS	-	expression tag	UNP Q94A76
A	826	HIS	-	expression tag	UNP Q94A76
B	-7	MET	-	initiating methionine	UNP Q94A76
B	-6	ASP	-	expression tag	UNP Q94A76
B	-5	TYR	-	expression tag	UNP Q94A76
B	-4	LYS	-	expression tag	UNP Q94A76
B	-3	ASP	-	expression tag	UNP Q94A76
B	-2	ASP	-	expression tag	UNP Q94A76
B	-1	ASP	-	expression tag	UNP Q94A76

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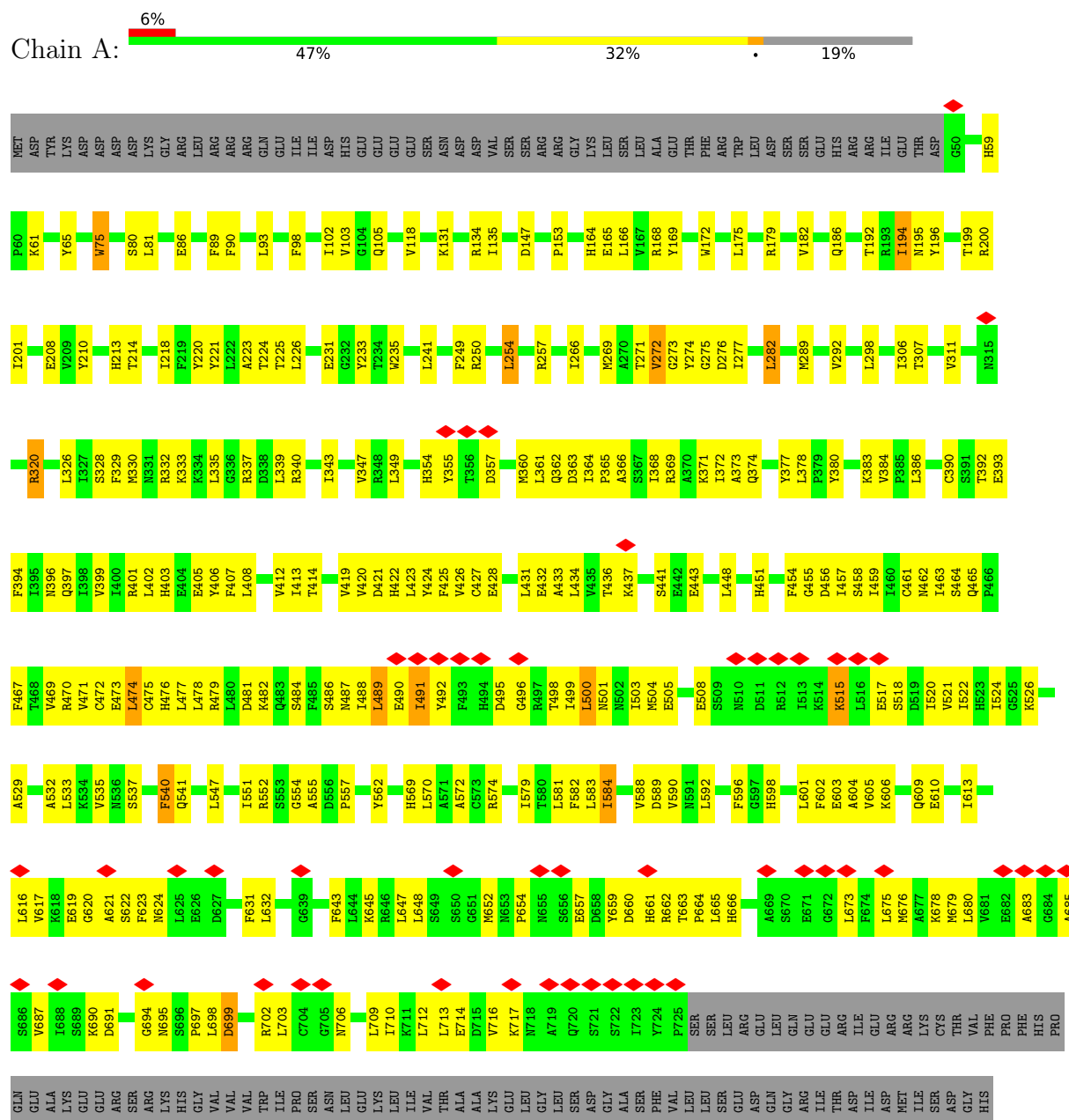
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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ASP	-	expression tag	UNP Q94A76
B	1	LYS	-	expression tag	UNP Q94A76
B	821	HIS	-	expression tag	UNP Q94A76
B	822	HIS	-	expression tag	UNP Q94A76
B	823	HIS	-	expression tag	UNP Q94A76
B	824	HIS	-	expression tag	UNP Q94A76
B	825	HIS	-	expression tag	UNP Q94A76
B	826	HIS	-	expression tag	UNP Q94A76
C	-7	MET	-	initiating methionine	UNP Q94A76
C	-6	ASP	-	expression tag	UNP Q94A76
C	-5	TYR	-	expression tag	UNP Q94A76
C	-4	LYS	-	expression tag	UNP Q94A76
C	-3	ASP	-	expression tag	UNP Q94A76
C	-2	ASP	-	expression tag	UNP Q94A76
C	-1	ASP	-	expression tag	UNP Q94A76
C	0	ASP	-	expression tag	UNP Q94A76
C	1	LYS	-	expression tag	UNP Q94A76
C	821	HIS	-	expression tag	UNP Q94A76
C	822	HIS	-	expression tag	UNP Q94A76
C	823	HIS	-	expression tag	UNP Q94A76
C	824	HIS	-	expression tag	UNP Q94A76
C	825	HIS	-	expression tag	UNP Q94A76
C	826	HIS	-	expression tag	UNP Q94A76
D	-7	MET	-	initiating methionine	UNP Q94A76
D	-6	ASP	-	expression tag	UNP Q94A76
D	-5	TYR	-	expression tag	UNP Q94A76
D	-4	LYS	-	expression tag	UNP Q94A76
D	-3	ASP	-	expression tag	UNP Q94A76
D	-2	ASP	-	expression tag	UNP Q94A76
D	-1	ASP	-	expression tag	UNP Q94A76
D	0	ASP	-	expression tag	UNP Q94A76
D	1	LYS	-	expression tag	UNP Q94A76
D	821	HIS	-	expression tag	UNP Q94A76
D	822	HIS	-	expression tag	UNP Q94A76
D	823	HIS	-	expression tag	UNP Q94A76
D	824	HIS	-	expression tag	UNP Q94A76
D	825	HIS	-	expression tag	UNP Q94A76
D	826	HIS	-	expression tag	UNP Q94A76

3 Residue-property plots

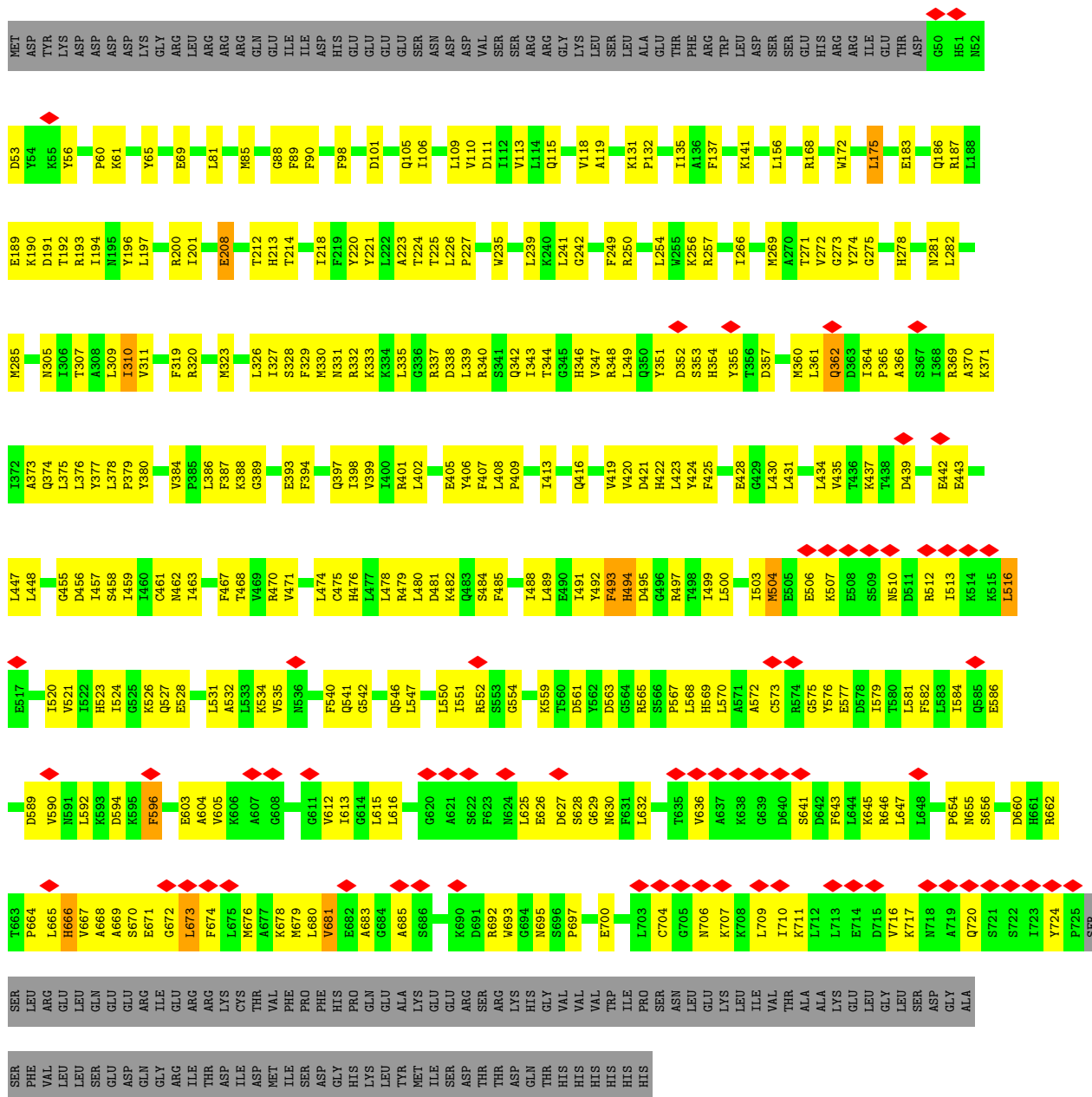
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

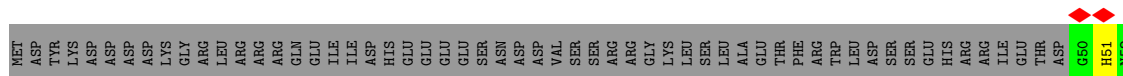


LYS
LEU
TYR
MET
LYS
ILE
SER
ASP
ASP
THR
THR
LYS
ASP
GLN
THR
THR
HIS
HIS
HIS
HIS
HIS

• Molecule 1: Potassium channel GORK



• Molecule 1: Potassium channel GORK



LYS	GLN	I688	V612	L531	V469	Y880
LEU	GLU	S689	I613	A532	R470	I381
TRR	ALA	K690	G614	L533	V471	K382
MET	LYS	D691	L615	K534	C472	K383
ILE	GLU	R692	L616	V535	E473	V384
SER	GLU	W693	V617	N536	L474	P385
ASP	ARG	G694	K618	A539	C475	L386
THR	SER	N695	E619	A539	H476	F387
THR	ARG	S696	G620	D543	L477	
THR	LYS	P697	A621	F544	R478	F394
GLN	HIS	I698	S622	D544	R479	I395
THR	GLY	D699	F623	Y545	L480	N396
HIS	VAL	E700	N624	Q546	D481	Q397
HIS	VAL	A701	L625	L547	K482	I398
HIS	VAL	R702	E626		Q483	V399
HIS	TRP		D627	I551	M487	I400
HIS	ILE	G705	S628	R552	I488	L401
HIS	PRO	N706	L632	S553	E489	L402
	SER	K707	A637	Q554	F493	H403
	ASN	K708	S641	A555	E490	Y406
	LEU	L709	D642	D556		F407
	GLU	I710	F643	P557	F493	L408
	LYS	K711	L644	N558	E411	
	LEU	L712		Y562	V419	
	ILE	L713	L648	R565	H422	
	VAL	E714	M652	P567	E428	
	THR	D715	N655	L568	C429	
	ALA	V716	D658	H569	L430	
	LYS	K717	Y659	L570	L431	
	LYS	N718	D660		L434	
	GLU	A719	H661	R574	V435	
	LEU	Q720	R662	Y576	T436	
	GLY	S721	T663	E577	K437	
	LEU	S722	P664	D578	T438	
	ASP	I723	L665	I579	D439	
	GLY	Y724	H666	T580	E442	
	SER	P725	A669	L581	E443	
	PHE	SER	L673	F582	S444	
	VAL	LEU	F674	I584	V445	
	LEU	SER	I675	Q585	T446	
	LEU	LEU	M676	E586	L447	
	LEU	LEU	A677	G587	F454	
	SER	ARG	K678	V588	G455	
	GLU	ILE	M679	D589	D456	
	ASP	GLU	L680	V590	I457	
	GLN	ARG	V681	N591	S458	
	GLY	ARG	E682	L592	I459	
	GLY	ARG	L683	K593	Q465	
	ILE	LYS	G684	D594	P466	
	THR	CYS	A685	L601	F467	
	SER	THR	S686	V605	T468	
	ASP	VAL	V687	K606		
	GLY	PHE				
	HIS	PRO				
	HIS	HIS				
	HIS	PRO				
	HIS	HIS				
	HIS	PRO				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31734	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	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	0.686	Depositor
Minimum map value	-0.417	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	315.19998, 315.19998, 315.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7879999, 0.7879999, 0.7879999	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	0.41	0/5615	0.61	0/7596
1	B	0.33	0/5615	0.52	0/7596
1	C	0.25	0/5615	0.46	0/7596
1	D	0.41	0/5615	0.61	0/7596
All	All	0.36	0/22460	0.55	0/30384

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	5486	0	5502	252	0
1	B	5486	0	5502	277	0
1	C	5486	0	5502	236	0
1	D	5486	0	5502	235	0
All	All	21944	0	22008	927	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 21.

All (927) 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:489:LEU:CA	1:A:496:GLY:HA3	1.78	1.14
1:A:489:LEU:HA	1:A:496:GLY:CA	1.82	1.08
1:B:676:MET:HA	1:B:679:MET:HE2	1.44	0.96
1:B:513:ILE:HA	1:B:516:LEU:HD12	1.51	0.91
1:D:526:LYS:HB3	1:D:530:GLU:HB3	1.53	0.90
1:A:489:LEU:HA	1:A:496:GLY:HA3	0.89	0.87
1:A:714:GLU:HB3	1:A:717:LYS:HZ2	1.38	0.86
1:B:364:ILE:HD13	1:C:343:ILE:HG13	1.58	0.85
1:D:59:HIS:HE1	1:D:61:LYS:HG2	1.42	0.83
1:C:699:ASP:HA	1:C:702:ARG:HD3	1.60	0.83
1:B:613:ILE:HG21	1:B:646:ARG:HH21	1.42	0.82
1:D:658:ASP:OD1	1:D:659:TYR:N	2.13	0.81
1:B:196:TYR:HB2	1:C:320:ARG:HG3	1.60	0.81
1:B:551:ILE:HD12	1:B:552:ARG:HE	1.46	0.80
1:A:687:VAL:HG11	1:A:713:LEU:HB3	1.64	0.80
1:A:372:ILE:HG23	1:D:335:LEU:HD11	1.64	0.79
1:B:346:HIS:CD2	1:D:365:PRO:HD3	2.18	0.78
1:C:106:ILE:HA	1:C:109:LEU:HD12	1.65	0.78
1:B:674:PHE:O	1:B:678:LYS:HB2	1.85	0.77
1:A:551:ILE:HA	1:A:555:ALA:HB3	1.67	0.76
1:B:422:HIS:HB3	1:B:479:ARG:HD3	1.66	0.76
1:D:720:GLN:HA	1:D:723:ILE:HB	1.68	0.76
1:C:572:ALA:HA	1:C:612:VAL:HG11	1.67	0.76
1:B:348:ARG:O	1:B:352:ASP:HB2	1.87	0.75
1:A:515:LYS:HZ1	1:A:518:SER:HB3	1.51	0.75
1:B:271:THR:HA	1:C:272:VAL:HG13	1.67	0.75
1:B:275:GLY:HA3	1:C:274:TYR:O	1.87	0.75
1:A:687:VAL:HG12	1:A:698:LEU:HG	1.69	0.74
1:A:461:CYS:SG	1:A:515:LYS:HD2	2.28	0.74
1:C:434:LEU:HB3	1:C:442:GLU:HB3	1.69	0.73
1:C:330:MET:HG2	1:C:335:LEU:HD12	1.70	0.73
1:D:497:ARG:NH1	1:D:520:ILE:O	2.21	0.73
1:A:613:ILE:O	1:A:617:VAL:HG23	1.89	0.73
1:D:526:LYS:O	1:D:530:GLU:N	2.21	0.73
1:C:109:LEU:HA	1:C:112:ILE:HD12	1.70	0.73
1:B:673:LEU:HD13	1:B:676:MET:HB2	1.71	0.72
1:C:431:LEU:HD23	1:C:471:VAL:HA	1.71	0.72
1:B:459:ILE:HG23	1:B:482:LYS:HG2	1.72	0.72
1:A:275:GLY:HA3	1:D:274:TYR:O	1.89	0.72
1:A:675:LEU:HA	1:A:678:LYS:HG3	1.71	0.72
1:B:551:ILE:HD11	1:B:582:PHE:HE2	1.55	0.72
1:B:434:LEU:HB3	1:B:442:GLU:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:ASP:HA	1:C:645:LYS:HE3	1.70	0.72
1:B:194:ILE:O	1:C:320:ARG:NH2	2.21	0.71
1:D:459:ILE:HD11	1:D:482:LYS:HA	1.70	0.71
1:C:195:ASN:OD1	1:C:195:ASN:N	2.22	0.71
1:D:606:LYS:HD2	1:D:643:PHE:HE1	1.54	0.71
1:A:390:CYS:HB3	1:A:499:ILE:HG23	1.71	0.71
1:A:605:VAL:HG11	1:A:647:LEU:HD23	1.73	0.70
1:D:536:ASN:HB3	1:D:570:LEU:HD12	1.73	0.70
1:B:90:PHE:O	1:B:168:ARG:NH1	2.24	0.70
1:B:354:HIS:HB3	1:B:357:ASP:HB2	1.72	0.70
1:B:377:TYR:HB2	1:B:399:VAL:HG13	1.73	0.70
1:A:540:PHE:CD2	1:D:562:TYR:HB2	2.27	0.70
1:A:377:TYR:HB2	1:A:399:VAL:HG13	1.73	0.69
1:A:504:MET:HA	1:A:504:MET:HE3	1.73	0.69
1:B:81:LEU:O	1:B:213:HIS:NE2	2.25	0.69
1:D:123:THR:HB	1:D:127:ARG:HB2	1.75	0.69
1:C:698:LEU:HD11	1:C:714:GLU:HG3	1.73	0.69
1:A:272:VAL:O	1:C:273:GLY:HA3	1.92	0.69
1:B:131:LYS:HD3	1:B:132:PRO:HD2	1.75	0.69
1:D:346:HIS:HE1	1:D:411:GLU:OE1	1.75	0.69
1:B:430:LEU:HD11	1:B:447:LEU:HB3	1.75	0.68
1:D:379:PRO:O	1:D:383:LYS:NZ	2.21	0.68
1:D:407:PHE:HB2	1:D:475:CYS:SG	2.33	0.68
1:A:632:LEU:HG	1:A:652:MET:HE2	1.76	0.68
1:B:507:LYS:HG2	1:B:513:ILE:HG12	1.75	0.68
1:B:589:ASP:HB3	1:B:592:LEU:HB2	1.74	0.68
1:B:674:PHE:HB2	1:B:706:ASN:HD21	1.59	0.68
1:D:500:LEU:HA	1:D:503:ILE:HG12	1.76	0.68
1:D:125:THR:HG22	1:D:126:TYR:HD1	1.58	0.68
1:A:226:LEU:O	1:A:250:ARG:NH2	2.26	0.68
1:A:517:GLU:HB2	1:A:522:ILE:HD11	1.75	0.67
1:B:353:SER:HA	1:C:332:ARG:HH22	1.58	0.67
1:C:377:TYR:HB2	1:C:399:VAL:HG13	1.77	0.67
1:C:598:HIS:HB3	1:C:603:GLU:OE1	1.95	0.67
1:B:373:ALA:HB1	1:B:399:VAL:HG12	1.76	0.67
1:B:456:ASP:OD1	1:B:457:ILE:N	2.28	0.66
1:C:397:GLN:OE1	1:C:401:ARG:NH2	2.28	0.66
1:D:81:LEU:O	1:D:213:HIS:NE2	2.27	0.66
1:B:357:ASP:HB3	1:B:360:MET:HE3	1.76	0.66
1:C:654:PRO:HB2	1:C:685:ALA:HB2	1.76	0.66
1:A:147:ASP:OD1	1:A:179:ARG:NH2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:662:ARG:HH21	1:C:666:HIS:HB3	1.59	0.66
1:D:59:HIS:CE1	1:D:61:LYS:HG2	2.30	0.66
1:A:632:LEU:HD11	1:A:652:MET:HG2	1.78	0.66
1:B:484:SER:O	1:B:488:ILE:HD12	1.94	0.66
1:C:361:LEU:HD23	1:C:364:ILE:HD12	1.76	0.66
1:D:430:LEU:HD11	1:D:447:LEU:HB3	1.77	0.66
1:D:522:ILE:HG22	1:D:526:LYS:HE2	1.78	0.66
1:A:520:ILE:O	1:A:524:ILE:HG13	1.95	0.66
1:A:489:LEU:HD22	1:A:500:LEU:HD23	1.78	0.66
1:A:601:LEU:HG	1:A:623:PHE:HE1	1.60	0.66
1:B:193:ARG:HG3	1:B:194:ILE:HG12	1.78	0.65
1:B:431:LEU:HB2	1:B:448:LEU:HB2	1.77	0.65
1:B:569:HIS:HE1	1:B:592:LEU:HB3	1.62	0.65
1:C:427:CYS:HB2	1:C:476:HIS:O	1.97	0.65
1:D:632:LEU:HD21	1:D:652:MET:HG2	1.78	0.65
1:A:368:ILE:O	1:A:372:ILE:HG13	1.97	0.65
1:A:274:TYR:O	1:C:275:GLY:HA3	1.97	0.65
1:B:320:ARG:NH1	1:D:189:GLU:O	2.27	0.65
1:D:497:ARG:NH1	1:D:524:ILE:HB	2.11	0.65
1:D:539:ALA:HA	1:D:579:ILE:HD13	1.77	0.65
1:B:671:GLU:HA	1:C:692:ARG:HH22	1.62	0.65
1:C:131:LYS:HD2	1:C:132:PRO:HD2	1.77	0.65
1:A:648:LEU:HD11	1:A:680:LEU:HD23	1.79	0.65
1:C:285:MET:O	1:C:289:MET:HG3	1.96	0.65
1:C:688:ILE:HG22	1:C:717:LYS:HG3	1.79	0.65
1:D:500:LEU:HB3	1:D:520:ILE:HG12	1.77	0.65
1:B:266:ILE:HG13	1:D:289:MET:HG2	1.79	0.65
1:C:605:VAL:O	1:C:646:ARG:NH2	2.29	0.65
1:C:634:THR:HG22	1:C:638:LYS:HE3	1.79	0.64
1:A:601:LEU:HD12	1:A:613:ILE:HG22	1.78	0.64
1:B:423:LEU:HB2	1:B:459:ILE:HD12	1.79	0.64
1:A:710:ILE:O	1:A:714:GLU:HG3	1.97	0.64
1:B:374:GLN:HA	1:B:378:LEU:HB2	1.79	0.64
1:D:510:ASN:HB2	1:D:513:ILE:HB	1.78	0.64
1:B:191:ASP:O	1:C:320:ARG:NH2	2.30	0.64
1:B:330:MET:HE3	1:B:340:ARG:HE	1.61	0.64
1:C:339:LEU:O	1:C:343:ILE:HG22	1.98	0.64
1:B:551:ILE:HD12	1:B:552:ARG:NE	2.12	0.64
1:D:669:ALA:HA	1:D:709:LEU:HD21	1.80	0.64
1:B:707:LYS:HA	1:B:710:ILE:HD13	1.80	0.64
1:D:623:PHE:HB3	1:D:625:LEU:HG	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:PRO:HD3	1:D:119:ALA:HB3	1.80	0.64
1:D:590:VAL:HG13	1:D:616:LEU:HD22	1.80	0.64
1:D:641:SER:HA	1:D:676:MET:HE3	1.80	0.64
1:D:677:ALA:O	1:D:681:VAL:HG23	1.97	0.64
1:B:338:ASP:OD1	1:B:339:LEU:N	2.30	0.64
1:B:523:HIS:NE2	1:B:527:GLN:OE1	2.31	0.64
1:D:85:MET:HG3	1:D:213:HIS:HE1	1.63	0.64
1:A:428:GLU:HB3	1:A:476:HIS:HB3	1.80	0.63
1:B:528:GLU:HG2	1:B:559:LYS:HE2	1.79	0.63
1:A:673:LEU:HB3	1:A:676:MET:HG2	1.79	0.63
1:A:392:THR:HG22	1:A:396:ASN:HD21	1.63	0.63
1:C:368:ILE:HD12	1:C:368:ILE:H	1.64	0.63
1:C:327:ILE:HA	1:C:330:MET:HE3	1.79	0.63
1:D:403:HIS:CD2	1:D:479:ARG:HH21	2.17	0.63
1:B:364:ILE:HG13	1:B:365:PRO:HD2	1.81	0.63
1:A:461:CYS:HB3	1:A:463:ILE:HG23	1.81	0.63
1:B:516:LEU:HB3	1:B:521:VAL:HG11	1.81	0.63
1:C:434:LEU:HA	1:C:443:GLU:O	1.99	0.63
1:B:442:GLU:OE1	1:B:470:ARG:NH2	2.32	0.62
1:A:90:PHE:O	1:A:168:ARG:NH1	2.32	0.62
1:A:540:PHE:HD2	1:D:562:TYR:HB2	1.64	0.62
1:B:665:LEU:HD22	1:B:685:ALA:HB3	1.81	0.62
1:D:402:LEU:HD13	1:D:478:LEU:HD13	1.82	0.62
1:D:715:ASP:HA	1:D:718:ASN:HD22	1.65	0.62
1:B:226:LEU:O	1:B:250:ARG:NH2	2.29	0.62
1:C:194:ILE:HD11	1:C:198:PHE:HD2	1.65	0.61
1:C:572:ALA:HB1	1:C:604:ALA:HB2	1.82	0.61
1:A:462:ASN:ND2	1:A:518:SER:HB2	2.15	0.61
1:B:431:LEU:HD23	1:B:471:VAL:HA	1.81	0.61
1:B:461:CYS:HA	1:B:516:LEU:HD21	1.80	0.61
1:B:613:ILE:HG21	1:B:646:ARG:NH2	2.15	0.61
1:D:484:SER:O	1:D:488:ILE:HG13	2.00	0.61
1:A:131:LYS:HB3	1:A:134:ARG:HG3	1.82	0.61
1:A:456:ASP:OD2	1:A:457:ILE:N	2.32	0.61
1:A:330:MET:HE3	1:A:340:ARG:HB2	1.82	0.61
1:C:461:CYS:HB2	1:C:463:ILE:HG22	1.82	0.61
1:A:80:SER:HB2	1:A:210:TYR:OH	2.01	0.61
1:B:710:ILE:HD12	1:B:710:ILE:H	1.65	0.60
1:C:556:ASP:HB3	1:C:559:LYS:HG2	1.83	0.60
1:B:660:ASP:HA	1:B:692:ARG:HH22	1.65	0.60
1:B:366:ALA:HB2	1:C:479:ARG:HH11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:LYS:HA	1:D:282:LEU:HD21	1.82	0.60
1:D:644:LEU:HD13	1:D:676:MET:HE2	1.83	0.60
1:A:401:ARG:HG3	1:A:488:ILE:HD11	1.84	0.60
1:B:435:VAL:HB	1:B:443:GLU:HB3	1.83	0.60
1:C:465:GLN:NE2	1:C:467:PHE:O	2.32	0.60
1:D:431:LEU:HD23	1:D:471:VAL:HA	1.83	0.60
1:B:275:GLY:CA	1:C:274:TYR:O	2.50	0.60
1:C:306:ILE:O	1:C:310:ILE:HG12	2.02	0.60
1:C:153:PRO:HB2	1:C:156:LEU:HB2	1.84	0.60
1:C:323:MET:HE1	1:C:347:VAL:HG12	1.83	0.60
1:D:687:VAL:H	1:D:720:GLN:HE22	1.49	0.60
1:C:59:HIS:ND1	1:C:60:PRO:HD2	2.16	0.59
1:A:365:PRO:HD3	1:D:346:HIS:CD2	2.37	0.59
1:B:361:LEU:HD23	1:B:361:LEU:H	1.67	0.59
1:C:456:ASP:OD1	1:C:457:ILE:N	2.36	0.59
1:D:326:LEU:HD22	1:D:347:VAL:HG21	1.83	0.59
1:A:488:ILE:HA	1:A:492:TYR:HB2	1.84	0.59
1:D:124:GLN:HG3	1:D:125:THR:H	1.68	0.59
1:D:648:LEU:HD21	1:D:679:MET:HB3	1.84	0.59
1:C:596:PHE:HB2	1:C:598:HIS:CD2	2.38	0.59
1:B:401:ARG:HD2	1:B:488:ILE:HD11	1.84	0.58
1:D:402:LEU:HD22	1:D:478:LEU:HB3	1.84	0.58
1:B:60:PRO:HD3	1:B:119:ALA:HB3	1.85	0.58
1:C:319:PHE:HA	1:C:351:TYR:CE2	2.38	0.58
1:D:179:ARG:HH11	1:D:182:VAL:HG11	1.68	0.58
1:A:665:LEU:HD21	1:A:687:VAL:HG22	1.85	0.58
1:A:90:PHE:HZ	1:A:254:LEU:HD13	1.68	0.58
1:A:420:VAL:HG23	1:A:465:GLN:HB2	1.84	0.58
1:A:498:THR:HG21	1:A:554:GLY:HA3	1.86	0.58
1:B:274:TYR:O	1:D:275:GLY:HA3	2.04	0.58
1:B:507:LYS:HA	1:B:510:ASN:HB2	1.85	0.58
1:B:319:PHE:CE1	1:B:323:MET:HG2	2.39	0.58
1:A:423:LEU:HD22	1:A:425:PHE:CE1	2.38	0.58
1:B:612:VAL:HA	1:B:615:LEU:HD23	1.86	0.57
1:A:547:LEU:HD11	1:A:583:LEU:HD21	1.85	0.57
1:B:355:TYR:HE1	1:B:405:GLU:HG2	1.68	0.57
1:B:495:ASP:O	1:B:499:ILE:HG12	2.04	0.57
1:B:540:PHE:HB2	1:B:570:LEU:HD22	1.87	0.57
1:A:420:VAL:HB	1:A:458:SER:HB3	1.86	0.57
1:C:413:ILE:HD13	1:C:477:LEU:HD11	1.86	0.57
1:D:240:LYS:NZ	1:D:245:SER:OG	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:THR:HG23	1:D:442:GLU:HG2	1.84	0.57
1:D:497:ARG:HH12	1:D:524:ILE:HB	1.68	0.57
1:B:500:LEU:HD12	1:B:503:ILE:HD11	1.84	0.57
1:A:241:LEU:HD21	1:A:276:ASP:HB2	1.85	0.57
1:A:643:PHE:CE1	1:A:647:LEU:HD21	2.40	0.57
1:B:681:VAL:HG11	1:B:716:VAL:HG21	1.86	0.57
1:D:568:LEU:HA	1:D:583:LEU:HD13	1.86	0.57
1:B:101:ASP:OD1	1:B:105:GLN:NE2	2.38	0.57
1:B:471:VAL:HG13	1:B:475:CYS:SG	2.44	0.57
1:B:605:VAL:HG13	1:B:646:ARG:HB3	1.86	0.57
1:C:395:ILE:O	1:C:399:VAL:HG23	2.04	0.57
1:D:119:ALA:HA	1:D:135:ILE:HD11	1.86	0.57
1:D:397:GLN:HB3	1:D:488:ILE:HD13	1.86	0.57
1:A:659:TYR:HB3	1:D:637:ALA:HB2	1.86	0.57
1:A:622:SER:OG	1:A:624:ASN:OD1	2.20	0.57
1:B:494:HIS:HD1	1:B:554:GLY:HA3	1.68	0.57
1:D:338:ASP:O	1:D:342:GLN:HG3	2.04	0.57
1:D:501:ASN:O	1:D:505:GLU:HG2	2.05	0.57
1:B:85:MET:HG3	1:B:213:HIS:CE1	2.40	0.56
1:A:662:ARG:NH1	1:D:660:ASP:OD2	2.38	0.56
1:C:691:ASP:OD1	1:C:695:ASN:N	2.34	0.56
1:A:714:GLU:HB3	1:A:717:LYS:NZ	2.17	0.56
1:B:348:ARG:O	1:B:352:ASP:CB	2.52	0.56
1:B:366:ALA:HB2	1:C:479:ARG:NH1	2.20	0.56
1:D:533:LEU:HD21	1:D:562:TYR:CE1	2.40	0.56
1:C:105:GLN:NE2	1:C:151:CYS:O	2.38	0.56
1:D:533:LEU:HD21	1:D:562:TYR:HE1	1.71	0.56
1:B:402:LEU:HD13	1:B:478:LEU:HD13	1.88	0.56
1:A:492:TYR:HB3	1:A:495:ASP:HB2	1.87	0.56
1:C:350:GLN:HG2	1:C:355:TYR:CE2	2.40	0.56
1:D:381:ILE:O	1:D:384:VAL:HG12	2.06	0.56
1:C:121:ARG:HG2	1:C:128:THR:HG22	1.86	0.56
1:A:433:ALA:HB1	1:A:467:PHE:CD1	2.40	0.56
1:A:414:THR:HG23	1:A:465:GLN:HG2	1.86	0.55
1:A:471:VAL:HG13	1:A:475:CYS:SG	2.46	0.55
1:A:569:HIS:NE2	1:A:598:HIS:O	2.39	0.55
1:B:361:LEU:O	1:B:364:ILE:HG22	2.06	0.55
1:C:530:GLU:O	1:C:534:LYS:HG3	2.07	0.55
1:D:384:VAL:HG22	1:D:386:LEU:H	1.71	0.55
1:D:513:ILE:O	1:D:515:LYS:NZ	2.39	0.55
1:D:673:LEU:HD21	1:D:676:MET:SD	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:662:ARG:HE	1:D:666:HIS:HB3	1.69	0.55
1:B:327:ILE:O	1:B:331:ASN:ND2	2.40	0.55
1:B:497:ARG:NH2	1:B:500:LEU:HB3	2.21	0.55
1:B:119:ALA:HA	1:B:135:ILE:HD11	1.88	0.55
1:D:126:TYR:O	1:D:127:ARG:HD3	2.07	0.55
1:B:281:ASN:O	1:B:285:MET:HG3	2.06	0.55
1:B:670:SER:HB3	1:B:700:GLU:HB3	1.89	0.55
1:B:693:TRP:HB2	1:B:695:ASN:HD21	1.71	0.55
1:A:515:LYS:HE3	1:A:521:VAL:HG21	1.88	0.55
1:A:455:GLY:O	1:A:459:ILE:HG13	2.06	0.55
1:A:490:GLU:HG3	1:A:491:ILE:H	1.71	0.55
1:A:406:TYR:HD2	1:A:474:LEU:HD11	1.72	0.54
1:C:195:ASN:O	1:C:199:THR:HG23	2.07	0.54
1:A:357:ASP:HA	1:A:360:MET:HB2	1.89	0.54
1:A:394:PHE:CG	1:A:499:ILE:HG21	2.42	0.54
1:A:657:GLU:OE2	1:A:661:HIS:ND1	2.40	0.54
1:B:656:SER:O	1:B:664:PRO:HD3	2.08	0.54
1:C:189:GLU:OE1	1:C:199:THR:OG1	2.23	0.54
1:C:196:TYR:HD1	1:C:197:LEU:HD22	1.72	0.54
1:C:463:ILE:HD12	1:C:464:SER:H	1.73	0.54
1:A:373:ALA:HB1	1:A:399:VAL:HG12	1.90	0.54
1:B:565:ARG:HH22	1:B:603:GLU:HG3	1.72	0.54
1:D:406:TYR:HE2	1:D:474:LEU:HB3	1.72	0.54
1:C:286:ILE:HA	1:C:289:MET:HE2	1.90	0.54
1:C:690:LYS:HD2	1:C:694:GLY:C	2.32	0.54
1:D:208:GLU:O	1:D:212:THR:HG23	2.08	0.54
1:D:673:LEU:HG	1:D:676:MET:HB2	1.90	0.54
1:A:105:GLN:NE2	1:A:153:PRO:HA	2.22	0.54
1:C:457:ILE:HD11	1:C:466:PRO:HG3	1.89	0.54
1:D:618:LYS:HD2	1:D:618:LYS:O	2.08	0.54
1:B:335:LEU:HB3	1:B:339:LEU:HD23	1.88	0.54
1:B:85:MET:HG3	1:B:213:HIS:HE1	1.73	0.54
1:B:520:ILE:O	1:B:524:ILE:HG13	2.07	0.54
1:C:56:TYR:O	1:C:57:ILE:HD13	2.07	0.54
1:A:486:SER:HB3	1:A:520:ILE:HD11	1.88	0.54
1:A:521:VAL:HA	1:A:524:ILE:HD12	1.90	0.54
1:D:86:GLU:HA	1:D:90:PHE:HD2	1.73	0.54
1:C:582:PHE:O	1:C:586:GLU:HG2	2.08	0.53
1:C:675:LEU:O	1:C:679:MET:HG3	2.08	0.53
1:D:131:LYS:HG2	1:D:134:ARG:HG2	1.90	0.53
1:C:666:HIS:CE1	1:C:691:ASP:HB3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:VAL:HA	1:A:402:LEU:HD12	1.91	0.53
1:C:611:GLY:O	1:C:615:LEU:HG	2.09	0.53
1:B:249:PHE:O	1:B:257:ARG:HD3	2.08	0.53
1:B:329:PHE:CD2	1:D:357:ASP:HB3	2.44	0.53
1:A:361:LEU:HD12	1:A:361:LEU:N	2.24	0.53
1:A:484:SER:O	1:A:488:ILE:HG12	2.08	0.53
1:C:368:ILE:O	1:C:372:ILE:HD12	2.08	0.53
1:C:388:LYS:HB3	1:C:502:ASN:ND2	2.23	0.53
1:D:399:VAL:HA	1:D:402:LEU:HD12	1.90	0.53
1:C:66:LYS:HA	1:C:69:GLU:HG3	1.90	0.53
1:D:434:LEU:HD23	1:D:444:SER:HA	1.89	0.53
1:A:384:VAL:HG21	1:A:425:PHE:HD2	1.74	0.53
1:B:355:TYR:CE1	1:B:405:GLU:HG2	2.43	0.53
1:D:699:ASP:HA	1:D:702:ARG:HD2	1.91	0.53
1:B:581:LEU:HA	1:B:584:ILE:HD12	1.90	0.53
1:B:660:ASP:HA	1:B:692:ARG:NH2	2.24	0.53
1:C:642:ASP:OD1	1:C:642:ASP:N	2.40	0.53
1:D:557:PRO:HB3	1:D:567:PRO:HG2	1.90	0.53
1:D:712:LEU:O	1:D:716:VAL:HG23	2.09	0.53
1:A:271:THR:HA	1:D:272:VAL:HG13	1.90	0.53
1:A:393:GLU:HG2	1:D:419:VAL:HG11	1.91	0.53
1:A:423:LEU:HB2	1:A:459:ILE:CD1	2.39	0.53
1:C:60:PRO:HD3	1:C:119:ALA:HB3	1.91	0.53
1:C:402:LEU:HD13	1:C:478:LEU:HD13	1.91	0.53
1:C:623:PHE:HZ	1:C:650:SER:HB2	1.74	0.53
1:A:362:GLN:N	1:A:362:GLN:OE1	2.42	0.52
1:A:552:ARG:HH21	1:A:582:PHE:HE1	1.57	0.52
1:A:654:PRO:HB2	1:A:685:ALA:HB2	1.90	0.52
1:B:398:ILE:HG23	1:B:480:LEU:HD22	1.91	0.52
1:A:343:ILE:HG13	1:C:368:ILE:HG21	1.91	0.52
1:A:426:VAL:HA	1:A:477:LEU:HD22	1.91	0.52
1:C:495:ASP:OD1	1:C:495:ASP:N	2.41	0.52
1:D:329:PHE:CE2	1:D:333:LYS:HG3	2.45	0.52
1:D:497:ARG:HH22	1:D:524:ILE:CA	2.21	0.52
1:A:609:GLN:O	1:A:613:ILE:HG12	2.10	0.52
1:A:643:PHE:O	1:A:647:LEU:HG	2.09	0.52
1:B:272:VAL:O	1:D:273:GLY:HA3	2.08	0.52
1:C:401:ARG:HE	1:C:488:ILE:HD11	1.74	0.52
1:B:428:GLU:O	1:B:475:CYS:HA	2.09	0.52
1:B:85:MET:HE3	1:B:254:LEU:HD11	1.91	0.52
1:D:526:LYS:HA	1:D:529:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ILE:HG21	1:C:289:MET:HA	1.90	0.52
1:A:333:LYS:HB3	1:C:376:LEU:HD21	1.90	0.52
1:A:330:MET:CE	1:A:340:ARG:HB2	2.39	0.52
1:B:208:GLU:O	1:B:212:THR:HG23	2.10	0.52
1:B:329:PHE:HD2	1:D:357:ASP:HB3	1.75	0.52
1:B:470:ARG:HG3	1:B:471:VAL:N	2.25	0.52
1:B:570:LEU:HD23	1:B:573:CYS:SG	2.50	0.52
1:B:594:ASP:OD1	1:B:596:PHE:N	2.42	0.52
1:C:530:GLU:O	1:C:533:LEU:N	2.43	0.52
1:B:256:LYS:HE3	1:D:282:LEU:HD13	1.91	0.52
1:D:618:LYS:HG3	1:D:619:GLU:OE2	2.09	0.52
1:B:310:ILE:HD11	1:D:304:GLY:HA3	1.91	0.52
1:B:326:LEU:O	1:B:330:MET:HG3	2.10	0.52
1:B:516:LEU:HD22	1:B:521:VAL:CG1	2.40	0.52
1:A:282:LEU:HD21	1:D:256:LYS:HA	1.92	0.51
1:B:361:LEU:O	1:B:369:ARG:NE	2.43	0.51
1:A:437:LYS:HE2	1:A:441:SER:HB3	1.92	0.51
1:D:497:ARG:HH22	1:D:524:ILE:HA	1.73	0.51
1:B:380:TYR:O	1:B:384:VAL:HG23	2.09	0.51
1:B:481:ASP:OD1	1:B:482:LYS:N	2.43	0.51
1:C:86:GLU:HA	1:C:90:PHE:HD2	1.75	0.51
1:A:272:VAL:HG13	1:C:271:THR:HA	1.91	0.51
1:A:380:TYR:CD2	1:A:427:CYS:HB3	2.46	0.51
1:D:578:ASP:O	1:D:581:LEU:HG	2.11	0.51
1:A:437:LYS:NZ	1:A:443:GLU:HB2	2.26	0.51
1:B:494:HIS:H	1:B:494:HIS:CD2	2.28	0.51
1:B:573:CYS:HB2	1:B:603:GLU:OE1	2.11	0.51
1:C:674:PHE:HA	1:C:709:LEU:HD12	1.92	0.51
1:B:420:VAL:HB	1:B:458:SER:HB3	1.93	0.51
1:D:519:ASP:HA	1:D:522:ILE:HD12	1.93	0.51
1:A:529:ALA:O	1:A:533:LEU:HG	2.10	0.51
1:A:648:LEU:HD13	1:A:683:ALA:HB2	1.93	0.51
1:D:62:ASN:OD1	1:D:63:ARG:N	2.44	0.51
1:D:207:VAL:HG12	1:D:298:LEU:HD21	1.92	0.51
1:D:223:ALA:HB2	1:D:235:TRP:NE1	2.25	0.51
1:A:431:LEU:HD23	1:A:471:VAL:HA	1.93	0.51
1:B:457:ILE:HG22	1:B:463:ILE:HD11	1.92	0.51
1:D:165:GLU:OE2	1:D:168:ARG:NH2	2.42	0.51
1:D:535:VAL:HG13	1:D:547:LEU:HD23	1.92	0.51
1:A:458:SER:OG	1:A:463:ILE:O	2.23	0.50
1:A:540:PHE:CG	1:A:570:LEU:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:HIS:CE1	1:A:697:PRO:HD3	2.46	0.50
1:C:665:LEU:HD23	1:C:697:PRO:HG2	1.93	0.50
1:D:565:ARG:HA	1:D:594:ASP:OD1	2.11	0.50
1:A:706:ASN:HB3	1:A:709:LEU:HB3	1.92	0.50
1:B:516:LEU:HD22	1:B:521:VAL:HG11	1.93	0.50
1:B:547:LEU:HD13	1:B:579:ILE:HD13	1.92	0.50
1:C:337:ARG:HA	1:C:340:ARG:HD3	1.93	0.50
1:C:665:LEU:HD13	1:C:680:LEU:HB3	1.93	0.50
1:B:88:GLY:HA2	1:B:221:TYR:HB2	1.93	0.50
1:D:557:PRO:HB2	1:D:588:VAL:HG21	1.92	0.50
1:D:606:LYS:HD2	1:D:643:PHE:CE1	2.39	0.50
1:A:676:MET:HA	1:A:679:MET:HE3	1.94	0.50
1:B:641:SER:HB2	1:B:676:MET:HE2	1.93	0.50
1:C:498:THR:HA	1:C:501:ASN:HD21	1.76	0.50
1:D:379:PRO:HA	1:D:382:LYS:HZ1	1.76	0.50
1:D:605:VAL:HA	1:D:613:ILE:HD11	1.94	0.50
1:A:329:PHE:HA	1:A:332:ARG:HD2	1.93	0.50
1:A:361:LEU:HD11	1:D:329:PHE:CD1	2.46	0.50
1:A:712:LEU:O	1:A:716:VAL:HG23	2.12	0.50
1:B:223:ALA:HB2	1:B:235:TRP:NE1	2.27	0.50
1:C:324:ASN:O	1:C:327:ILE:HG22	2.11	0.50
1:A:320:ARG:HD2	1:C:196:TYR:HB2	1.94	0.50
1:B:370:ALA:O	1:B:374:GLN:HG2	2.12	0.50
1:B:371:LYS:O	1:B:375:LEU:HB2	2.12	0.50
1:B:612:VAL:O	1:B:616:LEU:HG	2.12	0.50
1:D:357:ASP:O	1:D:360:MET:HG2	2.12	0.50
1:A:537:SER:O	1:A:541:GLN:HB2	2.12	0.50
1:B:220:TYR:O	1:B:224:THR:HG23	2.12	0.50
1:B:386:LEU:HD13	1:B:456:ASP:OD2	2.11	0.50
1:B:532:ALA:HB2	1:B:559:LYS:HE3	1.93	0.50
1:A:584:ILE:HG23	1:A:619:GLU:OE2	2.11	0.49
1:B:338:ASP:O	1:B:342:GLN:HG3	2.12	0.49
1:D:115:GLN:HB3	1:D:139:TYR:CE2	2.48	0.49
1:A:337:ARG:HA	1:A:340:ARG:HD2	1.94	0.49
1:A:366:ALA:HB2	1:D:479:ARG:HH11	1.77	0.49
1:A:397:GLN:O	1:A:401:ARG:HG2	2.13	0.49
1:A:457:ILE:O	1:A:461:CYS:HB2	2.12	0.49
1:B:172:TRP:O	1:B:175:LEU:HB2	2.13	0.49
1:C:223:ALA:HB2	1:C:235:TRP:NE1	2.27	0.49
1:B:353:SER:C	1:C:332:ARG:HH12	2.20	0.49
1:B:551:ILE:CD1	1:B:552:ARG:HE	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ASP:O	1:A:422:HIS:ND1	2.45	0.49
1:B:183:GLU:O	1:B:186:GLN:HG2	2.12	0.49
1:B:282:LEU:HD21	1:C:256:LYS:HA	1.95	0.49
1:D:321:ASP:HA	1:D:324:ASN:HD22	1.77	0.49
1:D:349:LEU:HD22	1:D:408:LEU:HG	1.94	0.49
1:D:584:ILE:HD12	1:D:619:GLU:HG3	1.94	0.49
1:A:714:GLU:O	1:A:717:LYS:HG2	2.13	0.49
1:C:536:ASN:HD22	1:C:561:ASP:HB3	1.77	0.49
1:C:358:THR:O	1:C:361:LEU:HB2	2.11	0.49
1:A:518:SER:O	1:A:522:ILE:HG12	2.13	0.49
1:C:667:VAL:O	1:C:671:GLU:HG2	2.12	0.49
1:A:307:THR:O	1:A:311:VAL:HG23	2.12	0.49
1:A:504:MET:O	1:A:508:GLU:HG2	2.12	0.49
1:A:433:ALA:HB2	1:A:448:LEU:HD11	1.93	0.49
1:B:69:GLU:OE2	1:B:187:ARG:NH2	2.45	0.49
1:C:402:LEU:HD21	1:C:425:PHE:CE2	2.48	0.49
1:C:502:ASN:O	1:C:505:GLU:HG2	2.12	0.49
1:D:493:PHE:HD2	1:D:527:GLN:HG2	1.77	0.49
1:D:707:LYS:HA	1:D:710:ILE:HB	1.95	0.49
1:A:486:SER:O	1:A:490:GLU:HG2	2.13	0.49
1:C:380:TYR:HA	1:C:383:LYS:HD2	1.94	0.49
1:C:426:VAL:HG12	1:C:450:PRO:HA	1.95	0.49
1:A:414:THR:HG22	1:A:469:VAL:HB	1.95	0.48
1:B:384:VAL:HG12	1:B:386:LEU:H	1.78	0.48
1:B:457:ILE:O	1:B:461:CYS:HB2	2.12	0.48
1:B:462:ASN:CG	1:B:462:ASN:O	2.56	0.48
1:B:575:GLY:HA2	1:B:612:VAL:HG21	1.95	0.48
1:C:491:ILE:HG22	1:C:492:TYR:CD1	2.47	0.48
1:D:220:TYR:O	1:D:224:THR:HG23	2.13	0.48
1:D:581:LEU:HB3	1:D:615:LEU:HD21	1.94	0.48
1:B:407:PHE:HB3	1:B:471:VAL:HG21	1.96	0.48
1:C:513:ILE:HD13	1:C:513:ILE:H	1.77	0.48
1:B:328:SER:O	1:B:332:ARG:HG2	2.13	0.48
1:C:465:GLN:HE21	1:C:467:PHE:H	1.61	0.48
1:A:590:VAL:HB	1:A:621:ALA:HB2	1.94	0.48
1:C:456:ASP:O	1:C:460:ILE:HG12	2.13	0.48
1:D:436:THR:HA	1:D:442:GLU:HA	1.94	0.48
1:D:497:ARG:HH22	1:D:523:HIS:C	2.21	0.48
1:A:392:THR:HG22	1:A:396:ASN:ND2	2.27	0.48
1:B:342:GLN:HE22	1:D:371:LYS:HD2	1.77	0.48
1:B:352:ASP:O	1:C:332:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:590:VAL:HG11	1:C:619:GLU:HB3	1.95	0.48
1:A:220:TYR:O	1:A:224:THR:HG23	2.13	0.48
1:A:487:ASN:CB	1:A:491:ILE:HB	2.43	0.48
1:B:534:LYS:HE2	1:C:530:GLU:HG2	1.95	0.48
1:C:497:ARG:NH2	1:C:524:ILE:HA	2.29	0.48
1:D:346:HIS:CE1	1:D:411:GLU:OE1	2.62	0.48
1:A:214:THR:O	1:A:218:ILE:HG13	2.14	0.48
1:A:249:PHE:O	1:A:257:ARG:HD3	2.14	0.48
1:A:368:ILE:HA	1:A:371:LYS:HD2	1.96	0.48
1:B:542:GLY:HA3	1:B:576:TYR:CE1	2.49	0.48
1:D:543:ASP:O	1:D:547:LEU:HD12	2.14	0.48
1:D:601:LEU:HB2	1:D:621:ALA:HB1	1.96	0.48
1:B:89:PHE:HA	1:B:220:TYR:CE2	2.49	0.48
1:C:81:LEU:O	1:C:213:HIS:NE2	2.42	0.48
1:A:208:GLU:HG2	1:A:298:LEU:HD23	1.95	0.48
1:B:630:ASN:HD22	1:B:630:ASN:H	1.62	0.48
1:C:385:PRO:O	1:C:502:ASN:ND2	2.47	0.48
1:D:85:MET:HG3	1:D:213:HIS:CE1	2.45	0.48
1:A:59:HIS:HD2	1:A:61:LYS:H	1.61	0.47
1:A:81:LEU:O	1:A:213:HIS:NE2	2.46	0.47
1:A:487:ASN:HB3	1:A:491:ILE:HB	1.94	0.47
1:C:349:LEU:HD21	1:C:474:LEU:HD11	1.95	0.47
1:D:430:LEU:HB3	1:D:473:GLU:OE2	2.13	0.47
1:D:626:GLU:H	1:D:626:GLU:CD	2.22	0.47
1:A:233:TYR:OH	1:D:256:LYS:NZ	2.37	0.47
1:A:421:ASP:HA	1:A:482:LYS:HB2	1.95	0.47
1:B:282:LEU:HD11	1:C:256:LYS:HD2	1.96	0.47
1:B:349:LEU:HD12	1:B:349:LEU:HA	1.73	0.47
1:C:87:PHE:O	1:C:168:ARG:NH1	2.47	0.47
1:C:220:TYR:O	1:C:224:THR:HG23	2.13	0.47
1:D:569:HIS:HE1	1:D:592:LEU:HG	1.77	0.47
1:B:409:PRO:HD3	1:B:474:LEU:HD23	1.96	0.47
1:B:491:ILE:HD12	1:C:483:GLN:HG2	1.96	0.47
1:B:632:LEU:HD23	1:B:647:LEU:HD12	1.95	0.47
1:B:669:ALA:HA	1:B:709:LEU:HD21	1.96	0.47
1:C:407:PHE:HB2	1:C:475:CYS:SG	2.54	0.47
1:C:590:VAL:HB	1:C:621:ALA:HB2	1.96	0.47
1:D:486:SER:O	1:D:490:GLU:HG3	2.14	0.47
1:D:693:TRP:HB2	1:D:695:ASN:HD21	1.79	0.47
1:A:532:ALA:HA	1:A:535:VAL:HG12	1.96	0.47
1:B:197:LEU:HB3	1:B:309:LEU:HG	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:MET:HE1	1:B:344:THR:HG22	1.96	0.47
1:C:322:LYS:HD3	1:C:351:TYR:CE2	2.49	0.47
1:C:350:GLN:HG2	1:C:355:TYR:HE2	1.78	0.47
1:C:388:LYS:HB3	1:C:502:ASN:HD21	1.78	0.47
1:C:628:SER:O	1:C:632:LEU:HD13	2.14	0.47
1:D:213:HIS:ND1	1:D:258:TYR:OH	2.34	0.47
1:D:236:ILE:HG12	1:D:249:PHE:HB2	1.96	0.47
1:A:335:LEU:HD21	1:C:372:ILE:HG23	1.96	0.47
1:B:461:CYS:SG	1:B:512:ARG:HB3	2.54	0.47
1:B:551:ILE:HD11	1:B:582:PHE:CE2	2.43	0.47
1:D:187:ARG:O	1:D:190:LYS:HG2	2.15	0.47
1:D:544:PHE:HE1	1:D:582:PHE:HB2	1.78	0.47
1:D:706:ASN:HB3	1:D:709:LEU:HB3	1.97	0.47
1:A:231:GLU:HG2	1:A:249:PHE:HE2	1.80	0.47
1:B:387:PHE:CD1	1:B:394:PHE:HE2	2.32	0.47
1:C:95:GLU:H	1:C:95:GLU:CD	2.22	0.47
1:C:714:GLU:O	1:C:718:ASN:ND2	2.47	0.47
1:D:507:LYS:HG3	1:D:517:GLU:OE2	2.14	0.47
1:A:366:ALA:HB2	1:D:479:ARG:NH1	2.29	0.47
1:A:610:GLU:HA	1:A:613:ILE:CG1	2.44	0.47
1:C:394:PHE:HB2	1:C:495:ASP:OD2	2.14	0.47
1:C:465:GLN:NE2	1:C:467:PHE:H	2.12	0.47
1:D:665:LEU:HD11	1:D:685:ALA:HB3	1.96	0.47
1:B:106:ILE:O	1:B:110:VAL:HG13	2.15	0.47
1:B:214:THR:O	1:B:218:ILE:HG13	2.15	0.47
1:D:361:LEU:HA	1:D:364:ILE:HG13	1.96	0.47
1:A:427:CYS:SG	1:A:478:LEU:HD23	2.55	0.47
1:B:273:GLY:HA3	1:C:272:VAL:O	2.14	0.47
1:B:540:PHE:HD2	1:B:541:GLN:HE21	1.62	0.47
1:B:629:GLY:O	1:B:630:ASN:C	2.58	0.47
1:C:662:ARG:HA	1:C:666:HIS:ND1	2.30	0.47
1:C:706:ASN:ND2	1:C:709:LEU:H	2.13	0.47
1:D:601:LEU:O	1:D:605:VAL:HG12	2.14	0.47
1:A:454:PHE:CZ	1:A:469:VAL:HG11	2.50	0.47
1:A:457:ILE:HD12	1:A:457:ILE:H	1.80	0.47
1:D:428:GLU:HG2	1:D:476:HIS:HB3	1.96	0.47
1:D:642:ASP:N	1:D:642:ASP:OD1	2.46	0.47
1:A:645:LYS:HB3	1:A:645:LYS:HE3	1.80	0.46
1:A:659:TYR:HD1	1:A:660:ASP:N	2.14	0.46
1:B:192:THR:HA	1:C:320:ARG:CZ	2.45	0.46
1:C:456:ASP:OD1	1:C:457:ILE:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:551:ILE:HG21	1:D:586:GLU:HG3	1.96	0.46
1:A:432:GLU:HB3	1:A:472:CYS:SG	2.56	0.46
1:A:489:LEU:HD13	1:A:500:LEU:HG	1.96	0.46
1:A:675:LEU:HD23	1:A:675:LEU:H	1.79	0.46
1:B:503:ILE:O	1:B:507:LYS:HD3	2.15	0.46
1:D:315:ASN:HA	1:D:318:ARG:NH1	2.31	0.46
1:D:344:THR:O	1:D:348:ARG:HG3	2.16	0.46
1:D:536:ASN:HB3	1:D:570:LEU:CD1	2.44	0.46
1:B:572:ALA:HB1	1:B:604:ALA:HB2	1.97	0.46
1:C:423:LEU:HB2	1:C:459:ILE:HD12	1.97	0.46
1:D:497:ARG:HH21	1:D:527:GLN:NE2	2.14	0.46
1:A:274:TYR:O	1:C:275:GLY:CA	2.63	0.46
1:A:706:ASN:HD22	1:A:709:LEU:HB2	1.79	0.46
1:A:714:GLU:CB	1:A:717:LYS:HZ2	2.21	0.46
1:C:196:TYR:CD1	1:C:197:LEU:HD22	2.51	0.46
1:D:504:MET:HA	1:D:507:LYS:HG2	1.98	0.46
1:A:386:LEU:HD13	1:A:456:ASP:OD1	2.15	0.46
1:A:393:GLU:O	1:A:397:GLN:HG2	2.16	0.46
1:A:690:LYS:HB3	1:A:694:GLY:HA2	1.96	0.46
1:B:625:LEU:HB2	1:B:628:SER:HB3	1.98	0.46
1:C:120:TYR:HE2	1:C:135:ILE:HA	1.80	0.46
1:C:208:GLU:HG2	1:C:298:LEU:HD23	1.97	0.46
1:C:319:PHE:CE1	1:C:323:MET:HE3	2.50	0.46
1:C:648:LEU:HD23	1:C:648:LEU:HA	1.73	0.46
1:D:179:ARG:NH1	1:D:182:VAL:HG11	2.31	0.46
1:D:504:MET:HG3	1:D:520:ILE:HD11	1.96	0.46
1:D:701:ALA:HB2	1:D:713:LEU:HD12	1.97	0.46
1:A:192:THR:HG21	1:D:327:ILE:HD12	1.96	0.46
1:A:383:LYS:HD2	1:A:451:HIS:CD2	2.51	0.46
1:A:431:LEU:HD22	1:A:469:VAL:HG13	1.98	0.46
1:A:610:GLU:HA	1:A:613:ILE:HD11	1.98	0.46
1:B:388:LYS:HD3	1:B:389:GLY:N	2.31	0.46
1:C:678:LYS:HB2	1:C:712:LEU:HD11	1.97	0.46
1:A:354:HIS:ND1	1:A:357:ASP:HB2	2.31	0.46
1:B:329:PHE:HA	1:B:332:ARG:CG	2.46	0.46
1:B:526:LYS:HE2	1:B:526:LYS:HB2	1.77	0.46
1:B:570:LEU:HD11	1:C:562:TYR:CD1	2.50	0.46
1:C:172:TRP:O	1:C:175:LEU:HB2	2.16	0.46
1:C:497:ARG:HH12	1:C:523:HIS:C	2.24	0.46
1:C:539:ALA:HA	1:C:579:ILE:HD13	1.98	0.46
1:D:397:GLN:O	1:D:401:ARG:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:LEU:HD12	1:A:347:VAL:HG21	1.98	0.46
1:A:337:ARG:O	1:A:340:ARG:HG2	2.15	0.46
1:A:428:GLU:O	1:A:475:CYS:HA	2.16	0.46
1:A:687:VAL:HG13	1:A:697:PRO:HB2	1.98	0.46
1:C:319:PHE:HE1	1:C:348:ARG:HE	1.64	0.46
1:C:526:LYS:O	1:C:530:GLU:HG3	2.15	0.46
1:C:701:ALA:HB1	1:C:710:ILE:HG12	1.98	0.46
1:D:544:PHE:CE1	1:D:582:PHE:HB2	2.51	0.46
1:A:330:MET:HG2	1:A:335:LEU:HD12	1.98	0.46
1:A:709:LEU:O	1:A:713:LEU:HG	2.16	0.46
1:B:111:ASP:O	1:B:115:GLN:HG2	2.15	0.46
1:B:333:LYS:HB3	1:D:376:LEU:HD21	1.97	0.46
1:C:662:ARG:NH2	1:C:666:HIS:HB3	2.28	0.46
1:C:716:VAL:O	1:C:720:GLN:HG3	2.16	0.46
1:A:522:ILE:HG22	1:A:526:LYS:HE3	1.97	0.45
1:B:437:LYS:HG3	1:B:439:ASP:H	1.80	0.45
1:B:693:TRP:HB2	1:B:695:ASN:ND2	2.30	0.45
1:B:720:GLN:HB3	1:B:724:TYR:CZ	2.52	0.45
1:C:373:ALA:HB1	1:C:399:VAL:HG12	1.98	0.45
1:D:315:ASN:HB3	1:D:351:TYR:HE1	1.81	0.45
1:A:337:ARG:HA	1:A:340:ARG:HG2	1.97	0.45
1:A:431:LEU:HG	1:A:475:CYS:SG	2.56	0.45
1:C:179:ARG:HH11	1:C:180:LYS:HE2	1.81	0.45
1:D:652:MET:HE3	1:D:652:MET:HA	1.99	0.45
1:A:691:ASP:OD1	1:A:695:ASN:N	2.44	0.45
1:A:289:MET:HA	1:D:266:ILE:HG21	1.99	0.45
1:A:365:PRO:HG2	1:A:368:ILE:HG13	1.99	0.45
1:B:393:GLU:O	1:B:397:GLN:HG2	2.16	0.45
1:C:698:LEU:HD13	1:C:717:LYS:HD3	1.97	0.45
1:A:200:ARG:HD3	1:A:200:ARG:HA	1.77	0.45
1:A:223:ALA:HB2	1:A:235:TRP:NE1	2.31	0.45
1:A:706:ASN:O	1:A:710:ILE:HG13	2.16	0.45
1:B:201:ILE:HD12	1:B:309:LEU:HD12	1.99	0.45
1:B:416:GLN:N	1:B:468:THR:OG1	2.43	0.45
1:B:605:VAL:HA	1:B:613:ILE:HD11	1.99	0.45
1:C:78:TYR:CE2	1:C:100:LEU:HD11	2.52	0.45
1:D:454:PHE:CD2	1:D:469:VAL:HG21	2.51	0.45
1:A:349:LEU:HD22	1:A:408:LEU:HG	1.99	0.45
1:B:402:LEU:HD21	1:B:425:PHE:HE2	1.81	0.45
1:B:499:ILE:O	1:B:503:ILE:HG12	2.16	0.45
1:C:568:LEU:HD11	1:C:616:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:644:LEU:O	1:C:644:LEU:HD12	2.16	0.45
1:C:662:ARG:HE	1:C:666:HIS:HB3	1.80	0.45
1:A:339:LEU:O	1:A:343:ILE:HD12	2.16	0.45
1:B:189:GLU:O	1:C:320:ARG:NH1	2.50	0.45
1:B:493:PHE:CD1	1:B:531:LEU:HD11	2.52	0.45
1:C:66:LYS:HD3	1:C:66:LYS:C	2.42	0.45
1:C:112:ILE:HG23	1:C:139:TYR:OH	2.16	0.45
1:C:279:ALA:HB2	1:C:288:VAL:HG21	1.98	0.45
1:C:338:ASP:OD2	1:C:338:ASP:N	2.49	0.45
1:C:398:ILE:O	1:C:402:LEU:HG	2.16	0.45
1:C:416:GLN:OE1	1:C:436:THR:N	2.50	0.45
1:C:460:ILE:HG13	1:C:461:CYS:N	2.31	0.45
1:D:494:HIS:O	1:D:497:ARG:HB3	2.17	0.45
1:A:475:CYS:HB3	1:A:477:LEU:HD21	1.98	0.45
1:A:501:ASN:O	1:A:505:GLU:HG2	2.17	0.45
1:A:589:ASP:HB3	1:A:592:LEU:HB2	1.97	0.45
1:A:663:THR:O	1:A:666:HIS:HB2	2.17	0.45
1:A:714:GLU:HA	1:A:717:LYS:HD3	1.98	0.45
1:B:668:ALA:HA	1:B:673:LEU:HD11	1.99	0.45
1:C:530:GLU:C	1:C:534:LYS:HG3	2.42	0.45
1:D:527:GLN:HA	1:D:531:LEU:HD13	1.98	0.45
1:C:411:GLU:O	1:C:471:VAL:HG23	2.17	0.45
1:D:497:ARG:HH22	1:D:524:ILE:N	2.15	0.45
1:D:498:THR:O	1:D:502:ASN:ND2	2.50	0.45
1:B:200:ARG:HG3	1:B:305:ASN:ND2	2.31	0.44
1:C:361:LEU:HD21	1:C:372:ILE:HD13	1.98	0.44
1:C:394:PHE:O	1:C:398:ILE:HG12	2.16	0.44
1:D:379:PRO:HA	1:D:382:LYS:NZ	2.32	0.44
1:D:459:ILE:HD13	1:D:485:PHE:HD2	1.82	0.44
1:A:194:ILE:O	1:D:320:ARG:NH1	2.44	0.44
1:A:431:LEU:HD13	1:A:454:PHE:CE2	2.52	0.44
1:B:339:LEU:O	1:B:343:ILE:HG13	2.16	0.44
1:B:461:CYS:SG	1:B:516:LEU:HD11	2.56	0.44
1:B:577:GLU:HB3	1:B:615:LEU:HD21	1.99	0.44
1:C:85:MET:HE3	1:C:85:MET:HB2	1.83	0.44
1:C:394:PHE:CE2	1:C:488:ILE:HG22	2.52	0.44
1:B:221:TYR:O	1:B:225:THR:HG23	2.17	0.44
1:B:320:ARG:HG2	1:D:196:TYR:CD1	2.51	0.44
1:C:387:PHE:HE2	1:C:425:PHE:CE1	2.36	0.44
1:A:431:LEU:HD11	1:A:477:LEU:HD11	1.98	0.44
1:D:495:ASP:O	1:D:499:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:688:ILE:HG22	1:D:717:LYS:HE3	2.00	0.44
1:A:165:GLU:HG3	1:A:169:TYR:HE1	1.82	0.44
1:B:362:GLN:HE21	1:B:362:GLN:HA	1.83	0.44
1:B:626:GLU:O	1:B:627:ASP:C	2.61	0.44
1:A:273:GLY:HA3	1:D:272:VAL:HG12	1.99	0.44
1:B:641:SER:HB2	1:B:676:MET:CE	2.47	0.44
1:B:673:LEU:HD22	1:B:676:MET:SD	2.58	0.44
1:C:131:LYS:HD2	1:C:131:LYS:HA	1.69	0.44
1:D:315:ASN:HB3	1:D:351:TYR:CE1	2.52	0.44
1:B:494:HIS:ND1	1:B:554:GLY:HA3	2.32	0.44
1:B:666:HIS:HD2	1:B:697:PRO:HG3	1.82	0.44
1:D:65:TYR:CE2	1:D:118:VAL:HG11	2.53	0.44
1:D:529:ALA:O	1:D:532:ALA:N	2.51	0.44
1:A:65:TYR:CE1	1:A:118:VAL:HG11	2.53	0.44
1:A:623:PHE:HD2	1:A:652:MET:SD	2.41	0.44
1:A:648:LEU:HD23	1:A:648:LEU:HA	1.83	0.44
1:B:339:LEU:HD11	1:D:372:ILE:HG13	1.99	0.44
1:B:662:ARG:HH22	1:B:670:SER:CB	2.30	0.44
1:A:172:TRP:O	1:A:175:LEU:HB2	2.17	0.44
1:B:402:LEU:HD21	1:B:425:PHE:CE2	2.53	0.44
1:C:420:VAL:O	1:C:482:LYS:HD2	2.18	0.44
1:D:592:LEU:HD12	1:D:593:LYS:N	2.33	0.44
1:A:220:TYR:OH	1:A:257:ARG:NH1	2.38	0.43
1:A:659:TYR:HD1	1:A:660:ASP:H	1.65	0.43
1:B:456:ASP:OD1	1:B:456:ASP:C	2.60	0.43
1:B:504:MET:HA	1:B:507:LYS:HB2	1.98	0.43
1:B:641:SER:O	1:B:645:LYS:HD3	2.18	0.43
1:C:80:SER:O	1:C:210:TYR:OH	2.29	0.43
1:D:76:ALA:HA	1:D:108:PHE:HZ	1.83	0.43
1:D:323:MET:SD	1:D:344:THR:HG22	2.58	0.43
1:A:699:ASP:HA	1:A:702:ARG:NE	2.33	0.43
1:B:357:ASP:HB3	1:B:360:MET:CE	2.45	0.43
1:B:654:PRO:O	1:B:664:PRO:HD2	2.16	0.43
1:D:456:ASP:HA	1:D:459:ILE:HG22	2.00	0.43
1:B:527:GLN:O	1:B:531:LEU:HG	2.17	0.43
1:B:667:VAL:HG21	1:C:659:TYR:CE1	2.52	0.43
1:C:221:TYR:O	1:C:225:THR:HG23	2.17	0.43
1:C:357:ASP:OD1	1:C:357:ASP:C	2.61	0.43
1:C:498:THR:HA	1:C:501:ASN:ND2	2.34	0.43
1:D:172:TRP:O	1:D:175:LEU:HB2	2.18	0.43
1:D:648:LEU:HB2	1:D:683:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:GLU:HG2	1:A:249:PHE:CE2	2.53	0.43
1:A:328:SER:O	1:A:332:ARG:HG3	2.18	0.43
1:A:392:THR:O	1:A:396:ASN:ND2	2.52	0.43
1:B:406:TYR:CE1	1:B:476:HIS:HB2	2.53	0.43
1:C:229:GLU:HG3	1:C:230:ASN:H	1.82	0.43
1:C:365:PRO:HD2	1:C:368:ILE:HD13	2.01	0.43
1:C:433:ALA:HB3	1:C:446:THR:H	1.84	0.43
1:C:687:VAL:O	1:C:697:PRO:HD2	2.18	0.43
1:C:707:LYS:HE3	1:D:705:GLY:HA3	1.99	0.43
1:D:408:LEU:HB2	1:D:411:GLU:OE2	2.18	0.43
1:D:422:HIS:ND1	1:D:481:ASP:HA	2.32	0.43
1:D:458:SER:OG	1:D:466:PRO:HD3	2.19	0.43
1:B:310:ILE:H	1:B:310:ILE:HG12	1.67	0.43
1:B:354:HIS:HB3	1:B:357:ASP:CB	2.46	0.43
1:B:568:LEU:HD21	1:B:590:VAL:HG12	2.00	0.43
1:C:61:LYS:HA	1:C:61:LYS:HD2	1.60	0.43
1:B:463:ILE:HD13	1:B:512:ARG:HD2	2.01	0.43
1:C:529:ALA:O	1:C:533:LEU:HG	2.19	0.43
1:A:364:ILE:HG12	1:A:369:ARG:HG3	2.00	0.43
1:A:500:LEU:HD12	1:A:524:ILE:CD1	2.49	0.43
1:B:349:LEU:HD22	1:B:408:LEU:HD23	2.00	0.43
1:B:402:LEU:HD23	1:B:402:LEU:HA	1.87	0.43
1:D:164:HIS:O	1:D:167:VAL:HG12	2.19	0.43
1:A:364:ILE:O	1:A:369:ARG:NE	2.52	0.43
1:B:494:HIS:CD2	1:B:494:HIS:N	2.86	0.43
1:C:687:VAL:HG11	1:C:713:LEU:HB3	2.01	0.43
1:C:698:LEU:O	1:C:702:ARG:HG3	2.19	0.43
1:D:396:ASN:O	1:D:400:ILE:HG13	2.19	0.43
1:A:515:LYS:HZ1	1:A:518:SER:CB	2.26	0.43
1:B:456:ASP:OD1	1:B:457:ILE:HD12	2.18	0.43
1:C:346:HIS:O	1:C:350:GLN:HG3	2.18	0.43
1:D:663:THR:O	1:D:666:HIS:HB2	2.19	0.43
1:A:135:ILE:H	1:A:135:ILE:HG13	1.66	0.43
1:B:337:ARG:HA	1:B:340:ARG:HD3	2.01	0.43
1:B:662:ARG:NH2	1:B:700:GLU:OE2	2.52	0.43
1:B:672:GLY:HA2	1:B:704:CYS:SG	2.59	0.43
1:C:51:HIS:NE2	1:C:57:ILE:O	2.49	0.43
1:C:255:TRP:O	1:C:259:THR:OG1	2.25	0.43
1:D:145:LEU:O	1:D:149:ILE:HG12	2.18	0.43
1:D:435:VAL:HG23	1:D:445:VAL:CG2	2.48	0.43
1:A:405:GLU:HB2	1:A:407:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:VAL:HG22	1:A:470:ARG:HG2	2.01	0.42
1:A:413:ILE:HG21	1:A:454:PHE:HZ	1.83	0.42
1:B:307:THR:O	1:B:311:VAL:HB	2.19	0.42
1:B:364:ILE:CG1	1:B:365:PRO:HD2	2.49	0.42
1:D:606:LYS:HA	1:D:643:PHE:CE1	2.54	0.42
1:A:86:GLU:HG3	1:A:93:LEU:HD21	2.00	0.42
1:A:424:TYR:HB2	1:A:454:PHE:CZ	2.54	0.42
1:A:631:PHE:CD2	1:A:652:MET:HE1	2.54	0.42
1:B:636:VAL:HG13	1:B:673:LEU:HD21	2.01	0.42
1:C:530:GLU:O	1:C:531:LEU:C	2.61	0.42
1:D:89:PHE:HA	1:D:220:TYR:CE2	2.54	0.42
1:D:205:LEU:HD13	1:D:205:LEU:HA	1.90	0.42
1:A:164:HIS:CE1	1:A:166:LEU:HD23	2.55	0.42
1:A:540:PHE:CE1	1:A:574:ARG:HB2	2.54	0.42
1:A:616:LEU:O	1:A:620:GLY:N	2.47	0.42
1:B:351:TYR:CD1	1:B:351:TYR:C	2.98	0.42
1:A:572:ALA:HB1	1:A:604:ALA:HB2	2.00	0.42
1:A:699:ASP:O	1:A:703:LEU:HG	2.20	0.42
1:A:702:ARG:HE	1:A:702:ARG:HB2	1.58	0.42
1:B:272:VAL:HG13	1:D:271:THR:HA	2.00	0.42
1:C:594:ASP:OD1	1:C:598:HIS:N	2.51	0.42
1:A:403:HIS:CD2	1:A:479:ARG:HH12	2.36	0.42
1:B:53:ASP:OD1	1:B:53:ASP:N	2.52	0.42
1:B:61:LYS:HE3	1:B:61:LYS:HB3	1.64	0.42
1:B:196:TYR:HD2	1:B:197:LEU:HD22	1.84	0.42
1:B:420:VAL:HG11	1:B:455:GLY:HA3	2.02	0.42
1:C:139:TYR:CE1	1:C:143:HIS:HB2	2.54	0.42
1:C:706:ASN:O	1:C:710:ILE:HG13	2.20	0.42
1:D:681:VAL:HG11	1:D:716:VAL:HG21	2.00	0.42
1:D:691:ASP:OD1	1:D:695:ASN:N	2.41	0.42
1:B:457:ILE:HG13	1:B:507:LYS:NZ	2.34	0.42
1:C:99:VAL:O	1:C:103:VAL:HG12	2.20	0.42
1:D:319:PHE:CD1	1:D:351:TYR:HD1	2.37	0.42
1:D:387:PHE:CE2	1:D:398:ILE:HG21	2.55	0.42
1:A:59:HIS:CD2	1:A:61:LYS:HG2	2.55	0.42
1:B:109:LEU:O	1:B:113:VAL:HG23	2.20	0.42
1:C:90:PHE:O	1:C:168:ARG:NH1	2.52	0.42
1:C:139:TYR:HE1	1:C:143:HIS:HB2	1.82	0.42
1:C:439:ASP:OD1	1:C:440:GLY:N	2.53	0.42
1:C:491:ILE:HD13	1:C:491:ILE:HA	1.88	0.42
1:D:687:VAL:O	1:D:717:LYS:NZ	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:GLN:O	1:A:378:LEU:HB3	2.20	0.42
1:A:481:ASP:HB2	1:A:484:SER:OG	2.18	0.42
1:A:522:ILE:O	1:A:526:LYS:HG3	2.20	0.42
1:A:547:LEU:HD22	1:A:579:ILE:HG23	2.00	0.42
1:B:98:PHE:HE1	1:B:156:LEU:HD11	1.84	0.42
1:B:319:PHE:CE1	1:B:351:TYR:HE2	2.37	0.42
1:B:376:LEU:HD11	1:C:335:LEU:HD21	2.01	0.42
1:B:378:LEU:HB3	1:B:379:PRO:HD3	2.01	0.42
1:C:108:PHE:O	1:C:111:ASP:HB3	2.19	0.42
1:D:354:HIS:C	1:D:356:THR:N	2.77	0.42
1:D:456:ASP:O	1:D:459:ILE:HG22	2.20	0.42
1:D:687:VAL:O	1:D:696:SER:HB2	2.20	0.42
1:A:665:LEU:CD2	1:A:687:VAL:HG22	2.49	0.42
1:B:327:ILE:O	1:B:330:MET:HB2	2.19	0.42
1:B:419:VAL:HG23	1:B:463:ILE:O	2.19	0.42
1:B:421:ASP:C	1:B:422:HIS:ND1	2.77	0.42
1:C:229:GLU:HG3	1:C:230:ASN:N	2.35	0.42
1:C:423:LEU:HD12	1:C:456:ASP:HA	2.02	0.42
1:C:540:PHE:O	1:C:574:ARG:NE	2.53	0.42
1:D:172:TRP:HE3	1:D:175:LEU:HG	1.85	0.42
1:D:279:ALA:HB2	1:D:288:VAL:HG21	2.02	0.42
1:D:706:ASN:O	1:D:710:ILE:N	2.34	0.42
1:B:361:LEU:H	1:B:361:LEU:CD2	2.32	0.42
1:C:551:ILE:HG23	1:C:557:PRO:HD3	2.00	0.42
1:D:666:HIS:NE2	1:D:695:ASN:O	2.47	0.42
1:A:394:PHE:CD2	1:A:499:ILE:HG21	2.55	0.41
1:B:492:TYR:HB3	1:B:495:ASP:HB2	2.02	0.41
1:B:552:ARG:NH2	1:B:586:GLU:OE1	2.53	0.41
1:C:405:GLU:OE2	1:C:405:GLU:HA	2.19	0.41
1:D:465:GLN:NE2	1:D:467:PHE:O	2.38	0.41
1:D:569:HIS:NE2	1:D:592:LEU:O	2.53	0.41
1:A:195:ASN:O	1:A:199:THR:HG23	2.20	0.41
1:B:643:PHE:O	1:B:647:LEU:HG	2.19	0.41
1:B:673:LEU:HD13	1:B:676:MET:CB	2.45	0.41
1:D:459:ILE:HG13	1:D:482:LYS:HG3	2.02	0.41
1:D:662:ARG:HH21	1:D:666:HIS:C	2.28	0.41
1:A:75:TRP:CH2	1:A:103:VAL:HG12	2.55	0.41
1:A:221:TYR:O	1:A:225:THR:HG23	2.20	0.41
1:A:408:LEU:HD23	1:A:408:LEU:HA	1.87	0.41
1:A:423:LEU:HB2	1:A:459:ILE:HD12	2.00	0.41
1:A:581:LEU:HA	1:A:584:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ILE:CD1	1:B:309:LEU:HD12	2.50	0.41
1:B:239:LEU:HG	1:B:241:LEU:HG	2.00	0.41
1:B:485:PHE:CE2	1:B:489:LEU:HD11	2.55	0.41
1:B:535:VAL:HG13	1:B:567:PRO:HG3	2.01	0.41
1:B:717:LYS:HE3	1:B:717:LYS:HB3	1.87	0.41
1:C:241:LEU:HD21	1:C:276:ASP:HB2	2.02	0.41
1:A:500:LEU:HA	1:A:500:LEU:HD22	1.69	0.41
1:A:602:PHE:CD1	1:A:602:PHE:C	2.98	0.41
1:A:603:GLU:O	1:A:606:LYS:HG2	2.20	0.41
1:B:422:HIS:HB2	1:B:424:TYR:CE1	2.56	0.41
1:B:645:LYS:HE2	1:B:645:LYS:HB2	1.82	0.41
1:C:90:PHE:HZ	1:C:254:LEU:HD22	1.86	0.41
1:C:500:LEU:HD13	1:C:500:LEU:HA	1.82	0.41
1:C:584:ILE:HG23	1:C:619:GLU:OE1	2.21	0.41
1:C:664:PRO:HB2	1:C:680:LEU:HD11	2.02	0.41
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.92	0.41
1:B:197:LEU:O	1:B:201:ILE:HG13	2.21	0.41
1:B:546:GLN:O	1:B:550:LEU:HD23	2.21	0.41
1:B:594:ASP:OD1	1:B:594:ASP:C	2.62	0.41
1:B:710:ILE:HD12	1:B:710:ILE:N	2.31	0.41
1:C:240:LYS:HD3	1:C:245:SER:HB2	2.03	0.41
1:A:90:PHE:CZ	1:A:254:LEU:HD13	2.51	0.41
1:A:98:PHE:CZ	1:A:102:ILE:HD11	2.54	0.41
1:A:196:TYR:O	1:A:199:THR:N	2.54	0.41
1:A:201:ILE:HD11	1:A:306:ILE:HA	2.03	0.41
1:A:419:VAL:HA	1:A:464:SER:HA	2.03	0.41
1:A:675:LEU:HD21	1:A:676:MET:HE2	2.02	0.41
1:B:497:ARG:HH12	1:B:500:LEU:HD23	1.85	0.41
1:B:711:LYS:HE3	1:B:711:LYS:HB3	1.88	0.41
1:C:57:ILE:HG13	1:C:130:TYR:O	2.21	0.41
1:C:121:ARG:HB3	1:C:126:TYR:HB3	2.03	0.41
1:C:426:VAL:HG21	1:C:431:LEU:HD12	2.02	0.41
1:C:641:SER:HA	1:C:676:MET:SD	2.61	0.41
1:D:535:VAL:HG12	1:D:567:PRO:HB3	2.02	0.41
1:D:574:ARG:HB3	1:D:576:TYR:CD2	2.55	0.41
1:B:65:TYR:CE1	1:B:118:VAL:HG21	2.56	0.41
1:B:137:PHE:CE2	1:B:141:LYS:HD3	2.55	0.41
1:B:186:GLN:O	1:B:190:LYS:NZ	2.53	0.41
1:B:223:ALA:HB2	1:B:235:TRP:CD1	2.55	0.41
1:C:662:ARG:HG2	1:C:691:ASP:HB2	2.02	0.41
1:D:221:TYR:O	1:D:225:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:529:ALA:O	1:D:533:LEU:HD12	2.21	0.41
1:A:275:GLY:CA	1:D:274:TYR:O	2.65	0.41
1:A:326:LEU:CD1	1:A:347:VAL:HG21	2.50	0.41
1:C:327:ILE:HA	1:C:330:MET:CE	2.50	0.41
1:C:458:SER:OG	1:C:463:ILE:O	2.26	0.41
1:C:526:LYS:HG2	1:C:530:GLU:HG3	2.03	0.41
1:C:618:LYS:HD3	1:C:618:LYS:N	2.35	0.41
1:A:182:VAL:O	1:A:186:GLN:HG3	2.21	0.41
1:A:490:GLU:HG3	1:A:491:ILE:N	2.33	0.41
1:A:533:LEU:HB3	1:D:533:LEU:HD23	2.03	0.41
1:A:659:TYR:CD1	1:A:660:ASP:N	2.89	0.41
1:A:675:LEU:O	1:A:679:MET:HG3	2.20	0.41
1:B:364:ILE:HG13	1:B:365:PRO:CD	2.49	0.41
1:B:692:ARG:HB2	1:B:692:ARG:NH1	2.36	0.41
1:C:424:TYR:HB2	1:C:454:PHE:CE1	2.56	0.41
1:C:593:LYS:HZ2	1:C:593:LYS:HG2	1.68	0.41
1:D:253:ASP:OD1	1:D:254:LEU:N	2.54	0.41
1:D:435:VAL:N	1:D:443:GLU:O	2.50	0.41
1:A:437:LYS:HZ3	1:A:443:GLU:HB2	1.85	0.41
1:A:557:PRO:HB2	1:A:588:VAL:HG22	2.03	0.41
1:A:654:PRO:O	1:A:664:PRO:HD2	2.21	0.41
1:B:330:MET:CE	1:B:340:ARG:HB3	2.51	0.41
1:B:378:LEU:O	1:B:378:LEU:HD12	2.21	0.41
1:B:413:ILE:HD11	1:B:471:VAL:HG22	2.01	0.41
1:B:506:GLU:H	1:B:506:GLU:HG3	1.70	0.41
1:B:680:LEU:O	1:B:683:ALA:HB3	2.20	0.41
1:C:85:MET:HE2	1:C:213:HIS:HE1	1.86	0.41
1:C:128:THR:O	1:C:128:THR:OG1	2.39	0.41
1:C:371:LYS:HB3	1:C:371:LYS:HE3	1.78	0.41
1:D:170:LEU:HA	1:D:170:LEU:HD23	1.86	0.41
1:D:557:PRO:CB	1:D:567:PRO:HG2	2.51	0.41
1:A:659:TYR:OH	1:D:658:ASP:OD2	2.38	0.40
1:B:534:LYS:HA	1:B:534:LYS:HD3	1.88	0.40
1:C:601:LEU:HB2	1:C:621:ALA:HB1	2.03	0.40
1:C:626:GLU:OE1	1:C:626:GLU:HA	2.21	0.40
1:D:437:LYS:HD3	1:D:437:LYS:HA	2.00	0.40
1:D:507:LYS:HD3	1:D:513:ILE:HD13	2.02	0.40
1:D:628:SER:O	1:D:632:LEU:HG	2.21	0.40
1:A:208:GLU:HG2	1:A:298:LEU:CD2	2.52	0.40
1:A:500:LEU:HD22	1:A:503:ILE:HG13	2.02	0.40
1:B:226:LEU:HD22	1:B:227:PRO:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:ASP:HB2	1:B:565:ARG:HG2	2.02	0.40
1:C:72:ILE:HD12	1:C:72:ILE:HA	1.83	0.40
1:D:314:SER:H	1:D:317:GLU:HG2	1.85	0.40
1:D:383:LYS:HE2	1:D:383:LYS:HB2	1.87	0.40
1:D:616:LEU:HD23	1:D:616:LEU:HA	1.89	0.40
1:B:85:MET:HE2	1:B:85:MET:HB3	1.97	0.40
1:B:242:GLY:HA3	1:D:280:VAL:HG11	2.04	0.40
1:B:275:GLY:O	1:B:278:HIS:HD2	2.05	0.40
1:B:320:ARG:HH22	1:D:190:LYS:HA	1.86	0.40
1:B:346:HIS:HA	1:B:408:LEU:HD11	2.04	0.40
1:B:662:ARG:NH1	1:C:660:ASP:OD1	2.55	0.40
1:C:149:ILE:O	1:C:154:TRP:NE1	2.52	0.40
1:C:281:ASN:HB2	1:C:284:GLU:CD	2.46	0.40
1:D:267:VAL:HG13	1:D:272:VAL:HB	2.03	0.40
1:D:689:SER:O	1:D:697:PRO:HD3	2.21	0.40
1:A:89:PHE:HA	1:A:220:TYR:CE2	2.56	0.40
1:B:201:ILE:HG12	1:B:305:ASN:HB3	2.03	0.40
1:C:396:ASN:O	1:C:400:ILE:HG13	2.21	0.40
1:D:394:PHE:O	1:D:398:ILE:HG12	2.20	0.40
1:B:329:PHE:HA	1:B:332:ARG:HG2	2.03	0.40
1:C:205:LEU:HD13	1:C:205:LEU:HA	1.84	0.40
1:C:704:CYS:HA	1:D:707:LYS:HE2	2.03	0.40
1:D:352:ASP:C	1:D:354:HIS:N	2.78	0.40
1:D:471:VAL:HG13	1:D:475:CYS:SG	2.62	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	674/834 (81%)	646 (96%)	28 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	674/834 (81%)	653 (97%)	21 (3%)	0	100	100
1	C	674/834 (81%)	650 (96%)	24 (4%)	0	100	100
1	D	674/834 (81%)	652 (97%)	22 (3%)	0	100	100
All	All	2696/3336 (81%)	2601 (96%)	95 (4%)	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	597/743 (80%)	573 (96%)	24 (4%)	28	60
1	B	597/743 (80%)	579 (97%)	18 (3%)	36	65
1	C	597/743 (80%)	576 (96%)	21 (4%)	32	62
1	D	597/743 (80%)	578 (97%)	19 (3%)	34	64
All	All	2388/2972 (80%)	2306 (97%)	82 (3%)	33	63

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	TRP
1	A	194	ILE
1	A	254	LEU
1	A	269	MET
1	A	272	VAL
1	A	277	ILE
1	A	282	LEU
1	A	292	VAL
1	A	320	ARG
1	A	355	TYR
1	A	363	ASP
1	A	434	LEU
1	A	436	THR

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Mol	Chain	Res	Type
1	A	473	GLU
1	A	474	LEU
1	A	489	LEU
1	A	491	ILE
1	A	500	LEU
1	A	515	LYS
1	A	540	PHE
1	A	562	TYR
1	A	584	ILE
1	A	596	PHE
1	A	699	ASP
1	B	56	TYR
1	B	175	LEU
1	B	208	GLU
1	B	269	MET
1	B	310	ILE
1	B	347	VAL
1	B	362	GLN
1	B	467	PHE
1	B	493	PHE
1	B	494	HIS
1	B	504	MET
1	B	516	LEU
1	B	561	ASP
1	B	596	PHE
1	B	655	ASN
1	B	666	HIS
1	B	673	LEU
1	B	681	VAL
1	C	53	ASP
1	C	114	LEU
1	C	126	TYR
1	C	179	ARG
1	C	195	ASN
1	C	197	LEU
1	C	204	LEU
1	C	205	LEU
1	C	266	ILE
1	C	272	VAL
1	C	277	ILE
1	C	281	ASN
1	C	343	ILE

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Mol	Chain	Res	Type
1	C	346	HIS
1	C	495	ASP
1	C	500	LEU
1	C	512	ARG
1	C	513	ILE
1	C	520	ILE
1	C	581	LEU
1	C	642	ASP
1	D	100	LEU
1	D	109	LEU
1	D	128	THR
1	D	192	THR
1	D	205	LEU
1	D	272	VAL
1	D	276	ASP
1	D	316	THR
1	D	318	ARG
1	D	320	ARG
1	D	355	TYR
1	D	406	TYR
1	D	514	LYS
1	D	528	GLU
1	D	547	LEU
1	D	578	ASP
1	D	612	VAL
1	D	642	ASP
1	D	655	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS
1	A	281	ASN
1	A	315	ASN
1	A	342	GLN
1	A	396	ASN
1	A	403	HIS
1	A	502	ASN
1	A	510	ASN
1	A	558	ASN
1	A	706	ASN
1	A	718	ASN

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Mol	Chain	Res	Type
1	B	105	GLN
1	B	186	GLN
1	B	278	HIS
1	B	324	ASN
1	B	331	ASN
1	B	342	GLN
1	B	346	HIS
1	B	354	HIS
1	B	362	GLN
1	B	416	GLN
1	B	546	GLN
1	B	558	ASN
1	B	624	ASN
1	B	630	ASN
1	B	655	ASN
1	B	695	ASN
1	C	52	ASN
1	C	281	ASN
1	C	342	GLN
1	C	354	HIS
1	C	462	ASN
1	C	483	GLN
1	C	501	ASN
1	C	510	ASN
1	C	523	HIS
1	C	598	HIS
1	C	695	ASN
1	C	718	ASN
1	D	59	HIS
1	D	324	ASN
1	D	346	HIS
1	D	350	GLN
1	D	403	HIS
1	D	502	ASN
1	D	527	GLN
1	D	655	ASN
1	D	695	ASN
1	D	718	ASN
1	D	720	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.

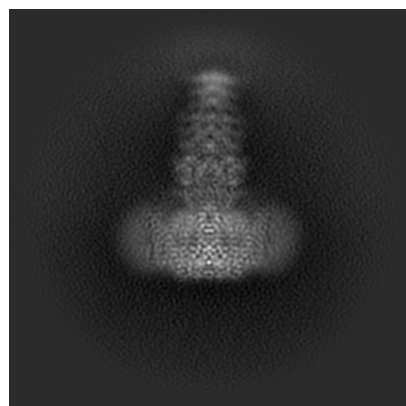
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62915. These allow visual inspection of the internal detail of the map and identification of artifacts.

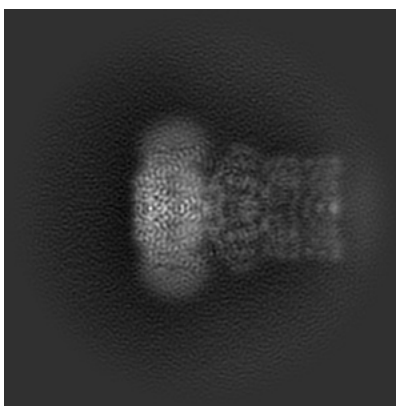
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

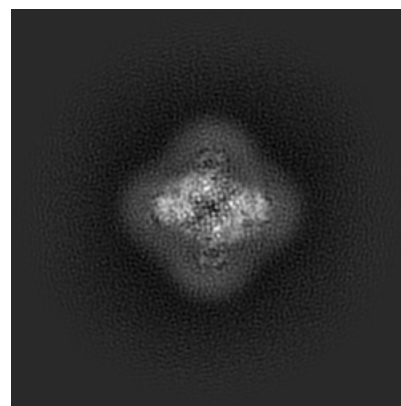
6.1.1 Primary map



X

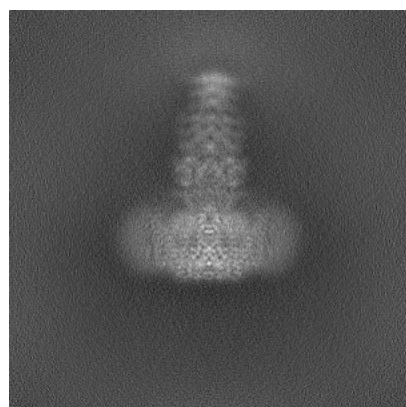


Y

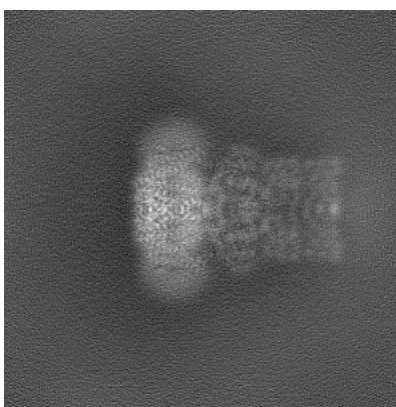


Z

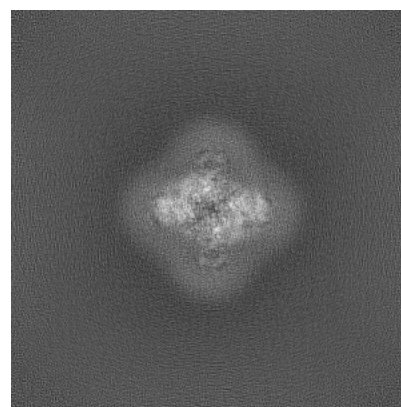
6.1.2 Raw map



X



Y

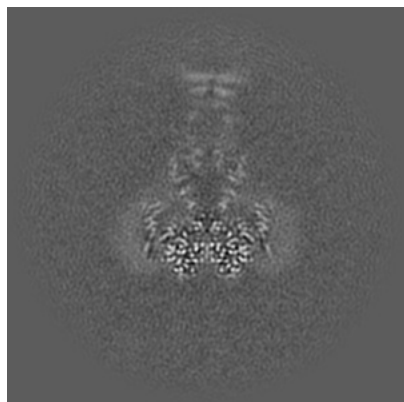


Z

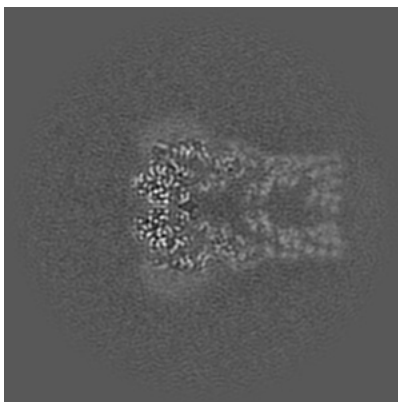
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

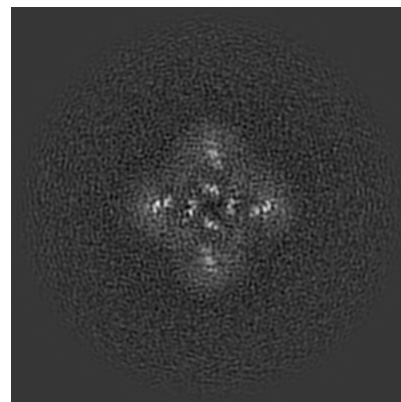
6.2.1 Primary map



X Index: 200

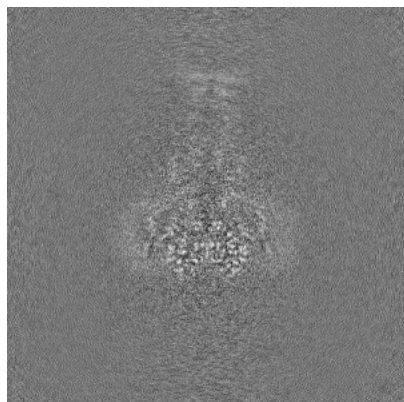


Y Index: 200

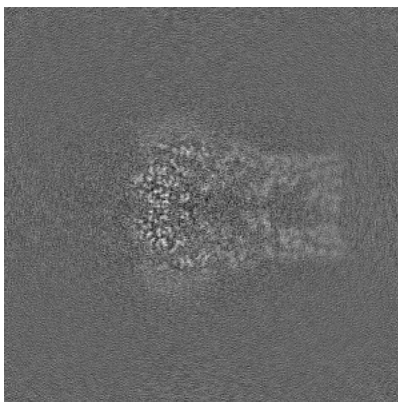


Z Index: 200

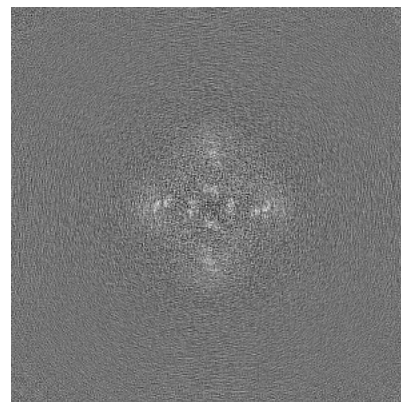
6.2.2 Raw map



X Index: 200



Y Index: 200

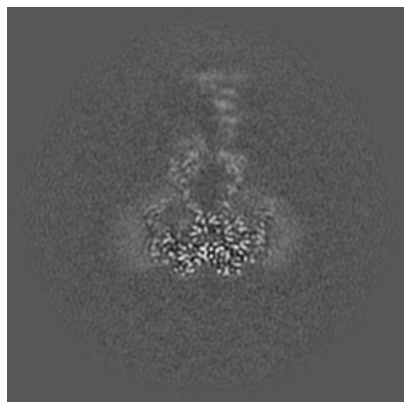


Z Index: 200

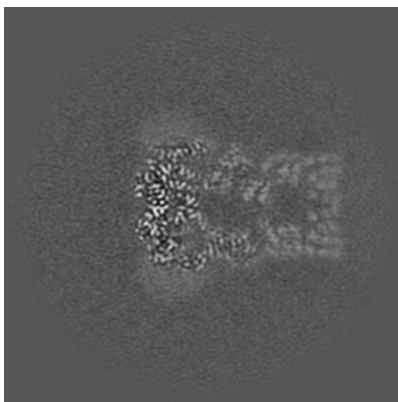
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

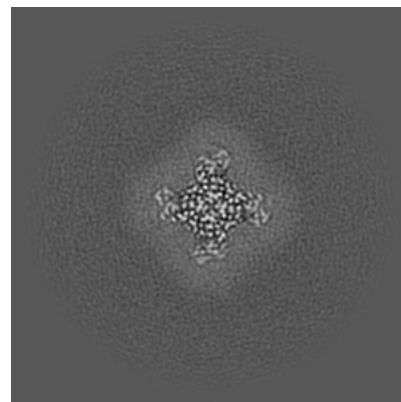
6.3.1 Primary map



X Index: 196

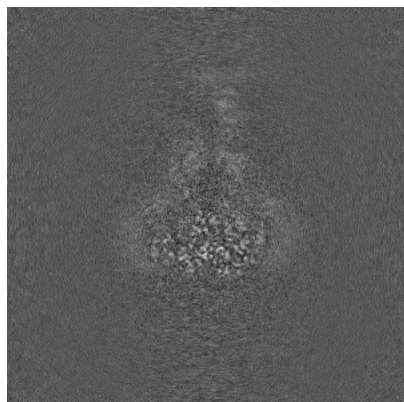


Y Index: 204

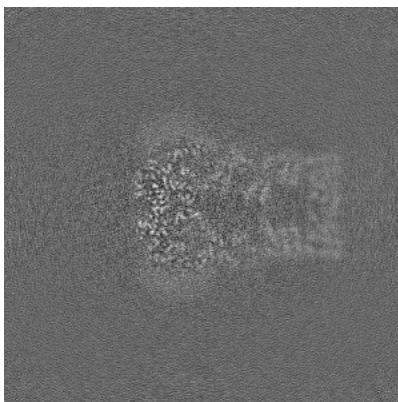


Z Index: 146

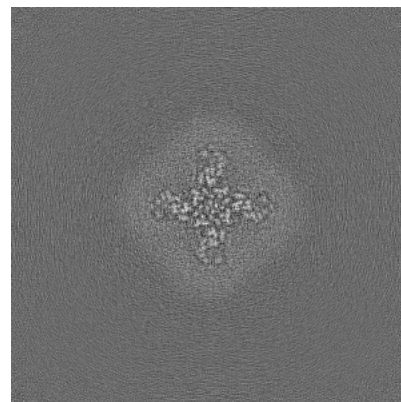
6.3.2 Raw map



X Index: 196



Y Index: 203

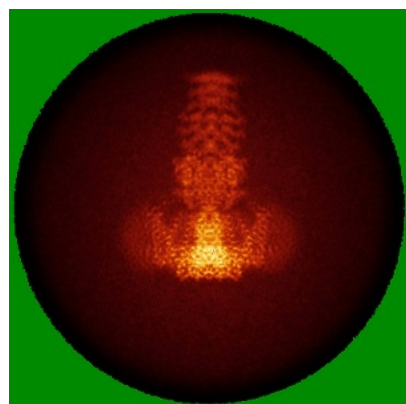


Z Index: 160

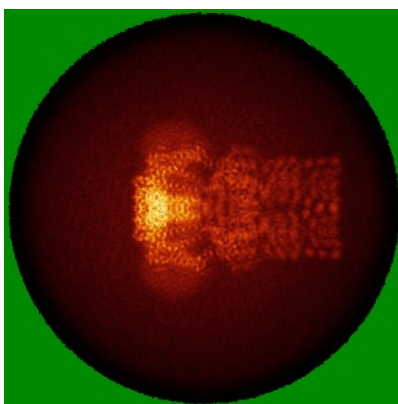
The images above show the largest variance slices of the map in three orthogonal directions.

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

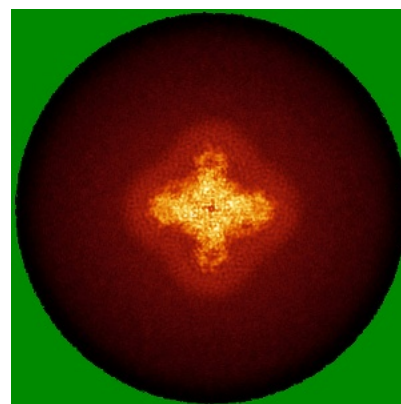
6.4.1 Primary map



X

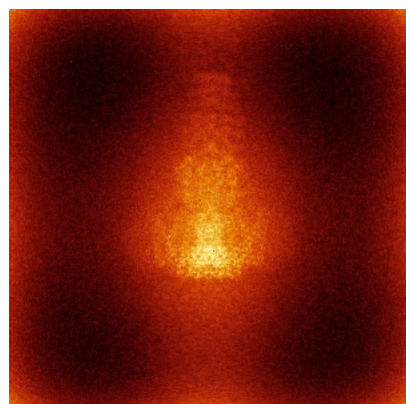


Y

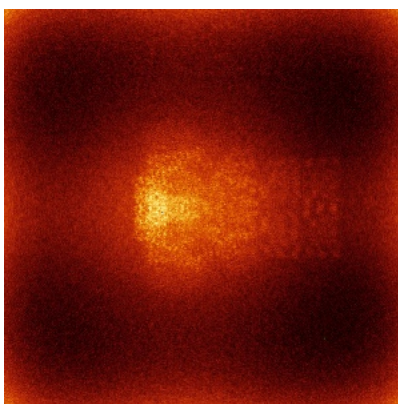


Z

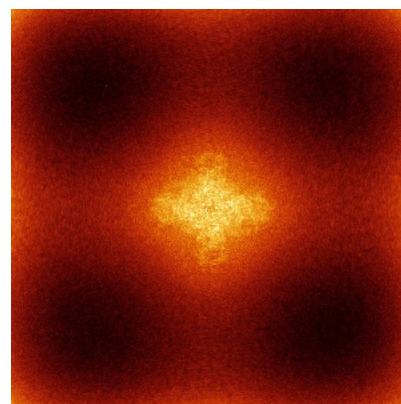
6.4.2 Raw map



X



Y

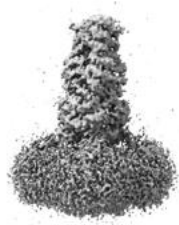


Z

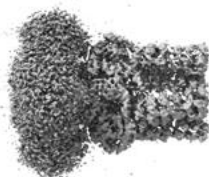
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



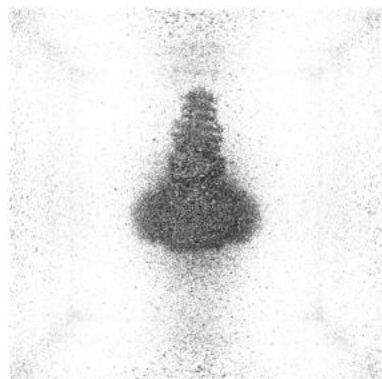
Y



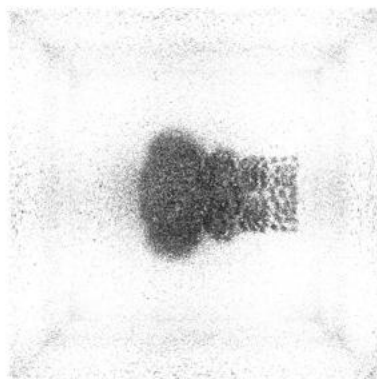
Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

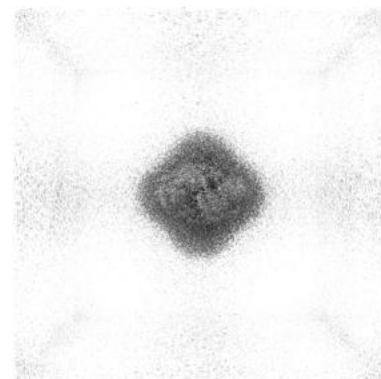
6.5.2 Raw map



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.

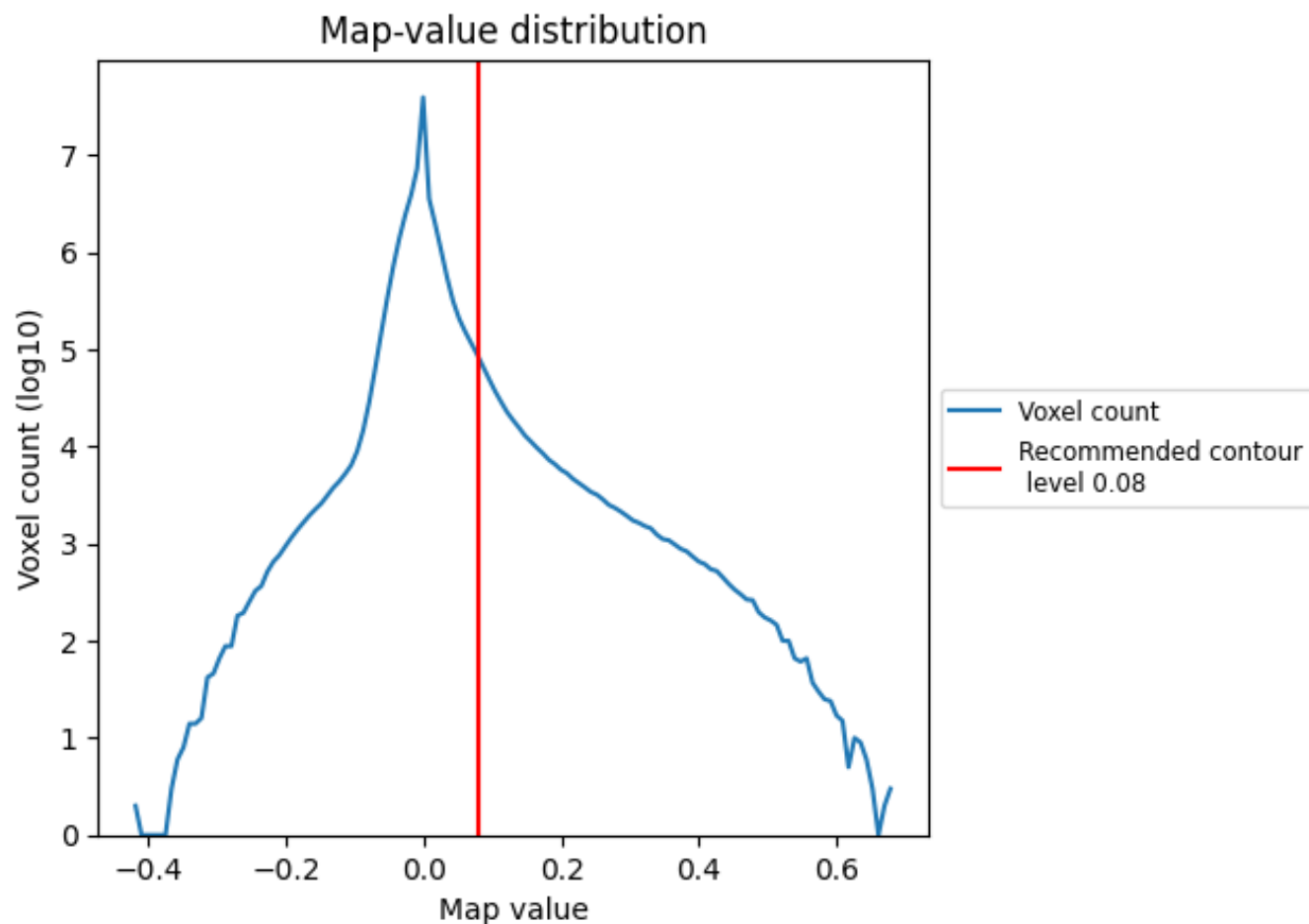
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

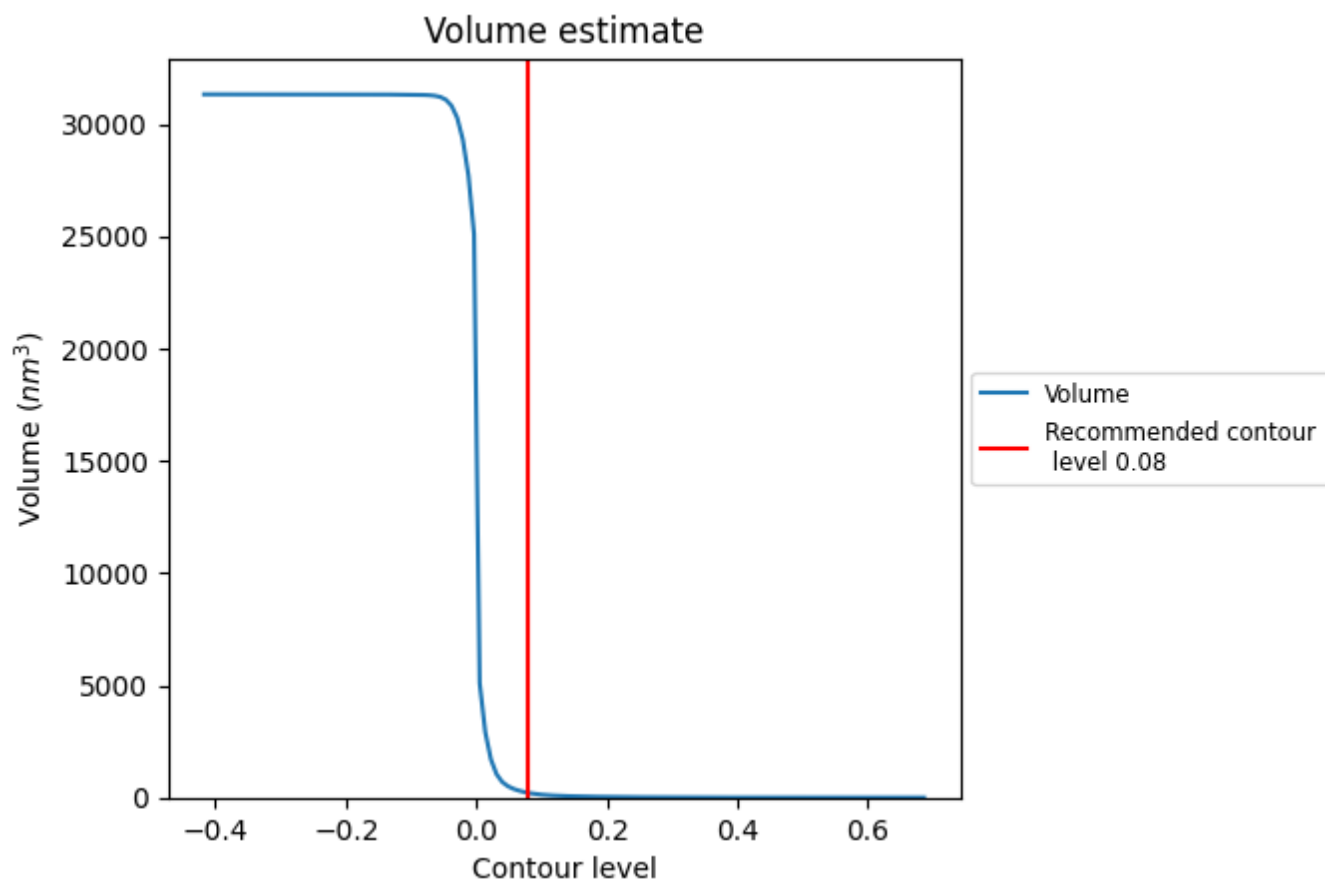
This section contains the results of statistical analysis of the map.

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.

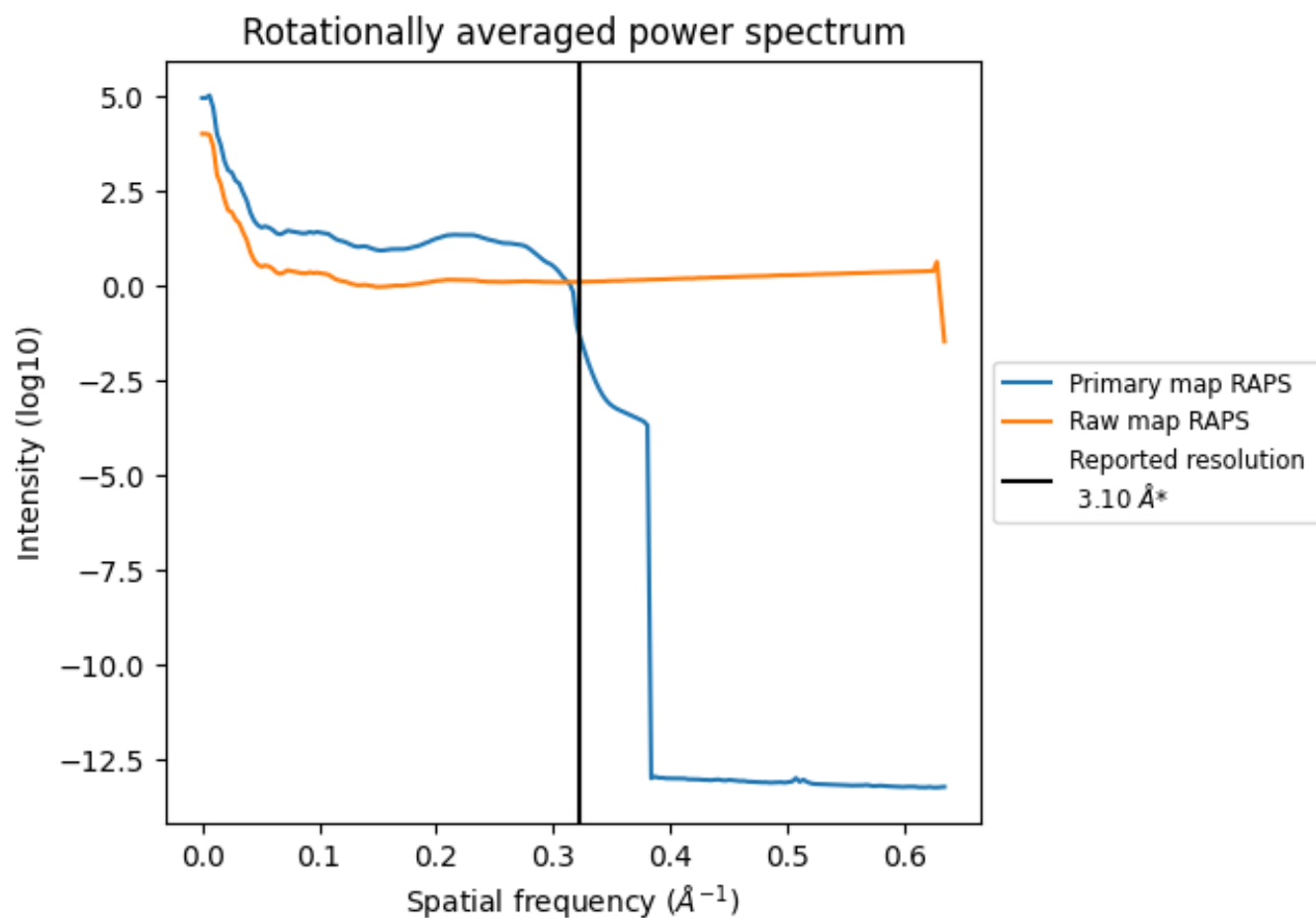
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 207 nm³; this corresponds to an approximate mass of 187 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 ⓘ

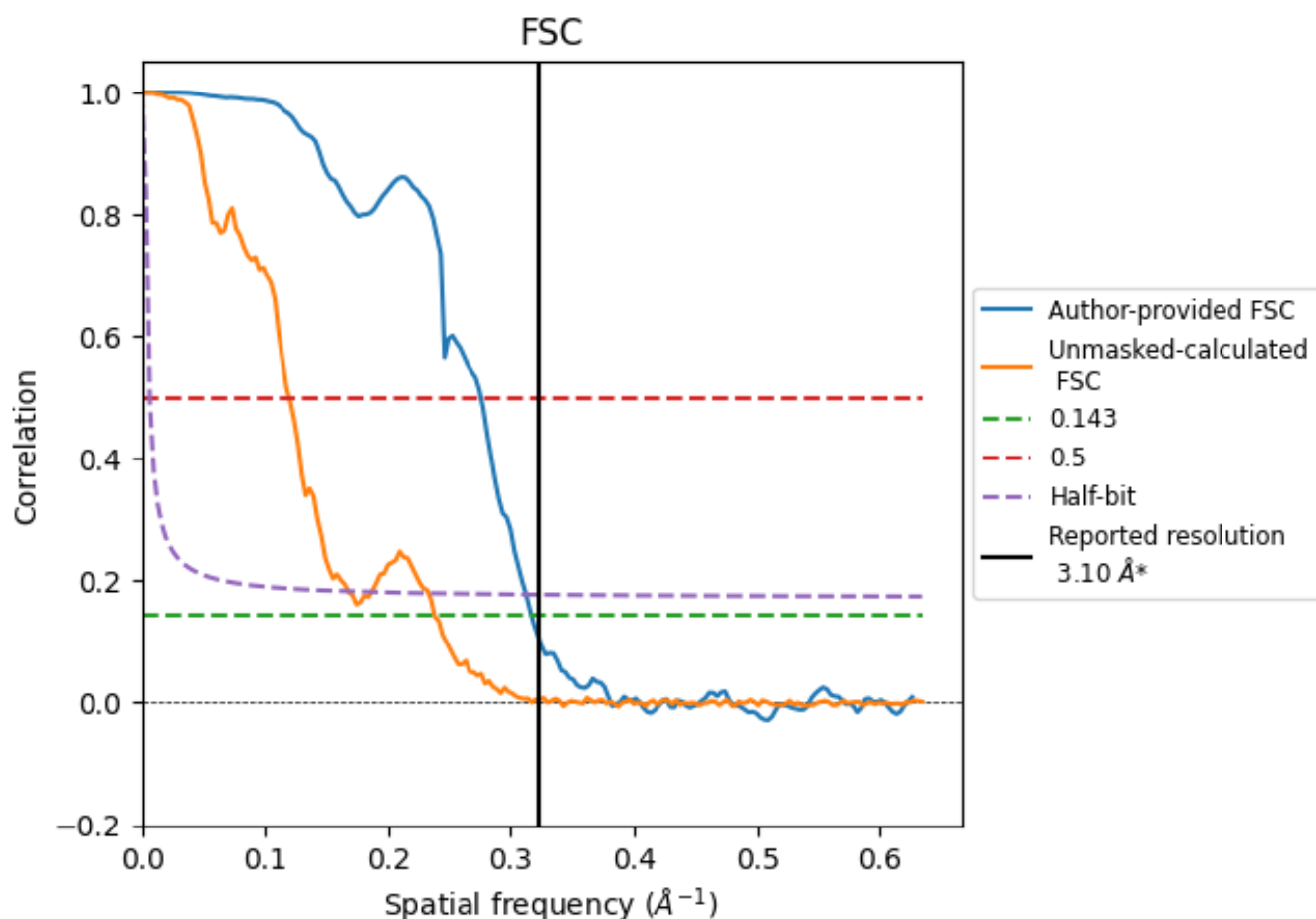


*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.323 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

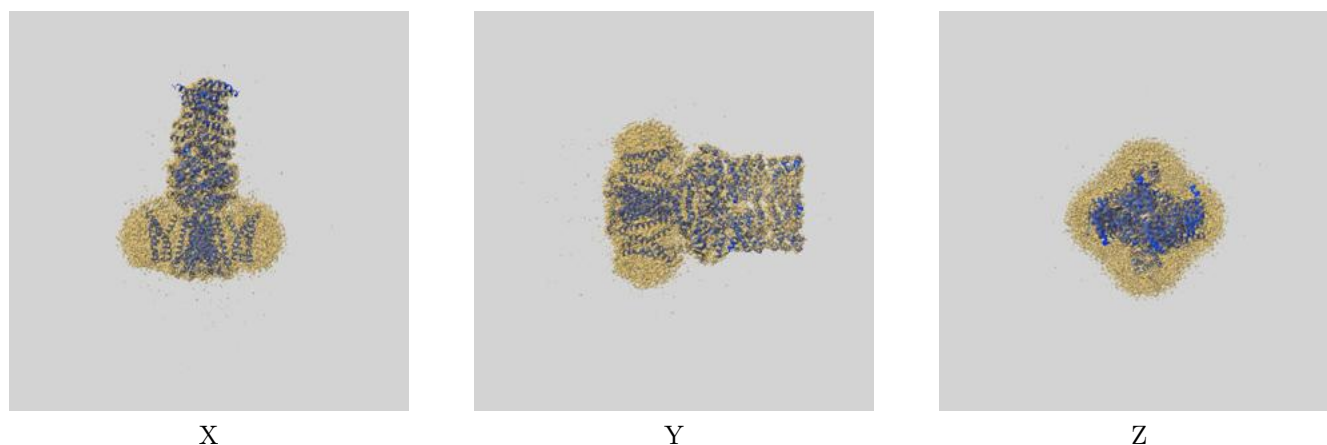
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.16	3.63	3.20
Unmasked-calculated*	4.21	8.36	5.96

*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 4.21 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

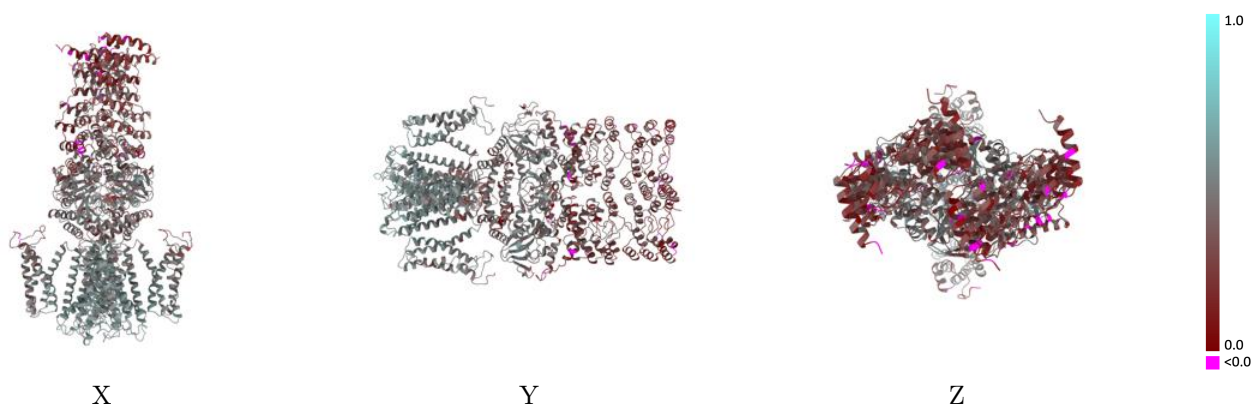
This section contains information regarding the fit between EMDB map EMD-62915 and PDB model 9LA0. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



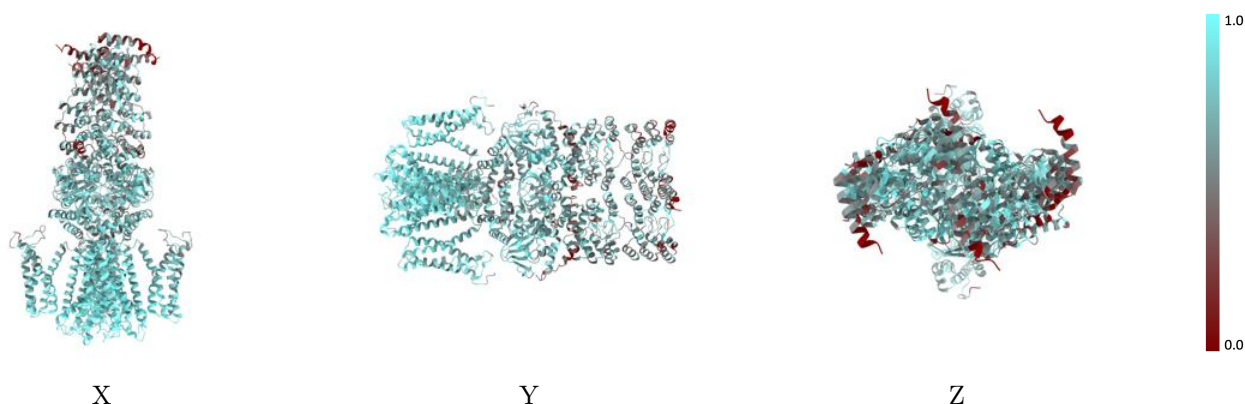
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



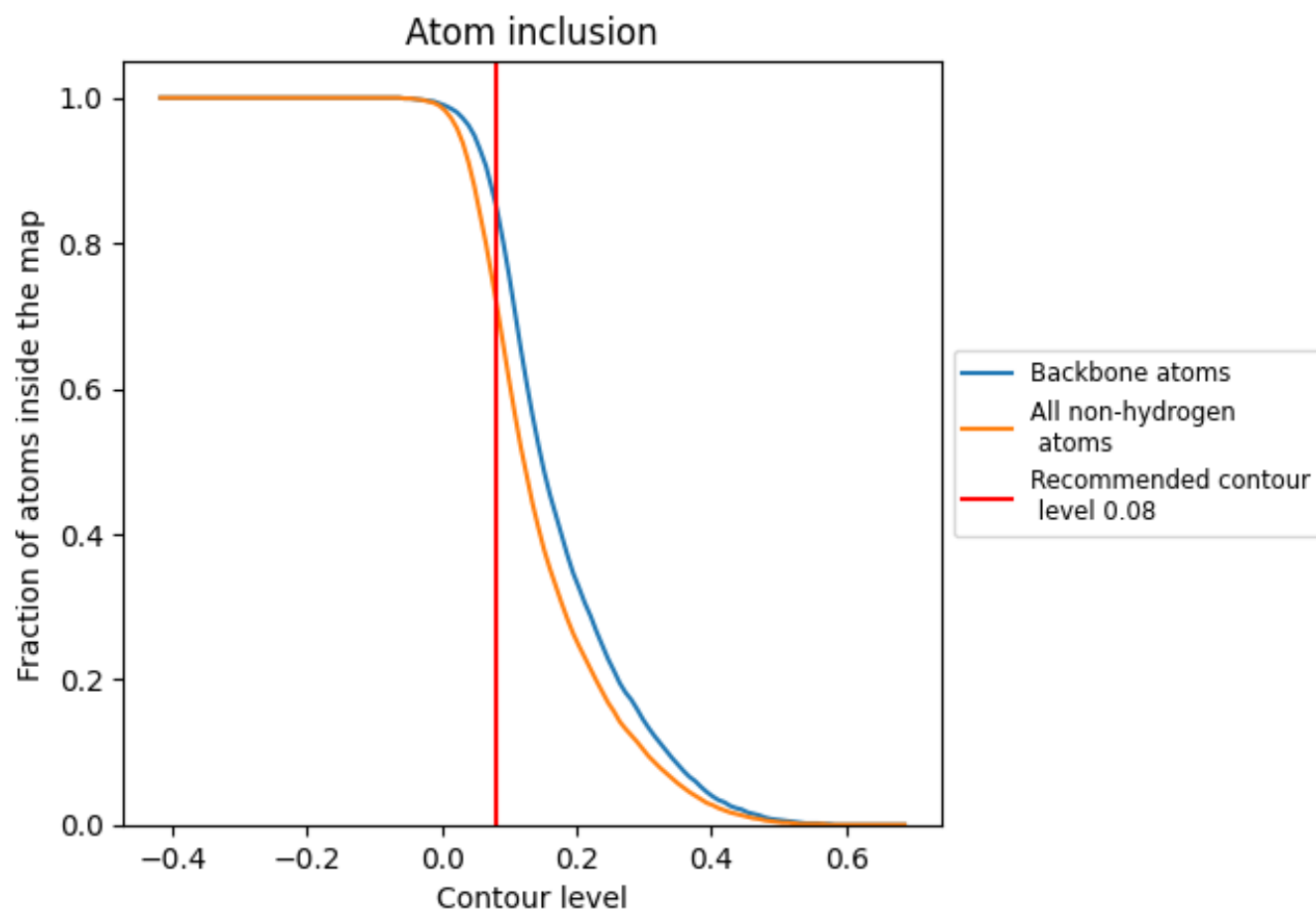
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 72% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7220	0.4000
A	0.7260	0.4050
B	0.7250	0.4050
C	0.7120	0.3910
D	0.7260	0.3990

