



Full wwPDB EM Validation Report ⓘ

Jul 9, 2025 – 08:25 PM JST

PDB ID : 9LA1 / pdb_00009la1
EMDB ID : EMD-62916
Title : Arabidopsis GORK WT4
Authors : Yamanashi, T.; Kume, T.; Sekido, N.; Muraoka, Y.; Yokoyama, T.; Tanaka, Y.; Uozumi, N.
Deposited on : 2025-01-01
Resolution : 3.15 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

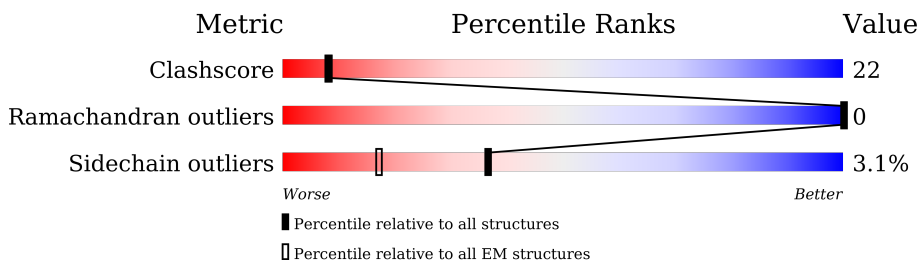
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.15 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	834	<div> <div>11%</div> <div>43%</div> <div>36%</div> <div>•</div> <div>19%</div> </div>
1	B	834	<div> <div>9%</div> <div>45%</div> <div>35%</div> <div>•</div> <div>19%</div> </div>
1	C	834	<div> <div>9%</div> <div>47%</div> <div>33%</div> <div>•</div> <div>19%</div> </div>
1	D	834	<div> <div>9%</div> <div>42%</div> <div>38%</div> <div>•</div> <div>19%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21940 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	675	Total	C	N	O	S	0	0
			5482	3557	913	987	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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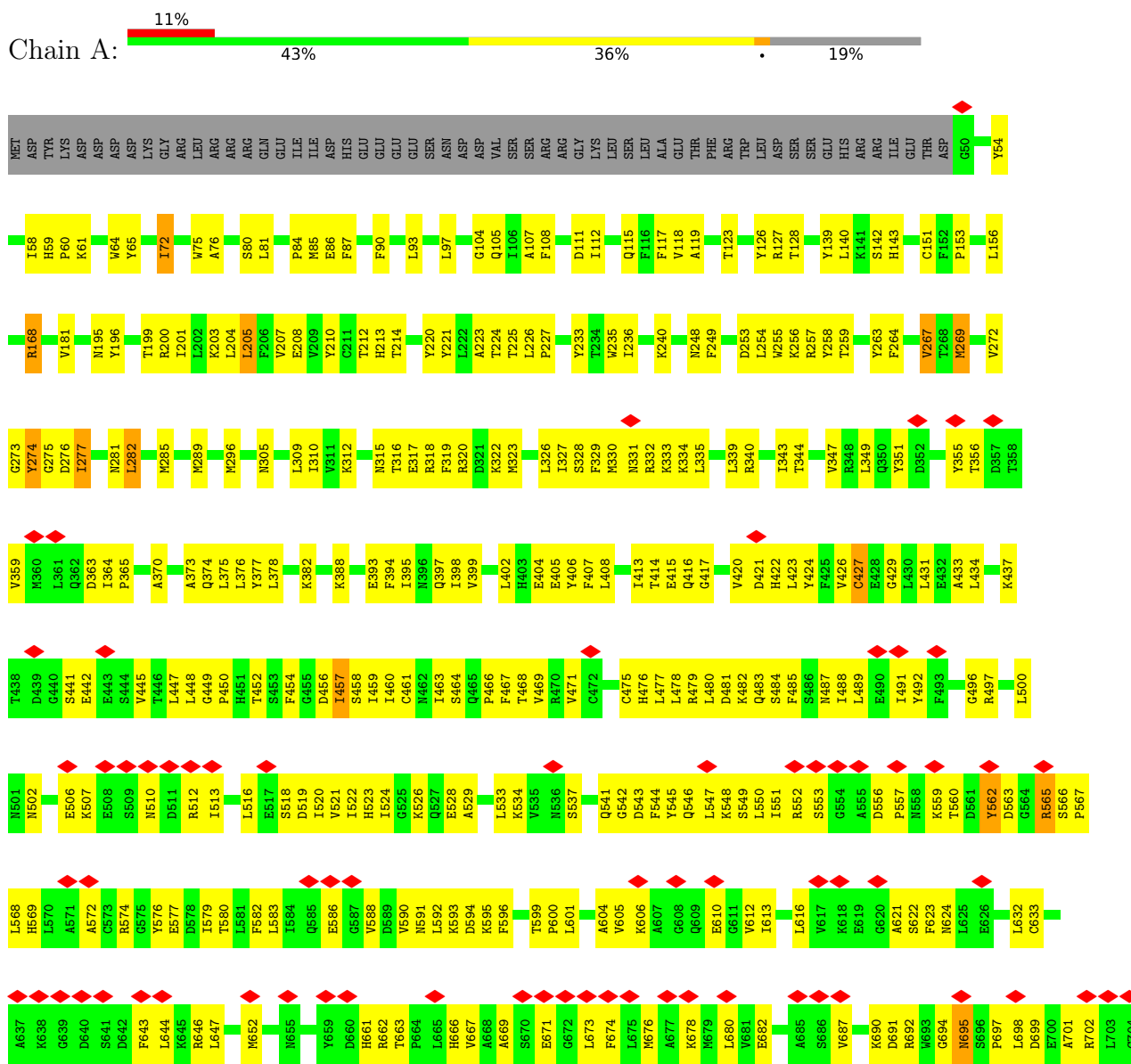
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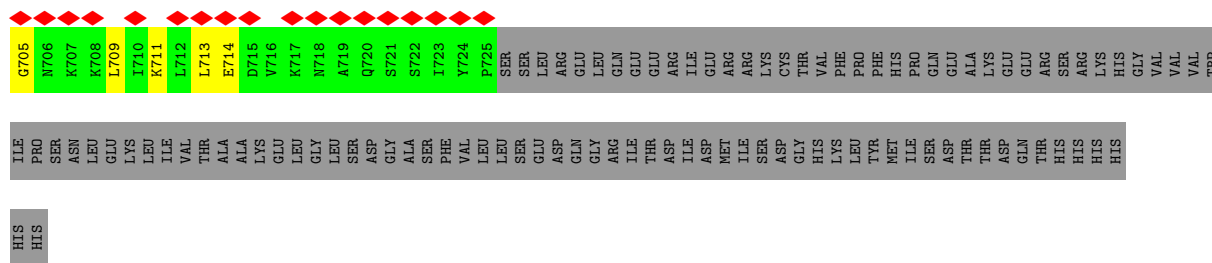
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ASP	-	expression tag	UNP Q94A76
B	1	LYS	-	expression tag	UNP Q94A76
B	821	HIS	-	expression tag	UNP Q94A76
B	822	HIS	-	expression tag	UNP Q94A76
B	823	HIS	-	expression tag	UNP Q94A76
B	824	HIS	-	expression tag	UNP Q94A76
B	825	HIS	-	expression tag	UNP 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

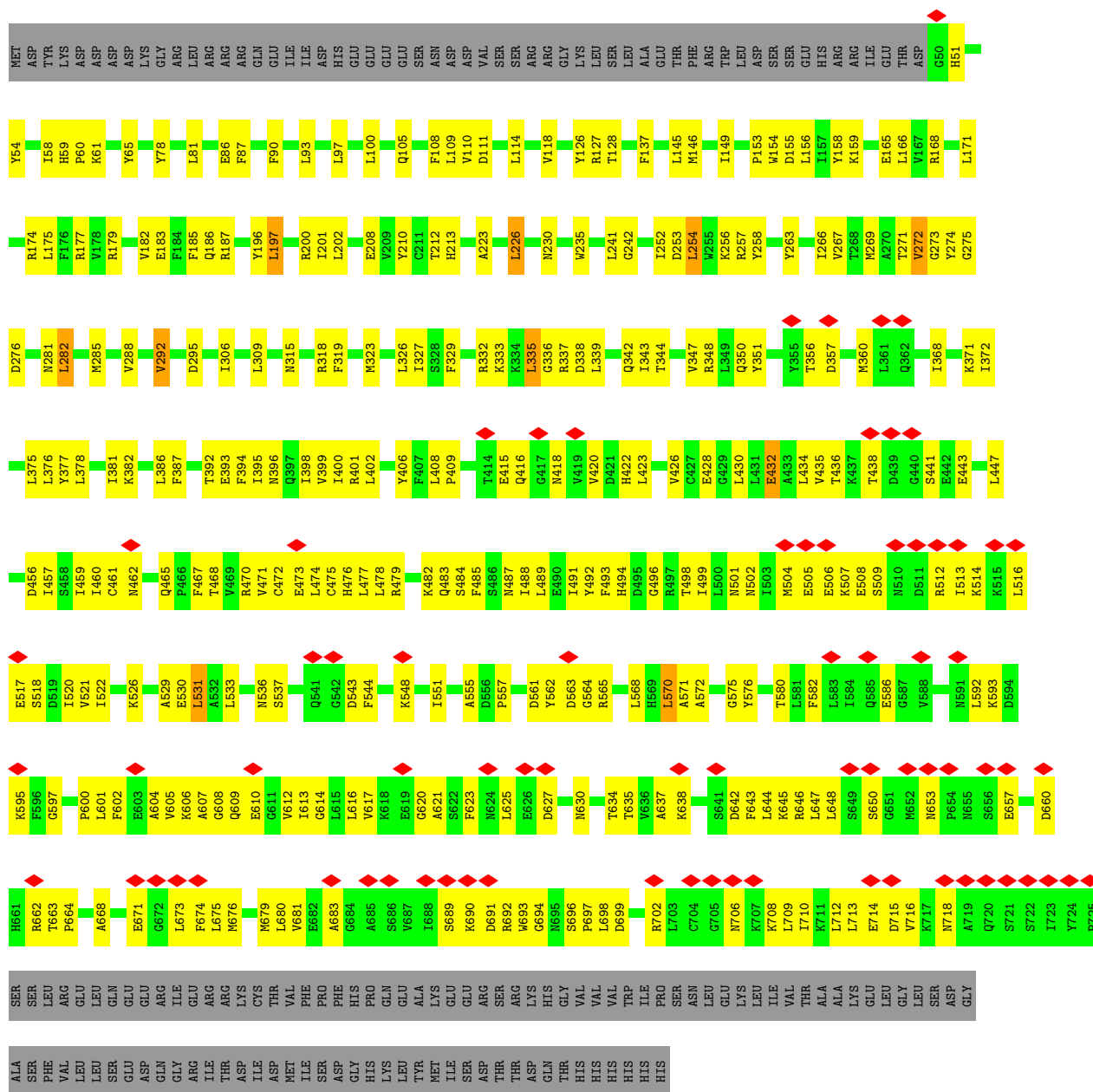
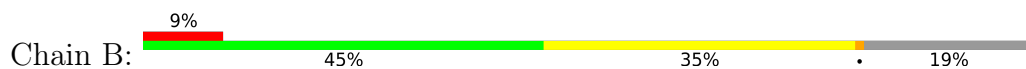
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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





Molecule 1: Potassium channel GORK



Molecule 1: Potassium channel GORK



SER	GLU	D691	S622	I551	Q483	E415	K334	L286	A136
ASP	ARG	R692	F623	R552	S484	Q416	L335	L239	F137
THR	SER	W693	F624	S553	F485	G417	G336	K240	R138
THR	ARG	G694	N624	S554	I488	M418	R337	L241	Y139
GLN	LYS	N695	E626	G554	D495	V419	D338	Y244	L140
THR	GLY	S696	D627	A555	G496	V420	L339	Y245	K141
HIS	VAL	P697	S628	D556	R497	D421	R340	S246	L145
HIS	VAL	D698	G629	P557	T498	H422	L343	Y249	M146
HIS	VAL	D699	N630	M558	I499	L423	T344	F249	D147
HIS	TRP	R702	F631	K559	T498	V426	G345	Y253	F148
HIS	ILE	L703	L632	T560	L500	C427	H346	L254	I149
HIS	PRO	C704	C833	D561	N501	L430	V347	D253	G150
SER	SER	G705	T634	Y562	N502	L431	R348	L255	W154
ASN	ASN	N706	T635	D563	I503	L434	L349	K256	D155
LEU	LEU	K707	V636	G564	M504	L435	Q350	R257	
GLU	GLU	K708	A637	R565	E506	L436	Y351	Y263	K159
LEU	LEU	I710	G639	P567	E507	T436	D352		
ILE	ILE	L713	F643	L568	E508	K437	S353		
VAL	THR	E714	L644	H569	S509	T438	H354	R168	
ALA	ALA			L570	N510	D439	Y355	L171	
LYS	LYS	K717	L647	A571	D511	G440	T358	W172	
GLU	GLU	N718	L648	C573	R512	S441	L361	I173	
LEU	LEU	A719	S649	R574	I513	E442	Q362	R174	
GLY	GLY	Q720	S650	E577	K514	E443	D363	R177	
LEU	LEU	S721	G651	D578	K515	S444	I364	V178	
SER	SER	S722	M652	I579	L516	V445	L364	R179	
ASP	ASP	I723	N653	T580	E517	L448	K371	E189	
GLY	GLY	Y724	P654	L581	S518	G449	L372	T192	
ALA	ALA	P725	N655	F582	D519	P450	A373	L277	
SER	PHE		S656		I520	F454	L376	H278	
VAL	VAL		E657		V521	G455	V280	A279	
LEU	LEU		H661	Q585	I522	D456	L281	N281	
LEU	LEU		R662	E586	H523	I457	L282	Y196	
ARG	ARG		T663	G587	I524	S458	R283	L197	
SER	SER		P664	V588	I524	F467	E284	F198	
GLU	GLU		L665	D589	G525	T468	M285	T199	
GLN	GLN		H666	V590	K526	R470			
GLY	GLY			N591	C461	V469	K382	H213	
ARG	ARG		A669	L592	I463	V471	K383	T214	
ILE	ILE			K593	S464		M289	F219	
THR	THR		L673	D594	Q465		I310	Y220	
ASP	ASP		F674	K595	Q466		F319	Y221	
ILE	ILE		L675		F467			L222	
ASP	ASP		M676	P600	T468		K322	A223	
MET	MET		A677	L601	V469		M323	T224	
ILE	ILE		K678	F602	R470		K324	T225	
SER	SER		M679				L402	L226	
ASP	ASP		L680	V605	N536		Y406	P227	
GLY	GLY		V681		S537		F407	D325	
PRO	PRO		E682	V612	A538		L327	L326	
HIS	HIS			I613			F407	L327	
LYS	LYS		A685	G614	L477		L408	P228	
LEU	LEU		S686	L615	L478		P409	S328	
TYR	TYR		V687	L616	R479		F329	N230	
MET	MET		I688	K618	L480		M330	E231	
ILE	ILE		S689	E619	D481		N331	G332	
			K690	G620	K482		R332	Y233	
				A621			K333	T234	
								W235	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24520	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	0.637	Depositor
Minimum map value	-0.341	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	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	0.34	0/5615	0.52	0/7596
1	B	0.29	0/5615	0.47	0/7596
1	C	0.36	0/5615	0.57	0/7596
1	D	0.45	0/5611	0.63	0/7591
All	All	0.36	0/22456	0.55	0/30379

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	267	0
1	B	5486	0	5502	249	0
1	C	5486	0	5502	243	0
1	D	5482	0	5499	268	0
All	All	21940	0	22005	948	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 22.

All (948) 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:491:ILE:HG23	1:D:483:GLN:HG2	1.48	0.92
1:D:361:LEU:HA	1:D:364:ILE:HD12	1.51	0.92
1:A:335:LEU:HD12	1:A:339:LEU:HD22	1.53	0.91
1:A:610:GLU:HA	1:A:613:ILE:HB	1.57	0.87
1:B:462:ASN:HB2	1:B:518:SER:HB3	1.57	0.85
1:B:402:LEU:HD13	1:B:478:LEU:HD13	1.60	0.83
1:B:460:ILE:HA	1:B:520:ILE:HD11	1.60	0.83
1:B:108:PHE:O	1:B:111:ASP:HB3	1.78	0.82
1:D:687:VAL:HB	1:D:717:LYS:HB2	1.63	0.79
1:A:330:MET:HE3	1:A:340:ARG:HD2	1.65	0.78
1:A:427:CYS:HG	1:A:476:HIS:HD1	1.29	0.78
1:D:674:PHE:HA	1:D:709:LEU:HD21	1.67	0.77
1:A:485:PHE:HA	1:A:488:ILE:HD12	1.65	0.77
1:B:59:HIS:HD2	1:B:61:LYS:HB3	1.48	0.77
1:C:605:VAL:HG23	1:C:646:ARG:HB3	1.65	0.77
1:B:197:LEU:H	1:B:197:LEU:HD23	1.50	0.76
1:D:556:ASP:HB3	1:D:559:LYS:HB2	1.67	0.76
1:A:289:MET:HA	1:D:266:ILE:HG21	1.68	0.76
1:B:537:SER:HB3	1:C:533:LEU:HD11	1.68	0.75
1:B:402:LEU:HB3	1:B:478:LEU:HD22	1.68	0.75
1:D:409:PRO:HA	1:D:471:VAL:HG12	1.69	0.74
1:C:575:GLY:HA2	1:C:612:VAL:HG21	1.69	0.74
1:D:690:LYS:HE2	1:D:696:SER:HB3	1.69	0.74
1:D:90:PHE:O	1:D:168:ARG:NH2	2.20	0.74
1:B:434:LEU:HD12	1:B:470:ARG:HE	1.52	0.73
1:B:580:THR:HG21	1:B:612:VAL:HG22	1.69	0.73
1:C:434:LEU:HB3	1:C:442:GLU:HB3	1.70	0.73
1:D:120:TYR:HD1	1:D:135:ILE:HG22	1.53	0.73
1:B:637:ALA:HB2	1:C:659:TYR:HB3	1.71	0.73
1:B:491:ILE:HG12	1:C:483:GLN:HE21	1.54	0.73
1:B:274:TYR:O	1:D:275:GLY:HA3	1.88	0.73
1:D:60:PRO:HD3	1:D:119:ALA:HB3	1.70	0.72
1:D:688:ILE:HG22	1:D:717:LYS:HE3	1.70	0.72
1:D:138:ARG:HA	1:D:141:LYS:HE3	1.70	0.72
1:D:687:VAL:HG11	1:D:713:LEU:HB3	1.70	0.72
1:B:376:LEU:HD11	1:C:335:LEU:HD11	1.70	0.72
1:B:401:ARG:HD2	1:B:488:ILE:HD11	1.70	0.72
1:C:659:TYR:O	1:C:692:ARG:NH2	2.23	0.72
1:A:424:TYR:HB3	1:A:477:LEU:HD23	1.70	0.71
1:B:197:LEU:HD12	1:B:309:LEU:HA	1.72	0.71
1:B:571:ALA:HB1	1:B:580:THR:HG22	1.73	0.71
1:A:524:ILE:O	1:A:528:GLU:HG3	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ILE:HA	1:A:523:HIS:HD2	1.56	0.71
1:B:87:PHE:HA	1:B:168:ARG:HH12	1.56	0.70
1:B:273:GLY:HA3	1:C:272:VAL:O	1.91	0.70
1:A:272:VAL:O	1:C:273:GLY:HA3	1.92	0.70
1:D:326:LEU:HB3	1:D:330:MET:HE3	1.73	0.70
1:B:395:ILE:O	1:B:399:VAL:HG23	1.92	0.70
1:C:551:ILE:HB	1:C:552:ARG:HH21	1.57	0.70
1:D:569:HIS:NE2	1:D:592:LEU:O	2.22	0.69
1:A:431:LEU:HD23	1:A:471:VAL:HA	1.73	0.69
1:D:507:LYS:HG3	1:D:514:LYS:HA	1.74	0.69
1:D:93:LEU:HD22	1:D:97:LEU:HD12	1.74	0.69
1:C:551:ILE:HG12	1:C:555:ALA:HB3	1.74	0.69
1:A:112:ILE:HG23	1:A:139:TYR:HE2	1.58	0.69
1:B:256:LYS:HA	1:D:282:LEU:HD21	1.75	0.69
1:A:484:SER:O	1:A:488:ILE:HG13	1.93	0.68
1:B:271:THR:HA	1:C:272:VAL:HG13	1.74	0.68
1:C:58:ILE:HB	1:C:118:VAL:HG22	1.74	0.68
1:D:402:LEU:HD13	1:D:478:LEU:HD23	1.75	0.68
1:B:267:VAL:HG13	1:B:272:VAL:HG22	1.76	0.68
1:B:430:LEU:HD11	1:B:447:LEU:HB3	1.74	0.68
1:B:179:ARG:O	1:B:183:GLU:HG2	1.94	0.68
1:A:520:ILE:O	1:A:524:ILE:HG13	1.94	0.67
1:A:423:LEU:HB2	1:A:459:ILE:HD12	1.75	0.67
1:C:548:LYS:HA	1:C:552:ARG:HH22	1.59	0.67
1:A:376:LEU:HD21	1:D:333:LYS:HB3	1.75	0.67
1:B:692:ARG:HH12	1:C:662:ARG:HH12	1.43	0.67
1:D:507:LYS:HD2	1:D:517:GLU:HA	1.76	0.67
1:A:643:PHE:HA	1:A:646:ARG:HE	1.59	0.67
1:A:497:ARG:NH2	1:A:528:GLU:OE2	2.27	0.66
1:B:145:LEU:O	1:B:149:ILE:HG13	1.95	0.66
1:C:124:GLN:CD	1:C:124:GLN:H	2.03	0.66
1:C:660:ASP:HA	1:C:692:ARG:HH21	1.59	0.66
1:A:213:HIS:ND1	1:A:258:TYR:OH	2.28	0.66
1:A:323:MET:HE1	1:A:344:THR:HG22	1.78	0.66
1:C:610:GLU:N	1:C:610:GLU:OE1	2.29	0.66
1:D:431:LEU:HD23	1:D:471:VAL:HA	1.78	0.66
1:B:241:LEU:HD21	1:B:276:ASP:HB2	1.78	0.65
1:A:377:TYR:HB2	1:A:399:VAL:HG13	1.78	0.65
1:B:105:GLN:OE1	1:B:177:ARG:NH2	2.25	0.65
1:C:411:GLU:N	1:C:411:GLU:OE1	2.30	0.65
1:C:465:GLN:NE2	1:C:467:PHE:O	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:PHE:HB2	1:C:475:CYS:SG	2.37	0.65
1:C:695:ASN:HD21	1:C:703:LEU:HD11	1.60	0.65
1:B:59:HIS:CD2	1:B:61:LYS:HB3	2.32	0.65
1:B:78:TYR:OH	1:B:100:LEU:HD21	1.97	0.65
1:B:396:ASN:O	1:B:400:ILE:HG13	1.97	0.65
1:B:533:LEU:HD21	1:C:537:SER:HB2	1.77	0.65
1:C:623:PHE:HB3	1:C:625:LEU:HG	1.79	0.65
1:A:599:THR:HG21	1:A:624:ASN:HD22	1.61	0.64
1:A:691:ASP:OD2	1:A:695:ASN:ND2	2.30	0.64
1:B:155:ASP:O	1:B:159:LYS:HG2	1.97	0.64
1:A:395:ILE:O	1:A:399:VAL:HG23	1.97	0.64
1:B:690:LYS:HB3	1:B:694:GLY:HA2	1.80	0.64
1:A:273:GLY:HA3	1:D:272:VAL:O	1.97	0.64
1:D:561:ASP:OD1	1:D:565:ARG:N	2.31	0.64
1:D:699:ASP:HA	1:D:702:ARG:HD2	1.79	0.64
1:A:378:LEU:HD11	1:A:382:LYS:HE3	1.79	0.64
1:B:501:ASN:O	1:B:505:GLU:HB2	1.98	0.64
1:D:634:THR:HG22	1:D:638:LYS:HE3	1.79	0.64
1:B:485:PHE:O	1:B:489:LEU:HD23	1.97	0.64
1:C:560:THR:HA	1:C:566:SER:HA	1.79	0.63
1:C:610:GLU:HA	1:C:613:ILE:HD12	1.80	0.63
1:B:406:TYR:CE1	1:B:476:HIS:HB2	2.33	0.63
1:D:698:LEU:HD22	1:D:717:LYS:HD3	1.80	0.63
1:C:557:PRO:HG3	1:C:588:VAL:HG22	1.81	0.63
1:B:572:ALA:HA	1:B:612:VAL:HG11	1.79	0.63
1:A:393:GLU:O	1:A:397:GLN:HG3	1.98	0.63
1:B:426:VAL:HG22	1:B:477:LEU:HD23	1.81	0.63
1:B:657:GLU:HA	1:B:663:THR:HA	1.81	0.63
1:B:196:TYR:HB2	1:C:320:ARG:HE	1.64	0.63
1:B:673:LEU:HD13	1:B:676:MET:HE2	1.81	0.63
1:C:548:LYS:HA	1:C:552:ARG:NH2	2.14	0.63
1:D:519:ASP:O	1:D:523:HIS:ND1	2.32	0.62
1:A:500:LEU:HD11	1:A:521:VAL:HG13	1.80	0.62
1:D:636:VAL:HG12	1:D:673:LEU:HD12	1.81	0.62
1:C:398:ILE:HG23	1:C:480:LEU:HD22	1.81	0.62
1:B:368:ILE:HA	1:B:371:LYS:HZ2	1.63	0.62
1:B:459:ILE:HG23	1:B:482:LYS:HG3	1.81	0.62
1:C:334:LYS:HE3	1:C:334:LYS:HA	1.80	0.62
1:C:712:LEU:O	1:C:716:VAL:HG23	1.99	0.62
1:A:84:PRO:HG2	1:A:214:THR:HG22	1.80	0.62
1:D:145:LEU:O	1:D:149:ILE:HG13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:ALA:HA	1:A:612:VAL:HG21	1.82	0.62
1:B:630:ASN:O	1:B:634:THR:HG23	2.00	0.62
1:C:315:ASN:HA	1:C:318:ARG:HG3	1.81	0.62
1:A:90:PHE:HZ	1:A:254:LEU:HD22	1.64	0.62
1:A:556:ASP:HB3	1:A:559:LYS:HG2	1.81	0.62
1:D:115:GLN:HB2	1:D:139:TYR:CE2	2.35	0.62
1:B:664:PRO:HB2	1:B:680:LEU:HD11	1.81	0.62
1:C:185:PHE:HB3	1:C:203:LYS:HE2	1.81	0.62
1:A:60:PRO:HD3	1:A:119:ALA:HB3	1.81	0.61
1:B:344:THR:O	1:B:348:ARG:HG2	1.99	0.61
1:C:658:ASP:OD1	1:C:662:ARG:N	2.21	0.61
1:A:373:ALA:HB1	1:A:399:VAL:HG12	1.82	0.61
1:B:275:GLY:HA3	1:C:274:TYR:O	2.01	0.61
1:D:196:TYR:HD1	1:D:197:LEU:HD22	1.66	0.61
1:D:350:GLN:HG2	1:D:355:TYR:HE1	1.65	0.61
1:D:572:ALA:HB1	1:D:616:LEU:HD11	1.82	0.61
1:A:420:VAL:HG13	1:A:459:ILE:HG13	1.82	0.61
1:A:669:ALA:HA	1:A:709:LEU:HD21	1.82	0.61
1:D:423:LEU:HD12	1:D:459:ILE:HD12	1.83	0.61
1:C:676:MET:HE2	1:C:676:MET:HA	1.83	0.61
1:B:657:GLU:HG2	1:B:663:THR:HG22	1.83	0.61
1:D:460:ILE:HD12	1:D:503:ILE:HD11	1.82	0.61
1:B:327:ILE:HG21	1:D:192:THR:HG21	1.83	0.60
1:D:687:VAL:HG13	1:D:697:PRO:HB2	1.82	0.60
1:A:562:TYR:HD2	1:D:537:SER:HA	1.67	0.60
1:A:394:PHE:O	1:A:398:ILE:HG22	2.01	0.60
1:B:252:ILE:O	1:B:257:ARG:NH1	2.34	0.60
1:B:456:ASP:OD1	1:B:457:ILE:N	2.34	0.60
1:D:319:PHE:HA	1:D:322:LYS:CE	2.31	0.60
1:B:282:LEU:HD21	1:C:256:LYS:HA	1.84	0.60
1:A:319:PHE:HB2	1:A:351:TYR:CD2	2.36	0.59
1:D:495:ASP:O	1:D:499:ILE:HG13	2.02	0.59
1:C:492:TYR:HB3	1:C:495:ASP:HB2	1.82	0.59
1:C:605:VAL:O	1:C:646:ARG:NH1	2.35	0.59
1:A:427:CYS:SG	1:A:476:HIS:ND1	2.67	0.59
1:A:80:SER:HB2	1:A:210:TYR:OH	2.01	0.59
1:A:457:ILE:HG21	1:A:512:ARG:NH2	2.17	0.59
1:C:385:PRO:HA	1:C:388:LYS:HG2	1.84	0.59
1:B:572:ALA:HB1	1:B:604:ALA:HB2	1.82	0.59
1:C:299:GLY:O	1:C:303:ILE:HD12	2.02	0.59
1:D:565:ARG:HA	1:D:569:HIS:ND1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:LYS:HG3	1:A:512:ARG:HB3	1.84	0.59
1:D:337:ARG:HA	1:D:340:ARG:HD2	1.82	0.59
1:A:563:ASP:HA	1:A:595:LYS:HE3	1.84	0.59
1:A:59:HIS:HE1	1:A:61:LYS:HD3	1.66	0.59
1:A:256:LYS:HA	1:C:282:LEU:HD11	1.85	0.59
1:C:691:ASP:OD1	1:C:692:ARG:N	2.36	0.59
1:A:565:ARG:HD3	1:A:569:HIS:CG	2.38	0.59
1:B:698:LEU:HD13	1:B:713:LEU:HB2	1.84	0.59
1:A:331:ASN:OD1	1:A:340:ARG:NH1	2.36	0.58
1:A:355:TYR:HA	1:D:332:ARG:HH22	1.68	0.58
1:B:377:TYR:HB2	1:B:399:VAL:HG13	1.84	0.58
1:B:601:LEU:HD21	1:B:650:SER:HB3	1.85	0.58
1:C:520:ILE:O	1:C:523:HIS:ND1	2.36	0.58
1:D:569:HIS:HD2	1:D:600:PRO:HG3	1.68	0.58
1:A:394:PHE:HA	1:A:397:GLN:NE2	2.17	0.58
1:A:547:LEU:O	1:A:551:ILE:HG12	2.02	0.58
1:D:339:LEU:O	1:D:343:ILE:HG13	2.03	0.58
1:A:377:TYR:HB2	1:A:399:VAL:CG1	2.32	0.58
1:A:463:ILE:HG21	1:A:513:ILE:HG13	1.83	0.58
1:A:376:LEU:HD11	1:D:333:LYS:HG3	1.86	0.58
1:C:319:PHE:HA	1:C:322:LYS:HE3	1.85	0.58
1:A:388:LYS:HB3	1:A:502:ASN:HD21	1.67	0.58
1:C:59:HIS:HD2	1:C:60:PRO:HD2	1.69	0.58
1:C:577:GLU:OE1	1:C:577:GLU:N	2.25	0.58
1:D:569:HIS:CD2	1:D:600:PRO:HG3	2.38	0.58
1:D:632:LEU:HD23	1:D:647:LEU:HD12	1.85	0.58
1:D:644:LEU:O	1:D:648:LEU:HG	2.04	0.58
1:D:236:ILE:HG12	1:D:249:PHE:HB3	1.86	0.58
1:D:323:MET:HE1	1:D:344:THR:HG22	1.85	0.58
1:A:126:TYR:OH	1:D:352:ASP:OD2	2.21	0.58
1:B:415:GLU:N	1:B:415:GLU:OE2	2.37	0.58
1:C:500:LEU:HD22	1:C:520:ILE:HB	1.86	0.58
1:A:65:TYR:CE2	1:A:118:VAL:HG21	2.39	0.58
1:B:185:PHE:HE1	1:B:202:LEU:HG	1.69	0.58
1:C:609:GLN:O	1:C:613:ILE:HG13	2.04	0.58
1:A:422:HIS:CD2	1:A:479:ARG:HD2	2.38	0.57
1:C:197:LEU:O	1:C:201:ILE:HG13	2.04	0.57
1:C:456:ASP:O	1:C:460:ILE:HG22	2.04	0.57
1:A:569:HIS:CE1	1:A:600:PRO:HG3	2.39	0.57
1:B:319:PHE:HE1	1:B:323:MET:HE2	1.69	0.57
1:B:498:THR:O	1:B:502:ASN:ND2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:ILE:HG13	1:D:107:ALA:N	2.18	0.57
1:C:356:THR:O	1:C:359:VAL:HG12	2.04	0.57
1:B:517:GLU:H	1:B:521:VAL:HB	1.69	0.57
1:B:642:ASP:HA	1:B:645:LYS:HE2	1.87	0.57
1:D:632:LEU:O	1:D:636:VAL:HG23	2.04	0.57
1:A:522:ILE:H	1:A:522:ILE:HD12	1.69	0.57
1:D:231:GLU:HA	1:D:234:THR:HG23	1.87	0.57
1:C:445:VAL:O	1:C:512:ARG:NH2	2.38	0.57
1:C:226:LEU:O	1:C:250:ARG:NH2	2.34	0.57
1:C:507:LYS:HG2	1:C:514:LYS:HD2	1.86	0.57
1:D:414:THR:OG1	1:D:465:GLN:NE2	2.35	0.57
1:A:437:LYS:HD2	1:A:441:SER:HB3	1.86	0.57
1:B:81:LEU:O	1:B:213:HIS:NE2	2.38	0.57
1:B:536:ASN:ND2	1:B:561:ASP:HB3	2.20	0.57
1:C:698:LEU:HD13	1:C:713:LEU:HB2	1.85	0.57
1:D:219:PHE:HA	1:D:222:LEU:HD12	1.87	0.57
1:A:111:ASP:O	1:A:115:GLN:HG2	2.05	0.56
1:C:674:PHE:HA	1:C:709:LEU:HD13	1.87	0.56
1:D:625:LEU:HB2	1:D:628:SER:HB3	1.87	0.56
1:A:203:LYS:O	1:A:207:VAL:HG23	2.04	0.56
1:A:590:VAL:HB	1:A:621:ALA:HB2	1.85	0.56
1:C:325:ASP:OD2	1:C:326:LEU:N	2.38	0.56
1:B:487:ASN:O	1:B:491:ILE:HG13	2.05	0.56
1:C:644:LEU:HD13	1:C:676:MET:SD	2.46	0.56
1:D:106:ILE:O	1:D:110:VAL:HG23	2.06	0.56
1:A:370:ALA:O	1:A:374:GLN:HG3	2.06	0.56
1:C:437:LYS:HE2	1:C:443:GLU:HG3	1.86	0.56
1:C:658:ASP:OD1	1:C:661:HIS:N	2.39	0.56
1:D:427:CYS:HB2	1:D:476:HIS:O	2.06	0.56
1:D:675:LEU:O	1:D:679:MET:HG3	2.06	0.56
1:A:481:ASP:HB3	1:A:484:SER:OG	2.06	0.56
1:D:435:VAL:HG13	1:D:443:GLU:HB3	1.88	0.56
1:B:59:HIS:HE1	1:B:128:THR:HG21	1.70	0.56
1:A:421:ASP:HA	1:A:482:LYS:HE3	1.88	0.55
1:A:520:ILE:HA	1:A:523:HIS:CD2	2.37	0.55
1:D:417:GLY:H	1:D:465:GLN:HB3	1.71	0.55
1:D:532:ALA:HB2	1:D:559:LYS:HD3	1.88	0.55
1:B:526:LYS:O	1:B:530:GLU:HG2	2.05	0.55
1:C:551:ILE:HB	1:C:552:ARG:NH2	2.22	0.55
1:D:379:PRO:C	1:D:383:LYS:HZ1	2.14	0.55
1:A:81:LEU:O	1:A:213:HIS:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:LEU:HD11	1:B:616:LEU:HD21	1.87	0.55
1:B:662:ARG:HG3	1:B:691:ASP:HB2	1.86	0.55
1:B:676:MET:HA	1:B:679:MET:CE	2.36	0.55
1:B:692:ARG:NH1	1:C:662:ARG:HH12	2.04	0.55
1:C:203:LYS:O	1:C:207:VAL:HG12	2.06	0.55
1:C:641:SER:O	1:C:645:LYS:HG3	2.06	0.55
1:D:457:ILE:H	1:D:457:ILE:HD12	1.70	0.55
1:A:568:LEU:HD13	1:A:588:VAL:HB	1.88	0.55
1:D:374:GLN:NE2	1:D:396:ASN:OD1	2.40	0.55
1:D:407:PHE:HB2	1:D:475:CYS:SG	2.46	0.55
1:D:434:LEU:H	1:D:434:LEU:HD23	1.70	0.55
1:D:497:ARG:HG2	1:D:527:GLN:OE1	2.05	0.55
1:D:698:LEU:HD21	1:D:714:GLU:HG2	1.88	0.55
1:C:457:ILE:O	1:C:461:CYS:HB2	2.05	0.55
1:D:344:THR:O	1:D:348:ARG:HG3	2.06	0.55
1:D:630:ASN:OD1	1:D:630:ASN:N	2.38	0.55
1:A:449:GLY:O	1:A:452:THR:HG22	2.06	0.55
1:D:654:PRO:HB2	1:D:685:ALA:HB2	1.86	0.55
1:A:305:ASN:OD1	1:D:310:ILE:HD13	2.07	0.55
1:A:316:THR:O	1:A:320:ARG:HG2	2.07	0.55
1:A:378:LEU:HD12	1:A:382:LYS:HG3	1.88	0.55
1:A:413:ILE:HG22	1:A:414:THR:HG23	1.88	0.55
1:A:663:THR:H	1:A:666:HIS:HB2	1.71	0.55
1:D:435:VAL:HB	1:D:467:PHE:HB3	1.87	0.55
1:D:563:ASP:HA	1:D:595:LYS:HD2	1.88	0.55
1:B:372:ILE:O	1:B:376:LEU:HD13	2.07	0.55
1:B:576:TYR:O	1:B:580:THR:HG23	2.07	0.55
1:B:699:ASP:HA	1:B:702:ARG:HD2	1.89	0.55
1:C:59:HIS:HB3	1:C:62:ASN:HB2	1.89	0.55
1:C:346:HIS:HE2	1:C:411:GLU:HG2	1.72	0.55
1:D:484:SER:O	1:D:488:ILE:HG13	2.07	0.55
1:D:510:ASN:HB3	1:D:513:ILE:HG12	1.88	0.54
1:A:466:PRO:HG2	1:A:467:PHE:CD2	2.42	0.54
1:A:255:TRP:O	1:A:259:THR:OG1	2.21	0.54
1:A:633:CYS:HB3	1:A:667:VAL:HG21	1.88	0.54
1:A:662:ARG:HG2	1:A:691:ASP:HB3	1.89	0.54
1:A:507:LYS:HE3	1:A:507:LYS:HA	1.88	0.54
1:B:398:ILE:O	1:B:402:LEU:HG	2.08	0.54
1:C:707:LYS:O	1:C:711:LYS:HG3	2.07	0.54
1:D:690:LYS:HB3	1:D:694:GLY:HA2	1.90	0.54
1:A:460:ILE:HG23	1:A:520:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:LYS:HD3	1:A:512:ARG:NH2	2.22	0.54
1:B:333:LYS:HB3	1:D:376:LEU:HD21	1.88	0.54
1:B:323:MET:O	1:B:327:ILE:HG12	2.07	0.54
1:D:189:GLU:HA	1:D:199:THR:HG21	1.89	0.54
1:B:602:PHE:CD2	1:B:625:LEU:HD21	2.43	0.54
1:C:602:PHE:HA	1:C:605:VAL:HG12	1.89	0.54
1:D:401:ARG:HD2	1:D:488:ILE:HD11	1.88	0.54
1:B:509:SER:HA	1:B:513:ILE:HD13	1.90	0.54
1:D:150:GLY:O	1:D:177:ARG:NH2	2.41	0.54
1:A:516:LEU:HD22	1:A:521:VAL:HG11	1.90	0.54
1:B:604:ALA:O	1:B:608:GLY:N	2.40	0.54
1:A:272:VAL:HG13	1:C:271:THR:HA	1.90	0.54
1:A:365:PRO:HD3	1:D:346:HIS:CE1	2.43	0.54
1:A:632:LEU:HD21	1:A:652:MET:SD	2.48	0.54
1:D:233:TYR:HD1	1:D:280:VAL:HG12	1.73	0.54
1:D:349:LEU:HD22	1:D:408:LEU:HD23	1.89	0.54
1:C:692:ARG:HG3	1:C:693:TRP:CE3	2.43	0.53
1:C:323:MET:HE1	1:C:344:THR:HG22	1.90	0.53
1:C:497:ARG:NH2	1:C:526:LYS:O	2.41	0.53
1:C:540:PHE:CE2	1:C:574:ARG:HD3	2.44	0.53
1:D:108:PHE:CE2	1:D:177:ARG:HD3	2.43	0.53
1:D:612:VAL:HA	1:D:615:LEU:HD12	1.90	0.53
1:B:126:TYR:CE1	1:C:474:LEU:HD22	2.44	0.53
1:C:61:LYS:HG2	1:C:66:LYS:HZ3	1.73	0.53
1:C:145:LEU:HD23	1:C:145:LEU:H	1.73	0.53
1:D:520:ILE:O	1:D:524:ILE:HG13	2.08	0.53
1:B:93:LEU:HD22	1:B:97:LEU:HD12	1.90	0.53
1:A:562:TYR:O	1:A:563:ASP:C	2.51	0.53
1:B:565:ARG:NH1	1:B:565:ARG:HB2	2.24	0.53
1:C:195:ASN:OD1	1:C:196:TYR:N	2.41	0.53
1:C:544:PHE:HB2	1:C:548:LYS:HZ3	1.74	0.53
1:D:415:GLU:HG3	1:D:418:ASN:HB2	1.91	0.53
1:A:565:ARG:HB2	1:A:569:HIS:CE1	2.43	0.53
1:B:368:ILE:HA	1:B:371:LYS:NZ	2.23	0.53
1:A:249:PHE:O	1:A:257:ARG:HD3	2.09	0.53
1:B:386:LEU:HD11	1:B:499:ILE:HG23	1.91	0.53
1:C:675:LEU:O	1:C:678:LYS:HG2	2.07	0.53
1:D:420:VAL:HG21	1:D:458:SER:HB3	1.90	0.53
1:B:226:LEU:HD12	1:B:230:ASN:HB2	1.90	0.53
1:B:551:ILE:HD12	1:B:582:PHE:CE2	2.43	0.53
1:B:660:ASP:HA	1:B:692:ARG:NH2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASP:OD2	1:A:254:LEU:N	2.42	0.53
1:A:574:ARG:NE	1:A:574:ARG:HA	2.22	0.53
1:B:343:ILE:HD11	1:D:372:ILE:HD11	1.91	0.53
1:A:485:PHE:O	1:A:489:LEU:HD23	2.09	0.52
1:A:661:HIS:HD2	1:A:692:ARG:HB2	1.73	0.52
1:C:532:ALA:HB2	1:C:559:LYS:HB3	1.91	0.52
1:A:76:ALA:HA	1:A:108:PHE:HZ	1.74	0.52
1:B:461:CYS:HA	1:B:517:GLU:HB3	1.90	0.52
1:B:606:LYS:HA	1:B:643:PHE:CZ	2.44	0.52
1:B:623:PHE:HB3	1:B:625:LEU:HG	1.90	0.52
1:C:420:VAL:HG13	1:C:459:ILE:HD12	1.92	0.52
1:D:406:TYR:HA	1:D:475:CYS:O	2.09	0.52
1:D:593:LYS:NZ	1:D:626:GLU:OE1	2.43	0.52
1:A:698:LEU:HD13	1:A:713:LEU:HB2	1.91	0.52
1:D:228:PRO:HA	1:D:231:GLU:HB3	1.90	0.52
1:B:59:HIS:CG	1:B:60:PRO:HD2	2.45	0.52
1:B:197:LEU:H	1:B:197:LEU:CD2	2.22	0.52
1:B:544:PHE:CE1	1:B:548:LYS:HE3	2.45	0.52
1:C:387:PHE:HE2	1:C:398:ILE:HG21	1.74	0.52
1:A:80:SER:O	1:A:210:TYR:OH	2.26	0.52
1:D:643:PHE:CE1	1:D:647:LEU:HD21	2.44	0.52
1:C:386:LEU:HG	1:C:387:PHE:CE1	2.44	0.52
1:D:675:LEU:HA	1:D:678:LYS:HE3	1.92	0.52
1:A:275:GLY:HA2	1:D:274:TYR:HB3	1.92	0.52
1:A:397:GLN:HG2	1:A:492:TYR:CD1	2.45	0.52
1:B:714:GLU:O	1:B:718:ASN:ND2	2.43	0.52
1:C:182:VAL:O	1:C:186:GLN:HG3	2.09	0.52
1:C:459:ILE:HD11	1:C:482:LYS:HG3	1.91	0.52
1:A:285:MET:O	1:A:289:MET:HG3	2.10	0.52
1:A:264:PHE:HD1	1:A:277:ILE:HB	1.75	0.51
1:A:330:MET:CE	1:A:340:ARG:HD2	2.37	0.51
1:A:572:ALA:HB1	1:A:604:ALA:HB2	1.92	0.51
1:B:483:GLN:NE2	1:B:487:ASN:OD1	2.43	0.51
1:B:536:ASN:HD22	1:B:561:ASP:HB3	1.75	0.51
1:D:222:LEU:HD13	1:D:284:GLU:HA	1.91	0.51
1:A:674:PHE:HA	1:A:709:LEU:HD13	1.92	0.51
1:D:698:LEU:CD2	1:D:717:LYS:HD3	2.40	0.51
1:D:643:PHE:O	1:D:647:LEU:HG	2.11	0.51
1:C:421:ASP:OD1	1:C:421:ASP:N	2.34	0.51
1:A:457:ILE:HG13	1:A:461:CYS:SG	2.50	0.51
1:B:393:GLU:OE2	1:B:393:GLU:N	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ILE:HG12	1:A:117:PHE:O	2.10	0.51
1:A:414:THR:O	1:A:468:THR:HG23	2.11	0.51
1:B:274:TYR:HE2	1:D:288:VAL:HG11	1.76	0.51
1:C:354:HIS:O	1:C:358:THR:HG23	2.11	0.51
1:A:281:ASN:O	1:A:285:MET:HG3	2.11	0.51
1:C:707:LYS:HA	1:C:710:ILE:HD12	1.92	0.51
1:D:426:VAL:HG12	1:D:450:PRO:HA	1.91	0.51
1:A:335:LEU:HD11	1:C:372:ILE:HG23	1.93	0.51
1:B:420:VAL:HG23	1:B:465:GLN:HB2	1.92	0.51
1:D:267:VAL:HA	1:D:272:VAL:HG13	1.93	0.51
1:D:87:PHE:O	1:D:168:ARG:NH2	2.30	0.50
1:D:101:ASP:O	1:D:105:GLN:HG2	2.11	0.50
1:A:545:TYR:CE2	1:D:522:ILE:HD13	2.47	0.50
1:A:711:LYS:HE3	1:A:711:LYS:HA	1.92	0.50
1:B:498:THR:HG22	1:B:502:ASN:HD21	1.75	0.50
1:B:570:LEU:HD21	1:C:562:TYR:CD1	2.45	0.50
1:D:350:GLN:HG2	1:D:355:TYR:CE1	2.45	0.50
1:D:698:LEU:HD11	1:D:714:GLU:HG3	1.93	0.50
1:A:434:LEU:HD23	1:A:442:GLU:HB2	1.93	0.50
1:B:642:ASP:OD1	1:B:646:ARG:NE	2.44	0.50
1:C:364:ILE:HG22	1:C:369:ARG:HG3	1.94	0.50
1:D:522:ILE:O	1:D:526:LYS:HG3	2.12	0.50
1:D:570:LEU:O	1:D:573:CYS:HB3	2.12	0.50
1:B:368:ILE:O	1:B:372:ILE:HG13	2.11	0.50
1:B:423:LEU:HB2	1:B:459:ILE:HD12	1.93	0.50
1:A:356:THR:O	1:A:359:VAL:HG12	2.11	0.50
1:B:681:VAL:HG11	1:B:716:VAL:HG21	1.93	0.50
1:C:359:VAL:O	1:C:362:GLN:HG2	2.11	0.50
1:C:634:THR:HG22	1:C:638:LYS:HZ2	1.76	0.50
1:D:168:ARG:O	1:D:171:LEU:HB2	2.11	0.50
1:D:358:THR:O	1:D:361:LEU:HB2	2.12	0.50
1:D:443:GLU:HG3	1:D:444:SER:H	1.77	0.50
1:D:623:PHE:HB2	1:D:652:MET:HE3	1.92	0.50
1:B:660:ASP:OD1	1:C:662:ARG:NH1	2.45	0.50
1:C:602:PHE:HA	1:C:605:VAL:CG1	2.42	0.50
1:B:531:LEU:HD21	1:B:555:ALA:HB1	1.94	0.50
1:A:691:ASP:OD1	1:A:694:GLY:N	2.44	0.50
1:A:90:PHE:CZ	1:A:254:LEU:HD22	2.45	0.49
1:A:565:ARG:H	1:A:565:ARG:HD2	1.77	0.49
1:B:183:GLU:O	1:B:187:ARG:HG3	2.12	0.49
1:B:266:ILE:HG21	1:D:289:MET:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:PHE:HA	1:B:332:ARG:HE	1.77	0.49
1:B:432:GLU:HB3	1:B:472:CYS:SG	2.52	0.49
1:D:378:LEU:O	1:D:382:LYS:HG2	2.12	0.49
1:A:226:LEU:HD22	1:A:227:PRO:HD2	1.94	0.49
1:C:524:ILE:HG13	1:C:525:GLY:N	2.27	0.49
1:A:483:GLN:O	1:A:487:ASN:ND2	2.46	0.49
1:B:434:LEU:HA	1:B:443:GLU:O	2.12	0.49
1:B:592:LEU:O	1:B:600:PRO:HD3	2.12	0.49
1:D:507:LYS:HA	1:D:513:ILE:HG13	1.93	0.49
1:A:562:TYR:O	1:A:562:TYR:HD1	1.94	0.49
1:B:61:LYS:HD2	1:B:61:LYS:O	2.12	0.49
1:C:556:ASP:OD1	1:C:557:PRO:HD2	2.13	0.49
1:C:630:ASN:N	1:C:630:ASN:OD1	2.44	0.49
1:C:698:LEU:HD21	1:C:714:GLU:OE2	2.13	0.49
1:D:233:TYR:CD1	1:D:280:VAL:HG12	2.47	0.49
1:A:220:TYR:O	1:A:224:THR:HG23	2.12	0.49
1:B:635:THR:HA	1:B:638:LYS:HD2	1.93	0.49
1:B:158:TYR:CE1	1:B:168:ARG:HD3	2.47	0.49
1:A:671:GLU:HB3	1:A:673:LEU:HG	1.93	0.49
1:B:689:SER:O	1:B:696:SER:HA	2.13	0.49
1:C:364:ILE:HG23	1:C:368:ILE:HB	1.94	0.49
1:A:330:MET:HB3	1:A:340:ARG:HD3	1.94	0.49
1:A:349:LEU:HD11	1:A:406:TYR:HB2	1.94	0.49
1:C:552:ARG:NH2	1:C:582:PHE:CZ	2.81	0.49
1:B:564:GLY:HA3	1:B:595:LYS:HG3	1.94	0.49
1:C:561:ASP:OD1	1:C:565:ARG:N	2.45	0.49
1:C:605:VAL:HG23	1:C:646:ARG:CB	2.41	0.49
1:D:346:HIS:NE2	1:D:406:TYR:O	2.46	0.49
1:A:507:LYS:HB2	1:A:510:ASN:HA	1.95	0.49
1:B:281:ASN:O	1:B:285:MET:HG3	2.13	0.49
1:D:331:ASN:HA	1:D:340:ARG:HH22	1.77	0.49
1:D:663:THR:O	1:D:666:HIS:HB2	2.13	0.49
1:D:692:ARG:HB3	1:D:693:TRP:CE3	2.47	0.49
1:A:269:MET:SD	1:C:296:MET:HE1	2.52	0.48
1:C:223:ALA:HB2	1:C:235:TRP:NE1	2.28	0.48
1:D:525:GLY:HA2	1:D:528:GLU:HG2	1.95	0.48
1:D:590:VAL:HG22	1:D:619:GLU:HG3	1.95	0.48
1:A:142:SER:O	1:A:143:HIS:HB2	2.12	0.48
1:A:544:PHE:CD1	1:A:579:ILE:HG12	2.48	0.48
1:C:601:LEU:HB2	1:C:621:ALA:HB3	1.95	0.48
1:A:223:ALA:HB2	1:A:235:TRP:NE1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:ILE:O	1:A:526:LYS:HG3	2.13	0.48
1:C:281:ASN:HB3	1:C:283:ARG:HG2	1.94	0.48
1:C:327:ILE:HA	1:C:330:MET:HE3	1.95	0.48
1:C:423:LEU:HD13	1:C:456:ASP:HB2	1.95	0.48
1:D:131:LYS:HB3	1:D:134:ARG:HG2	1.96	0.48
1:D:665:LEU:HD21	1:D:680:LEU:HB2	1.94	0.48
1:B:562:TYR:HB3	1:C:540:PHE:HD1	1.78	0.48
1:C:62:ASN:ND2	1:C:64:TRP:HB2	2.28	0.48
1:D:154:TRP:HB2	1:D:174:ARG:HH22	1.79	0.48
1:D:602:PHE:CD1	1:D:625:LEU:HD11	2.48	0.48
1:B:110:VAL:O	1:B:114:LEU:N	2.34	0.48
1:B:208:GLU:O	1:B:212:THR:HG23	2.12	0.48
1:C:707:LYS:NZ	1:D:702:ARG:O	2.23	0.48
1:D:329:PHE:HA	1:D:332:ARG:HH11	1.79	0.48
1:D:434:LEU:HA	1:D:445:VAL:HG12	1.96	0.48
1:D:456:ASP:O	1:D:457:ILE:C	2.56	0.48
1:B:285:MET:HE3	1:C:259:THR:HG22	1.95	0.48
1:B:409:PRO:HA	1:B:471:VAL:HG12	1.95	0.48
1:C:212:THR:HG22	1:C:291:TYR:OH	2.13	0.48
1:C:548:LYS:HD3	1:C:552:ARG:HH22	1.78	0.48
1:C:712:LEU:HD12	1:C:712:LEU:HA	1.66	0.48
1:D:241:LEU:HB2	1:D:246:TYR:HE1	1.78	0.48
1:B:401:ARG:HD3	1:B:484:SER:HB3	1.96	0.48
1:B:409:PRO:HG3	1:B:473:GLU:C	2.39	0.48
1:C:78:TYR:OH	1:C:100:LEU:HD21	2.13	0.48
1:C:432:GLU:HG3	1:C:470:ARG:HB3	1.95	0.48
1:D:155:ASP:OD1	1:D:159:LYS:NZ	2.47	0.48
1:D:319:PHE:HA	1:D:322:LYS:HE2	1.95	0.48
1:D:536:ASN:HD22	1:D:561:ASP:HB3	1.79	0.48
1:A:201:ILE:HD12	1:A:309:LEU:HD13	1.96	0.48
1:A:320:ARG:NH2	1:C:189:GLU:O	2.47	0.48
1:A:461:CYS:C	1:A:518:SER:HB2	2.38	0.48
1:C:409:PRO:HG3	1:C:473:GLU:C	2.39	0.48
1:D:417:GLY:HA2	1:D:464:SER:HB2	1.96	0.48
1:A:601:LEU:O	1:A:605:VAL:HG23	2.14	0.48
1:B:551:ILE:HD12	1:B:582:PHE:HE2	1.78	0.48
1:C:76:ALA:HA	1:C:108:PHE:HZ	1.77	0.48
1:C:430:LEU:O	1:C:472:CYS:HB2	2.13	0.48
1:C:671:GLU:HA	1:D:708:LYS:NZ	2.29	0.48
1:B:333:LYS:HB2	1:B:335:LEU:HD13	1.96	0.48
1:D:195:ASN:OD1	1:D:196:TYR:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:HIS:ND1	1:B:258:TYR:OH	2.39	0.47
1:C:219:PHE:HE1	1:C:284:GLU:HB3	1.79	0.47
1:C:386:LEU:HG	1:C:387:PHE:CD1	2.49	0.47
1:A:335:LEU:HD12	1:A:339:LEU:CD2	2.36	0.47
1:B:242:GLY:HA3	1:D:280:VAL:HG11	1.96	0.47
1:D:511:ASP:O	1:D:514:LYS:HB3	2.14	0.47
1:B:109:LEU:O	1:B:110:VAL:HB	2.14	0.47
1:A:335:LEU:HD13	1:C:375:LEU:HD22	1.95	0.47
1:A:415:GLU:OE2	1:A:415:GLU:N	2.47	0.47
1:B:59:HIS:CE1	1:B:128:THR:HG21	2.49	0.47
1:A:329:PHE:CE2	1:C:358:THR:HB	2.50	0.47
1:D:398:ILE:O	1:D:402:LEU:HG	2.13	0.47
1:A:199:THR:HG22	1:A:203:LYS:HE2	1.97	0.47
1:B:368:ILE:HD13	1:C:342:GLN:HB3	1.95	0.47
1:B:401:ARG:CD	1:B:488:ILE:HD11	2.43	0.47
1:B:499:ILE:HA	1:B:502:ASN:HD22	1.77	0.47
1:B:504:MET:HA	1:B:508:GLU:HA	1.96	0.47
1:C:72:ILE:HA	1:C:72:ILE:HD12	1.70	0.47
1:C:90:PHE:CE2	1:C:254:LEU:HD13	2.50	0.47
1:A:333:LYS:HD2	1:C:376:LEU:HD21	1.96	0.47
1:A:375:LEU:HD23	1:D:335:LEU:HD22	1.96	0.47
1:A:458:SER:HA	1:A:463:ILE:HG12	1.97	0.47
1:A:481:ASP:O	1:A:484:SER:HB2	2.14	0.47
1:B:489:LEU:HD12	1:B:496:GLY:HA2	1.95	0.47
1:B:601:LEU:HD21	1:B:650:SER:CB	2.45	0.47
1:C:397:GLN:O	1:C:401:ARG:HG2	2.15	0.47
1:D:122:ASP:O	1:D:126:TYR:N	2.47	0.47
1:D:413:ILE:HG22	1:D:414:THR:HG23	1.97	0.47
1:D:657:GLU:HB3	1:D:661:HIS:HA	1.95	0.47
1:A:334:LYS:HD2	1:A:334:LYS:C	2.40	0.47
1:B:165:GLU:CD	1:B:168:ARG:HE	2.23	0.47
1:B:409:PRO:HG3	1:B:474:LEU:N	2.29	0.47
1:C:208:GLU:O	1:C:212:THR:HG23	2.15	0.47
1:D:266:ILE:HD13	1:D:266:ILE:HA	1.75	0.47
1:D:412:VAL:HG12	1:D:470:ARG:HG2	1.96	0.47
1:D:557:PRO:HB2	1:D:588:VAL:HG22	1.97	0.47
1:A:427:CYS:HG	1:A:476:HIS:CG	2.29	0.47
1:A:644:LEU:HD21	1:A:680:LEU:HD21	1.96	0.47
1:D:379:PRO:O	1:D:383:LYS:NZ	2.45	0.47
1:A:488:ILE:HG23	1:A:492:TYR:CD2	2.49	0.47
1:A:678:LYS:O	1:A:682:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ILE:HG21	1:B:256:LYS:HD2	1.97	0.47
1:B:484:SER:O	1:B:488:ILE:HG13	2.15	0.47
1:B:529:ALA:O	1:B:533:LEU:HD13	2.14	0.47
1:A:75:TRP:CH2	1:A:104:GLY:HA2	2.50	0.46
1:B:408:LEU:HD23	1:B:409:PRO:HD2	1.97	0.46
1:D:226:LEU:HG	1:D:230:ASN:HB3	1.97	0.46
1:D:674:PHE:CE1	1:D:678:LYS:HE2	2.49	0.46
1:B:660:ASP:HA	1:B:692:ARG:HH21	1.81	0.46
1:D:112:ILE:HG12	1:D:139:TYR:OH	2.14	0.46
1:D:270:ALA:HB3	1:D:272:VAL:HG12	1.96	0.46
1:D:431:LEU:HD21	1:D:471:VAL:HG22	1.97	0.46
1:D:461:CYS:HB3	1:D:463:ILE:HG12	1.95	0.46
1:D:614:GLY:O	1:D:618:LYS:HG2	2.15	0.46
1:A:574:ARG:HB3	1:A:576:TYR:CZ	2.50	0.46
1:B:393:GLU:H	1:B:393:GLU:CD	2.17	0.46
1:A:59:HIS:CG	1:A:60:PRO:HD2	2.49	0.46
1:A:426:VAL:HG12	1:A:450:PRO:HA	1.96	0.46
1:B:381:ILE:HG13	1:B:402:LEU:HD11	1.96	0.46
1:C:500:LEU:O	1:C:504:MET:HG2	2.15	0.46
1:A:326:LEU:O	1:A:330:MET:HG3	2.16	0.46
1:A:591:ASN:OD1	1:A:622:SER:N	2.23	0.46
1:B:623:PHE:HE2	1:B:650:SER:HB2	1.81	0.46
1:D:59:HIS:CG	1:D:60:PRO:HD2	2.51	0.46
1:A:489:LEU:HD11	1:A:496:GLY:HA3	1.97	0.46
1:B:158:TYR:CZ	1:B:168:ARG:HD3	2.51	0.46
1:B:339:LEU:HA	1:B:342:GLN:HG2	1.98	0.46
1:B:616:LEU:O	1:B:620:GLY:N	2.48	0.46
1:C:456:ASP:O	1:C:459:ILE:HG22	2.16	0.46
1:C:514:LYS:HG2	1:C:515:LYS:O	2.16	0.46
1:C:521:VAL:HA	1:C:524:ILE:HG12	1.97	0.46
1:D:430:LEU:HD12	1:D:431:LEU:N	2.30	0.46
1:C:269:MET:HE2	1:C:269:MET:HB3	1.75	0.46
1:C:384:VAL:HG12	1:C:386:LEU:HB3	1.97	0.46
1:D:63:ARG:HA	1:D:66:LYS:HZ3	1.81	0.46
1:D:549:SER:O	1:D:553:SER:OG	2.27	0.46
1:A:205:LEU:HD12	1:A:205:LEU:HA	1.80	0.46
1:A:533:LEU:HD11	1:D:537:SER:HB2	1.97	0.46
1:A:576:TYR:CD2	1:A:579:ILE:HD12	2.51	0.46
1:B:336:GLY:O	1:B:337:ARG:C	2.59	0.46
1:B:551:ILE:HD13	1:B:557:PRO:HG3	1.96	0.46
1:D:254:LEU:HG	1:D:255:TRP:N	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:ALA:HB1	1:D:284:GLU:HB3	1.96	0.46
1:D:414:THR:O	1:D:468:THR:HA	2.15	0.46
1:A:64:TRP:HA	1:A:64:TRP:CE3	2.51	0.46
1:A:208:GLU:O	1:A:212:THR:HG23	2.16	0.46
1:A:507:LYS:HD3	1:A:512:ARG:HH21	1.81	0.46
1:B:87:PHE:O	1:B:168:ARG:NH2	2.45	0.46
1:B:394:PHE:O	1:B:398:ILE:HG12	2.16	0.46
1:B:428:GLU:HB3	1:B:476:HIS:HB3	1.97	0.46
1:B:575:GLY:HA2	1:B:612:VAL:HG21	1.98	0.46
1:C:188:LEU:HD12	1:C:188:LEU:HA	1.75	0.46
1:C:387:PHE:CE2	1:C:398:ILE:HG21	2.50	0.46
1:A:105:GLN:HB2	1:A:151:CYS:SG	2.56	0.46
1:A:402:LEU:HD22	1:A:478:LEU:HB3	1.97	0.46
1:A:574:ARG:HB3	1:A:576:TYR:CE1	2.51	0.46
1:A:676:MET:O	1:A:680:LEU:HG	2.15	0.46
1:C:185:PHE:O	1:C:189:GLU:HG3	2.16	0.46
1:C:196:TYR:O	1:C:199:THR:OG1	2.27	0.46
1:D:570:LEU:HD12	1:D:570:LEU:H	1.81	0.46
1:A:577:GLU:HA	1:A:580:THR:HB	1.98	0.45
1:B:171:LEU:O	1:B:174:ARG:HB2	2.16	0.45
1:B:601:LEU:HD12	1:B:621:ALA:HB1	1.97	0.45
1:A:519:ASP:HB3	1:A:523:HIS:NE2	2.31	0.45
1:A:695:ASN:HD21	1:D:693:TRP:HE1	1.65	0.45
1:C:75:TRP:HE1	1:C:104:GLY:HA2	1.81	0.45
1:C:601:LEU:O	1:C:605:VAL:HG12	2.16	0.45
1:A:330:MET:SD	1:A:343:ILE:HD12	2.56	0.45
1:A:417:GLY:C	1:A:464:SER:HB2	2.42	0.45
1:B:644:LEU:HA	1:B:647:LEU:HD12	1.97	0.45
1:D:326:LEU:HD23	1:D:326:LEU:HA	1.79	0.45
1:D:458:SER:HB2	1:D:466:PRO:HD3	1.99	0.45
1:D:519:ASP:HA	1:D:522:ILE:HD12	1.98	0.45
1:A:329:PHE:CD2	1:C:358:THR:HB	2.50	0.45
1:A:632:LEU:HD11	1:A:652:MET:HG2	1.98	0.45
1:C:407:PHE:HB2	1:C:475:CYS:HG	1.79	0.45
1:C:633:CYS:HB3	1:C:667:VAL:HG21	1.98	0.45
1:D:115:GLN:HA	1:D:115:GLN:NE2	2.32	0.45
1:D:241:LEU:HD21	1:D:276:ASP:HB2	1.99	0.45
1:D:371:LYS:HB3	1:D:371:LYS:HE3	1.65	0.45
1:D:531:LEU:HD11	1:D:550:LEU:HD22	1.99	0.45
1:A:433:ALA:HB3	1:A:445:VAL:HB	1.97	0.45
1:B:614:GLY:HA2	1:B:617:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:TYR:CD1	1:C:138:ARG:HD3	2.52	0.45
1:B:90:PHE:CZ	1:B:254:LEU:HD13	2.52	0.45
1:B:253:ASP:OD1	1:B:253:ASP:N	2.49	0.45
1:C:86:GLU:HG3	1:C:93:LEU:HD23	1.99	0.45
1:C:398:ILE:O	1:C:402:LEU:HG	2.16	0.45
1:C:409:PRO:HG3	1:C:474:LEU:N	2.31	0.45
1:D:154:TRP:HB2	1:D:174:ARG:NH2	2.32	0.45
1:B:269:MET:HE2	1:B:269:MET:HB3	1.89	0.45
1:B:607:ALA:HB1	1:B:609:GLN:HE21	1.81	0.45
1:D:387:PHE:HE2	1:D:398:ILE:HG21	1.80	0.45
1:D:551:ILE:HG21	1:D:586:GLU:HG3	1.98	0.45
1:D:589:ASP:HB3	1:D:592:LEU:HB2	1.99	0.45
1:D:626:GLU:OE1	1:D:626:GLU:N	2.50	0.45
1:A:72:ILE:HD13	1:A:72:ILE:HA	1.65	0.45
1:A:240:LYS:O	1:A:240:LYS:HD3	2.17	0.45
1:A:322:LYS:HD3	1:A:351:TYR:OH	2.16	0.45
1:B:471:VAL:HG13	1:B:475:CYS:SG	2.57	0.45
1:B:712:LEU:O	1:B:716:VAL:HG23	2.16	0.45
1:C:431:LEU:HB2	1:C:448:LEU:HB2	1.97	0.45
1:C:461:CYS:SG	1:C:520:ILE:HD13	2.57	0.45
1:C:601:LEU:HD23	1:C:623:PHE:CE2	2.52	0.45
1:C:641:SER:HB2	1:C:645:LYS:NZ	2.31	0.45
1:D:196:TYR:CD1	1:D:197:LEU:HD22	2.51	0.45
1:A:690:LYS:HB3	1:A:694:GLY:HA2	1.99	0.45
1:B:492:TYR:HB3	1:B:494:HIS:CE1	2.51	0.45
1:C:233:TYR:CD1	1:C:280:VAL:HG12	2.52	0.45
1:D:85:MET:HE2	1:D:85:MET:HB2	1.78	0.45
1:A:195:ASN:OD1	1:A:196:TYR:N	2.50	0.44
1:A:285:MET:HE3	1:D:241:LEU:HD12	1.98	0.44
1:A:454:PHE:CE2	1:A:469:VAL:HG21	2.52	0.44
1:A:506:GLU:HG2	1:A:507:LYS:HD2	1.99	0.44
1:C:433:ALA:O	1:C:445:VAL:N	2.49	0.44
1:C:520:ILE:H	1:C:520:ILE:HG12	1.49	0.44
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.84	0.44
1:A:349:LEU:HD22	1:A:408:LEU:HG	1.99	0.44
1:B:100:LEU:C	1:B:100:LEU:HD23	2.43	0.44
1:B:288:VAL:O	1:B:292:VAL:HB	2.17	0.44
1:B:593:LYS:HD2	1:B:597:GLY:HA2	1.99	0.44
1:C:576:TYR:HB2	1:C:579:ILE:HG22	1.97	0.44
1:C:581:LEU:HD23	1:C:615:LEU:HD11	2.00	0.44
1:A:605:VAL:HA	1:A:613:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:LEU:HD13	1:B:166:LEU:HA	1.84	0.44
1:B:506:GLU:OE1	1:B:507:LYS:HD3	2.18	0.44
1:B:648:LEU:HD13	1:B:683:ALA:HB2	1.99	0.44
1:C:275:GLY:O	1:C:276:ASP:C	2.60	0.44
1:D:61:LYS:O	1:D:61:LYS:HG3	2.18	0.44
1:A:72:ILE:HD11	1:A:107:ALA:O	2.18	0.44
1:A:326:LEU:HD12	1:A:347:VAL:HG21	1.98	0.44
1:A:537:SER:O	1:A:541:GLN:HG2	2.17	0.44
1:B:241:LEU:HD23	1:B:241:LEU:HA	1.78	0.44
1:B:516:LEU:HB3	1:B:522:ILE:HG12	1.99	0.44
1:B:709:LEU:O	1:B:713:LEU:HG	2.18	0.44
1:A:545:TYR:CE2	1:A:546:GLN:NE2	2.82	0.44
1:A:644:LEU:HA	1:A:647:LEU:HD12	1.98	0.44
1:B:196:TYR:CD2	1:C:320:ARG:HG3	2.53	0.44
1:B:493:PHE:CE1	1:B:531:LEU:HD22	2.52	0.44
1:B:689:SER:O	1:B:697:PRO:HD3	2.17	0.44
1:C:583:LEU:CD2	1:C:588:VAL:HG21	2.47	0.44
1:C:601:LEU:HD22	1:C:621:ALA:O	2.17	0.44
1:D:431:LEU:HB2	1:D:448:LEU:HB2	2.00	0.44
1:B:387:PHE:HD1	1:B:499:ILE:HD11	1.83	0.44
1:B:516:LEU:HD22	1:B:522:ILE:HA	2.00	0.44
1:D:520:ILE:HD12	1:D:520:ILE:HA	1.82	0.44
1:A:701:ALA:O	1:A:705:GLY:N	2.44	0.44
1:C:396:ASN:O	1:C:400:ILE:HG13	2.18	0.44
1:D:81:LEU:O	1:D:213:HIS:NE2	2.51	0.44
1:D:353:SER:C	1:D:355:TYR:H	2.26	0.44
1:D:515:LYS:HD2	1:D:516:LEU:HG	2.00	0.44
1:A:233:TYR:CE1	1:D:244:TYR:HB3	2.53	0.44
1:A:328:SER:O	1:A:332:ARG:HG2	2.18	0.44
1:B:605:VAL:HG11	1:B:647:LEU:HD23	1.98	0.44
1:C:487:ASN:O	1:C:491:ILE:HG13	2.18	0.44
1:D:353:SER:C	1:D:355:TYR:N	2.76	0.44
1:D:618:LYS:HA	1:D:618:LYS:HD3	1.86	0.44
1:A:431:LEU:HB2	1:A:448:LEU:HB2	2.00	0.44
1:A:461:CYS:O	1:A:518:SER:HB2	2.18	0.44
1:B:149:ILE:HG22	1:B:154:TRP:HZ2	1.81	0.44
1:C:719:ALA:O	1:C:722:SER:OG	2.32	0.44
1:A:221:TYR:O	1:A:225:THR:HG23	2.18	0.43
1:A:274:TYR:O	1:C:275:GLY:CA	2.66	0.43
1:A:310:ILE:HD13	1:C:305:ASN:ND2	2.33	0.43
1:A:699:ASP:HA	1:A:702:ARG:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:601:LEU:HD11	1:C:617:VAL:HG23	1.99	0.43
1:D:437:LYS:HG2	1:D:438:THR:H	1.83	0.43
1:D:566:SER:HB2	1:D:567:PRO:HD2	2.00	0.43
1:A:87:PHE:O	1:A:168:ARG:NH1	2.45	0.43
1:A:542:GLY:HA2	1:A:576:TYR:CE2	2.53	0.43
1:B:315:ASN:OD1	1:B:318:ARG:NH1	2.51	0.43
1:D:52:ASN:OD1	1:D:52:ASN:O	2.37	0.43
1:D:239:LEU:HD11	1:D:241:LEU:HG	2.00	0.43
1:D:398:ILE:HG23	1:D:480:LEU:HD22	2.00	0.43
1:A:105:GLN:HE22	1:A:153:PRO:HB3	1.82	0.43
1:A:204:LEU:HA	1:A:204:LEU:HD13	1.69	0.43
1:A:529:ALA:O	1:A:533:LEU:HG	2.18	0.43
1:B:182:VAL:O	1:B:186:GLN:HG3	2.17	0.43
1:C:393:GLU:O	1:C:397:GLN:HG2	2.18	0.43
1:D:139:TYR:CD1	1:D:139:TYR:C	2.96	0.43
1:D:398:ILE:HD13	1:D:488:ILE:HD12	1.99	0.43
1:A:429:GLY:HA3	1:A:475:CYS:HA	2.00	0.43
1:A:466:PRO:HA	1:C:545:TYR:CE1	2.53	0.43
1:A:583:LEU:HA	1:A:586:GLU:HG3	2.01	0.43
1:B:153:PRO:HB2	1:B:156:LEU:HD23	2.01	0.43
1:C:308:ALA:O	1:C:312:LYS:HG2	2.18	0.43
1:D:75:TRP:CZ3	1:D:104:GLY:HA2	2.53	0.43
1:A:153:PRO:HB2	1:A:156:LEU:HD23	2.00	0.43
1:C:387:PHE:CE2	1:C:398:ILE:HG13	2.53	0.43
1:C:615:LEU:O	1:C:618:LYS:HB2	2.17	0.43
1:C:657:GLU:HB3	1:C:661:HIS:HA	2.00	0.43
1:D:512:ARG:HA	1:D:512:ARG:HD3	1.63	0.43
1:D:686:SER:OG	1:D:688:ILE:HG13	2.18	0.43
1:A:687:VAL:O	1:A:697:PRO:HD2	2.19	0.43
1:C:175:LEU:HG	1:C:210:TYR:OH	2.18	0.43
1:C:632:LEU:HD23	1:C:647:LEU:HD13	2.01	0.43
1:D:263:TYR:O	1:D:267:VAL:HG13	2.18	0.43
1:D:413:ILE:HB	1:D:469:VAL:HB	2.00	0.43
1:D:421:ASP:O	1:D:422:HIS:ND1	2.51	0.43
1:D:676:MET:O	1:D:680:LEU:HD12	2.19	0.43
1:A:623:PHE:CE1	1:A:652:MET:HB2	2.54	0.43
1:B:223:ALA:HB2	1:B:235:TRP:NE1	2.33	0.43
1:B:282:LEU:HD12	1:B:285:MET:HE2	2.00	0.43
1:B:378:LEU:HD13	1:B:399:VAL:HG21	2.01	0.43
1:B:491:ILE:HG23	1:C:483:GLN:NE2	2.34	0.43
1:C:435:VAL:HG23	1:C:467:PHE:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:LEU:HD13	1:D:485:PHE:CD2	2.54	0.43
1:D:590:VAL:CG2	1:D:619:GLU:HG3	2.49	0.43
1:A:274:TYR:CD1	1:C:273:GLY:HA2	2.54	0.43
1:A:463:ILE:HG21	1:A:513:ILE:CG1	2.49	0.43
1:B:671:GLU:HB2	1:B:673:LEU:HG	1.99	0.43
1:C:575:GLY:CA	1:C:612:VAL:HG21	2.46	0.43
1:C:666:HIS:CD2	1:C:700:GLU:HG3	2.54	0.43
1:D:220:TYR:O	1:D:224:THR:HG23	2.19	0.43
1:D:706:ASN:O	1:D:710:ILE:HG13	2.18	0.43
1:A:323:MET:HE2	1:A:327:ILE:HG12	2.01	0.43
1:B:570:LEU:HD21	1:C:562:TYR:CE1	2.53	0.43
1:C:197:LEU:HD23	1:C:200:ARG:NH2	2.34	0.43
1:D:699:ASP:O	1:D:703:LEU:HG	2.18	0.43
1:A:75:TRP:CZ3	1:A:104:GLY:HA2	2.53	0.43
1:A:282:LEU:HD21	1:D:256:LYS:HA	2.01	0.43
1:B:127:ARG:HG2	1:B:127:ARG:HH11	1.83	0.43
1:C:170:LEU:HD23	1:C:170:LEU:HA	1.72	0.43
1:C:385:PRO:HA	1:C:388:LYS:CG	2.49	0.43
1:C:418:ASN:OD1	1:C:419:VAL:N	2.51	0.43
1:A:592:LEU:O	1:A:600:PRO:HD3	2.19	0.42
1:A:593:LYS:HB3	1:A:599:THR:HG22	2.01	0.42
1:A:623:PHE:HE1	1:A:652:MET:HA	1.83	0.42
1:A:674:PHE:O	1:A:678:LYS:HB2	2.18	0.42
1:B:338:ASP:O	1:B:342:GLN:HG2	2.18	0.42
1:D:426:VAL:CG2	1:D:431:LEU:HD12	2.49	0.42
1:A:263:TYR:O	1:A:267:VAL:HB	2.19	0.42
1:A:317:GLU:HG2	1:C:196:TYR:CE2	2.54	0.42
1:B:357:ASP:HA	1:B:360:MET:HB2	2.02	0.42
1:B:422:HIS:HB3	1:B:479:ARG:HG3	2.01	0.42
1:B:660:ASP:OD1	1:B:692:ARG:NH2	2.51	0.42
1:C:466:PRO:HG2	1:C:467:PHE:CE2	2.54	0.42
1:C:671:GLU:HG2	1:C:673:LEU:HG	2.00	0.42
1:D:713:LEU:O	1:D:717:LYS:HB3	2.20	0.42
1:A:86:GLU:HG3	1:A:93:LEU:HD21	2.01	0.42
1:A:296:MET:HE2	1:A:296:MET:HB3	1.78	0.42
1:A:329:PHE:CD1	1:A:329:PHE:C	2.96	0.42
1:A:534:LYS:HA	1:A:534:LYS:HD3	1.90	0.42
1:A:548:LYS:HG2	1:A:582:PHE:CE2	2.54	0.42
1:B:175:LEU:HD22	1:B:210:TYR:OH	2.18	0.42
1:B:565:ARG:HB2	1:B:565:ARG:CZ	2.48	0.42
1:C:671:GLU:HA	1:D:708:LYS:HZ2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:LEU:HD12	1:A:616:LEU:HB3	2.01	0.42
1:A:647:LEU:HB3	1:A:652:MET:SD	2.59	0.42
1:B:201:ILE:HG13	1:B:306:ILE:HG12	2.01	0.42
1:B:402:LEU:HD22	1:B:478:LEU:HB3	2.02	0.42
1:B:507:LYS:H	1:B:507:LYS:HG2	1.61	0.42
1:C:108:PHE:CZ	1:C:177:ARG:HD3	2.55	0.42
1:C:120:TYR:CE2	1:C:129:VAL:HB	2.55	0.42
1:C:152:PHE:O	1:C:154:TRP:N	2.53	0.42
1:C:678:LYS:O	1:C:682:GLU:HG2	2.19	0.42
1:D:420:VAL:O	1:D:482:LYS:HD2	2.18	0.42
1:D:544:PHE:CD1	1:D:579:ILE:HG12	2.54	0.42
1:A:236:ILE:HG12	1:A:249:PHE:HB2	2.01	0.42
1:A:256:LYS:HE2	1:C:282:LEU:HG	2.00	0.42
1:B:93:LEU:HD23	1:B:93:LEU:HA	1.88	0.42
1:B:580:THR:HG21	1:B:612:VAL:CG2	2.43	0.42
1:C:102:ILE:O	1:C:106:ILE:HG13	2.20	0.42
1:C:501:ASN:O	1:C:505:GLU:HG3	2.20	0.42
1:D:635:THR:HA	1:D:638:LYS:HD2	2.02	0.42
1:A:605:VAL:HG12	1:A:643:PHE:HE1	1.84	0.42
1:C:165:GLU:OE2	1:C:168:ARG:NE	2.46	0.42
1:C:365:PRO:HD2	1:C:368:ILE:HD12	2.00	0.42
1:D:93:LEU:HD23	1:D:93:LEU:HA	1.84	0.42
1:D:118:VAL:O	1:D:135:ILE:HD12	2.20	0.42
1:D:267:VAL:HB	1:D:273:GLY:H	1.84	0.42
1:A:315:ASN:HA	1:A:318:ARG:HE	1.83	0.42
1:A:402:LEU:HD13	1:A:478:LEU:HG	2.02	0.42
1:A:420:VAL:CG1	1:A:459:ILE:HG13	2.47	0.42
1:A:623:PHE:CD1	1:A:652:MET:HE3	2.54	0.42
1:B:126:TYR:CD1	1:C:474:LEU:HD22	2.54	0.42
1:B:416:GLN:HG3	1:B:468:THR:OG1	2.19	0.42
1:B:435:VAL:HG22	1:B:467:PHE:HB3	2.01	0.42
1:C:365:PRO:HB2	1:C:368:ILE:HG13	2.02	0.42
1:C:544:PHE:O	1:C:547:LEU:HG	2.20	0.42
1:D:454:PHE:CD2	1:D:469:VAL:HG21	2.54	0.42
1:B:274:TYR:O	1:D:275:GLY:CA	2.63	0.42
1:C:226:LEU:HD23	1:C:226:LEU:HA	1.84	0.42
1:A:323:MET:CE	1:A:344:THR:HG22	2.49	0.42
1:B:109:LEU:C	1:B:111:ASP:H	2.27	0.42
1:C:63:ARG:O	1:C:63:ARG:NH1	2.52	0.42
1:C:483:GLN:OE1	1:C:483:GLN:HA	2.19	0.42
1:C:540:PHE:HE2	1:C:574:ARG:HD3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:601:LEU:HD12	1:C:616:LEU:HB2	2.02	0.42
1:D:231:GLU:HB2	1:D:249:PHE:CE1	2.55	0.42
1:A:463:ILE:HG21	1:A:513:ILE:CD1	2.50	0.42
1:A:534:LYS:HD2	1:D:530:GLU:OE2	2.20	0.42
1:B:693:TRP:HE1	1:C:693:TRP:NE1	2.18	0.42
1:C:80:SER:HB2	1:C:210:TYR:OH	2.20	0.42
1:C:557:PRO:CG	1:C:588:VAL:HG22	2.48	0.42
1:D:666:HIS:CE1	1:D:697:PRO:HD3	2.55	0.42
1:D:99:VAL:O	1:D:103:VAL:HG23	2.19	0.41
1:D:714:GLU:O	1:D:718:ASN:ND2	2.53	0.41
1:A:397:GLN:C	1:A:397:GLN:OE1	2.63	0.41
1:A:416:GLN:HB2	1:C:545:TYR:OH	2.19	0.41
1:A:488:ILE:HG13	1:A:488:ILE:H	1.67	0.41
1:B:197:LEU:O	1:B:200:ARG:HB3	2.20	0.41
1:B:483:GLN:HE21	1:B:487:ASN:CG	2.27	0.41
1:B:675:LEU:O	1:B:679:MET:HE2	2.20	0.41
1:B:706:ASN:O	1:B:710:ILE:HG13	2.20	0.41
1:C:367:SER:O	1:C:371:LYS:HG3	2.20	0.41
1:C:590:VAL:HG12	1:C:621:ALA:HB2	2.02	0.41
1:D:72:ILE:HD13	1:D:72:ILE:HA	1.78	0.41
1:D:173:ILE:HD13	1:D:173:ILE:HA	1.83	0.41
1:A:456:ASP:O	1:A:460:ILE:HG13	2.20	0.41
1:C:269:MET:HA	1:C:295:ASP:OD2	2.19	0.41
1:C:281:ASN:O	1:C:285:MET:HG3	2.19	0.41
1:C:435:VAL:HG23	1:C:445:VAL:HG21	2.02	0.41
1:C:599:THR:O	1:C:603:GLU:HG2	2.20	0.41
1:D:137:PHE:O	1:D:141:LYS:HG3	2.21	0.41
1:A:58:ILE:HG13	1:A:118:VAL:HG23	2.03	0.41
1:A:274:TYR:CE1	1:C:273:GLY:HA2	2.55	0.41
1:A:407:PHE:HB2	1:A:475:CYS:SG	2.59	0.41
1:B:197:LEU:HD22	1:C:317:GLU:OE2	2.20	0.41
1:B:634:THR:O	1:B:638:LYS:HG3	2.20	0.41
1:D:410:GLY:HA2	1:D:470:ARG:HH22	1.85	0.41
1:A:698:LEU:HD21	1:A:714:GLU:HG2	2.02	0.41
1:B:347:VAL:O	1:B:350:GLN:HG3	2.21	0.41
1:A:315:ASN:N	1:A:318:ARG:HH21	2.17	0.41
1:A:363:ASP:O	1:A:364:ILE:HD13	2.19	0.41
1:A:407:PHE:CZ	1:A:413:ILE:HD11	2.55	0.41
1:A:480:LEU:HD21	1:A:488:ILE:CD1	2.51	0.41
1:B:356:THR:O	1:B:360:MET:HG2	2.20	0.41
1:B:674:PHE:CD1	1:B:708:LYS:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:ASP:HA	1:B:718:ASN:HD22	1.86	0.41
1:C:347:VAL:O	1:C:350:GLN:HG2	2.20	0.41
1:C:690:LYS:HG3	1:C:694:GLY:O	2.21	0.41
1:D:325:ASP:O	1:D:328:SER:OG	2.35	0.41
1:D:577:GLU:O	1:D:581:LEU:HD13	2.19	0.41
1:D:623:PHE:HB3	1:D:625:LEU:HG	2.02	0.41
1:A:127:ARG:HD2	1:A:128:THR:N	2.35	0.41
1:A:200:ARG:HE	1:A:200:ARG:HB3	1.78	0.41
1:A:460:ILE:HG13	1:A:460:ILE:H	1.61	0.41
1:A:484:SER:O	1:A:485:PHE:C	2.62	0.41
1:A:545:TYR:HE2	1:D:522:ILE:HD13	1.86	0.41
1:B:59:HIS:ND1	1:B:60:PRO:HD2	2.35	0.41
1:B:382:LYS:NZ	1:B:392:THR:HG22	2.36	0.41
1:C:85:MET:HE3	1:C:85:MET:HB2	1.86	0.41
1:C:326:LEU:HD23	1:C:326:LEU:HA	1.88	0.41
1:D:98:PHE:C	1:D:98:PHE:CD2	2.99	0.41
1:D:544:PHE:O	1:D:548:LYS:HG3	2.20	0.41
1:A:566:SER:OG	1:A:569:HIS:ND1	2.44	0.41
1:B:326:LEU:HD12	1:B:347:VAL:HG21	2.01	0.41
1:B:653:ASN:HD22	1:B:683:ALA:HB3	1.86	0.41
1:C:172:TRP:O	1:C:175:LEU:HB2	2.20	0.41
1:D:546:GLN:O	1:D:550:LEU:HG	2.20	0.41
1:A:550:LEU:HA	1:A:553:SER:HB2	2.02	0.41
1:A:557:PRO:O	1:A:567:PRO:HD2	2.21	0.41
1:A:565:ARG:HD2	1:A:566:SER:H	1.86	0.41
1:A:594:ASP:C	1:A:596:PHE:H	2.29	0.41
1:B:65:TYR:CZ	1:B:118:VAL:HG21	2.55	0.41
1:B:86:GLU:HA	1:B:90:PHE:HD2	1.86	0.41
1:B:377:TYR:HB2	1:B:399:VAL:CG1	2.49	0.41
1:B:706:ASN:OD1	1:B:708:LYS:HG2	2.21	0.41
1:C:231:GLU:HG2	1:C:249:PHE:HE2	1.86	0.41
1:D:84:PRO:HG2	1:D:214:THR:HG22	2.03	0.41
1:D:95:GLU:O	1:D:98:PHE:HB2	2.20	0.41
1:D:269:MET:HE2	1:D:269:MET:HB3	1.99	0.41
1:D:605:VAL:HG21	1:D:623:PHE:HE1	1.86	0.41
1:D:664:PRO:HB2	1:D:680:LEU:CD2	2.51	0.41
1:D:687:VAL:O	1:D:696:SER:HB2	2.20	0.41
1:D:698:LEU:HD21	1:D:714:GLU:CG	2.50	0.41
1:A:606:LYS:HA	1:A:643:PHE:CE1	2.56	0.41
1:B:436:THR:HA	1:B:441:SER:O	2.21	0.41
1:B:493:PHE:CD1	1:B:493:PHE:C	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:ASP:OD1	1:B:630:ASN:HB2	2.20	0.41
1:C:548:LYS:HB3	1:C:552:ARG:HH12	1.85	0.41
1:C:615:LEU:HD23	1:C:615:LEU:HA	1.82	0.41
1:C:623:PHE:CD1	1:C:652:MET:HG2	2.55	0.41
1:D:662:ARG:HG2	1:D:691:ASP:HB2	2.03	0.41
1:A:404:GLU:C	1:A:405:GLU:HG2	2.47	0.40
1:A:463:ILE:HD13	1:A:513:ILE:HG13	2.03	0.40
1:B:610:GLU:HA	1:B:613:ILE:HB	2.03	0.40
1:C:687:VAL:HG13	1:C:698:LEU:HB2	2.03	0.40
1:D:253:ASP:O	1:D:257:ARG:HD3	2.21	0.40
1:D:319:PHE:O	1:D:322:LYS:HG2	2.21	0.40
1:D:499:ILE:HA	1:D:502:ASN:OD1	2.20	0.40
1:D:501:ASN:O	1:D:505:GLU:HG3	2.21	0.40
1:A:549:SER:HA	1:A:552:ARG:HD2	2.02	0.40
1:A:560:THR:HG22	1:A:565:ARG:O	2.21	0.40
1:B:263:TYR:CD2	1:D:285:MET:HG2	2.57	0.40
1:B:375:LEU:HD12	1:B:375:LEU:HA	1.85	0.40
1:C:208:GLU:HG3	1:C:298:LEU:HD21	2.02	0.40
1:D:147:ASP:OD2	1:D:179:ARG:NH2	2.37	0.40
1:D:279:ALA:HB2	1:D:288:VAL:HG21	2.02	0.40
1:D:339:LEU:HD12	1:D:339:LEU:HA	1.92	0.40
1:D:561:ASP:OD2	1:D:565:ARG:HB2	2.21	0.40
1:A:340:ARG:O	1:A:344:THR:HG23	2.21	0.40
1:A:543:ASP:OD2	1:A:546:GLN:HG2	2.22	0.40
1:B:582:PHE:O	1:B:586:GLU:HG2	2.21	0.40
1:B:668:ALA:HB1	1:B:673:LEU:HB2	2.04	0.40
1:C:122:ASP:O	1:C:126:TYR:N	2.54	0.40
1:C:599:THR:HG21	1:C:622:SER:O	2.21	0.40
1:D:496:GLY:O	1:D:500:LEU:HG	2.22	0.40
1:D:534:LYS:HB3	1:D:534:LYS:HE2	1.85	0.40
1:D:540:PHE:HB2	1:D:570:LEU:HD23	2.03	0.40
1:D:656:SER:O	1:D:664:PRO:HD3	2.21	0.40
1:B:418:ASN:O	1:B:465:GLN:N	2.45	0.40
1:B:514:LYS:HE2	1:B:514:LYS:HB3	1.85	0.40
1:B:533:LEU:CD2	1:C:537:SER:HB2	2.46	0.40
1:B:561:ASP:CG	1:B:563:ASP:H	2.30	0.40
1:C:454:PHE:CD2	1:C:469:VAL:HG21	2.55	0.40
1:D:387:PHE:CE2	1:D:398:ILE:HG21	2.56	0.40
1:D:665:LEU:CD2	1:D:680:LEU:HB2	2.52	0.40
1:A:85:MET:HE3	1:A:85:MET:HB2	1.74	0.40
1:B:145:LEU:HG	1:B:146:MET:CE	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:PHE:HE2	1:D:372:ILE:HD13	1.86	0.40
1:B:488:ILE:O	1:B:491:ILE:HB	2.22	0.40
1:B:543:ASP:OD2	1:C:523:HIS:HA	2.22	0.40
1:C:707:LYS:HE3	1:D:705:GLY:HA3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	674/834 (81%)	641 (95%)	33 (5%)	0	100	100
1	B	674/834 (81%)	648 (96%)	26 (4%)	0	100	100
1	C	674/834 (81%)	647 (96%)	27 (4%)	0	100	100
1	D	673/834 (81%)	638 (95%)	35 (5%)	0	100	100
All	All	2695/3336 (81%)	2574 (96%)	121 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	597/743 (80%)	575 (96%)	22 (4%)	29	57
1	B	597/743 (80%)	579 (97%)	18 (3%)	36	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	597/743 (80%)	585 (98%)	12 (2%)	50	72
1	D	597/743 (80%)	575 (96%)	22 (4%)	29	57
All	All	2388/2972 (80%)	2314 (97%)	74 (3%)	37	62

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	TYR
1	A	72	ILE
1	A	97	LEU
1	A	123	THR
1	A	140	LEU
1	A	168	ARG
1	A	181	VAL
1	A	205	LEU
1	A	248	ASN
1	A	267	VAL
1	A	269	MET
1	A	274	TYR
1	A	276	ASP
1	A	277	ILE
1	A	282	LEU
1	A	312	LYS
1	A	427	CYS
1	A	447	LEU
1	A	457	ILE
1	A	562	TYR
1	A	565	ARG
1	A	695	ASN
1	B	51	HIS
1	B	54	TYR
1	B	58	ILE
1	B	137	PHE
1	B	197	LEU
1	B	226	LEU
1	B	254	LEU
1	B	272	VAL
1	B	282	LEU
1	B	292	VAL
1	B	295	ASP
1	B	335	LEU

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Mol	Chain	Res	Type
1	B	351	TYR
1	B	432	GLU
1	B	438	THR
1	B	512	ARG
1	B	531	LEU
1	B	570	LEU
1	C	72	ILE
1	C	101	ASP
1	C	109	LEU
1	C	147	ASP
1	C	272	VAL
1	C	318	ARG
1	C	350	GLN
1	C	383	LYS
1	C	512	ARG
1	C	520	ILE
1	C	547	LEU
1	C	630	ASN
1	D	56	TYR
1	D	64	TRP
1	D	72	ILE
1	D	118	VAL
1	D	171	LEU
1	D	229	GLU
1	D	233	TYR
1	D	236	ILE
1	D	240	LYS
1	D	245	SER
1	D	253	ASP
1	D	254	LEU
1	D	266	ILE
1	D	272	VAL
1	D	277	ILE
1	D	351	TYR
1	D	355	TYR
1	D	436	THR
1	D	437	LYS
1	D	460	ILE
1	D	612	VAL
1	D	630	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	105	GLN
1	A	115	GLN
1	A	186	GLN
1	A	248	ASN
1	A	346	HIS
1	A	350	GLN
1	A	487	ASN
1	A	502	ASN
1	A	523	HIS
1	A	624	ASN
1	A	695	ASN
1	B	164	HIS
1	B	451	HIS
1	B	483	GLN
1	B	502	ASN
1	B	609	GLN
1	B	718	ASN
1	C	51	HIS
1	C	59	HIS
1	C	62	ASN
1	C	105	GLN
1	C	143	HIS
1	C	451	HIS
1	C	483	GLN
1	C	502	ASN
1	C	541	GLN
1	C	546	GLN
1	C	558	ASN
1	C	624	ASN
1	C	695	ASN
1	D	52	ASN
1	D	62	ASN
1	D	115	GLN
1	D	281	ASN
1	D	305	ASN
1	D	315	ASN
1	D	374	GLN
1	D	396	ASN
1	D	418	ASN
1	D	451	HIS
1	D	536	ASN
1	D	541	GLN

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Mol	Chain	Res	Type
1	D	546	GLN
1	D	695	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.

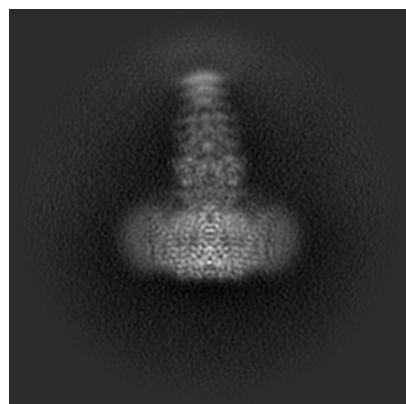
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62916. These allow visual inspection of the internal detail of the map and identification of artifacts.

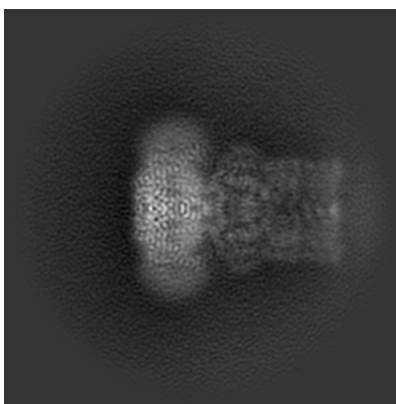
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

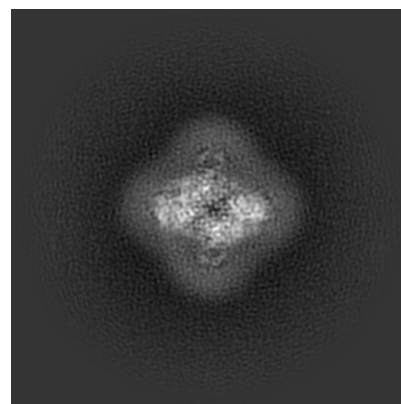
6.1.1 Primary map



X

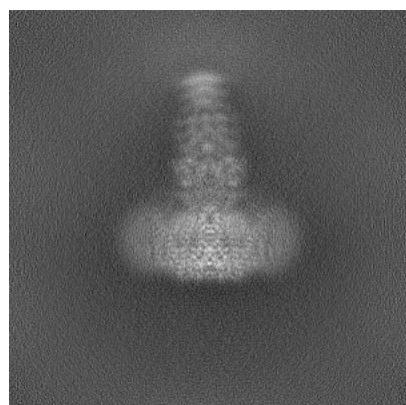


Y

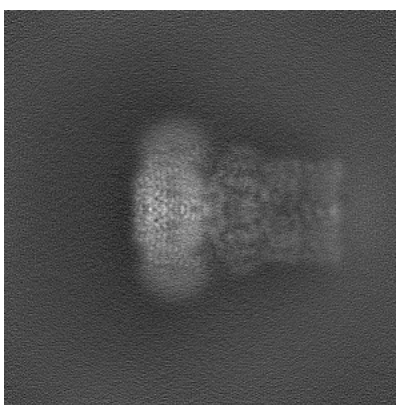


Z

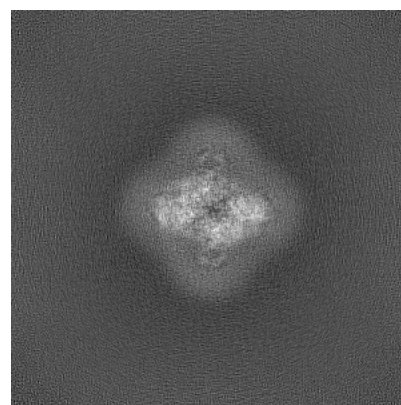
6.1.2 Raw map



X



Y

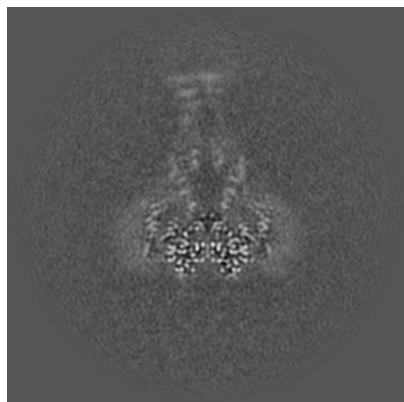


Z

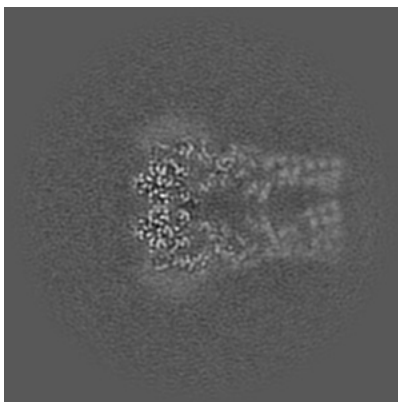
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

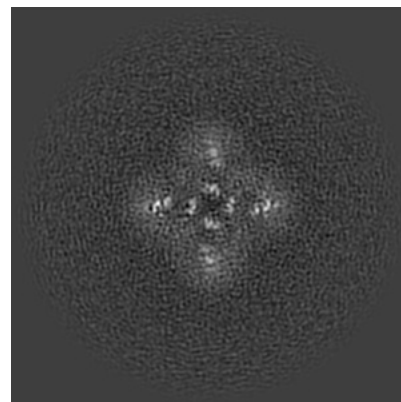
6.2.1 Primary map



X Index: 200

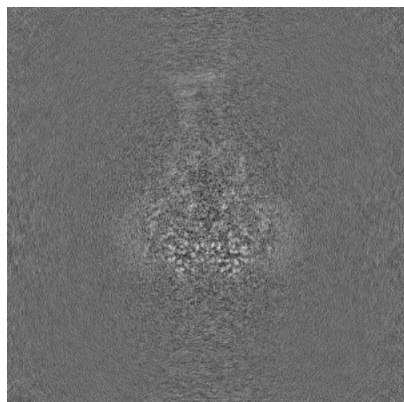


Y Index: 200

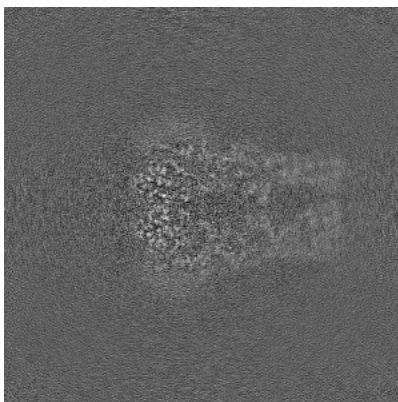


Z Index: 200

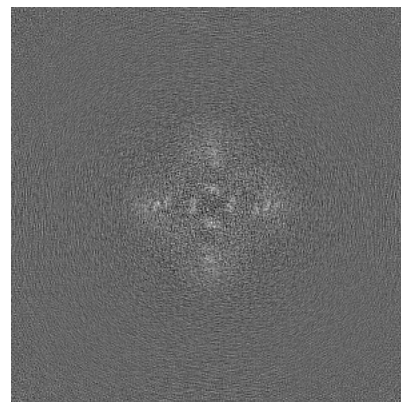
6.2.2 Raw map



X Index: 200



Y Index: 200

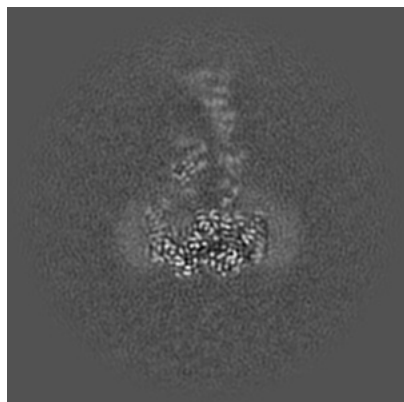


Z Index: 200

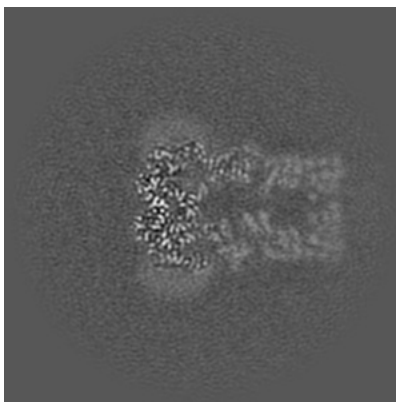
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

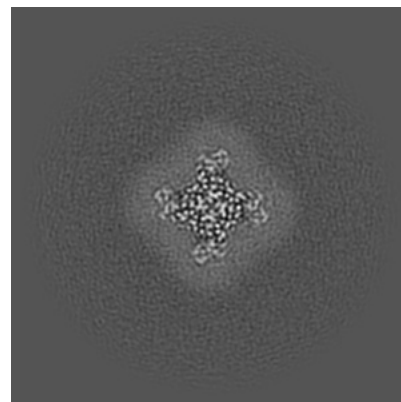
6.3.1 Primary map



X Index: 192

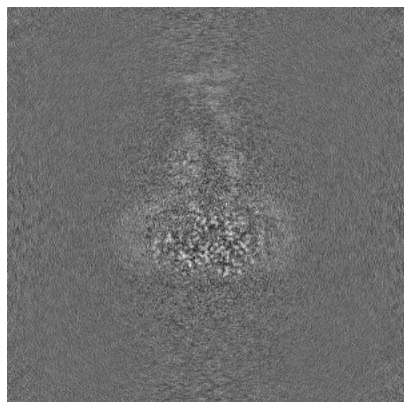


Y Index: 196

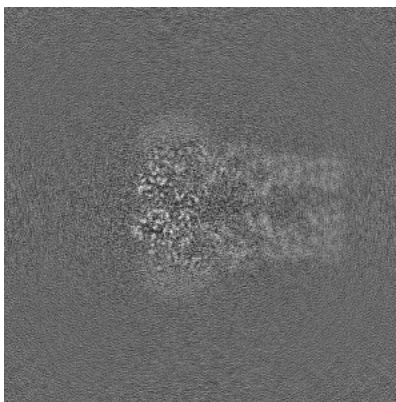


Z Index: 146

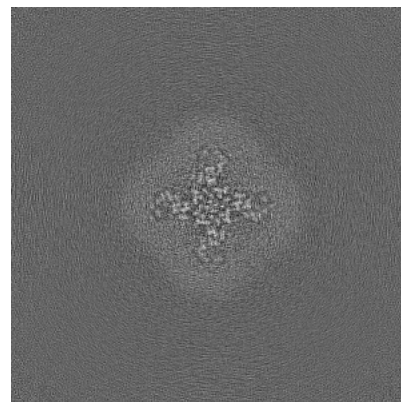
6.3.2 Raw map



X Index: 195



Y Index: 198

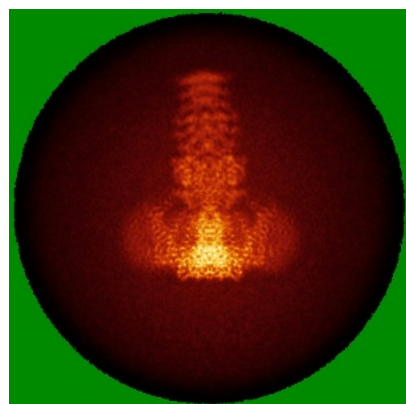


Z Index: 160

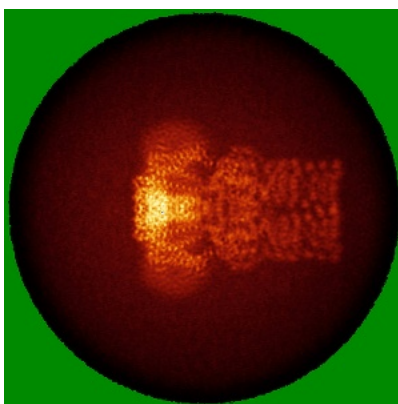
The images above show the largest variance slices of the map in three orthogonal directions.

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

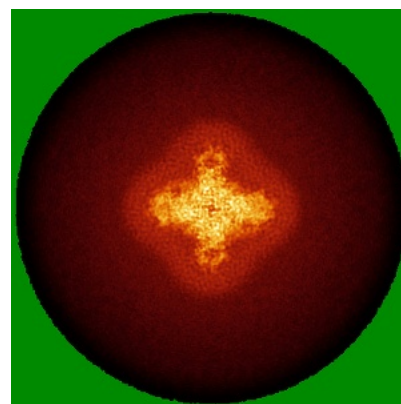
6.4.1 Primary map



X

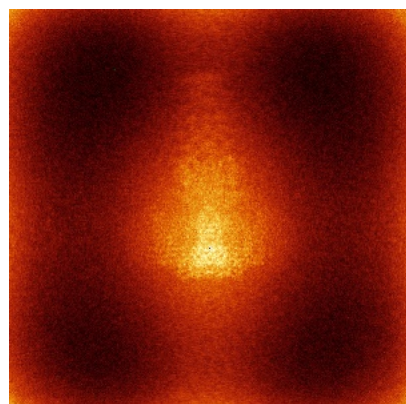


Y

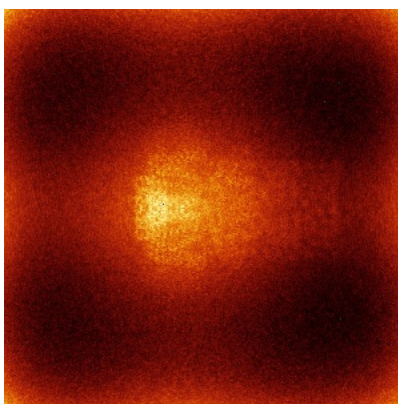


Z

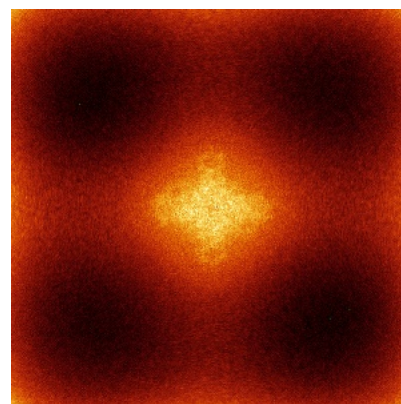
6.4.2 Raw map



X



Y

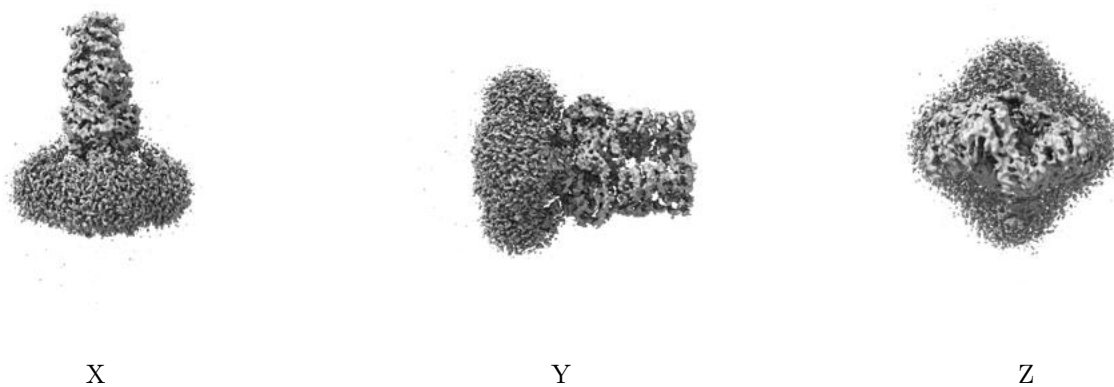


Z

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.

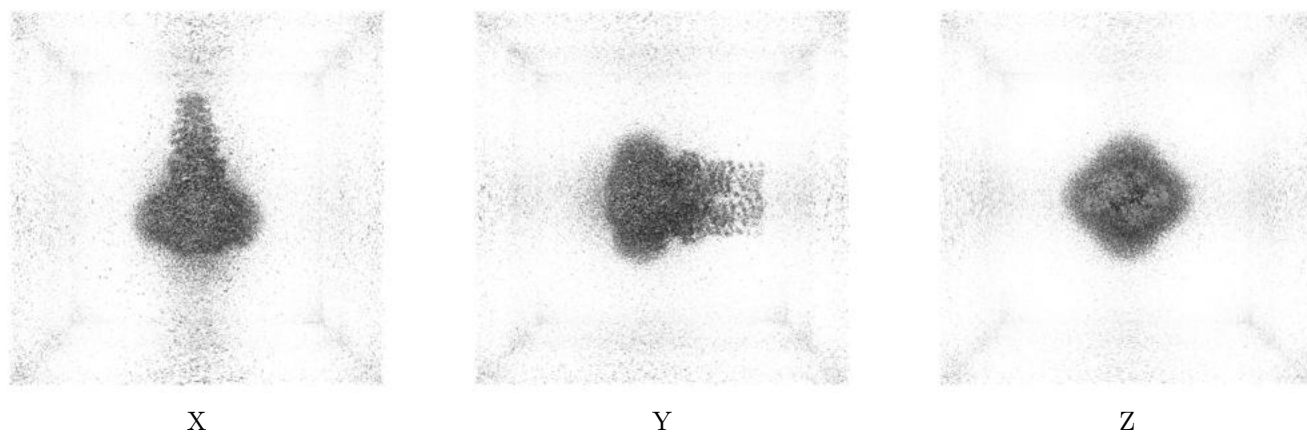
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

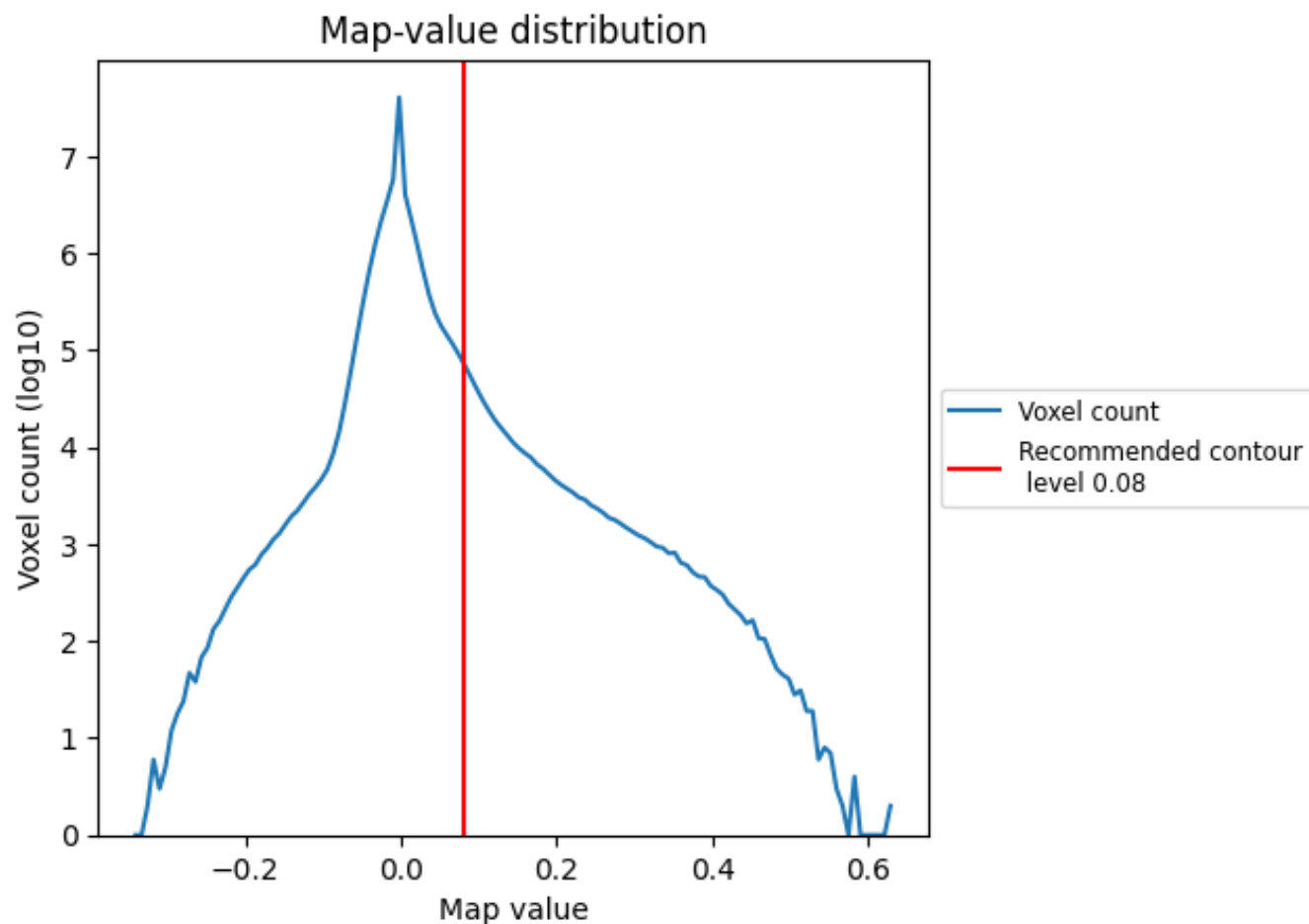
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

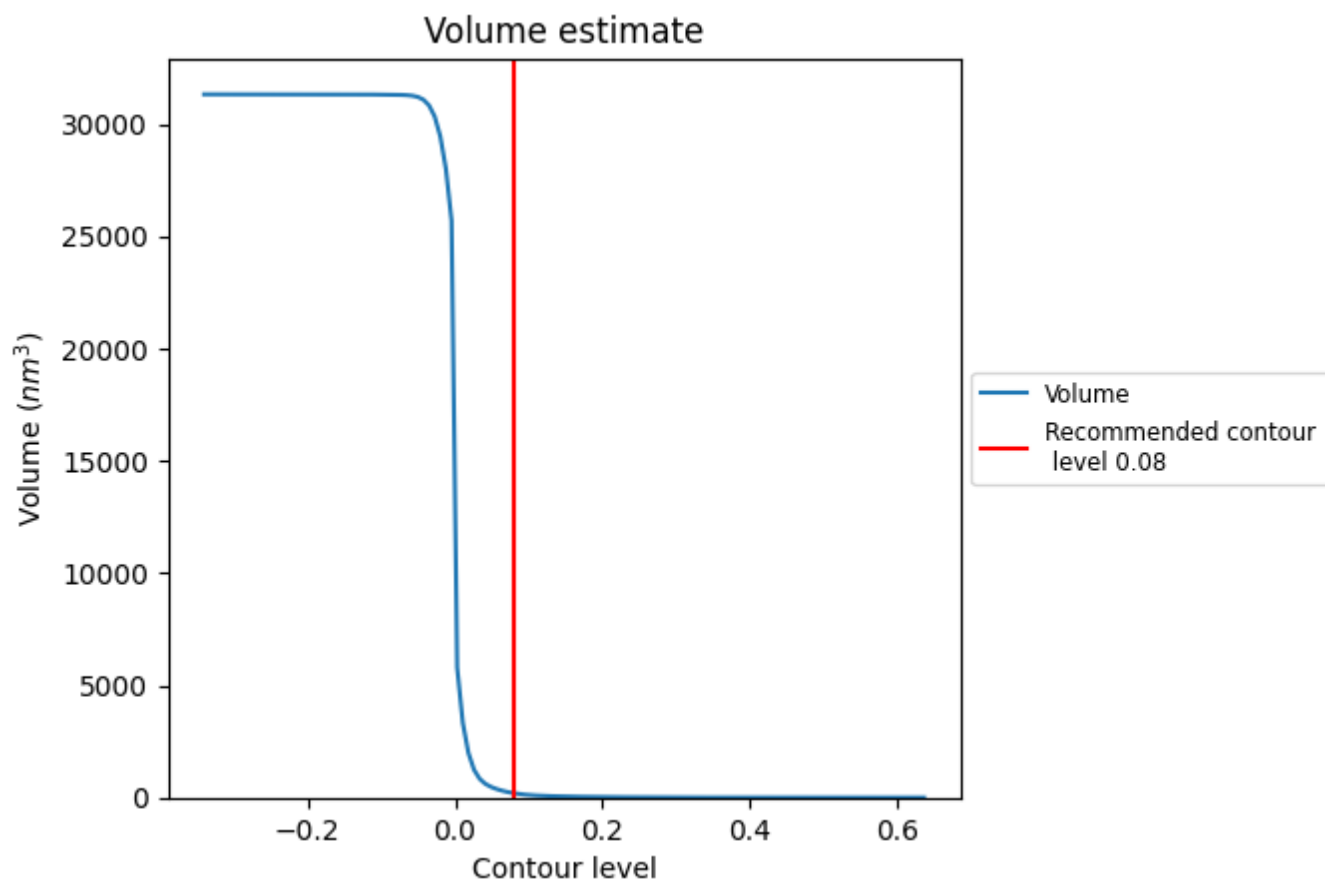
This section contains the results of statistical analysis of the map.

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.

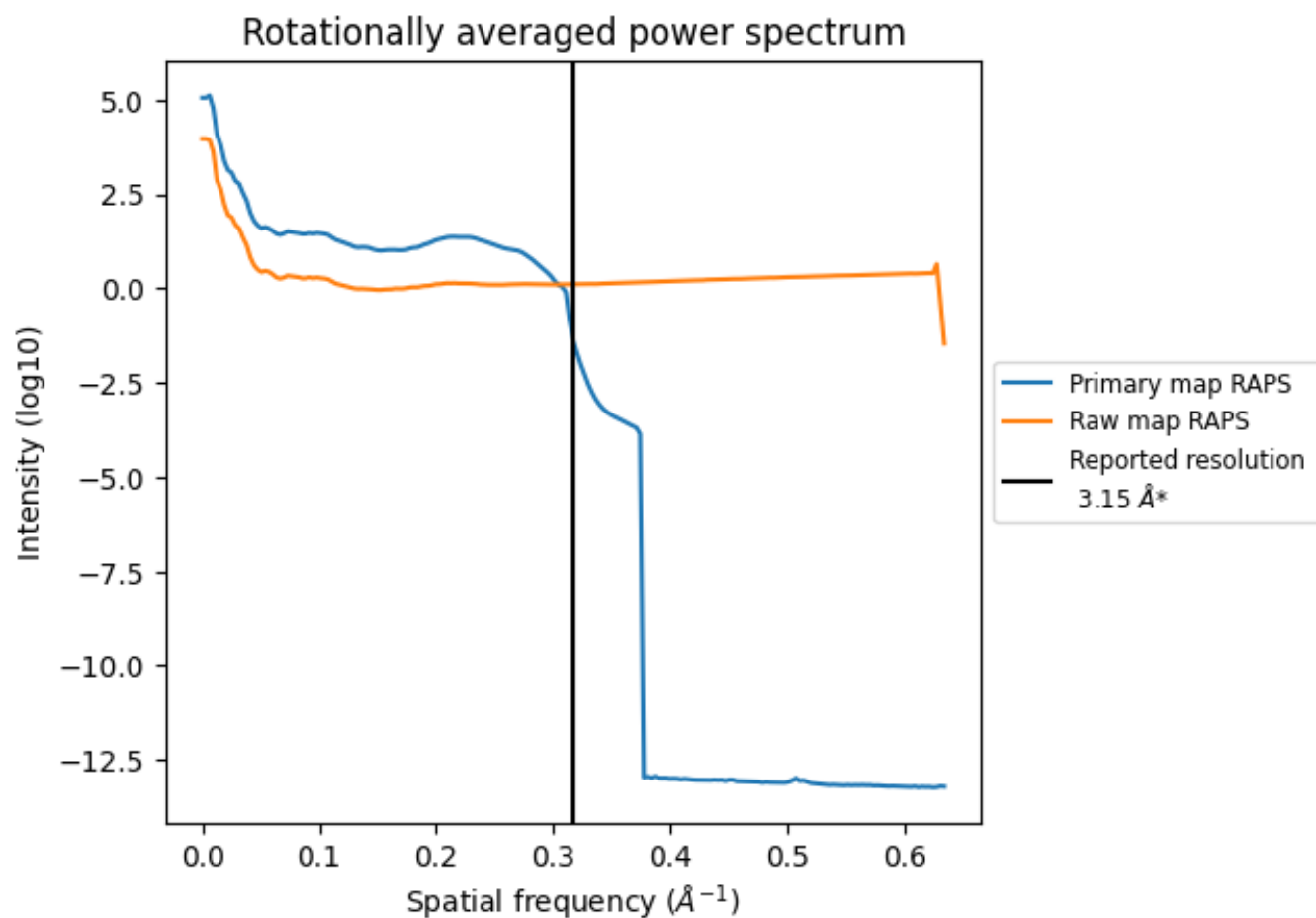
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 193 nm³; this corresponds to an approximate mass of 174 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 ⓘ

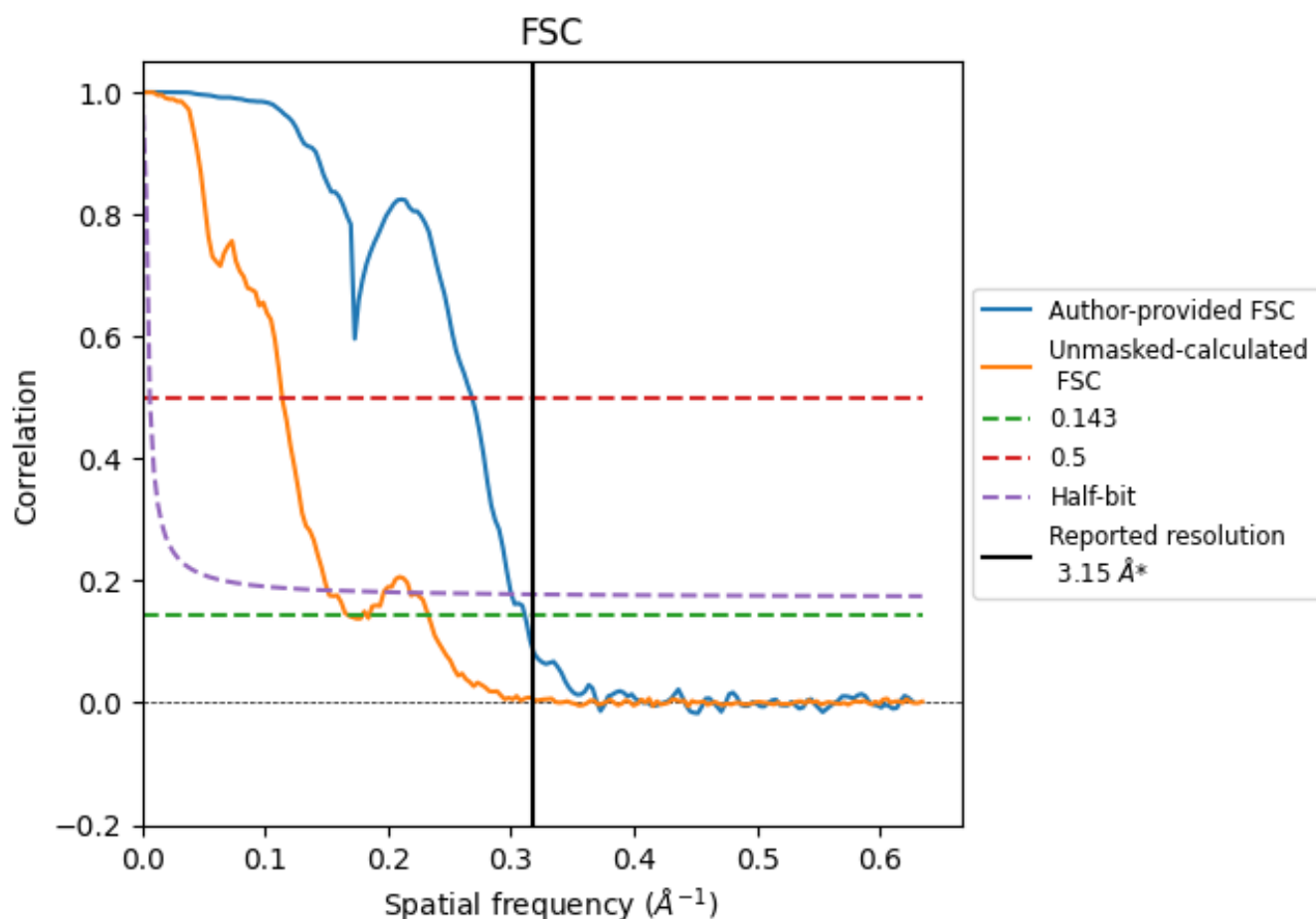


*Reported resolution corresponds to spatial frequency of 0.317 Å⁻¹

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 0.317 \AA^{-1}

8.2 Resolution estimates [i](#)

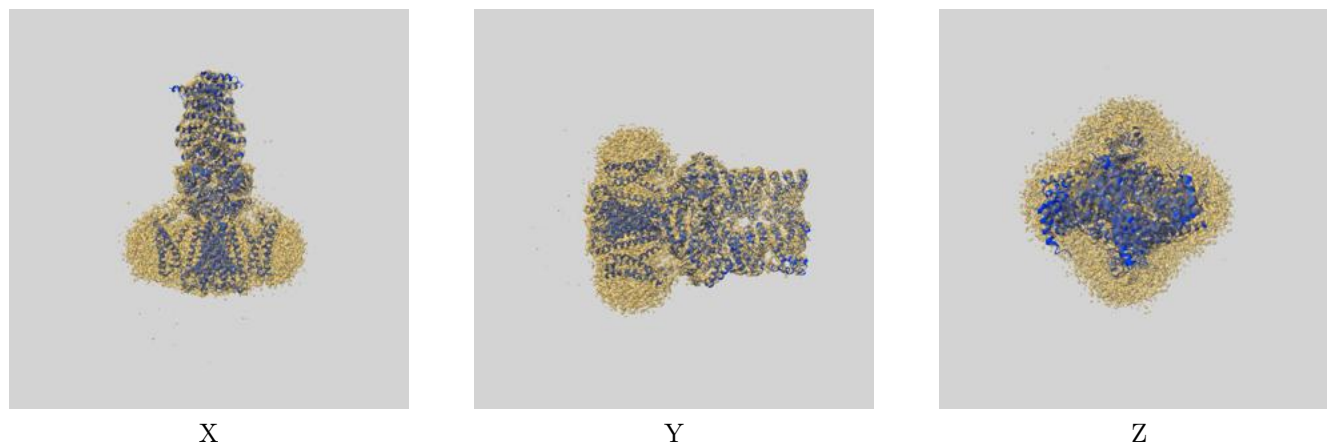
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	3.21	3.73	3.33
Unmasked-calculated*	5.96	8.78	6.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.96 differs from the reported value 3.15 by more than 10 %

9 Map-model fit [i](#)

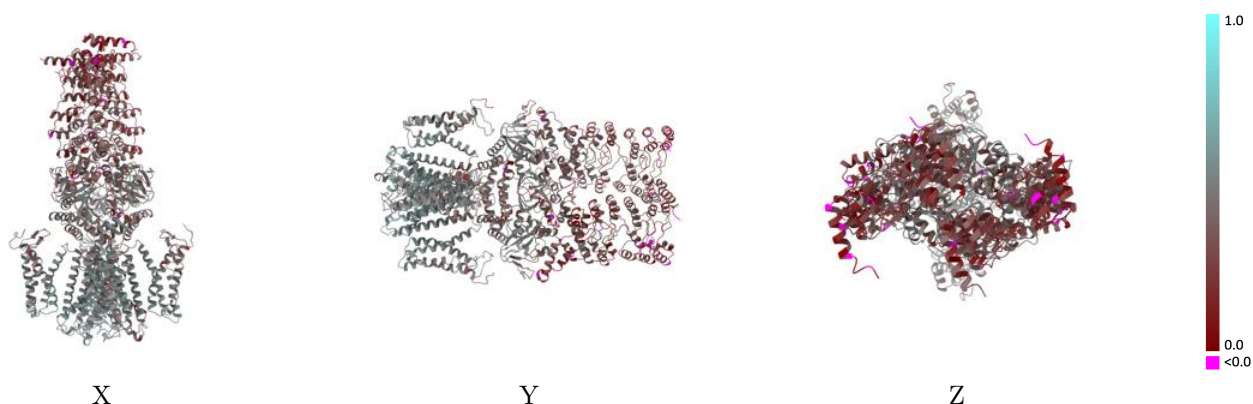
This section contains information regarding the fit between EMDB map EMD-62916 and PDB model 9LA1. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



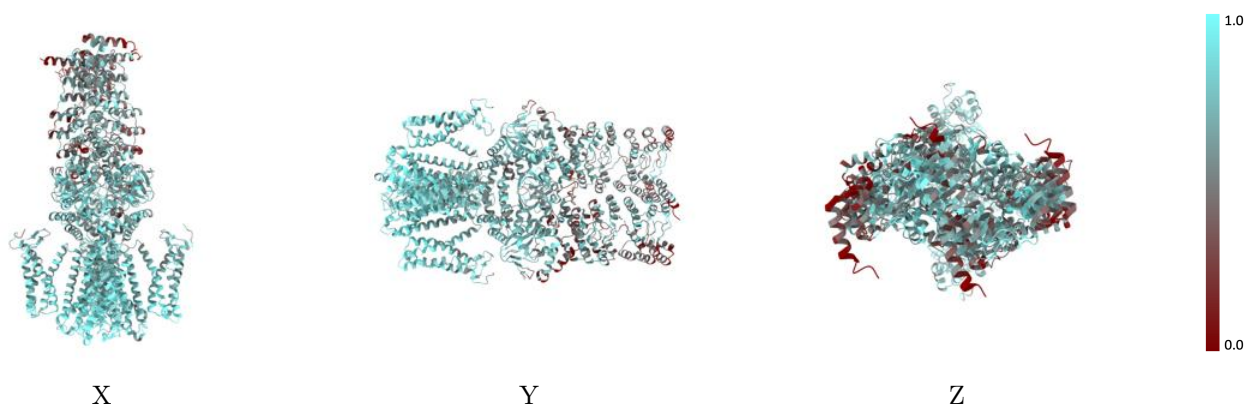
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



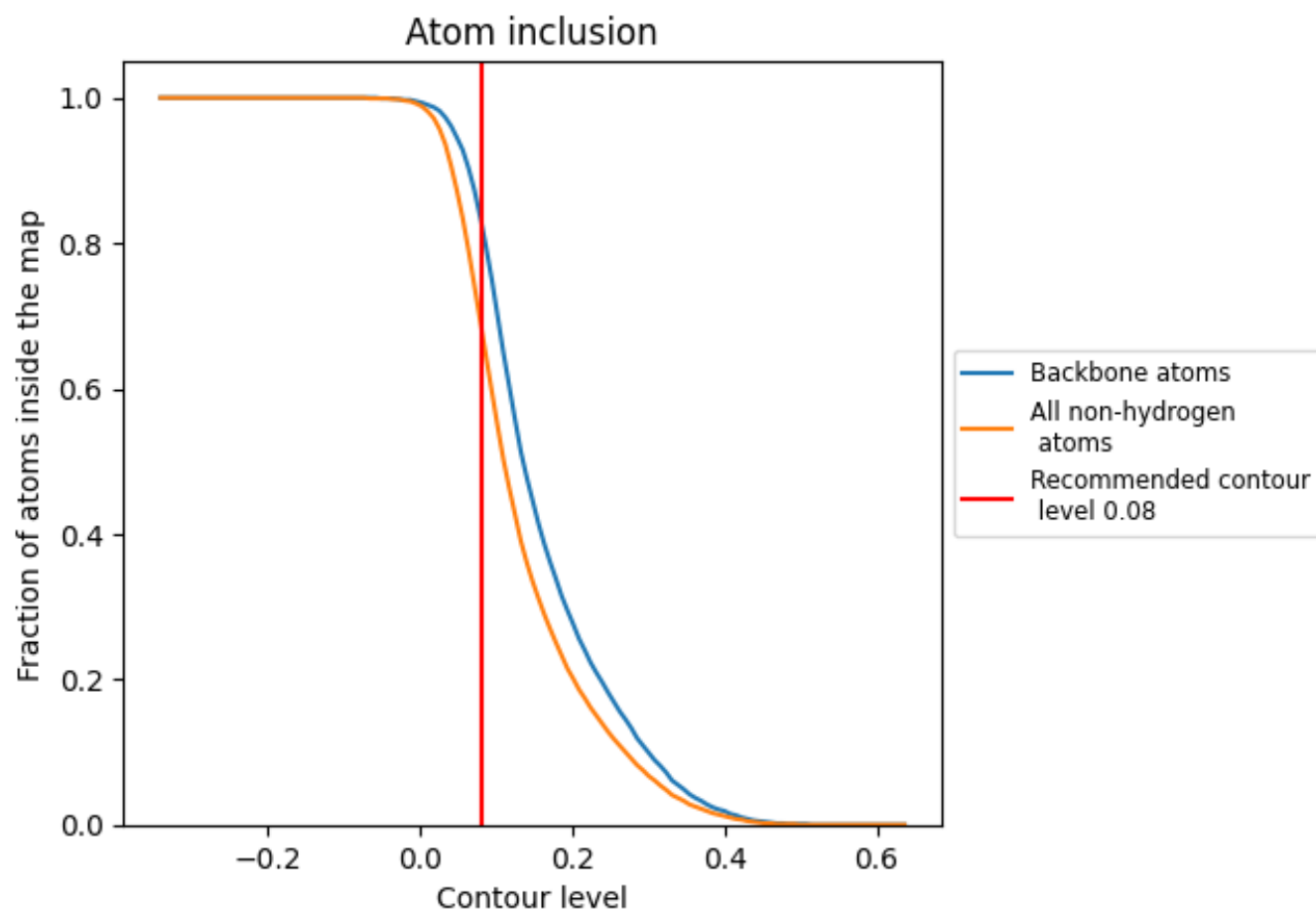
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 83% of all backbone atoms, 69% 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	<div></div> 0.6880	<div></div> 0.3920
A	<div></div> 0.6790	<div></div> 0.3900
B	<div></div> 0.6860	<div></div> 0.3890
C	<div></div> 0.6950	<div></div> 0.4060
D	<div></div> 0.6900	<div></div> 0.3820

