



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:42 PM UTC

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

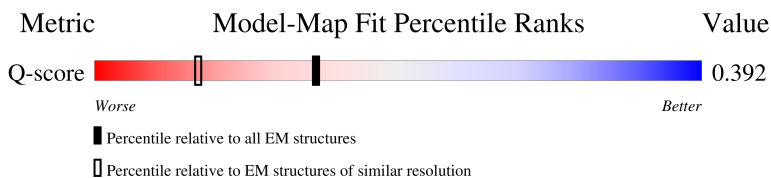
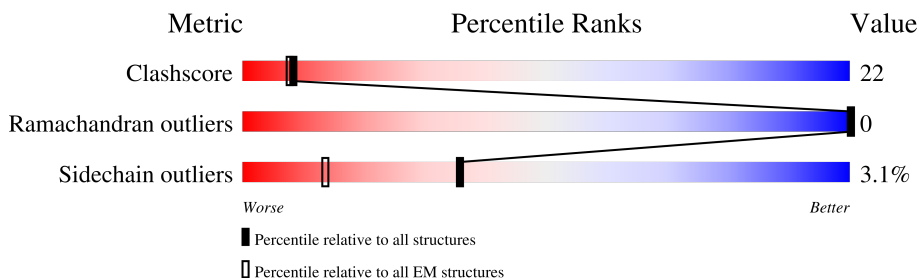
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.15 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14486 (2.65 - 3.65)

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	11% 43% 36% • 19%
1	B	834	9% 45% 35% • 19%
1	C	834	9% 47% 33% • 19%
1	D	834	9% 42% 38% • 19%

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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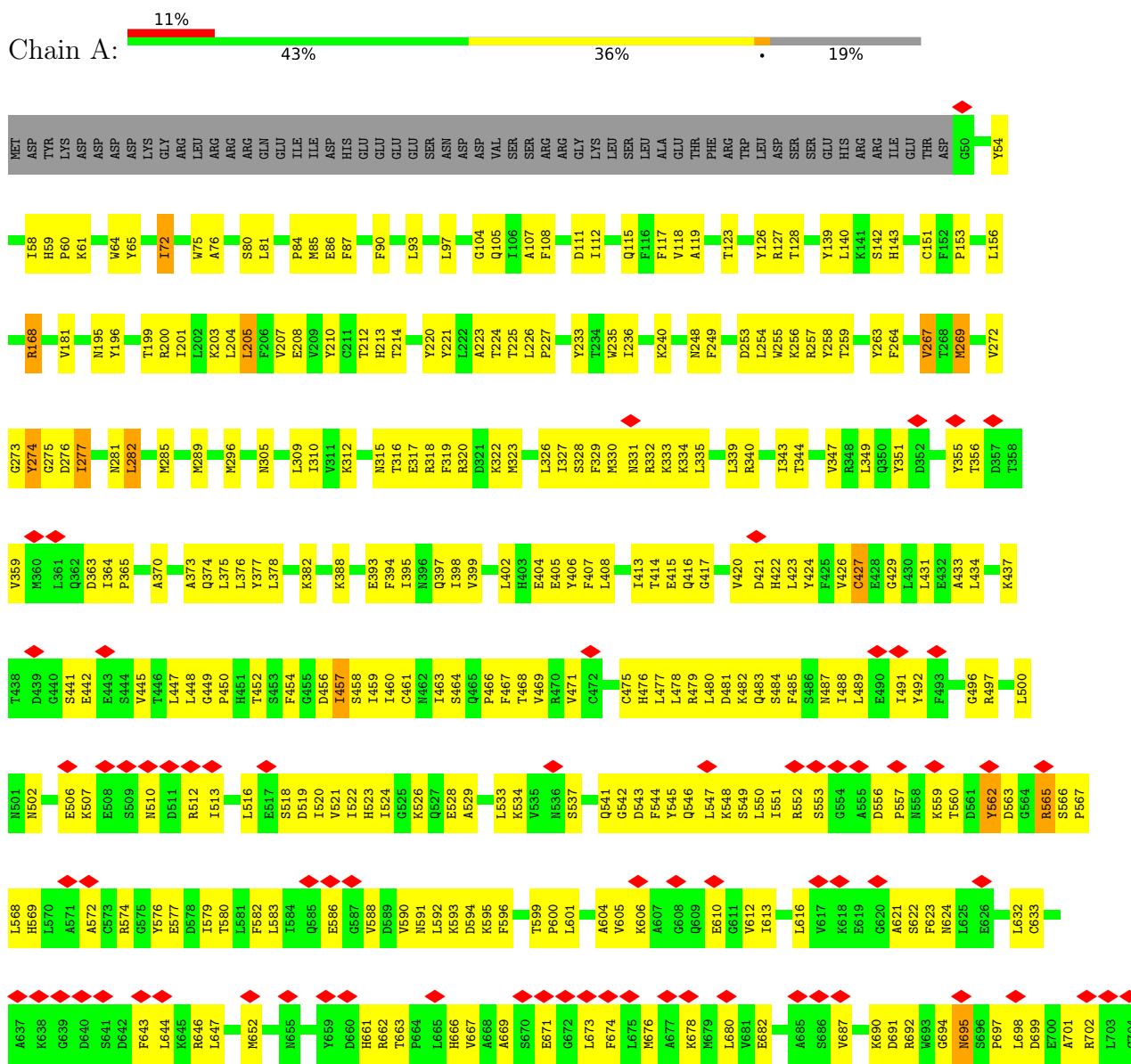
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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ASP	-	expression tag	UNP Q94A76
B	1	LYS	-	expression tag	UNP Q94A76
B	821	HIS	-	expression tag	UNP Q94A76
B	822	HIS	-	expression tag	UNP Q94A76
B	823	HIS	-	expression tag	UNP Q94A76
B	824	HIS	-	expression 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

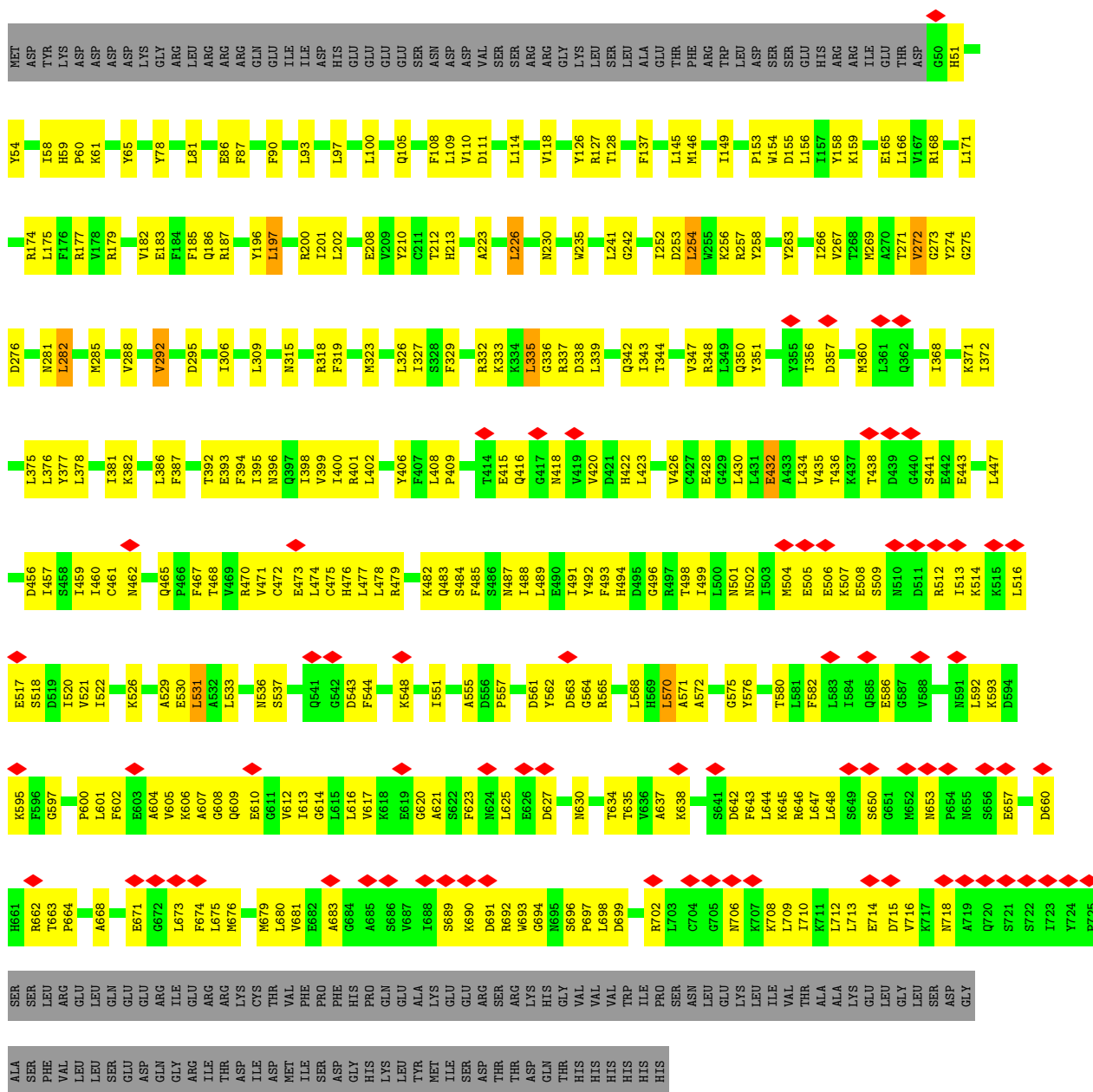
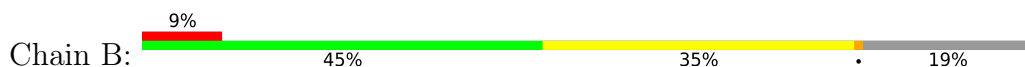
3 Residue-property plots

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	I489	V419	D338	L140	L141
THR	GLY	S696	D627	A555	D495	V420	L339	Y244	L145
HIS	VAL	P697	S628	D556	G496	D421	R340	S245	M146
HIS	VAL	L698	G629	P557	R497	H422	L343	Y246	D147
HIS	VAL	D999	N630	M558	T498	L423	T343	F249	F148
HIS	TRP	R702	F631	K559	I499	V426	G345	I149	I149
HIS	ILE	L703	L632	T560	L500	C427	H346	D253	G150
HIS	PRO	C704	C633	D561	N501	L430	V347	L254	
	SER	G705	T634	Y562	N502	L431	R348	W255	W154
	ASN	N706	T635	D563	I503	L434	L349	K256	D155
	LEU	K707	V636	G564	M504	L435	Q350	R257	
	GLU	K708	A637	R565	E506	T436	Y351	K159	
	LYS	L709	K638	S566	E507	T437	D352	Y263	
	LEU	I710	G639	P567	K507	D438	S353	R168	
	ILE	L713	F643	L568	E508	T439	H354	I266	
	VAL	E714	L644	H569	S509	D439	Y355	V267	
	THR			L570	N510	G440	T358	T268	
	ALA			A571	D511	S441	K361	M269	
	LYS	K717	L647	A572	R512	G442	Q362	I173	
	GLU	N718	L648	C573	I513	E443	D363	R174	
	LEU	A719	S649	R574	K514	S444	I364	R177	
	LEU	Q720	S650	E577	K515	V445	K371	V178	
	GLY	S721	G651	D578	L516	L448	L372	R179	
	LEU	S722	M652	I579	E517	G449	Q374	E189	
	SER	S723	N653	T580	S518	P450	L376	T192	
	ASP	I723	P654	L581	I520	F454	V280	N195	
	GLY	Y724	N655	F582	V521	G455	L281	Y196	
	ALA	P725	S656		I522	D456	L282	L197	
	SER		E657		H523	I457	R283	F198	
	PHE				I524	S458	E284	T199	
	VAL				G525	I459	M285		
	LEU				K526	C461	V288	H213	
	LEU				Q527	N462	M289	T214	
	ARG				E528	I463	I310	F219	
	ILE				A529	S464	F319	Y220	
	THR				E530	Q465	M396	Y221	
	ASP				L531	F466	Q397	L222	
	ASP				A532	F467	I398	A223	
	ILE				K533	T468	M323	T224	
	MET				V534	V469	N324	T225	
	THR				V535	R470	L402	L226	
	VAL				N536	V471	Y406	P227	
	ASP				S537	C475	F407	D325	
	GLY				A538	H476	L408	L326	
	LYS				A539	L477	S328	I327	
	PRO				F540	L478	N230	P228	
	LYS					R479	F329	E231	
	LEU					D480	M330	G332	
	TYR					L481	N331	Y233	
	GLU					K482	R332	T234	
	MET						E411	W235	
	ILE						V412		
							I413		
							T414		

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%)	30	58
1	B	597/743 (80%)	579 (97%)	18 (3%)	36	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	597/743 (80%)	585 (98%)	12 (2%)	48	68
1	D	597/743 (80%)	575 (96%)	22 (4%)	30	58
All	All	2388/2972 (80%)	2314 (97%)	74 (3%)	36	61

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.

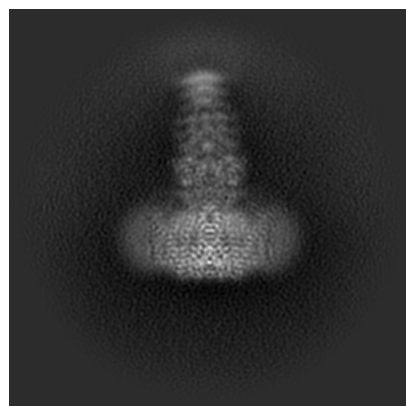
6 Map visualisation [i](#)

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.

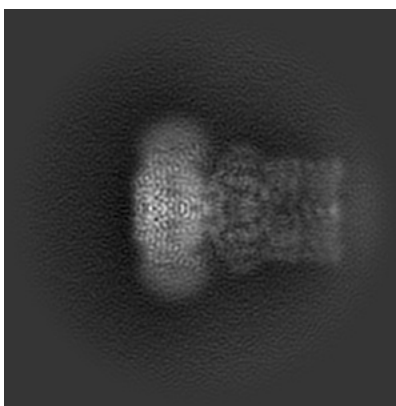
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

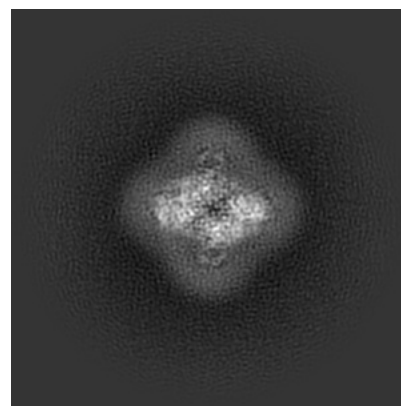
6.1.1 Primary map



X

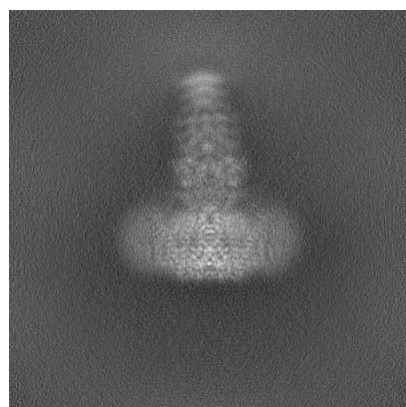


Y

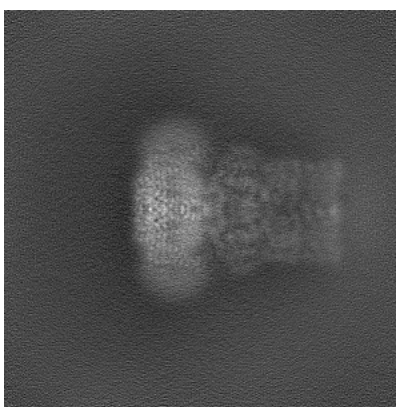


Z

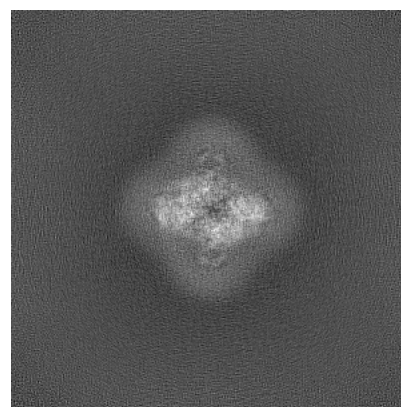
6.1.2 Raw map



X



Y

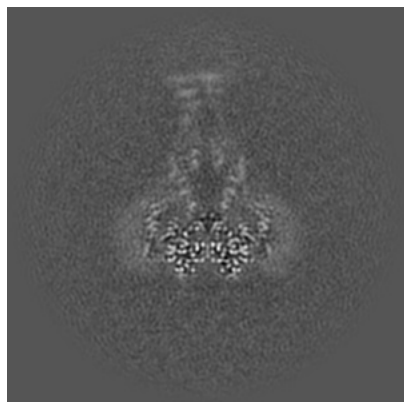


Z

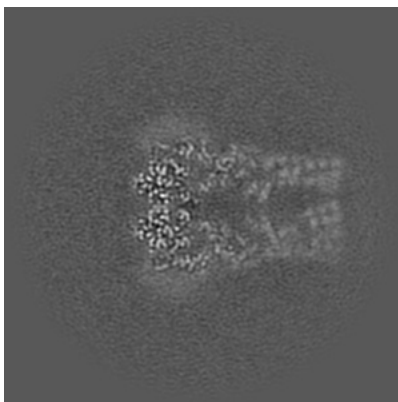
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

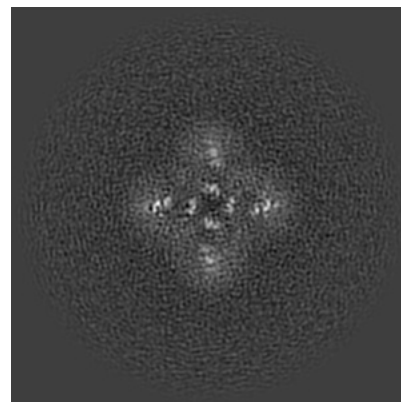
6.2.1 Primary map



X Index: 200

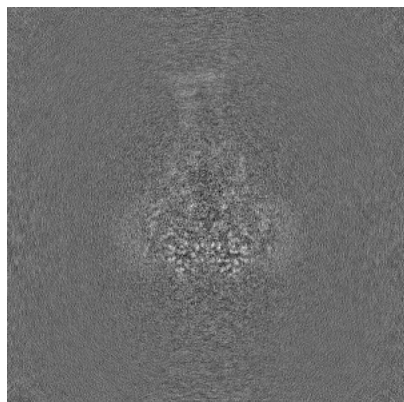


Y Index: 200

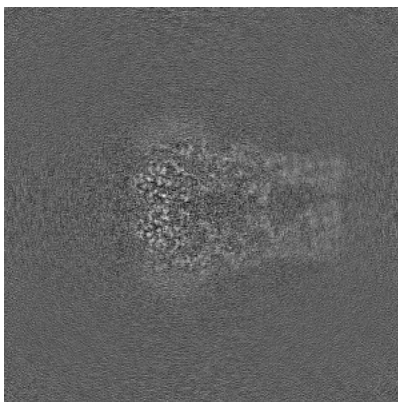


Z Index: 200

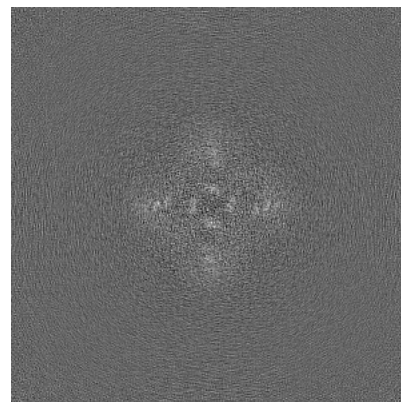
6.2.2 Raw map



X Index: 200



Y Index: 200

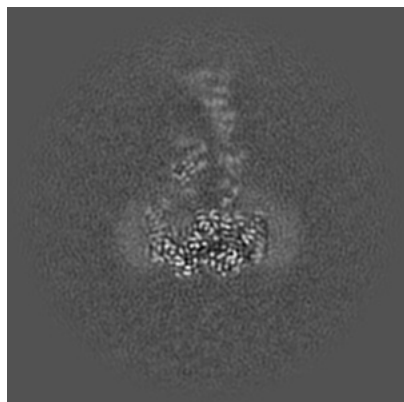


Z Index: 200

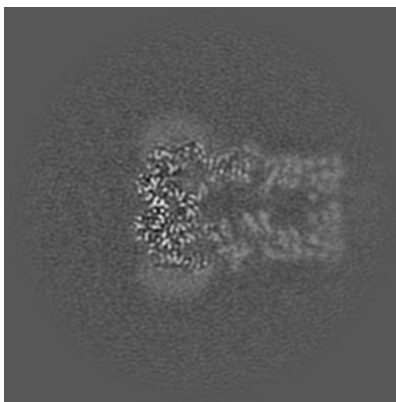
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

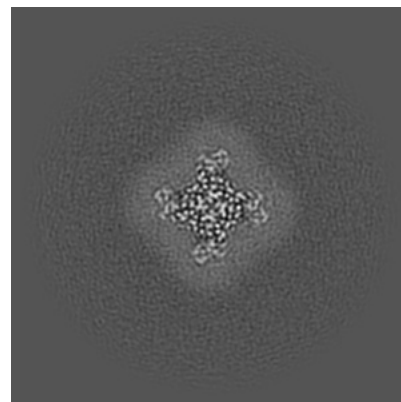
6.3.1 Primary map



X Index: 192

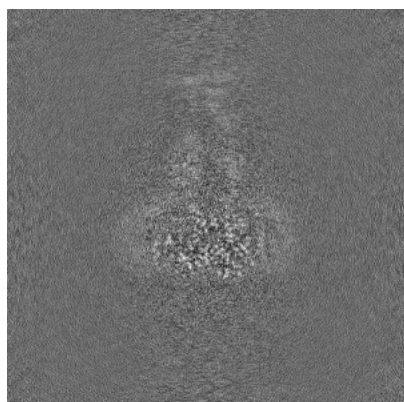


Y Index: 196

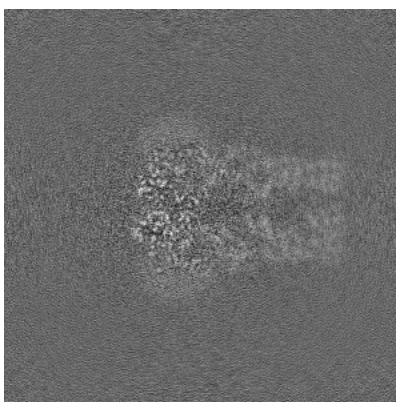


Z Index: 146

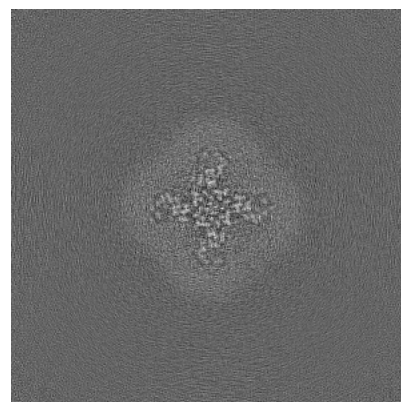
6.3.2 Raw map



X Index: 195



Y Index: 198

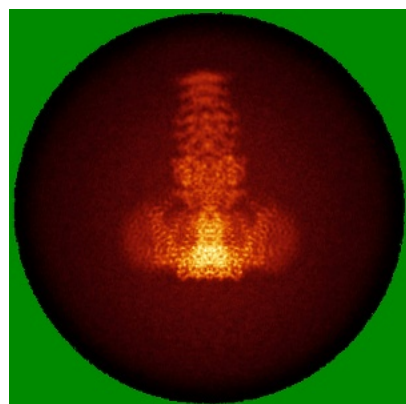


Z Index: 160

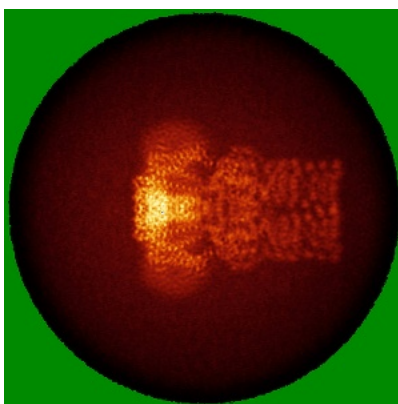
The images above show the largest variance slices of the map in three orthogonal directions.

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

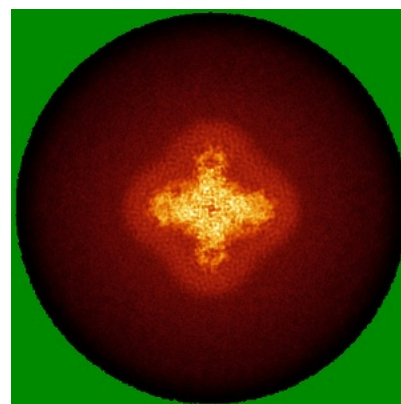
6.4.1 Primary map



X

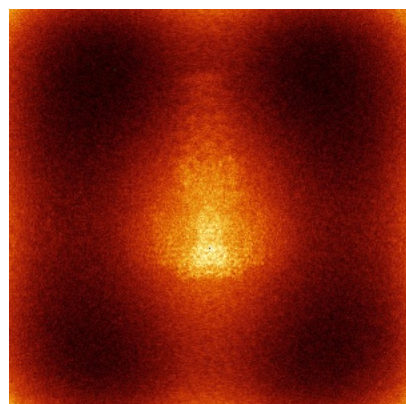


Y

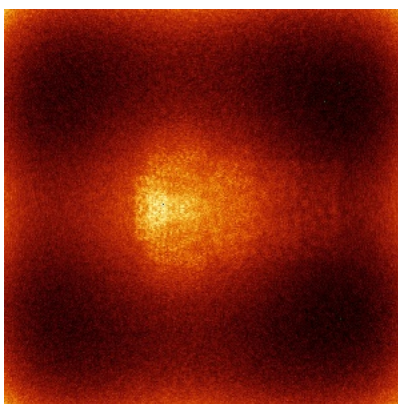


Z

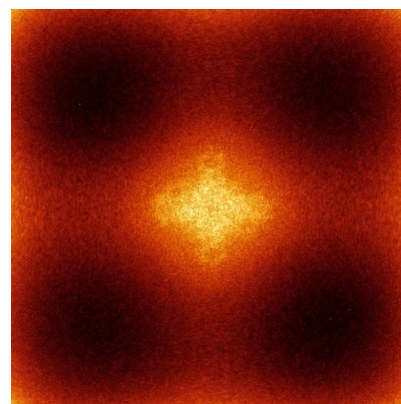
6.4.2 Raw map



X



Y

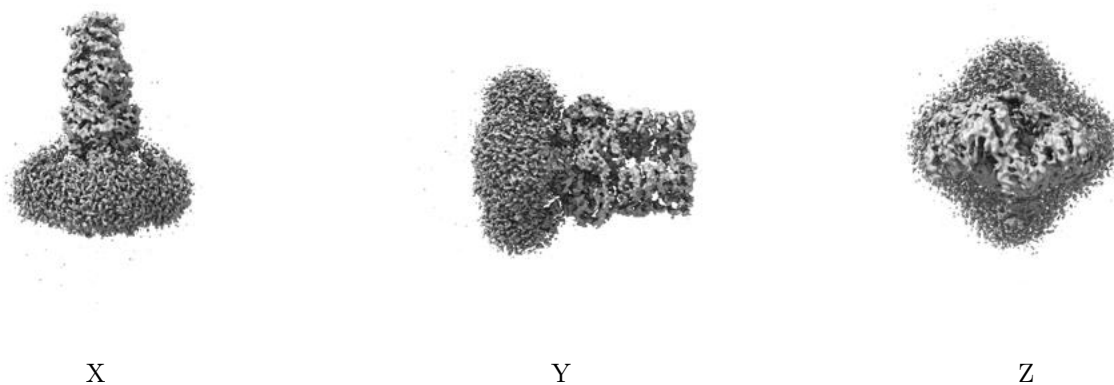


Z

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.

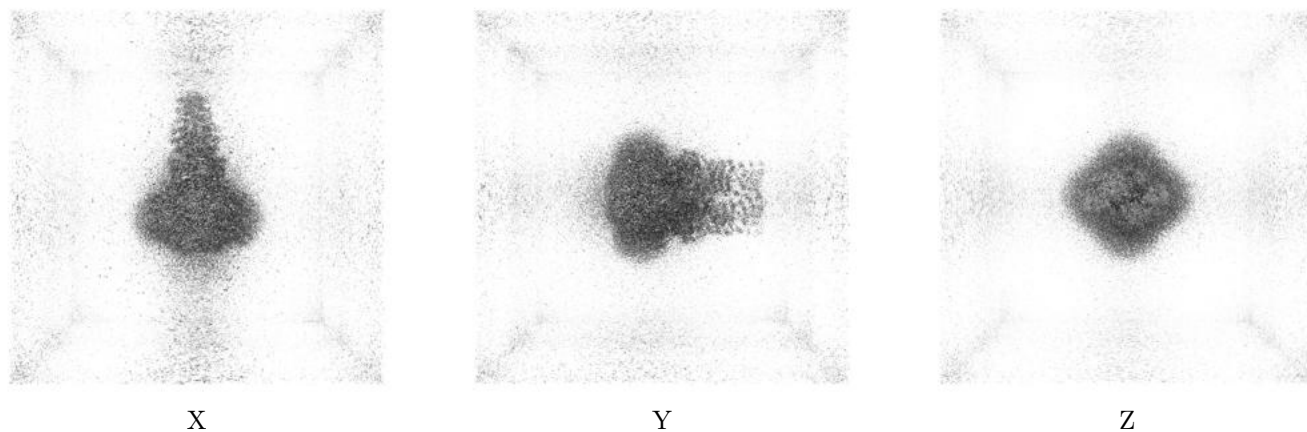
6.5 Orthogonal surface views [i](#)

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.

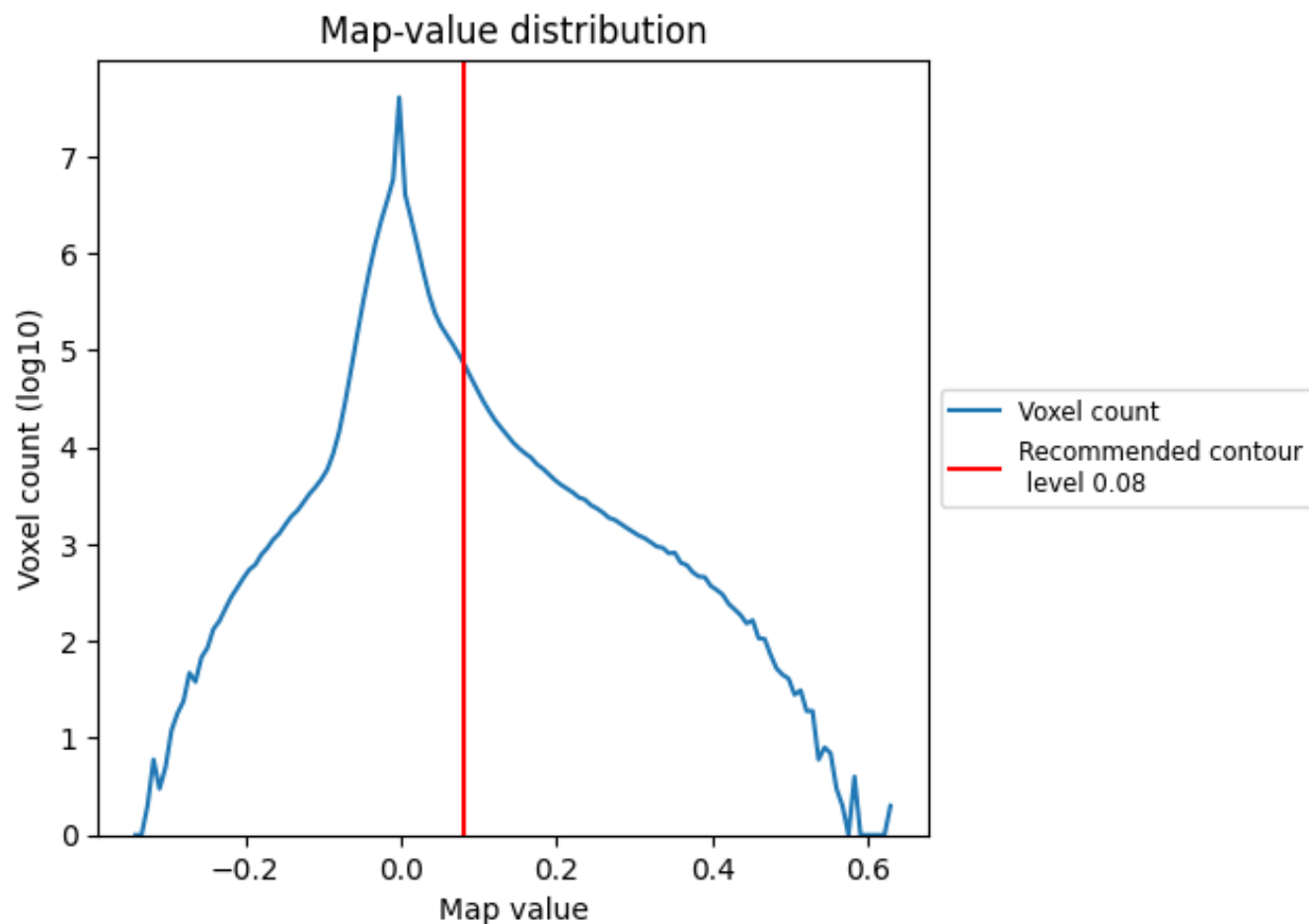
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

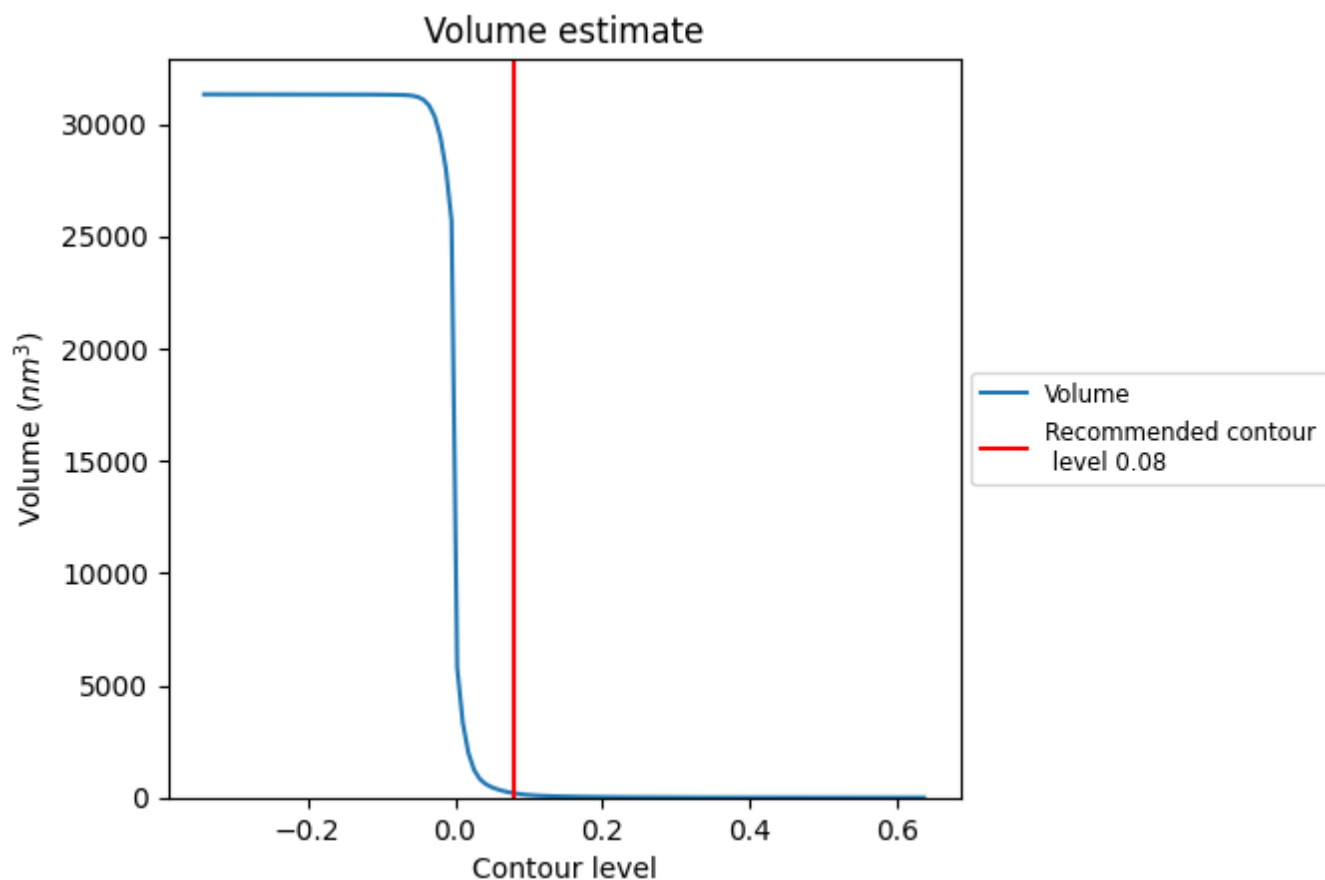
This section contains the results of statistical analysis of the map.

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.

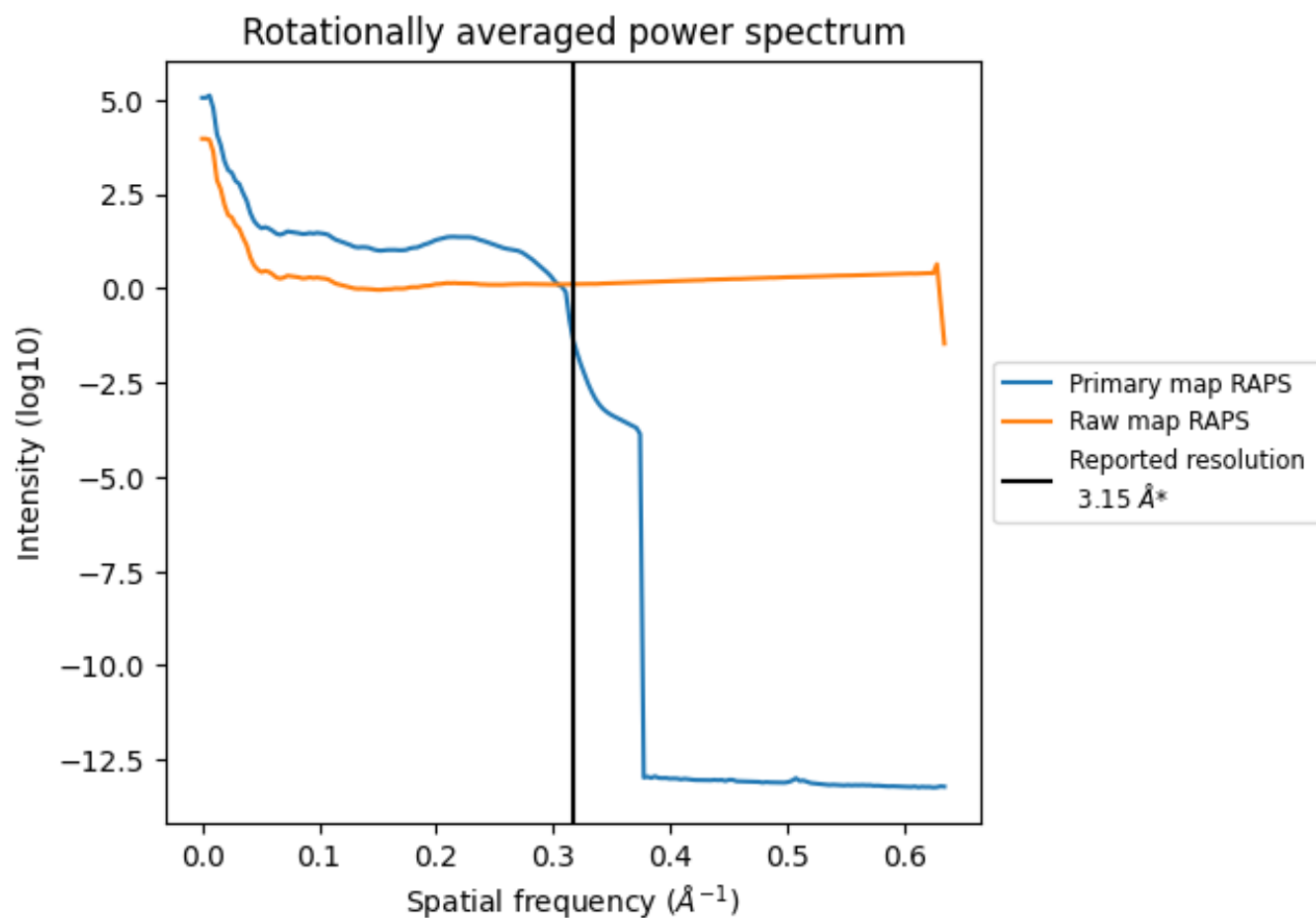
7.2 Volume estimate [i](#)



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 ⓘ

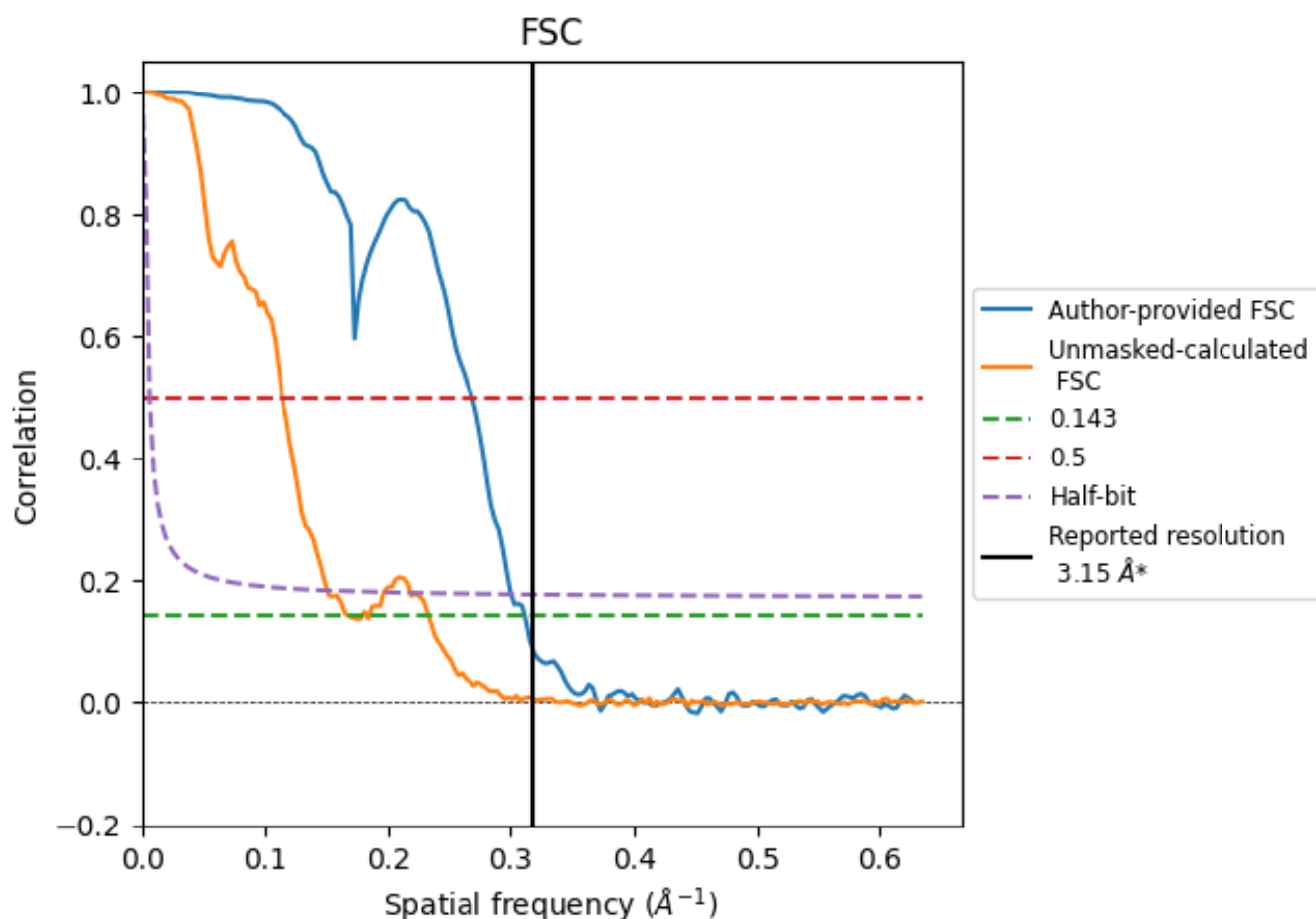


*Reported resolution corresponds to spatial frequency of 0.317 Å⁻¹

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 $0.317 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

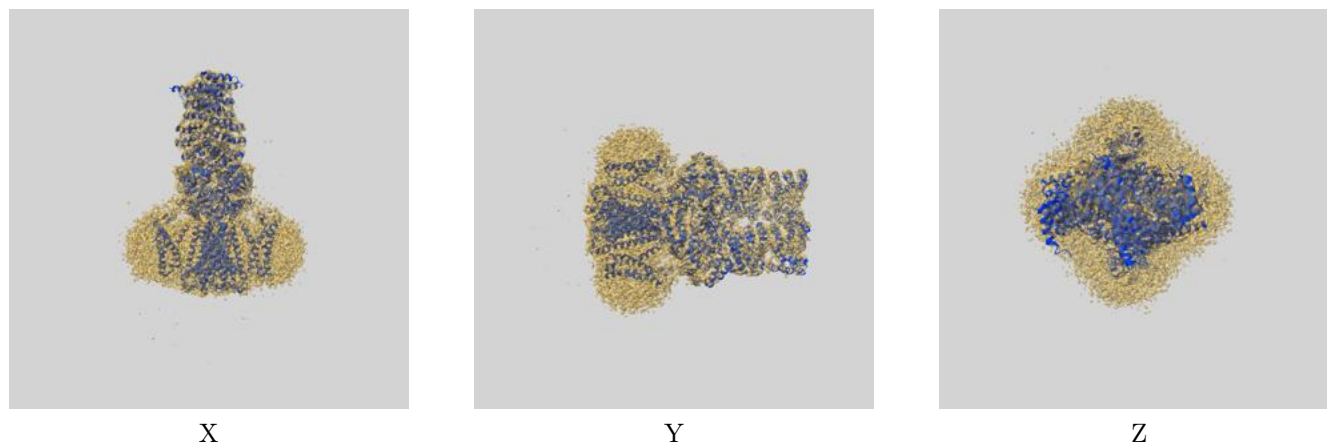
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	3.21	3.73	3.33
Unmasked-calculated*	5.96	8.78	6.63

*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](#)

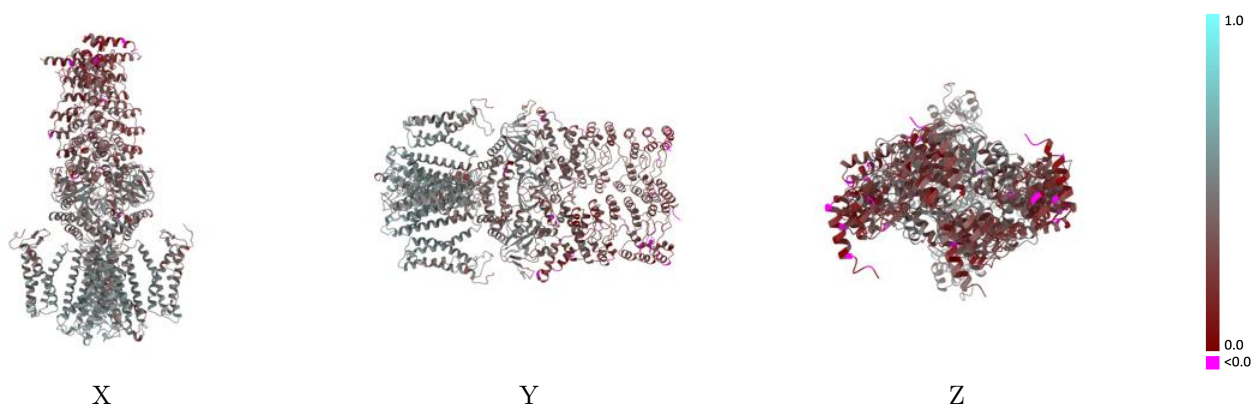
This section contains information regarding the fit between EMDB map EMD-62916 and PDB model 9LA1. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



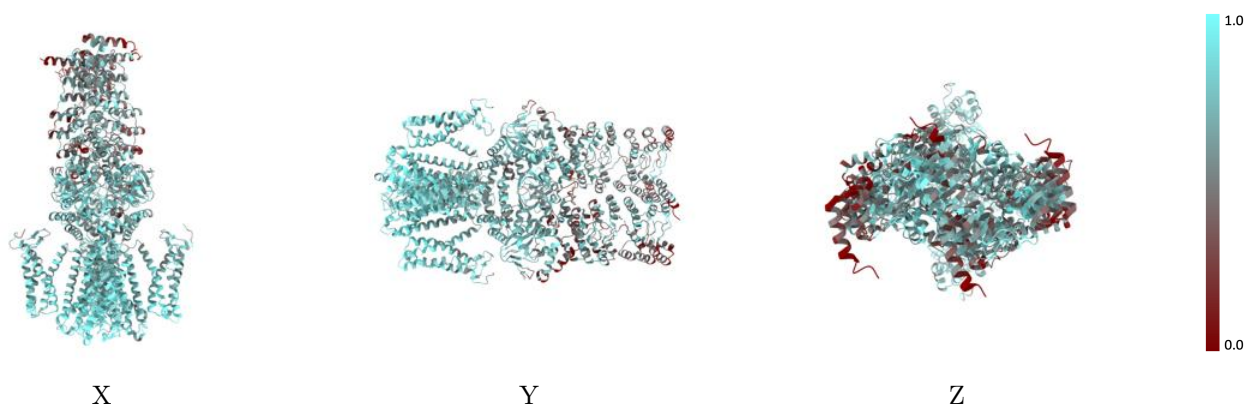
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



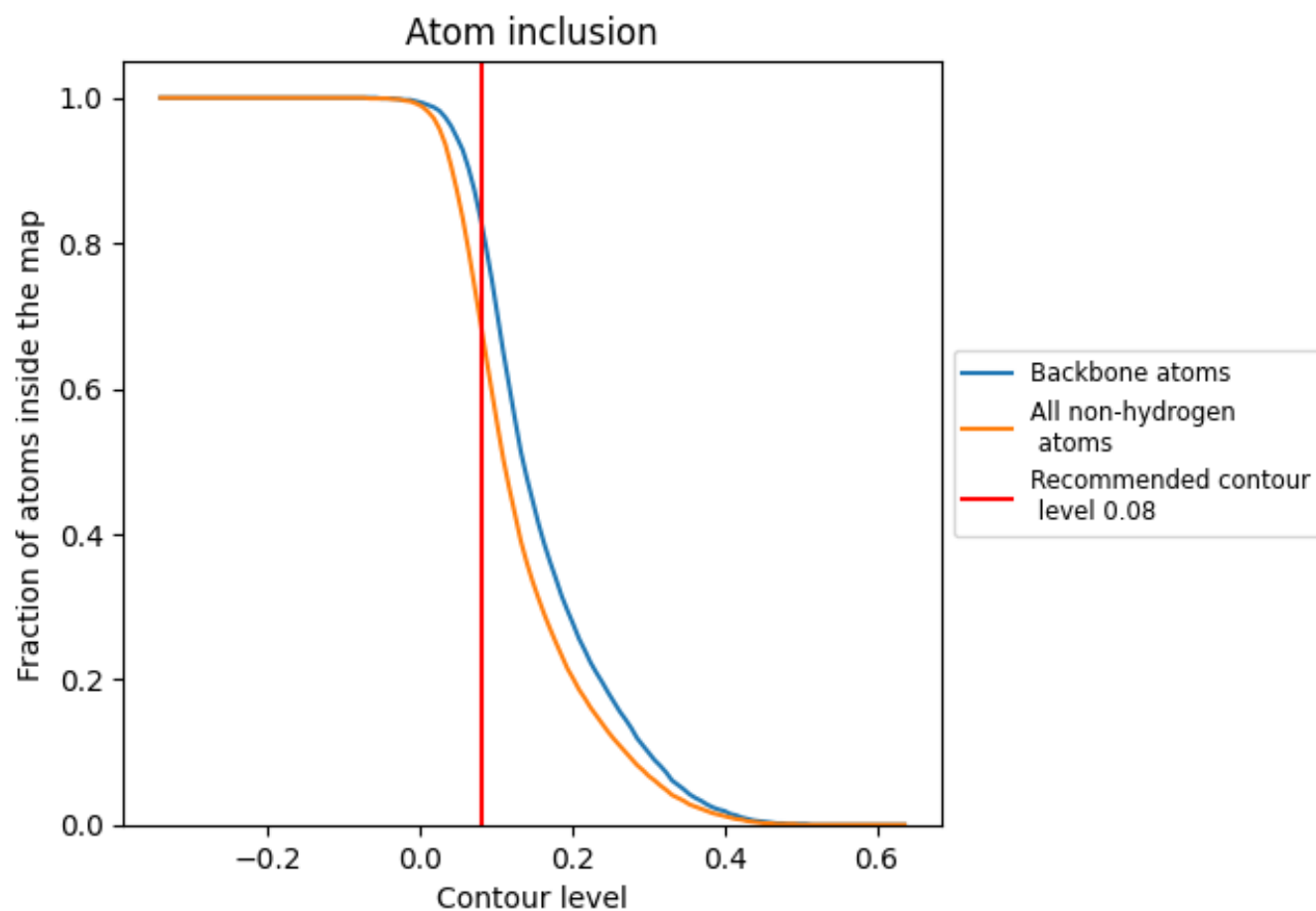
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

