



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 05:47 PM UTC

PDB ID : 8GK0 / pdb_00008gk0
EMDB ID : EMD-40177
Title : Multi-drug efflux pump RE-CmeB bound with Erythromycin
Authors : Zhang, Z.
Deposited on : 2023-03-16
Resolution : 3.44 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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

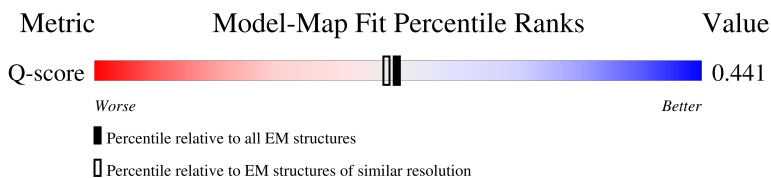
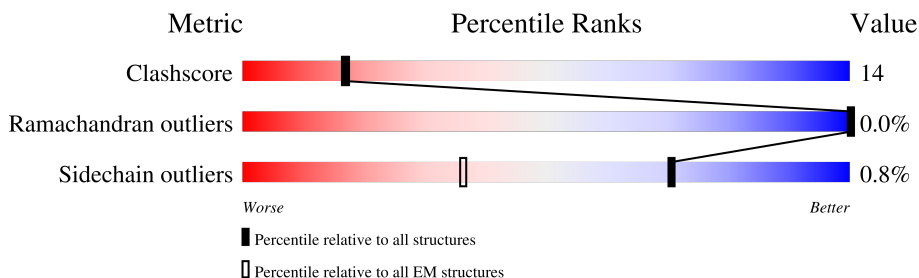
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.44 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	13877 (2.94 - 3.94)

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	1039	
1	B	1039	
1	C	1039	

2 Entry composition [i](#)

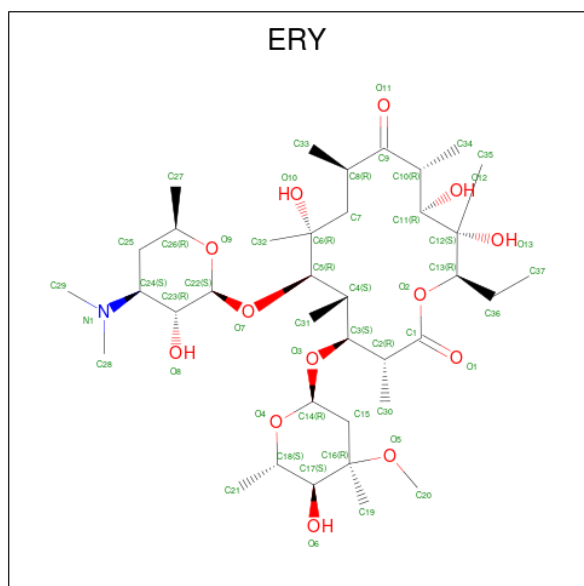
There are 2 unique types of molecules in this entry. The entry contains 23949 atoms, of which 67 are hydrogens and 0 are deuteriums.

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 Efflux pump membrane transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1025	Total	C	N	O	S	0	0
			7877	5110	1269	1470	28		
1	A	1032	Total	C	N	O	S	0	0
			7975	5173	1286	1488	28		
1	C	1032	Total	C	N	O	S	0	0
			7979	5174	1288	1489	28		

- Molecule 2 is ERYTHROMYCIN A (CCD ID: ERY) (formula: $C_{37}H_{67}NO_{13}$) (labeled as "Ligand of Interest" by depositor).

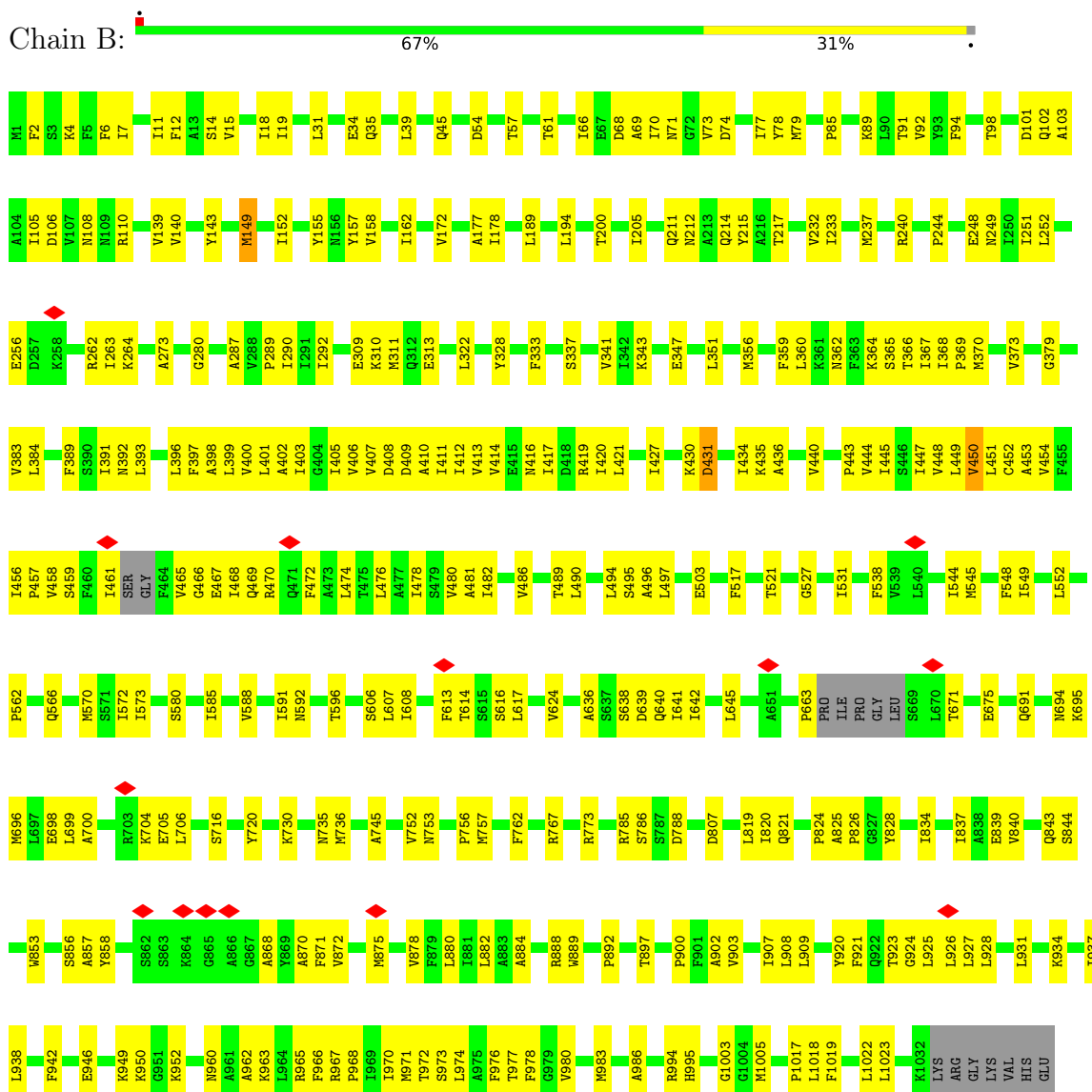


Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	H	N	O	0
			118	37	67	1	13	

3 Residue-property plots

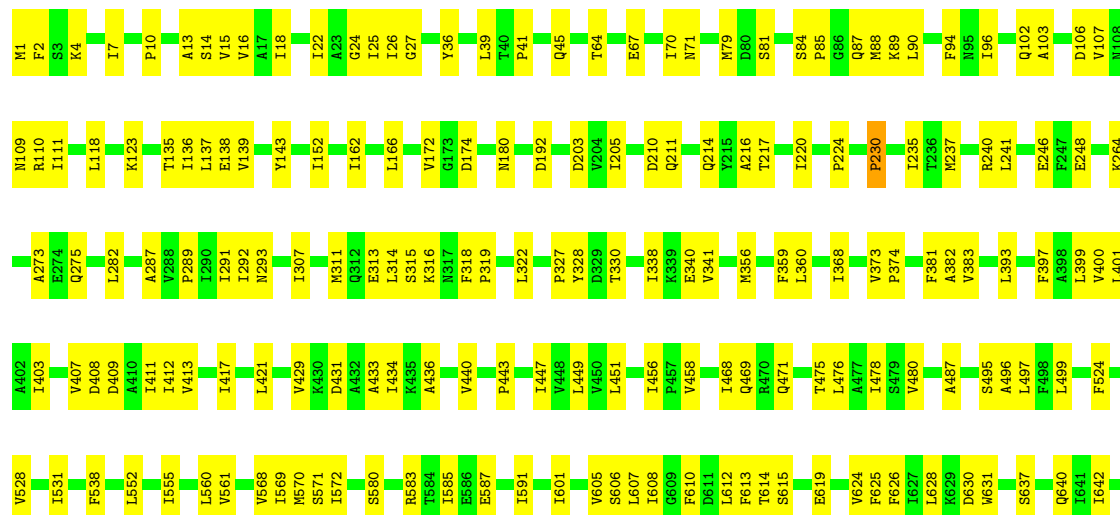
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

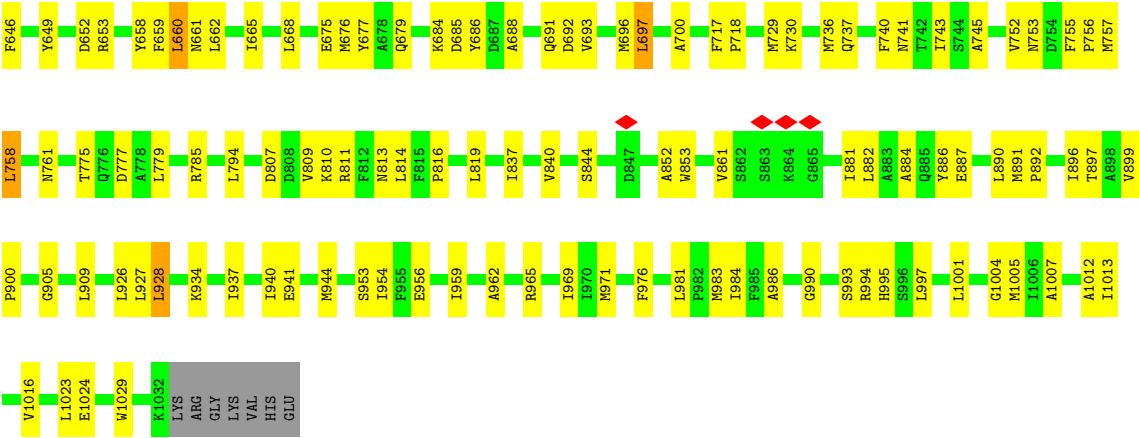
- Molecule 1: Efflux pump membrane transporter



A986	F879	M729	I601	I478	G379	K264	M1
R994	M736	M736	S604	S479	T380	L282	K4
L1001	L882	F740	V605	V480	V383	L290	I7
I1002	A884	M753	F610	G484	Y385	L291	P10
M1005	Q885	M753	D611	F485	S390	L292	P10
I1006	R888	P756	L612	L488	N391	N299	S14
A1007	R890	M757	E619	T491	L393	N302	V15
I1013	M891	F762	F625	L497	F397	K305	I18
F1014	P892	Q763	P626	T500	A398	E309	I19
L1023	L893	V764	D630	R501	L399	K310	G24
K1032	V895	L769	Q633	N502	V400	K311	L31
LYS	T897	F772	R634	K512	A402	L314	E34
ARG	R773	M774	Y649	F517	I403	S315	Q35
GLY	A902	M774	M654	F517	I405	F318	Y36
LYS	G905	A778	M654	F517	I405	F318	P37
VAL	D916	I782	L660	V523	I411	G321	S38
HIS	I919	M791	N661	I531	V413	L322	L39
GLU	T923	I792	L662	R534	I417	K323	T40
	T923	P793	P663	T535	I417	Y324	T43
	L794	L794	P664	T536	S425	L326	T44
L928	P666	L794	P665	R537	S425	L326	Q45
L929	P667	L800	G667	F538	I434	P327	V46
G930	V801	R802	L668	V539	K435	D329	Y50
L931	R802	R802	S669	L540	A436	D329	T51
			L670	L540	M437	L332	G52
N935	P806	P806	L670	L544	M438	L332	T205
A936	A936	P806	Y677	M545	E439	T344	I66
I937	I937	K810	Y677	I546	V440	F345	I70
L938	R811	R811	K684	I549	P443	L351	N71
L939	D685	F812	D685	I549	V444	V352	N75
N813	N813	N813	Y686	L552	I445	L353	N75
F942	F942	L814	Y686	L552	S446	V354	D80
K949	K949	L819	T689	I555	I447	M356	G221
K950	K950	L819	Q690	I555	I447	M356	V92
G951	G951	T829	Q691	S559	V450	N362	N95
K952	K952	T829	D692	S559	L451	F363	P100
A961	A961	A833	V693	S563	V454	K228	I105
R965	R965	T837	M696	E564	F455	V232	D106
F966	F966	V840	R701	D565	V458	L367	V107
R967	R967	V840	V709	V568	I569	P369	R110
P968	P968	L845	R710	M570	I461	M370	T115
I969	I969	L845	R710	M570	I461	L371	L118
		Y649	T715	T590	F464	A372	
L981	L981	Y649	T715	T590	F464	V373	
P982	P982	A868	Y720	M598	Q469	P374	
N983	N983	K721	L722	K599	R477	L377	
F984	F984	V871	L722	K599	R477	L377	
E985	E985	V871	L722	K599	R477	L377	

- Chain C:  71% 28%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17038	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	36.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.823	Depositor
Minimum map value	-0.331	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	376.64, 376.64, 376.64	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ERY

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	0.17	0/8129	0.38	0/11043
1	B	0.18	0/8025	0.43	0/10903
1	C	0.19	0/8133	0.43	0/11047
All	All	0.18	0/24287	0.41	0/32993

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	7975	0	8150	206	0
1	B	7877	0	8023	242	0
1	C	7979	0	8156	254	0
2	C	51	67	67	10	0
All	All	23882	67	24396	672	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 14.

All (672) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:LEU:HG	1:B:927:LEU:HD13	1.51	0.92
1:C:928:LEU:HD21	1:C:1004:GLY:HA3	1.52	0.90
1:C:166:LEU:HD21	1:C:311:MET:HE1	1.55	0.89
1:C:572:ILE:HG13	1:C:613:PHE:CE2	2.10	0.87
1:A:902:ALA:HB1	1:A:928:LEU:HD12	1.58	0.84
1:B:639:ASP:HA	1:B:642:ILE:HD12	1.63	0.81
1:C:172:VAL:HG13	1:C:292:ILE:HG23	1.62	0.81
1:C:560:LEU:HD21	1:C:668:LEU:HD11	1.61	0.80
1:C:665:ILE:HG12	1:C:668:LEU:HD22	1.63	0.80
1:C:572:ILE:HG13	1:C:613:PHE:HE2	1.46	0.79
1:A:214:GLN:HG3	1:A:240:ARG:HG3	1.66	0.77
1:A:455:PHE:HB3	1:A:473:ALA:HB1	1.66	0.77
1:C:757:MET:HG2	1:C:758:LEU:HD22	1.67	0.75
1:C:585:ILE:HG12	1:C:608:ILE:HD13	1.66	0.75
1:B:430:LYS:HD3	1:B:496:ALA:HB1	1.68	0.74
1:B:983:MET:HG3	1:B:994:ARG:HG2	1.70	0.74
1:B:517:PHE:HZ	1:B:967:ARG:HA	1.53	0.73
1:B:15:VAL:HG11	1:C:884:ALA:HB2	1.70	0.73
1:A:884:ALA:HB2	1:C:15:VAL:HG21	1.70	0.72
1:C:45:GLN:HG3	1:C:89:LYS:HE3	1.71	0.72
1:A:24:GLY:HA3	1:A:378:LEU:HB3	1.72	0.71
1:A:137:LEU:HG	1:A:138:GLU:HG2	1.71	0.71
1:C:591:ILE:HD12	1:C:649:TYR:CE2	2.25	0.71
1:B:467:GLU:OE1	1:B:467:GLU:N	2.21	0.71
1:A:353:LEU:HG	1:A:370:MET:HE3	1.73	0.71
1:A:434:ILE:O	1:A:438:ASN:ND2	2.24	0.70
1:A:405:ILE:HD11	1:A:931:LEU:HD21	1.72	0.70
1:A:969:ILE:HG21	1:A:1013:ILE:HG21	1.73	0.70
1:B:973:SER:HA	1:B:976:PHE:CE1	2.27	0.70
1:B:233:ILE:HD12	1:C:718:PRO:HB2	1.73	0.70
1:C:407:VAL:O	1:C:411:ILE:HG12	1.91	0.70
1:B:459:SER:HA	1:B:469:GLN:HE22	1.57	0.70
1:C:449:LEU:HB3	1:C:881:ILE:HD13	1.73	0.70
1:B:102:GLN:NE2	1:B:106:ASP:OD1	2.26	0.69
1:C:642:ILE:HD11	1:C:661:ASN:OD1	1.91	0.69
1:B:362:ASN:HD21	1:B:503:GLU:HB3	1.57	0.69
1:C:613:PHE:HZ	1:C:660:LEU:HD11	1.56	0.69
1:C:568:VAL:HG23	1:C:662:LEU:CD1	2.23	0.69
1:B:973:SER:HA	1:B:976:PHE:CZ	2.28	0.68
1:B:212:ASN:O	1:B:753:ASN:ND2	2.27	0.68
1:B:552:LEU:HD13	1:B:908:LEU:HA	1.75	0.68
1:C:443:PRO:O	1:C:447:ILE:HD12	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:570:MET:SD	1:C:612:LEU:HD23	2.34	0.68
1:A:446:SER:OG	1:A:885:GLN:NE2	2.27	0.68
1:B:968:PRO:HA	1:B:971:MET:HE2	1.76	0.68
1:B:451:LEU:O	1:B:454:VAL:HG12	1.94	0.67
1:A:413:VAL:O	1:A:417:ILE:HD12	1.94	0.67
1:C:729:MET:HE3	1:C:730:LYS:HE2	1.76	0.67
1:A:402:ALA:HA	1:A:405:ILE:HB	1.77	0.67
1:B:407:VAL:O	1:B:411:ILE:HG13	1.95	0.66
1:A:71:ASN:O	1:A:110:ARG:NH2	2.28	0.66
1:C:677:TYR:HB2	1:C:852:ALA:HB3	1.78	0.66
1:B:699:LEU:HD23	1:B:844:SER:HB2	1.77	0.66
1:C:612:LEU:HD22	1:C:625:PHE:HZ	1.58	0.66
1:C:139:VAL:O	1:C:327:PRO:HD2	1.96	0.65
1:B:412:ILE:HG23	1:B:965:ARG:HH22	1.61	0.65
1:B:108:ASN:HD22	1:C:109:ASN:HB3	1.61	0.65
1:B:573:ILE:HD11	1:B:591:ILE:HD13	1.79	0.64
1:B:671:THR:HB	1:B:856:SER:HB2	1.78	0.64
1:C:811:ARG:HH21	1:C:816:PRO:HD3	1.63	0.64
1:A:633:GLN:N	1:A:633:GLN:OE1	2.29	0.64
1:C:612:LEU:HG	2:C:1101:ERY:C26	2.28	0.64
1:C:443:PRO:HG3	1:C:941:GLU:HG3	1.80	0.64
1:C:591:ILE:HD12	1:C:649:TYR:HE2	1.63	0.64
1:C:659:PHE:C	1:C:660:LEU:HD23	2.22	0.64
1:B:942:PHE:HD2	1:B:965:ARG:HD3	1.62	0.63
1:C:665:ILE:HD11	1:C:668:LEU:HD13	1.79	0.63
1:B:907:ILE:HG12	1:B:921:PHE:HZ	1.63	0.63
1:A:660:LEU:HD21	1:A:710:ARG:HH22	1.63	0.63
1:A:729:MET:HE1	1:A:736:MET:SD	2.38	0.63
1:B:467:GLU:HA	1:B:470:ARG:HB3	1.81	0.63
1:A:677:TYR:HE2	1:A:810:LYS:HD3	1.64	0.63
1:B:162:ILE:HG23	1:B:311:MET:HE1	1.81	0.63
1:C:447:ILE:HG12	1:C:934:LYS:HG3	1.81	0.63
1:A:950:LYS:HB2	1:A:952:LYS:HG2	1.81	0.62
1:A:568:VAL:HG13	1:A:662:LEU:HD21	1.80	0.62
1:C:205:ILE:HD11	1:C:745:ALA:HB2	1.79	0.62
1:C:340:GLU:HG2	1:C:994:ARG:HH12	1.63	0.62
1:A:458:VAL:HA	1:A:461:ILE:HD12	1.82	0.62
1:C:610:PHE:CE2	1:C:612:LEU:HA	2.35	0.62
1:A:248:GLU:HB3	1:A:264:LYS:HB2	1.80	0.62
1:A:136:ILE:HG23	1:A:291:ILE:HG23	1.82	0.62
1:C:241:LEU:HD22	1:C:246:GLU:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:VAL:HG22	1:B:406:VAL:HG13	1.82	0.62
1:A:192:ASP:N	1:A:192:ASP:OD1	2.33	0.62
1:C:291:ILE:C	1:C:292:ILE:HD12	2.24	0.62
1:A:162:ILE:HD12	1:A:314:LEU:HD13	1.81	0.61
1:A:684:LYS:NZ	1:A:692:ASP:OD2	2.32	0.61
1:B:938:LEU:HD13	1:B:965:ARG:HH21	1.65	0.61
1:C:570:MET:HE3	1:C:660:LEU:HD12	1.81	0.61
1:B:383:VAL:HG11	1:B:478:ILE:HG21	1.82	0.61
1:C:471:GLN:O	1:C:475:THR:HG23	2.00	0.61
1:C:411:ILE:HG23	1:C:971:MET:HE3	1.83	0.61
1:B:466:GLY:HA2	1:B:469:GLN:HE21	1.65	0.61
1:B:466:GLY:O	1:B:470:ARG:N	2.32	0.61
1:A:4:LYS:HA	1:A:7:ILE:HG22	1.83	0.61
1:C:174:ASP:HB3	1:C:293:ASN:HB2	1.82	0.61
1:C:458:VAL:HG21	1:C:926:LEU:HD11	1.82	0.61
1:C:693:VAL:O	1:C:697:LEU:HD22	2.00	0.60
1:A:299:ASN:ND2	1:A:302:ASN:OD1	2.33	0.60
1:A:619:GLU:OE1	1:A:619:GLU:N	2.31	0.60
1:C:568:VAL:HG23	1:C:662:LEU:HD13	1.84	0.60
1:C:612:LEU:HG	2:C:1101:ERY:H26	1.83	0.60
1:C:686:TYR:CZ	1:C:809:VAL:HG13	2.35	0.60
1:C:976:PHE:HD2	1:C:1005:MET:HE1	1.66	0.60
1:C:139:VAL:HG22	1:C:291:ILE:CD1	2.31	0.60
1:C:610:PHE:CZ	1:C:612:LEU:HA	2.37	0.60
1:B:14:SER:O	1:B:18:ILE:HD12	2.01	0.60
1:C:528:VAL:HA	1:C:531:ILE:HG12	1.83	0.60
1:B:410:ALA:O	1:B:414:VAL:HG12	2.02	0.60
1:C:413:VAL:O	1:C:417:ILE:HG12	2.00	0.60
1:C:572:ILE:HG21	1:C:613:PHE:CE2	2.37	0.60
1:B:200:THR:HG21	1:B:785:ARG:H	1.67	0.59
1:B:699:LEU:HG	1:B:840:VAL:HG23	1.83	0.59
1:A:305:LYS:O	1:A:309:GLU:HG3	2.00	0.59
1:C:292:ILE:HD12	1:C:292:ILE:N	2.16	0.59
1:C:572:ILE:HB	1:C:658:TYR:HB2	1.84	0.59
1:B:694:ASN:O	1:B:698:GLU:HG3	2.03	0.59
1:A:40:THR:OG1	1:A:667:GLY:HA3	2.03	0.59
1:B:696:MET:HE2	1:B:820:ILE:HD13	1.84	0.59
1:C:71:ASN:O	1:C:110:ARG:NH2	2.35	0.59
1:B:450:VAL:HG23	1:B:878:VAL:HG22	1.84	0.59
1:B:531:ILE:HG12	1:B:538:PHE:CE2	2.38	0.59
1:C:81:SER:HB2	1:C:90:LEU:HG	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:VAL:HG13	1:C:959:ILE:HD12	1.85	0.59
1:B:448:VAL:HG13	1:B:480:VAL:HG13	1.84	0.58
1:C:289:PRO:HG2	1:C:607:LEU:HD21	1.85	0.58
1:C:328:TYR:CZ	1:C:330:THR:HG22	2.37	0.58
1:B:942:PHE:CD2	1:B:965:ARG:HD3	2.39	0.58
1:B:413:VAL:O	1:B:417:ILE:HG13	2.03	0.58
1:B:427:ILE:HD12	1:B:435:LYS:HZ1	1.68	0.58
1:B:447:ILE:HG21	1:B:934:LYS:HE2	1.86	0.58
1:C:652:ASP:OD1	1:C:653:ARG:N	2.37	0.58
1:A:685:ASP:OD1	1:A:686:TYR:N	2.36	0.58
1:B:252:LEU:HD21	1:B:263:ILE:HG12	1.86	0.58
1:B:960:ASN:HD22	1:B:963:LYS:HE3	1.69	0.58
1:B:962:ALA:HB2	1:B:1017:PRO:HG3	1.85	0.57
1:A:692:ASP:OD2	1:A:849:TYR:OH	2.20	0.57
1:B:11:ILE:HD13	1:C:887:GLU:HG3	1.86	0.57
1:B:251:ILE:HB	1:C:730:LYS:HG3	1.87	0.57
1:C:162:ILE:HD11	1:C:318:PHE:HE1	1.69	0.57
1:C:752:VAL:HG23	1:C:753:ASN:N	2.19	0.57
1:B:367:ILE:HA	1:B:370:MET:HB3	1.86	0.57
1:A:188:TRP:HB3	1:A:769:LEU:HB2	1.85	0.57
1:A:986:ALA:HB1	1:A:994:ARG:HH21	1.69	0.57
1:A:353:LEU:HA	1:A:370:MET:HE1	1.87	0.57
1:B:474:LEU:O	1:B:478:ILE:HG13	2.05	0.57
1:A:397:PHE:O	1:A:401:LEU:HG	2.04	0.57
1:B:309:GLU:O	1:B:313:GLU:HG2	2.05	0.56
1:B:6:PHE:HD2	1:B:489:THR:HB	1.70	0.56
1:B:73:VAL:HG22	1:B:110:ARG:HD3	1.87	0.56
1:B:205:ILE:HD11	1:B:745:ALA:HB2	1.87	0.56
2:C:1101:ERY:H193	2:C:1101:ERY:H213	1.87	0.56
1:B:71:ASN:OD1	1:A:168:ARG:NH1	2.38	0.56
1:A:220:ILE:HG13	1:A:235:ILE:HD11	1.86	0.56
1:A:938:LEU:HB3	1:A:969:ILE:HD11	1.87	0.56
1:C:700:ALA:HB2	1:C:840:VAL:HG11	1.88	0.56
1:B:105:ILE:HG21	1:A:105:ILE:HD11	1.88	0.56
1:B:636:ALA:HB1	1:B:640:GLN:HE21	1.71	0.56
1:A:443:PRO:O	1:A:447:ILE:HG13	2.05	0.56
1:B:158:VAL:HG11	1:B:290:ILE:HD11	1.88	0.56
1:C:383:VAL:HG12	1:C:478:ILE:HD13	1.87	0.56
1:C:646:PHE:CD1	1:C:659:PHE:HD2	2.24	0.56
1:B:31:LEU:HD13	1:B:391:ILE:HG23	1.86	0.55
1:A:540:LEU:O	1:A:544:ILE:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:THR:HG23	1:B:966:PHE:CD2	2.41	0.55
1:B:143:TYR:HB3	1:B:287:ALA:HB2	1.89	0.55
1:A:451:LEU:HD13	1:A:480:VAL:HG21	1.88	0.55
1:C:779:LEU:HD22	1:C:794:LEU:HD23	1.88	0.55
1:B:45:GLN:OE1	1:B:89:LYS:NZ	2.37	0.55
1:B:440:VAL:C	1:B:443:PRO:HD2	2.31	0.55
1:B:1019:PHE:O	1:B:1023:LEU:HD23	2.06	0.55
1:C:421:LEU:HD11	1:C:429:VAL:HG12	1.89	0.55
1:C:451:LEU:HD12	1:C:480:VAL:HG21	1.88	0.55
1:A:469:GLN:HG3	1:A:923:THR:HG22	1.87	0.55
1:C:665:ILE:HG13	1:C:668:LEU:HB2	1.89	0.55
1:A:100:PRO:HB2	1:A:131:LYS:HD2	1.89	0.55
1:C:10:PRO:HB3	1:C:497:LEU:HD11	1.89	0.55
1:B:66:ILE:O	1:B:70:ILE:HG12	2.07	0.54
1:B:976:PHE:HD1	1:B:1005:MET:SD	2.29	0.54
1:A:891:MET:HE2	1:A:891:MET:N	2.23	0.54
1:C:45:GLN:CG	1:C:89:LYS:HE3	2.36	0.54
1:B:482:ILE:HD12	1:B:482:ILE:H	1.73	0.54
1:B:902:ALA:HB1	1:B:928:LEU:HB3	1.90	0.54
1:A:52:GLY:HA2	1:C:217:THR:HG22	1.89	0.54
1:A:931:LEU:HB3	1:A:1005:MET:HE1	1.88	0.54
1:B:149:MET:HE3	1:B:322:LEU:HD13	1.87	0.54
1:A:383:VAL:HG11	1:A:478:ILE:HG12	1.89	0.54
1:C:14:SER:O	1:C:18:ILE:HG13	2.07	0.54
1:B:606:SER:HB3	1:B:624:VAL:HG13	1.88	0.54
1:B:966:PHE:O	1:B:970:ILE:HG12	2.08	0.54
1:A:145:GLU:OE1	1:A:323:LYS:NZ	2.41	0.54
1:B:445:ILE:O	1:B:449:LEU:HG	2.06	0.54
1:B:720:TYR:HB2	1:A:235:ILE:HD13	1.88	0.54
1:B:819:LEU:HD21	1:B:821:GLN:HE21	1.73	0.54
1:A:344:THR:HG23	1:A:982:PRO:HB2	1.89	0.54
1:C:135:THR:HG22	1:C:136:ILE:N	2.23	0.54
1:C:986:ALA:O	1:C:995:HIS:NE2	2.41	0.54
1:B:94:PHE:HB3	1:B:98:THR:HG21	1.89	0.54
1:A:565:ASP:OD2	1:A:634:ARG:NH2	2.40	0.54
1:B:396:LEU:HD23	1:B:399:LEU:HD12	1.89	0.54
1:C:139:VAL:HG22	1:C:291:ILE:HD13	1.89	0.54
1:A:942:PHE:HD2	1:A:961:ALA:HA	1.72	0.53
1:B:490:LEU:HG	1:B:494:LEU:HD11	1.90	0.53
1:B:825:ALA:HB1	1:B:826:PRO:HD2	1.91	0.53
1:A:435:LYS:HA	1:A:438:ASN:HD21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:VAL:HG23	1:C:400:VAL:HG23	1.89	0.53
1:C:476:LEU:O	1:C:480:VAL:HG12	2.07	0.53
1:B:248:GLU:HB2	1:B:264:LYS:HB3	1.90	0.53
1:B:980:VAL:HG21	1:B:1005:MET:HE1	1.90	0.53
1:C:665:ILE:CG1	1:C:668:LEU:HD22	2.38	0.53
1:B:54:ASP:OD1	1:B:54:ASP:N	2.39	0.53
1:A:34:GLU:O	1:A:392:ASN:HA	2.09	0.53
1:C:572:ILE:HG21	1:C:613:PHE:CD2	2.43	0.53
1:C:614:THR:O	1:C:615:SER:C	2.51	0.53
1:C:630:ASP:OD1	1:C:631:TRP:N	2.42	0.53
1:B:706:LEU:HA	1:B:824:PRO:O	2.09	0.53
1:C:417:ILE:HD12	1:C:433:ALA:HA	1.90	0.53
1:B:472:PHE:CZ	1:B:923:THR:HB	2.44	0.53
1:C:84:SER:OG	1:C:87:GLN:HG3	2.09	0.53
1:B:189:LEU:HB3	1:B:194:LEU:HD11	1.90	0.53
1:B:416:ASN:O	1:B:420:ILE:HG12	2.09	0.53
1:A:722:LEU:HB2	1:C:237:MET:HB2	1.90	0.53
1:C:368:ILE:HD13	1:C:495:SER:HA	1.91	0.53
1:C:891:MET:HG3	1:C:944:MET:HE1	1.89	0.53
1:A:458:VAL:HG21	1:A:469:GLN:HB3	1.90	0.53
1:B:675:GLU:OE1	1:B:675:GLU:N	2.41	0.53
1:C:41:PRO:HB3	1:C:96:ILE:HG12	1.91	0.53
1:A:345:PHE:CD1	1:A:403:ILE:HD11	2.44	0.52
1:A:185:MET:HB3	1:A:764:VAL:HG22	1.91	0.52
1:C:292:ILE:HG21	1:C:307:ILE:HD11	1.91	0.52
1:A:590:THR:HG22	1:A:649:TYR:OH	2.10	0.52
1:A:919:ILE:O	1:A:923:THR:HG23	2.09	0.52
1:A:450:VAL:O	1:A:454:VAL:HG23	2.10	0.52
1:C:90:LEU:C	1:C:90:LEU:HD23	2.35	0.52
1:B:478:ILE:O	1:B:482:ILE:HD12	2.09	0.52
1:B:924:GLY:O	1:B:928:LEU:HG	2.10	0.52
1:C:1:MET:SD	1:C:2:PHE:N	2.83	0.52
1:C:403:ILE:O	1:C:407:VAL:HG22	2.10	0.52
1:B:786:SER:OG	1:B:788:ASP:OD1	2.24	0.52
1:B:77:ILE:HD11	1:B:858:TYR:CZ	2.44	0.52
1:B:430:LYS:O	1:B:434:ILE:HG12	2.10	0.52
1:B:705:GLU:O	1:B:825:ALA:HB2	2.10	0.52
1:B:903:VAL:O	1:B:907:ILE:HG13	2.09	0.52
1:A:888:ARG:HE	1:A:889:TRP:H	1.57	0.52
1:C:313:GLU:OE1	1:C:316:LYS:NZ	2.30	0.52
1:C:637:SER:N	1:C:640:GLN:OE1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:973:SER:O	1:B:977:THR:HG23	2.11	0.51
1:C:969:ILE:HG13	1:C:1013:ILE:HD11	1.92	0.51
1:C:976:PHE:CD2	1:C:1005:MET:HE1	2.44	0.51
1:A:534:ARG:HB3	1:A:537:ARG:HE	1.75	0.51
1:C:39:LEU:HD22	1:C:468:ILE:HG13	1.93	0.51
1:B:39:LEU:HD11	1:B:467:GLU:OE2	2.10	0.51
1:B:613:PHE:CD1	1:B:614:THR:HG23	2.46	0.51
1:B:837:ILE:HA	1:B:840:VAL:HG12	1.92	0.51
1:C:413:VAL:HG21	1:C:487:ALA:HB1	1.92	0.51
1:C:192:ASP:N	1:C:192:ASP:OD1	2.41	0.51
1:C:755:PHE:CE2	1:C:757:MET:HE2	2.45	0.51
1:B:440:VAL:O	1:B:444:VAL:HG13	2.11	0.51
1:B:461:ILE:HD11	1:B:870:ALA:HB3	1.92	0.51
1:B:486:VAL:HG13	1:B:490:LEU:HB3	1.92	0.51
1:C:408:ASP:O	1:C:412:ILE:HG13	2.11	0.51
1:C:431:ASP:HA	1:C:434:ILE:HG22	1.93	0.51
1:A:201:ALA:O	1:A:205:ILE:HD12	2.11	0.51
1:A:326:ILE:O	1:A:326:ILE:HG13	2.11	0.51
1:A:356:MET:HG2	1:A:411:ILE:HD11	1.92	0.51
1:A:536:ILE:HG13	1:A:537:ARG:N	2.25	0.51
1:C:162:ILE:HD12	1:C:314:LEU:HD13	1.93	0.51
1:C:684:LYS:NZ	1:C:692:ASP:OD2	2.42	0.51
1:B:454:VAL:O	1:B:926:LEU:HD11	2.11	0.51
1:C:469:GLN:OE1	1:C:469:GLN:HA	2.11	0.51
1:A:612:LEU:HB3	1:A:670:LEU:HD21	1.92	0.51
1:C:568:VAL:O	1:C:569:ILE:HD13	2.11	0.51
1:A:373:VAL:O	1:A:377:LEU:HD23	2.10	0.50
1:C:675:GLU:OE2	1:C:675:GLU:N	2.43	0.50
1:C:752:VAL:HG23	1:C:753:ASN:H	1.76	0.50
1:B:527:GLY:O	1:B:531:ILE:HG13	2.11	0.50
1:B:616:SER:OG	1:B:617:LEU:N	2.43	0.50
1:B:834:ILE:HA	1:B:837:ILE:HG22	1.93	0.50
1:B:45:GLN:NE2	1:B:91:THR:OG1	2.44	0.50
1:B:700:ALA:O	1:B:706:LEU:HD11	2.12	0.50
1:A:241:LEU:HD22	1:A:246:GLU:HB3	1.92	0.50
1:A:895:VAL:HG21	1:A:937:ILE:HD13	1.93	0.50
1:C:289:PRO:HG2	1:C:607:LEU:CD2	2.41	0.50
1:C:571:SER:HB2	1:C:626:PHE:HE2	1.75	0.50
1:B:356:MET:HE3	1:B:369:PRO:HG2	1.94	0.50
1:B:450:VAL:HG11	1:B:937:ILE:CD1	2.42	0.50
1:C:319:PRO:HD2	1:C:322:LEU:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:665:ILE:CG1	1:C:668:LEU:HB2	2.41	0.50
1:C:64:THR:HG23	1:C:811:ARG:HH12	1.75	0.50
1:B:773:ARG:NH1	1:A:222:GLU:O	2.43	0.50
1:A:115:THR:HA	1:A:118:LEU:HD23	1.94	0.50
1:C:755:PHE:HE2	1:C:757:MET:HE2	1.76	0.50
1:B:77:ILE:HG13	1:B:78:TYR:CD2	2.47	0.50
1:C:136:ILE:HD13	1:C:291:ILE:HD12	1.93	0.50
1:C:568:VAL:HG23	1:C:662:LEU:HD11	1.93	0.50
1:B:232:VAL:HG23	1:C:580:SER:HA	1.94	0.49
1:A:598:MET:HB2	1:A:601:ILE:HD12	1.93	0.49
1:A:600:GLU:N	1:A:600:GLU:OE2	2.45	0.49
1:C:340:GLU:CG	1:C:994:ARG:HH12	2.25	0.49
1:C:571:SER:HB3	1:C:624:VAL:O	2.12	0.49
1:B:1018:LEU:O	1:B:1022:LEU:HG	2.12	0.49
1:B:4:LYS:O	1:B:7:ILE:HG22	2.12	0.49
1:B:736:MET:HG3	1:A:211:GLN:HA	1.93	0.49
1:A:740:PHE:HD2	1:C:216:ALA:HB2	1.77	0.49
1:B:6:PHE:CD2	1:B:489:THR:HB	2.47	0.49
1:B:403:ILE:O	1:B:407:VAL:HG13	2.12	0.49
1:B:613:PHE:HD1	1:B:614:THR:HG23	1.77	0.49
1:A:720:TYR:HB3	1:A:800:LEU:HD11	1.95	0.49
1:A:938:LEU:HD23	1:A:969:ILE:HD13	1.94	0.49
1:C:436:ALA:O	1:C:440:VAL:HG22	2.11	0.49
1:A:446:SER:HB2	1:A:937:ILE:HG21	1.94	0.49
1:B:853:TRP:HD1	1:B:857:ALA:HB1	1.78	0.49
1:C:458:VAL:HG13	1:C:469:GLN:HB3	1.94	0.49
1:A:145:GLU:N	1:A:321:GLY:O	2.43	0.49
1:A:315:SER:HA	1:A:318:PHE:CG	2.48	0.49
1:A:662:LEU:H	1:A:662:LEU:HD22	1.78	0.49
1:B:249:ASN:HA	1:B:262:ARG:HD3	1.95	0.49
1:B:641:ILE:O	1:B:645:LEU:HG	2.13	0.49
1:B:752:VAL:HG23	1:B:753:ASN:H	1.78	0.49
1:A:773:ARG:CZ	1:C:230:PRO:HD2	2.43	0.49
1:C:560:LEU:HG	1:C:561:VAL:HG23	1.95	0.49
1:B:638:SER:O	1:B:642:ILE:HG13	2.12	0.49
1:B:215:TYR:HE2	1:C:736:MET:HE2	1.78	0.49
1:A:172:VAL:HG13	1:A:292:ILE:HG23	1.93	0.49
1:A:401:LEU:HD22	1:A:1001:LEU:HD12	1.94	0.49
1:B:57:THR:O	1:B:61:THR:OG1	2.28	0.48
1:B:402:ALA:O	1:B:405:ILE:HG22	2.12	0.48
1:C:976:PHE:HB3	1:C:1005:MET:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1029:TRP:CD1	1:C:1029:TRP:C	2.91	0.48
1:B:880:LEU:HD23	1:A:19:ILE:HG13	1.94	0.48
1:C:447:ILE:HG21	1:C:934:LYS:HE2	1.95	0.48
1:C:282:LEU:HD12	1:C:605:VAL:HG22	1.95	0.48
1:C:524:PHE:CZ	1:C:962:ALA:HB1	2.48	0.48
1:C:685:ASP:OD1	1:C:686:TYR:N	2.46	0.48
2:C:1101:ERY:H11	2:C:1101:ERY:C7	2.43	0.48
1:B:108:ASN:ND2	1:C:109:ASN:HB3	2.27	0.48
1:B:172:VAL:HG13	1:B:292:ILE:HG23	1.96	0.48
1:B:178:ILE:HG13	1:B:607:LEU:HD22	1.96	0.48
1:B:465:VAL:HA	1:B:468:ILE:HD11	1.95	0.48
1:C:70:ILE:HD11	1:C:107:VAL:HG13	1.96	0.48
1:C:107:VAL:O	1:C:111:ILE:HG13	2.14	0.48
1:A:736:MET:HB2	1:C:210:ASP:OD1	2.14	0.48
1:C:106:ASP:O	1:C:110:ARG:HG2	2.14	0.48
1:C:397:PHE:HD2	1:C:997:LEU:HD13	1.78	0.48
1:A:938:LEU:HD12	1:A:965:ARG:NH1	2.28	0.48
1:B:882:LEU:HB2	1:B:892:PRO:HB3	1.94	0.48
1:B:946:GLU:HB3	1:B:952:LYS:HZ2	1.79	0.48
1:A:833:ALA:O	1:A:837:ILE:HG22	2.14	0.48
1:A:905:GLY:HA3	1:A:1007:ALA:HB2	1.95	0.48
1:B:459:SER:HB2	1:B:470:ARG:HD3	1.96	0.48
1:A:545:MET:O	1:A:549:ILE:HG13	2.14	0.48
1:C:137:LEU:HB3	1:C:292:ILE:O	2.14	0.48
1:C:409:ASP:HA	1:C:412:ILE:HD12	1.95	0.48
1:C:587:GLU:O	1:C:591:ILE:HG12	2.13	0.48
1:B:139:VAL:HG23	1:B:328:TYR:HD2	1.79	0.47
1:A:531:ILE:HD13	1:A:538:PHE:CE2	2.49	0.47
1:A:981:LEU:HA	1:A:1002:ILE:HD11	1.96	0.47
1:C:203:ASP:OD2	1:C:785:ARG:NH2	2.48	0.47
1:B:907:ILE:HG12	1:B:921:PHE:CZ	2.48	0.47
1:A:591:ILE:HA	1:A:649:TYR:HE2	1.79	0.47
1:A:630:ASP:O	1:A:634:ARG:HG2	2.14	0.47
1:C:775:THR:HG22	1:C:777:ASP:H	1.79	0.47
1:B:74:ASP:N	1:B:74:ASP:OD1	2.48	0.47
1:A:701:ARG:NH1	1:A:709:VAL:O	2.47	0.47
1:A:715:THR:HG22	1:A:806:PRO:HB3	1.97	0.47
1:C:892:PRO:O	1:C:896:ILE:HG12	2.14	0.47
1:B:868:ALA:HB1	1:B:871:PHE:HB2	1.96	0.47
1:C:613:PHE:CZ	1:C:660:LEU:HD11	2.45	0.47
1:B:152:ILE:HG12	1:B:273:ALA:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:888:ARG:HH11	1:B:889:TRP:H	1.62	0.47
1:A:80:ASP:HB3	1:A:812:PHE:HD1	1.78	0.47
1:C:328:TYR:OH	1:C:330:THR:HG22	2.15	0.47
1:C:338:ILE:O	1:C:341:VAL:HG12	2.15	0.47
1:C:531:ILE:HG22	1:C:538:PHE:CZ	2.49	0.47
1:B:35:GLN:O	1:B:393:LEU:HG	2.14	0.47
1:B:396:LEU:O	1:B:400:VAL:HG12	2.14	0.47
1:B:411:ILE:HD12	1:B:972:THR:HG22	1.95	0.47
1:C:717:PHE:CD2	1:C:807:ASP:HB2	2.50	0.47
1:B:256:GLU:N	1:B:256:GLU:OE2	2.47	0.47
1:B:408:ASP:O	1:B:412:ILE:HG12	2.15	0.47
1:A:43:THR:OG1	1:A:132:SER:O	2.33	0.47
1:A:366:THR:HG22	1:A:370:MET:HE2	1.97	0.47
1:A:484:GLY:O	1:A:488:LEU:HG	2.15	0.47
1:A:569:ILE:N	1:A:626:PHE:O	2.44	0.47
1:A:570:MET:HE2	1:A:662:LEU:HD13	1.96	0.47
1:C:24:GLY:HA2	1:C:382:ALA:HB2	1.97	0.47
1:C:569:ILE:HD11	1:C:628:LEU:HD11	1.97	0.47
1:C:899:VAL:HG22	1:C:900:PRO:HD3	1.97	0.47
1:B:364:LYS:O	1:B:368:ILE:HG13	2.15	0.47
1:C:583:ARG:O	1:C:587:GLU:HG2	2.15	0.47
1:B:359:PHE:HE2	1:B:974:LEU:HD13	1.78	0.47
1:B:379:GLY:O	1:B:383:VAL:HG12	2.15	0.47
1:B:986:ALA:O	1:B:995:HIS:NE2	2.47	0.47
1:A:37:PRO:O	1:A:39:LEU:HG	2.14	0.47
1:A:436:ALA:O	1:A:440:VAL:HG22	2.15	0.47
1:C:552:LEU:HA	1:C:555:ILE:HG22	1.97	0.47
1:B:839:GLU:O	1:B:843:GLN:HG2	2.15	0.46
1:C:570:MET:HG2	1:C:572:ILE:HD11	1.96	0.46
1:A:46:VAL:HG22	1:A:129:VAL:HG22	1.95	0.46
1:A:935:ASN:O	1:A:939:ILE:HG22	2.15	0.46
1:C:572:ILE:CG1	1:C:613:PHE:HE2	2.24	0.46
1:C:658:TYR:HD1	1:C:660:LEU:HD21	1.80	0.46
1:C:897:THR:O	1:C:900:PRO:HD2	2.15	0.46
1:B:157:TYR:CD1	1:B:157:TYR:C	2.94	0.46
1:A:31:LEU:HD22	1:A:390:SER:HA	1.97	0.46
1:B:140:VAL:O	1:B:290:ILE:N	2.39	0.46
1:B:368:ILE:HD13	1:B:495:SER:HA	1.98	0.46
1:C:45:GLN:HE21	1:C:89:LYS:HE3	1.79	0.46
1:B:360:LEU:HD21	1:B:365:SER:HB2	1.98	0.46
1:A:563:SER:HA	1:A:664:PRO:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:ILE:HG21	1:A:668:LEU:HD13	1.97	0.46
1:A:871:PHE:CE2	1:A:929:ILE:HD11	2.51	0.46
1:B:12:PHE:O	1:B:15:VAL:HG12	2.16	0.46
1:B:977:THR:HG22	1:B:1005:MET:SD	2.55	0.46
1:A:66:ILE:O	1:A:70:ILE:HG12	2.15	0.46
1:B:588:VAL:HA	1:B:591:ILE:HG22	1.98	0.46
1:A:485:PHE:CD1	1:A:485:PHE:C	2.94	0.46
1:C:152:ILE:HG12	1:C:273:ALA:HB2	1.97	0.46
1:C:976:PHE:HB3	1:C:1005:MET:HE3	1.97	0.46
1:B:417:ILE:O	1:B:421:LEU:HG	2.16	0.46
1:B:909:LEU:HD23	1:B:1003:GLY:N	2.30	0.46
1:C:45:GLN:HE21	1:C:89:LYS:CE	2.28	0.46
1:C:890:LEU:HB3	1:C:1023:LEU:HD12	1.97	0.46
1:B:2:PHE:CD1	1:B:2:PHE:C	2.93	0.46
1:B:157:TYR:O	1:B:157:TYR:HD1	1.98	0.46
1:B:458:VAL:O	1:B:469:GLN:NE2	2.49	0.46
1:B:545:MET:O	1:B:549:ILE:HG13	2.16	0.46
1:A:4:LYS:HB3	1:A:4:LYS:HE2	1.70	0.46
1:A:35:GLN:O	1:A:393:LEU:HB2	2.16	0.46
1:C:601:ILE:HG21	1:C:626:PHE:HB3	1.98	0.46
1:B:405:ILE:HD12	1:B:405:ILE:HA	1.82	0.45
1:A:568:VAL:HG13	1:A:662:LEU:CD2	2.43	0.45
1:C:809:VAL:HG12	1:C:810:LYS:N	2.30	0.45
1:B:968:PRO:O	1:B:972:THR:HG23	2.16	0.45
1:A:559:SER:HB3	1:A:829:THR:HB	1.98	0.45
1:A:677:TYR:CZ	1:A:819:LEU:HD13	2.51	0.45
1:A:894:ALA:HB2	1:A:1023:LEU:HD12	1.98	0.45
1:C:612:LEU:HD21	2:C:1101:ERY:O10	2.16	0.45
1:B:452:CYS:O	1:B:456:ILE:HG22	2.15	0.45
1:A:70:ILE:HG21	1:A:92:VAL:HG21	1.97	0.45
1:A:140:VAL:HB	1:A:290:ILE:HB	1.98	0.45
1:A:981:LEU:O	1:A:984:ILE:HG22	2.17	0.45
1:B:695:LYS:HA	1:B:698:GLU:OE1	2.17	0.45
1:A:188:TRP:CZ2	1:C:224:PRO:HG2	2.52	0.45
1:A:380:THR:O	1:A:384:LEU:HG	2.17	0.45
1:A:610:PHE:HE2	1:A:612:LEU:HD23	1.82	0.45
1:A:690:GLN:HA	1:A:693:VAL:HG22	1.98	0.45
1:C:356:MET:O	1:C:360:LEU:HB2	2.16	0.45
1:C:393:LEU:O	1:C:397:PHE:HD1	1.98	0.45
1:B:214:GLN:HG2	1:B:237:MET:SD	2.57	0.45
1:B:572:ILE:O	1:B:572:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:LYS:HG3	1:B:705:GLU:CD	2.42	0.45
1:A:720:TYR:HE1	1:A:802:ARG:HG2	1.81	0.45
1:C:954:ILE:HD13	1:C:1024:GLU:HB3	1.98	0.45
1:A:470:ARG:NH1	1:A:470:ARG:HB2	2.32	0.45
1:A:837:ILE:HA	1:A:840:VAL:HG12	1.99	0.45
1:C:136:ILE:HD12	2:C:1101:ERY:C33	2.47	0.45
1:B:211:GLN:NE2	1:C:730:LYS:HE3	2.32	0.45
1:B:566:GLN:NE2	1:B:663:PRO:HD3	2.31	0.45
1:B:977:THR:HA	1:B:1005:MET:SD	2.57	0.45
1:A:70:ILE:HD12	1:A:107:VAL:HG13	1.98	0.45
1:C:143:TYR:HB3	1:C:287:ALA:HB2	1.97	0.45
1:C:417:ILE:HD13	1:C:436:ALA:HB3	1.99	0.45
1:C:905:GLY:HA3	1:C:1007:ALA:HB2	1.99	0.45
1:A:351:LEU:O	1:A:354:VAL:HG12	2.17	0.45
1:A:599:LYS:HA	1:A:599:LYS:HD3	1.73	0.45
1:C:22:ILE:O	1:C:25:ILE:HG22	2.17	0.45
1:C:882:LEU:HB2	1:C:892:PRO:HB3	1.99	0.45
1:B:351:LEU:HD23	1:B:978:PHE:HB3	1.99	0.44
1:A:80:ASP:HB3	1:A:812:PHE:CD1	2.52	0.44
1:A:1005:MET:HE2	1:A:1005:MET:HA	1.99	0.44
1:C:4:LYS:O	1:C:7:ILE:HG22	2.17	0.44
1:C:994:ARG:HD2	1:C:994:ARG:N	2.32	0.44
1:B:356:MET:HE1	1:B:365:SER:O	2.17	0.44
1:B:443:PRO:O	1:B:447:ILE:HG13	2.17	0.44
1:A:377:LEU:HD13	1:A:399:LEU:HD22	1.99	0.44
1:B:903:VAL:HG22	1:B:925:LEU:HD11	1.99	0.44
1:A:782:ILE:HB	1:A:794:LEU:HD23	1.98	0.44
1:C:7:ILE:HD11	1:C:496:ALA:HB2	1.98	0.44
1:C:886:TYR:HB3	1:C:944:MET:HE3	1.98	0.44
1:B:472:PHE:CZ	1:B:476:LEU:HD11	2.51	0.44
1:A:536:ILE:O	1:A:539:VAL:HG12	2.17	0.44
1:C:1:MET:HE2	1:C:1:MET:HA	1.99	0.44
1:A:879:PHE:CD1	1:A:892:PRO:HB2	2.52	0.44
1:C:676:MET:HG2	1:C:853:TRP:CZ3	2.52	0.44
1:B:456:ILE:CG2	1:B:457:PRO:HD3	2.48	0.44
1:A:35:GLN:HG2	1:A:36:TYR:CD2	2.53	0.44
1:A:440:VAL:C	1:A:443:PRO:HD2	2.42	0.44
1:A:512:LYS:HD2	1:A:512:LYS:HA	1.85	0.44
1:A:689:ILE:O	1:A:693:VAL:HG13	2.18	0.44
1:B:101:ASP:HB3	1:C:102:GLN:NE2	2.32	0.44
1:B:544:ILE:O	1:B:548:PHE:HD1	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD21	1:A:385:TYR:HA	2.00	0.44
1:C:240:ARG:HD3	1:C:756:PRO:HD3	1.99	0.44
1:C:729:MET:SD	1:C:736:MET:HG3	2.58	0.44
1:B:155:TYR:CE2	1:B:177:ALA:HB3	2.52	0.44
1:B:427:ILE:HD12	1:B:435:LYS:NZ	2.32	0.44
1:C:891:MET:HE2	1:C:940:ILE:HG23	1.99	0.44
1:B:337:SER:O	1:B:341:VAL:HG23	2.17	0.44
1:A:500:THR:OG1	1:A:502:ASN:O	2.36	0.44
1:A:949:LYS:HE3	1:A:950:LYS:HD3	1.98	0.44
1:C:248:GLU:HB3	1:C:264:LYS:HB3	2.00	0.44
1:C:981:LEU:O	1:C:984:ILE:HG22	2.18	0.44
1:B:232:VAL:HG21	1:C:619:GLU:OE2	2.18	0.43
1:B:730:LYS:HA	1:B:730:LYS:HD3	1.73	0.43
1:A:604:SER:O	1:A:604:SER:OG	2.33	0.43
1:A:791:MET:O	1:A:792:ILE:HD13	2.18	0.43
1:C:118:LEU:O	1:C:123:LYS:NZ	2.48	0.43
1:A:150:ASN:OD1	1:A:150:ASN:N	2.47	0.43
1:A:368:ILE:HB	1:A:369:PRO:HD3	1.99	0.43
1:A:141:SER:OG	1:A:282:LEU:HD22	2.19	0.43
1:B:767:ARG:HH22	1:A:222:GLU:HB3	1.82	0.43
1:B:903:VAL:HA	1:B:925:LEU:HD11	1.99	0.43
1:A:967:ARG:HB3	1:A:968:PRO:HD3	2.00	0.43
1:C:677:TYR:CZ	1:C:819:LEU:HD12	2.54	0.43
1:B:158:VAL:HG22	1:B:162:ILE:HD12	2.00	0.43
1:C:180:ASN:ND2	1:C:275:GLN:OE1	2.50	0.43
1:B:341:VAL:HG11	1:B:396:LEU:HB3	1.99	0.43
1:A:139:VAL:HG23	1:A:328:TYR:HD2	1.82	0.43
1:A:564:GLU:OE1	1:A:564:GLU:HA	2.19	0.43
1:A:663:PRO:HG3	1:A:669:SER:O	2.19	0.43
1:C:36:TYR:CE1	1:C:393:LEU:HD12	2.54	0.43
1:C:612:LEU:HB3	2:C:1101:ERY:H271	2.01	0.43
1:C:340:GLU:OE1	1:C:340:GLU:HA	2.17	0.43
1:C:458:VAL:CG1	1:C:469:GLN:HB3	2.49	0.43
1:A:50:TYR:OH	1:C:214:GLN:NE2	2.52	0.43
1:A:413:VAL:HG11	1:A:491:THR:HG23	2.01	0.43
1:A:774:ASN:H	1:C:220:ILE:HG12	1.84	0.43
1:A:916:ASP:OD1	1:A:916:ASP:N	2.44	0.43
1:B:94:PHE:CZ	1:B:103:ALA:HB1	2.54	0.43
1:B:178:ILE:HB	1:B:289:PRO:HD2	2.01	0.43
1:B:459:SER:CA	1:B:469:GLN:HE22	2.29	0.43
1:A:605:VAL:HG12	1:A:625:PHE:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:THR:HG21	1:A:916:ASP:HB3	2.01	0.43
1:C:315:SER:HA	1:C:318:PHE:CG	2.54	0.43
1:C:381:PHE:CE1	1:C:399:LEU:HD11	2.53	0.43
1:B:872:VAL:HA	1:B:875:MET:HG2	2.01	0.43
1:C:26:ILE:HG13	1:C:27:GLY:N	2.32	0.43
1:C:983:MET:HE2	1:C:983:MET:HA	2.01	0.43
1:B:691:GLN:O	1:B:695:LYS:HG3	2.19	0.42
1:B:853:TRP:CD1	1:B:857:ALA:HB1	2.54	0.42
1:A:696:MET:HE2	1:A:845:LEU:HD22	2.01	0.42
1:C:84:SER:HB2	1:C:85:PRO:HD2	2.00	0.42
1:C:688:ALA:HA	1:C:691:GLN:OE1	2.19	0.42
1:C:737:GLN:HE22	1:C:741:ASN:HD21	1.67	0.42
1:B:359:PHE:CE2	1:B:974:LEU:HD13	2.55	0.42
1:B:453:ALA:O	1:B:457:PRO:HG2	2.20	0.42
1:A:677:TYR:CE2	1:A:810:LYS:HD3	2.49	0.42
1:C:897:THR:C	1:C:900:PRO:HD2	2.44	0.42
1:C:965:ARG:O	1:C:969:ILE:HG12	2.20	0.42
1:A:517:PHE:HE2	1:A:967:ARG:HG3	1.84	0.42
1:C:70:ILE:HD13	1:C:110:ARG:HB2	2.02	0.42
1:C:136:ILE:HD12	2:C:1101:ERY:H331	2.02	0.42
1:C:909:LEU:HD12	1:C:909:LEU:HA	1.89	0.42
1:B:735:ASN:HB3	1:A:210:ASP:OD2	2.19	0.42
1:B:884:ALA:HB2	1:A:15:VAL:HG11	2.01	0.42
1:A:75:ASN:HA	1:A:95:ASN:HD22	1.85	0.42
1:A:169:ILE:HD13	1:A:169:ILE:HA	1.90	0.42
1:A:969:ILE:HD13	1:A:969:ILE:HA	1.78	0.42
1:A:223:GLU:OE2	1:A:228:LYS:NZ	2.51	0.42
1:A:329:ASP:O	1:A:332:ILE:HG22	2.19	0.42
1:A:757:MET:HB3	1:A:762:PHE:HD2	1.85	0.42
1:C:612:LEU:O	2:C:1101:ERY:H211	2.20	0.42
1:C:891:MET:N	1:C:892:PRO:HD2	2.34	0.42
1:A:894:ALA:HA	1:A:897:THR:HG22	2.01	0.42
1:B:931:LEU:O	1:B:934:LYS:HG2	2.20	0.42
1:A:39:LEU:HB3	1:A:464:PHE:CE1	2.55	0.42
1:A:159:SER:HA	1:A:163:LEU:HD12	2.01	0.42
1:C:13:ALA:O	1:C:16:VAL:HG12	2.20	0.42
1:C:88:MET:SD	1:C:88:MET:C	3.03	0.42
1:C:138:GLU:OE2	1:C:307:ILE:HD12	2.20	0.42
1:A:14:SER:O	1:A:18:ILE:HG12	2.19	0.42
1:B:34:GLU:O	1:B:392:ASN:HA	2.19	0.42
1:B:497:LEU:HD12	1:B:497:LEU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:MET:HE2	1:A:324:TYR:CD2	2.55	0.42
1:A:882:LEU:HD22	1:A:937:ILE:HD11	2.02	0.42
1:C:813:ASN:C	1:C:814:LEU:HD12	2.45	0.42
1:B:356:MET:SD	1:B:366:THR:HG23	2.60	0.41
1:B:436:ALA:O	1:B:440:VAL:HG22	2.20	0.41
1:B:949:LYS:HD2	1:B:950:LYS:HB2	2.01	0.41
1:A:241:LEU:HB3	1:A:246:GLU:HB3	2.02	0.41
1:C:585:ILE:HG12	1:C:608:ILE:HG21	2.01	0.41
1:B:351:LEU:HD12	1:B:351:LEU:HA	1.86	0.41
1:B:447:ILE:O	1:B:451:LEU:HD23	2.20	0.41
1:A:10:PRO:HG2	1:A:497:LEU:HD13	2.01	0.41
1:A:552:LEU:HA	1:A:555:ILE:HG22	2.02	0.41
1:A:720:TYR:HB2	1:C:235:ILE:HG12	2.01	0.41
1:C:90:LEU:C	1:C:90:LEU:CD2	2.93	0.41
1:B:149:MET:HB2	1:B:149:MET:HE2	1.81	0.41
1:B:240:ARG:HB3	1:B:756:PRO:HD3	2.03	0.41
1:B:562:PRO:HD2	1:B:920:TYR:HE2	1.85	0.41
1:A:478:ILE:O	1:A:479:SER:C	2.64	0.41
1:C:214:GLN:NE2	1:C:214:GLN:HA	2.35	0.41
1:C:440:VAL:HA	1:C:443:PRO:HG2	2.02	0.41
1:C:456:ILE:HD13	1:C:456:ILE:HA	1.88	0.41
1:B:79:MET:HB2	1:B:92:VAL:HG22	2.02	0.41
1:B:85:PRO:HD3	1:B:807:ASP:O	2.21	0.41
1:B:396:LEU:HD23	1:B:396:LEU:HA	1.96	0.41
1:B:416:ASN:HA	1:B:419:ARG:HG2	2.02	0.41
1:B:478:ILE:O	1:B:481:ALA:N	2.52	0.41
1:A:546:ILE:HD13	1:A:549:ILE:HD12	2.03	0.41
1:A:942:PHE:CD2	1:A:961:ALA:HA	2.54	0.41
1:C:495:SER:O	1:C:499:LEU:HB2	2.21	0.41
1:C:752:VAL:CG2	1:C:753:ASN:N	2.82	0.41
1:B:217:THR:HG22	1:C:743:ILE:HG21	2.02	0.41
1:B:417:ILE:HG13	1:B:417:ILE:H	1.68	0.41
1:B:580:SER:HB3	1:A:232:VAL:HG23	2.03	0.41
1:C:412:ILE:HG23	1:C:965:ARG:HH12	1.84	0.41
1:C:568:VAL:CG2	1:C:662:LEU:HD22	2.50	0.41
1:C:679:GLN:OE1	1:C:852:ALA:HB2	2.20	0.41
1:C:730:LYS:HD3	1:C:730:LYS:HA	1.80	0.41
1:A:37:PRO:O	1:A:38:SER:C	2.64	0.41
1:A:367:ILE:HD12	1:A:367:ILE:HA	1.83	0.41
1:C:106:ASP:OD1	1:C:106:ASP:N	2.54	0.41
1:C:990:GLY:O	1:C:993:SER:OG	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LYS:O	1:B:347:GLU:HG3	2.19	0.41
1:B:409:ASP:N	1:B:409:ASP:OD1	2.53	0.41
1:C:615:SER:H	2:C:1101:ERY:H212	1.84	0.41
1:B:68:ASP:OD1	1:B:68:ASP:C	2.63	0.41
1:B:155:TYR:HE2	1:B:177:ALA:HB3	1.84	0.41
1:B:310:LYS:HD3	1:B:310:LYS:HA	1.91	0.41
1:B:825:ALA:HB1	1:B:828:TYR:HD1	1.86	0.41
1:B:897:THR:O	1:B:900:PRO:HD2	2.20	0.41
1:A:445:ILE:HD11	1:A:488:LEU:HD11	2.01	0.41
1:C:328:TYR:CE2	1:C:330:THR:HG22	2.56	0.41
1:C:926:LEU:HA	1:C:926:LEU:HD23	1.85	0.41
1:B:244:PRO:O	1:B:248:GLU:HG2	2.21	0.41
1:B:570:MET:HE2	1:B:663:PRO:HA	2.03	0.41
1:A:240:ARG:HB3	1:A:756:PRO:HD3	2.03	0.41
1:C:373:VAL:HB	1:C:374:PRO:HD3	2.03	0.41
1:C:606:SER:CB	1:C:624:VAL:HG22	2.51	0.41
1:C:837:ILE:HD12	1:C:837:ILE:HA	1.83	0.41
1:C:886:TYR:OH	1:C:937:ILE:HA	2.21	0.41
1:C:94:PHE:CE2	1:C:103:ALA:HB1	2.56	0.41
1:C:736:MET:HE3	1:C:740:PHE:CE1	2.56	0.41
1:B:280:GLY:HA3	1:B:289:PRO:HD3	2.03	0.40
1:B:362:ASN:O	1:B:366:THR:OG1	2.33	0.40
1:B:398:ALA:HB2	1:B:472:PHE:CD1	2.55	0.40
1:B:592:ASN:O	1:B:596:THR:HG23	2.21	0.40
1:A:362:ASN:O	1:A:366:THR:OG1	2.27	0.40
1:A:374:PRO:O	1:A:378:LEU:HD23	2.21	0.40
1:A:469:GLN:CG	1:A:923:THR:HG22	2.51	0.40
1:A:813:ASN:C	1:A:814:LEU:HD12	2.45	0.40
1:B:68:ASP:OD1	1:B:69:ALA:N	2.54	0.40
1:B:403:ILE:O	1:B:406:VAL:HG12	2.21	0.40
1:B:757:MET:HB3	1:B:762:PHE:HD2	1.86	0.40
1:A:45:GLN:HE21	1:A:45:GLN:HB2	1.61	0.40
1:A:310:LYS:HA	1:A:310:LYS:HD2	1.84	0.40
1:A:371:ILE:O	1:A:374:PRO:HD2	2.22	0.40
1:A:868:ALA:O	1:A:872:VAL:HG12	2.21	0.40
1:C:572:ILE:HG21	1:C:613:PHE:HE2	1.82	0.40
1:C:953:SER:HB2	1:C:956:GLU:HG2	2.03	0.40
1:B:431:ASP:O	1:B:434:ILE:HB	2.20	0.40
1:B:716:SER:O	1:B:716:SER:OG	2.31	0.40
1:A:890:LEU:HD23	1:A:1023:LEU:HD22	2.03	0.40
1:B:397:PHE:O	1:B:401:LEU:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:PHE:CE1	1:B:923:THR:HB	2.55	0.40
1:A:212:ASN:O	1:A:753:ASN:ND2	2.54	0.40
1:A:772:PHE:HD1	1:A:778:ALA:HB1	1.87	0.40
1:C:67:GLU:HG2	1:C:79:MET:HE3	2.03	0.40
1:C:359:PHE:CD2	1:C:971:MET:HG2	2.56	0.40
1:C:568:VAL:CG2	1:C:662:LEU:CD2	3.00	0.40
1:C:662:LEU:N	1:C:662:LEU:HD12	2.36	0.40
1:C:927:LEU:HD22	1:C:1001:LEU:HD11	2.03	0.40
1:B:384:LEU:HD13	1:B:389:PHE:HB2	2.02	0.40
1:B:585:ILE:HG12	1:B:608:ILE:HG21	2.02	0.40
1:A:425:SER:HA	1:A:501:ARG:NH1	2.36	0.40
1:C:401:LEU:HG	1:C:927:LEU:HD13	2.02	0.40
1:C:696:MET:HG3	1:C:844:SER:HB2	2.04	0.40
1:C:853:TRP:CD1	1:C:861:VAL:HG21	2.56	0.40
1:C:1012:ALA:O	1:C:1016:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1030/1039 (99%)	1016 (99%)	14 (1%)	0	100	100
1	B	1019/1039 (98%)	996 (98%)	23 (2%)	0	100	100
1	C	1030/1039 (99%)	1008 (98%)	21 (2%)	1 (0%)	48	78
All	All	3079/3117 (99%)	3020 (98%)	58 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	230	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	875/883 (99%)	866 (99%)	9 (1%)	68	75
1	B	859/883 (97%)	854 (99%)	5 (1%)	78	80
1	C	876/883 (99%)	870 (99%)	6 (1%)	76	78
All	All	2610/2649 (98%)	2590 (99%)	20 (1%)	70	77

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	19	ILE
1	B	149	MET
1	B	333	PHE
1	B	431	ASP
1	B	450	VAL
1	A	150	ASN
1	A	220	ILE
1	A	363	PHE
1	A	403	ILE
1	A	411	ILE
1	A	523	VAL
1	A	937	ILE
1	A	969	ILE
1	A	1014	PHE
1	C	211	GLN
1	C	660	LEU
1	C	697	LEU
1	C	758	LEU
1	C	761	ASN
1	C	928	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	231	GLN

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Mol	Chain	Res	Type
1	B	362	ASN
1	B	416	ASN
1	B	469	GLN
1	B	574	ASN
1	B	640	GLN
1	B	690	GLN
1	B	737	GLN
1	B	765	ASN
1	B	1027	ASN
1	A	161	ASN
1	A	438	ASN
1	A	469	GLN
1	A	582	HIS
1	A	594	ASN
1	A	679	GLN
1	C	45	GLN
1	C	161	ASN
1	C	180	ASN
1	C	214	GLN
1	C	275	GLN
1	C	708	ASN
1	C	737	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ERY	C	1101	-	53,53,53	0.94	1 (1%)	82,82,82	1.49	13 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ERY	C	1101	-	-	16/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	ERY	O2-C1	5.12	1.46	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1101	ERY	C22-O7-C5	-4.34	108.87	116.26
2	C	1101	ERY	O2-C1-C2	3.71	119.46	111.53
2	C	1101	ERY	O7-C5-C6	3.15	110.15	106.40
2	C	1101	ERY	C27-C26-C25	-3.13	108.53	113.27
2	C	1101	ERY	O5-C16-C15	-3.09	108.19	112.95
2	C	1101	ERY	O5-C16-C17	3.05	108.28	103.86
2	C	1101	ERY	C34-C10-C11	-2.73	110.84	114.30
2	C	1101	ERY	C15-C16-C17	2.53	111.97	107.64
2	C	1101	ERY	C16-C17-C18	2.50	114.76	111.12
2	C	1101	ERY	C7-C8-C9	-2.49	109.14	113.32
2	C	1101	ERY	O2-C1-O1	-2.36	119.69	123.95
2	C	1101	ERY	C13-O2-C1	-2.30	114.18	118.20
2	C	1101	ERY	C6-C5-C4	-2.12	110.81	113.89

There are no chirality outliers.

All (16) torsion outliers are listed below:

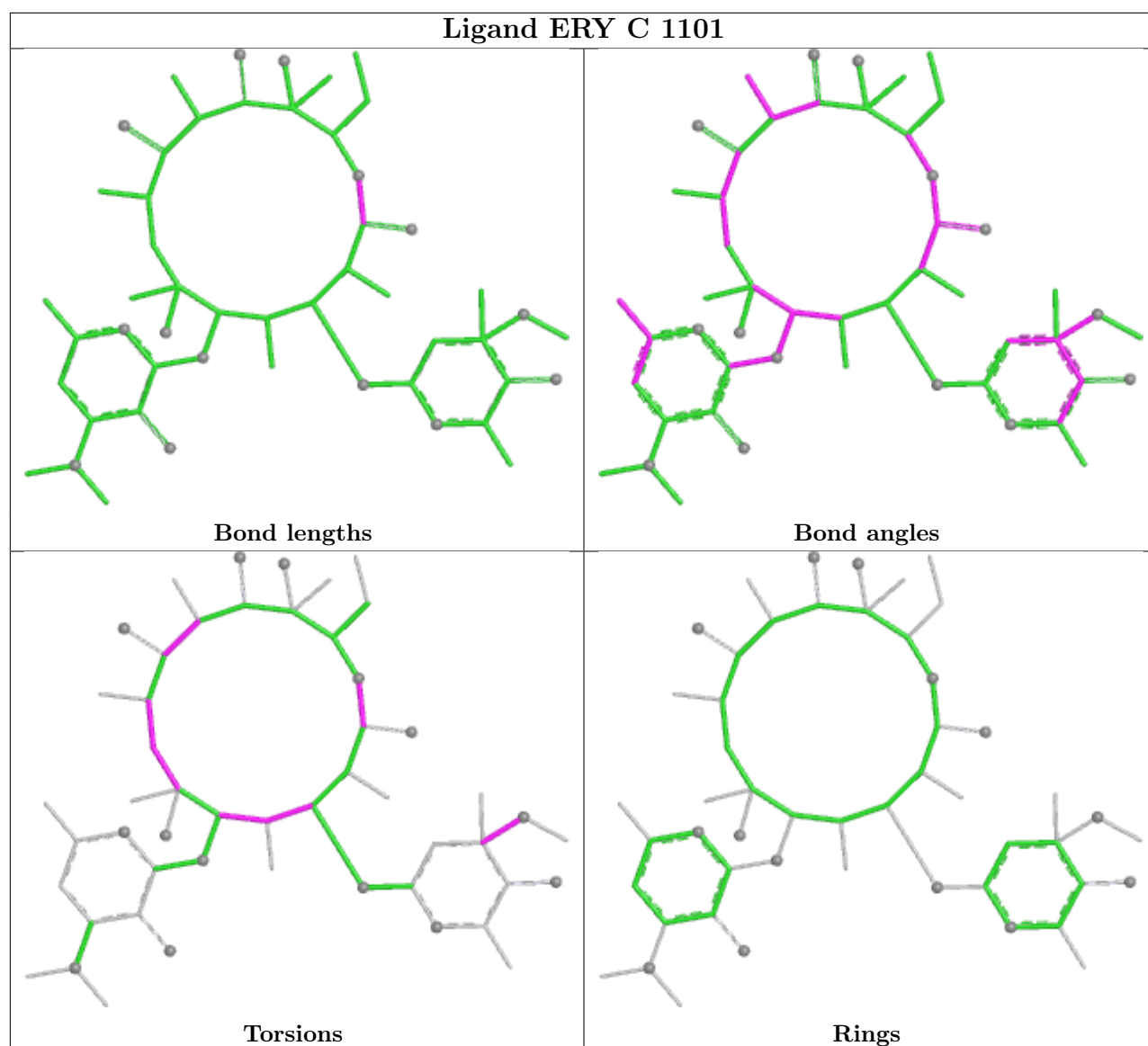
Mol	Chain	Res	Type	Atoms
2	C	1101	ERY	C17-C16-O5-C20
2	C	1101	ERY	C2-C1-O2-C13
2	C	1101	ERY	O3-C3-C4-C31
2	C	1101	ERY	C2-C3-C4-C31
2	C	1101	ERY	O3-C3-C4-C5
2	C	1101	ERY	C2-C3-C4-C5
2	C	1101	ERY	O1-C1-O2-C13
2	C	1101	ERY	C3-C4-C5-O7
2	C	1101	ERY	C32-C6-C7-C8
2	C	1101	ERY	O10-C6-C7-C8
2	C	1101	ERY	C11-C10-C9-C8
2	C	1101	ERY	C3-C4-C5-C6
2	C	1101	ERY	C11-C10-C9-O11
2	C	1101	ERY	C34-C10-C9-C8
2	C	1101	ERY	C6-C7-C8-C33
2	C	1101	ERY	C15-C16-O5-C20

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1101	ERY	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

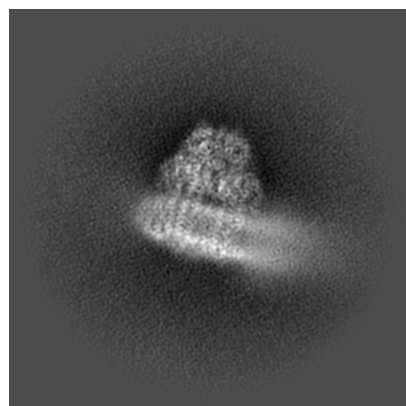
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40177. These allow visual inspection of the internal detail of the map and identification of artifacts.

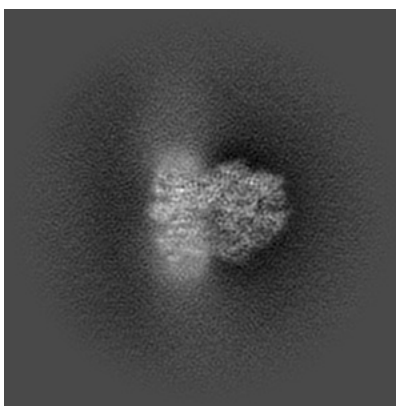
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

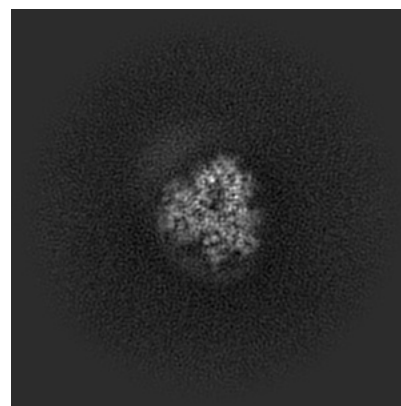
6.1.1 Primary map



X

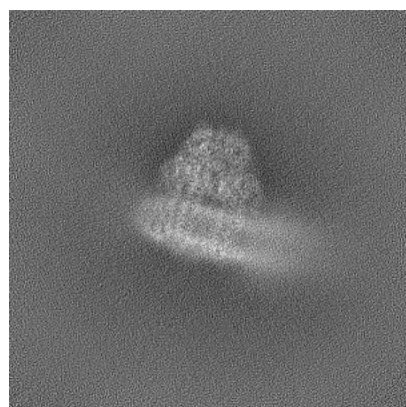


Y

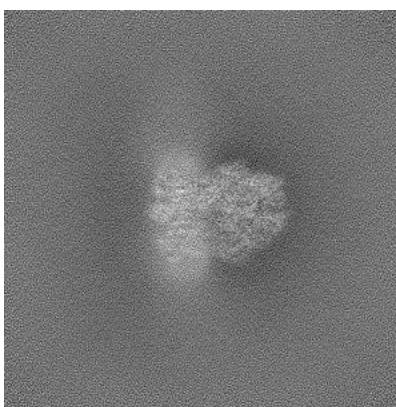


Z

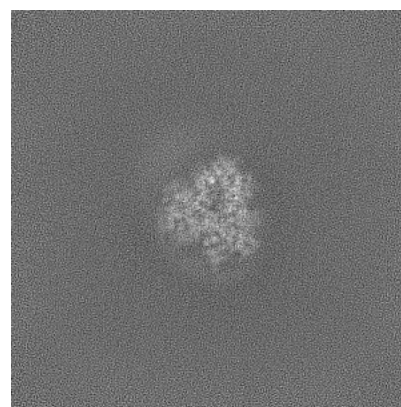
6.1.2 Raw map



X



Y

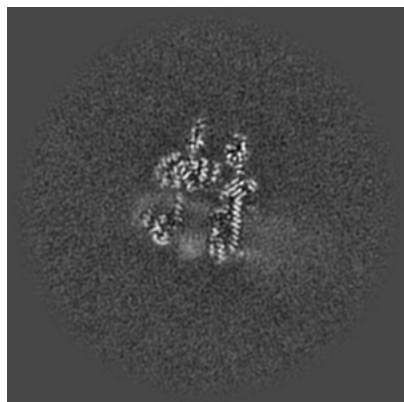


Z

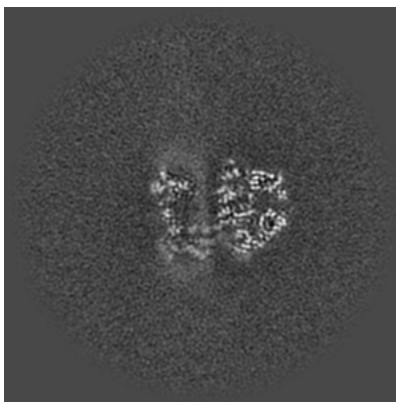
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

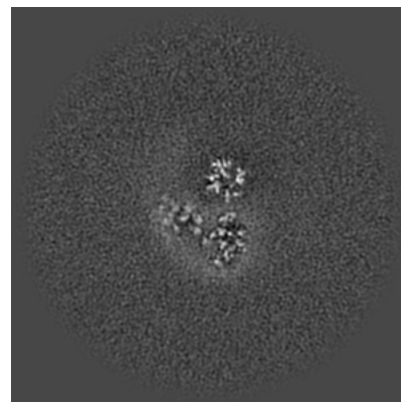
6.2.1 Primary map



X Index: 176

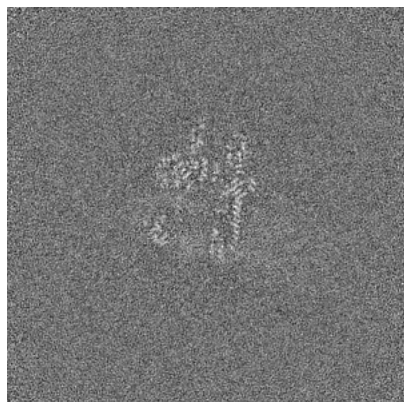


Y Index: 176

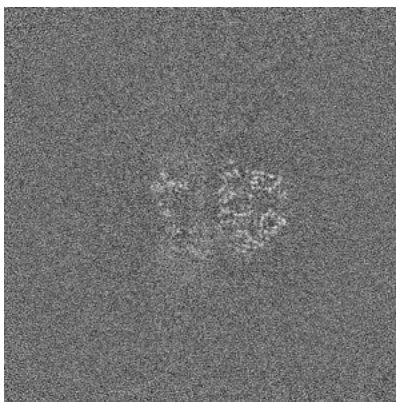


Z Index: 176

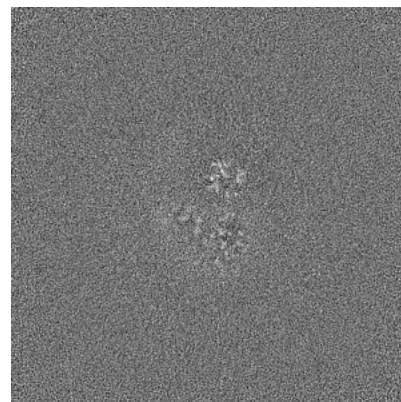
6.2.2 Raw map



X Index: 176



Y Index: 176

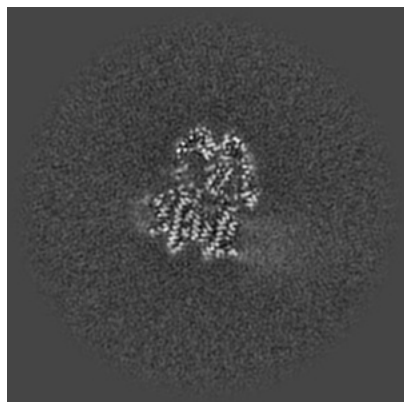


Z Index: 176

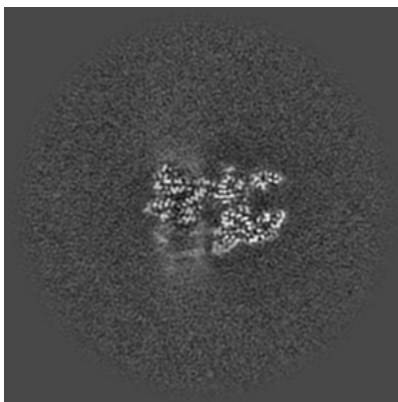
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

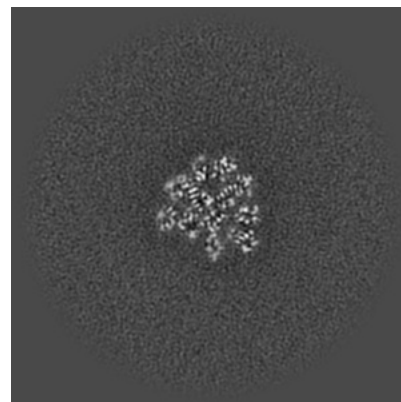
6.3.1 Primary map



X Index: 192

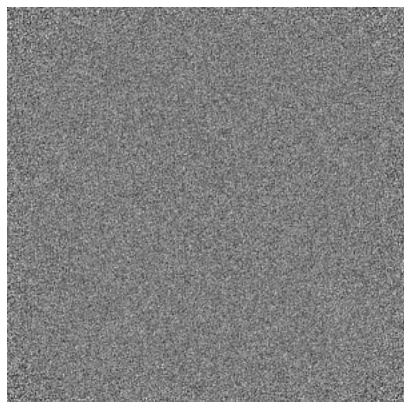


Y Index: 186

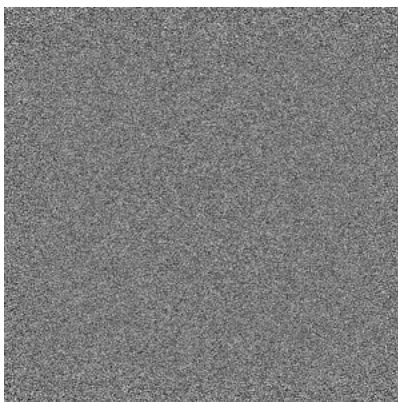


Z Index: 201

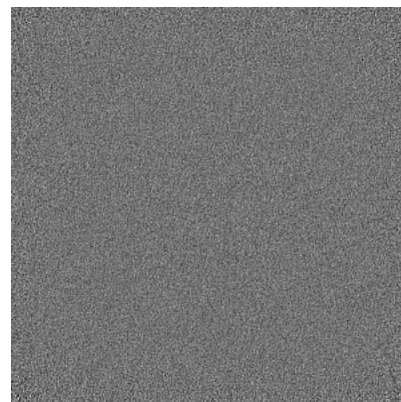
6.3.2 Raw map



X Index: 0



Y Index: 0

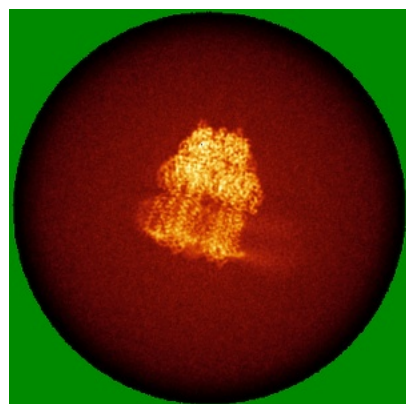


Z Index: 0

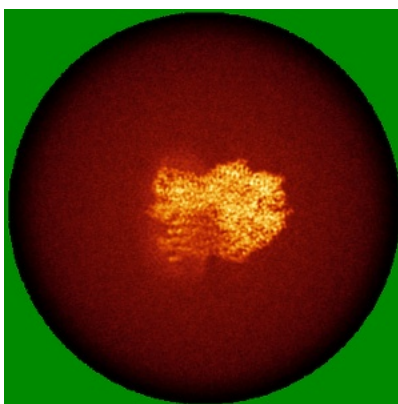
The images above show the largest variance slices of the map in three orthogonal directions.

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

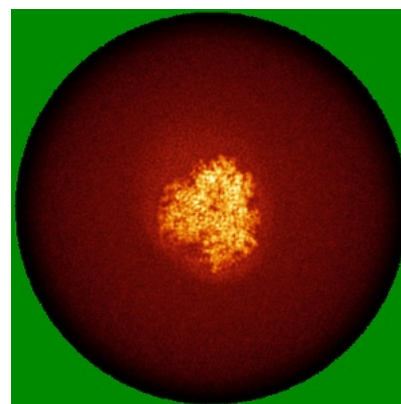
6.4.1 Primary map



X

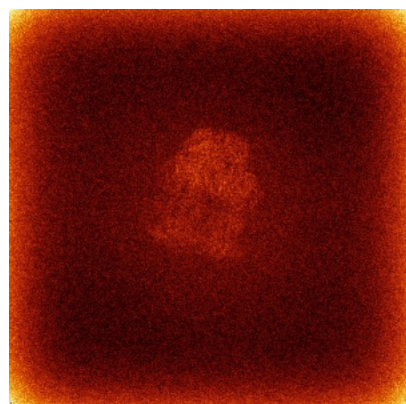


Y

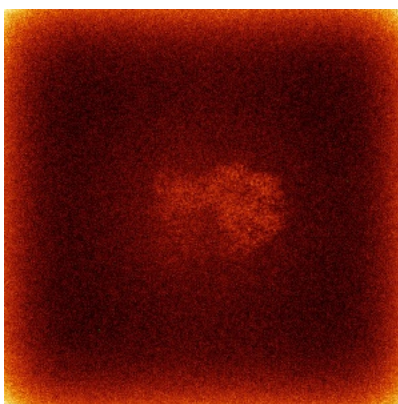


Z

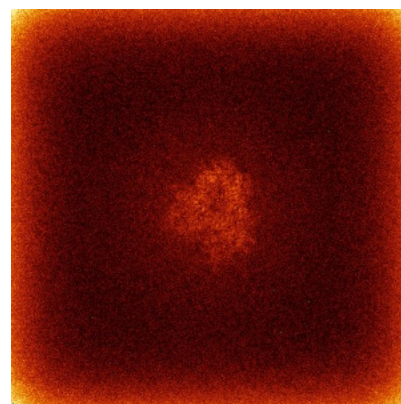
6.4.2 Raw map



X



Y

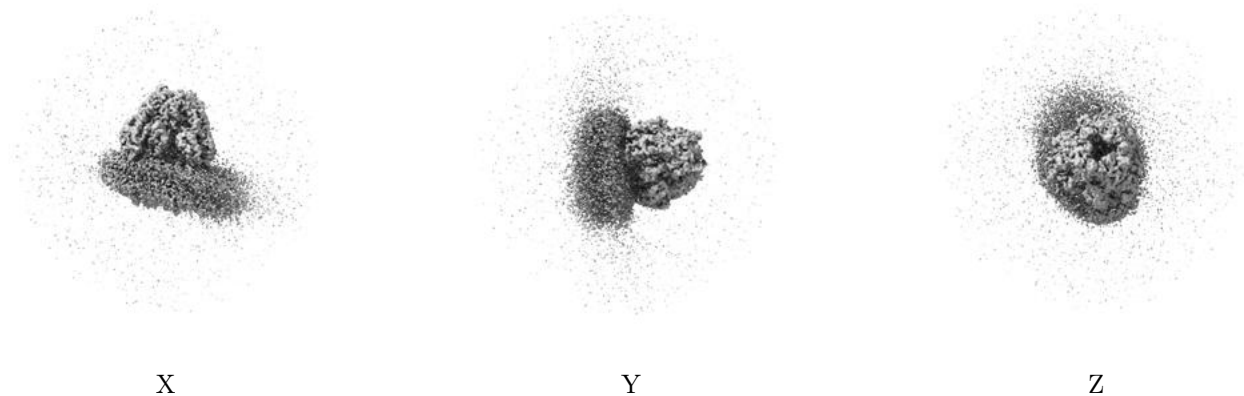


Z

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.

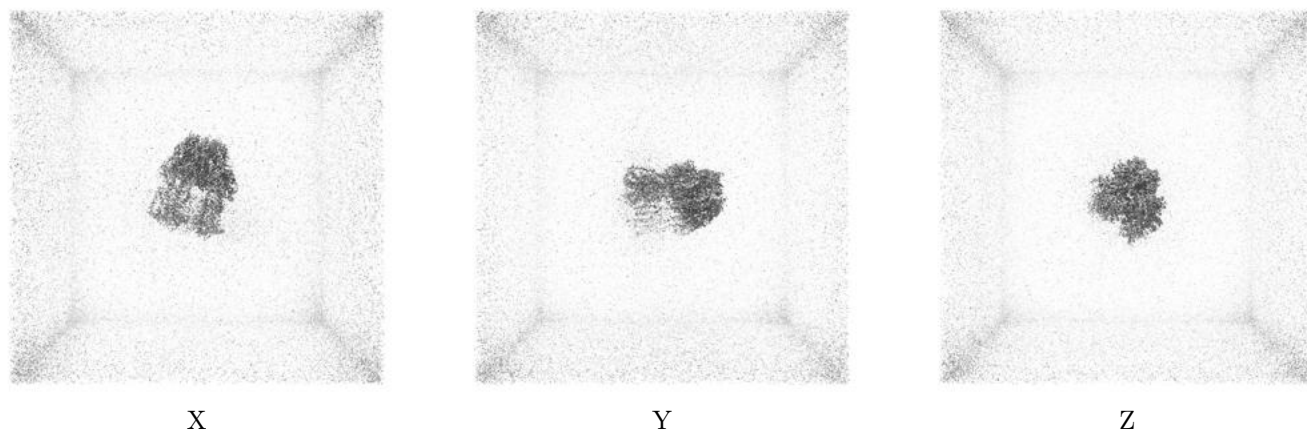
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

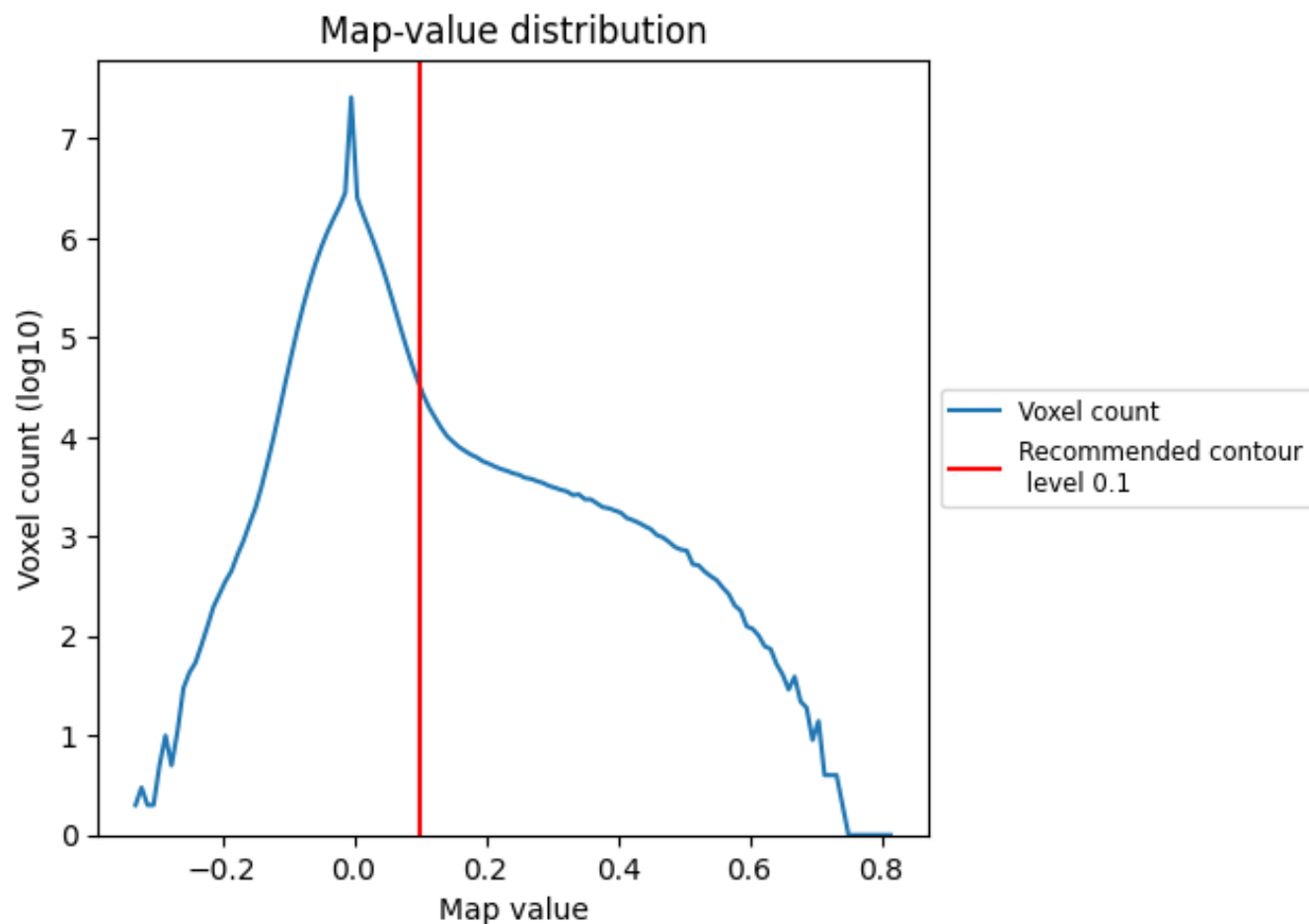
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

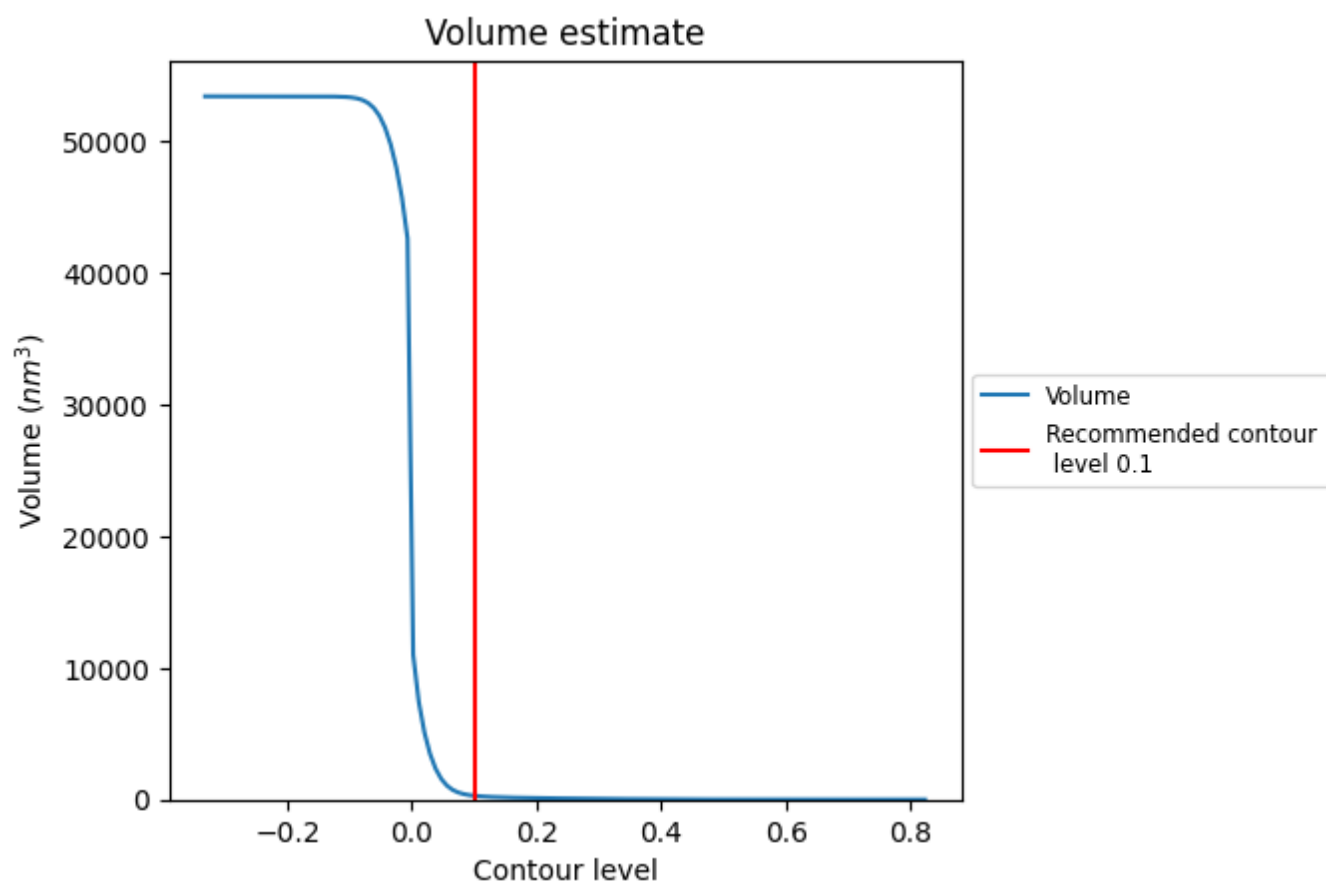
This section contains the results of statistical analysis of the map.

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.

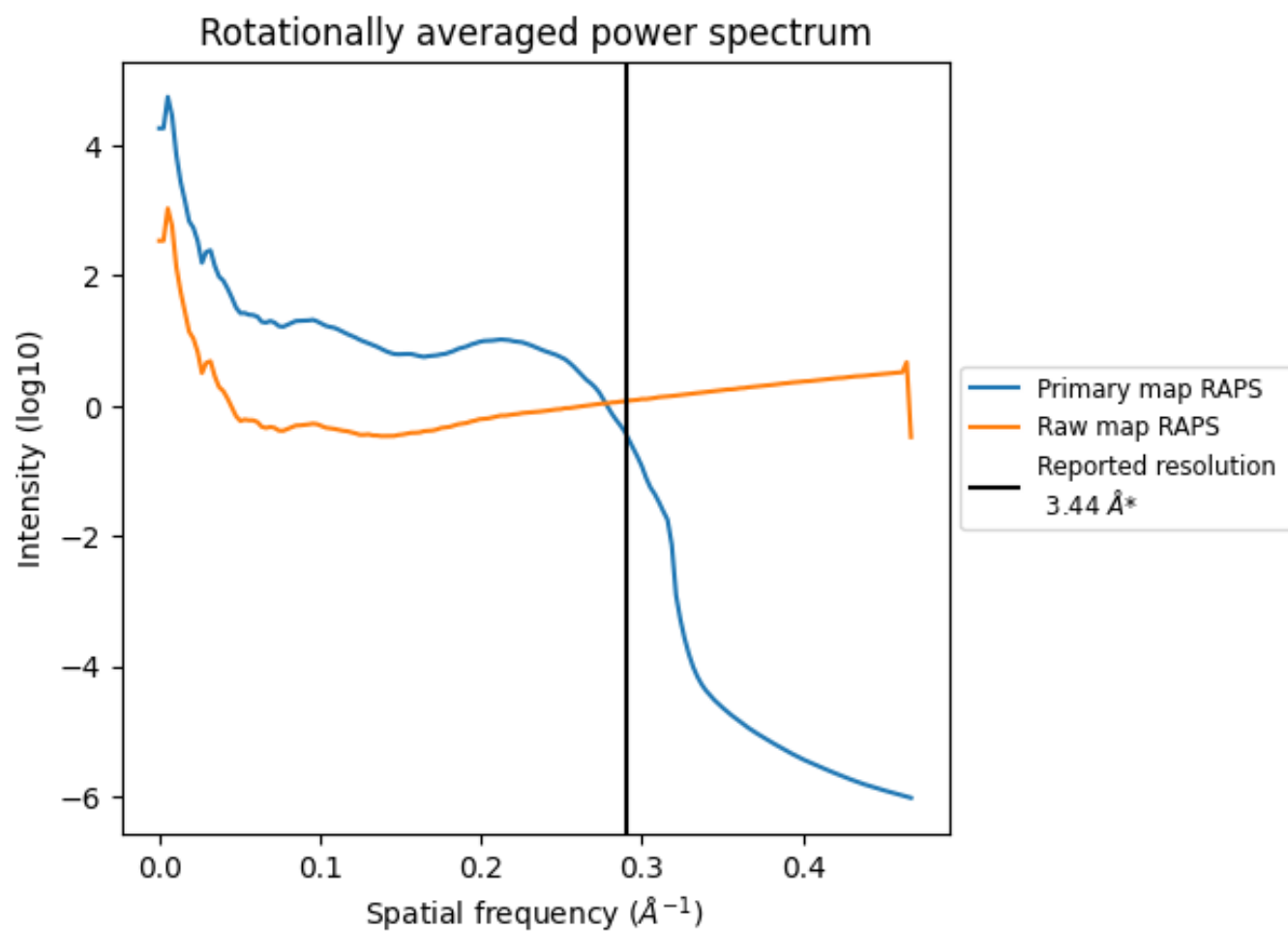
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 291 nm³; this corresponds to an approximate mass of 263 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 ⓘ

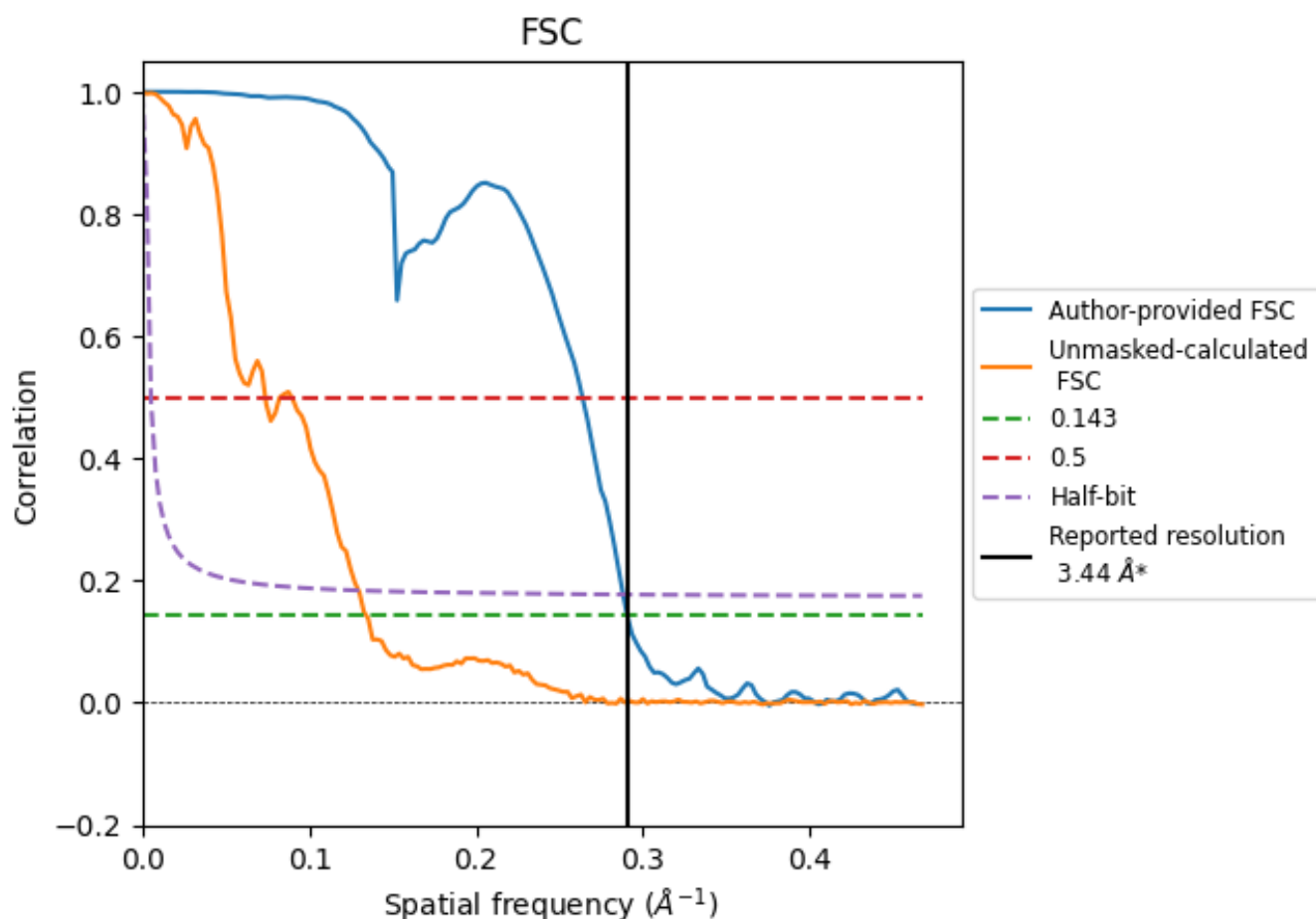


*Reported resolution corresponds to spatial frequency of 0.291 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.291 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

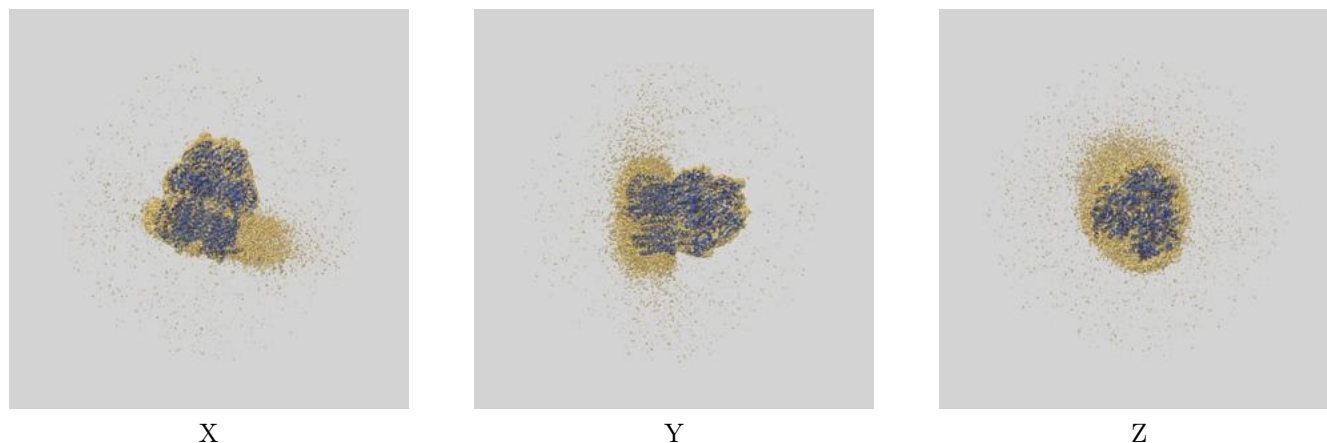
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.44	-	-
Author-provided FSC curve	3.44	3.79	3.47
Unmasked-calculated*	7.46	13.55	7.72

*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 7.46 differs from the reported value 3.44 by more than 10 %

9 Map-model fit [i](#)

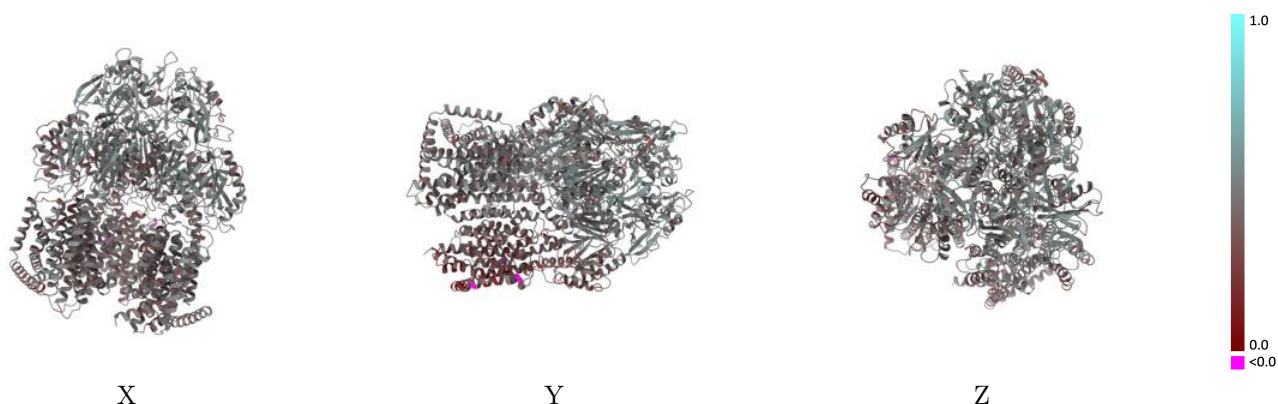
This section contains information regarding the fit between EMDB map EMD-40177 and PDB model 8GK0. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



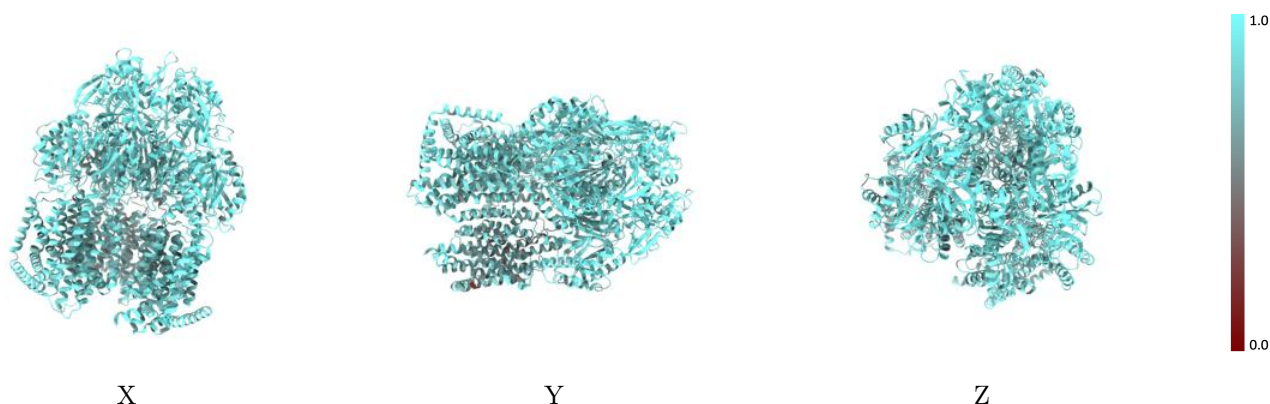
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



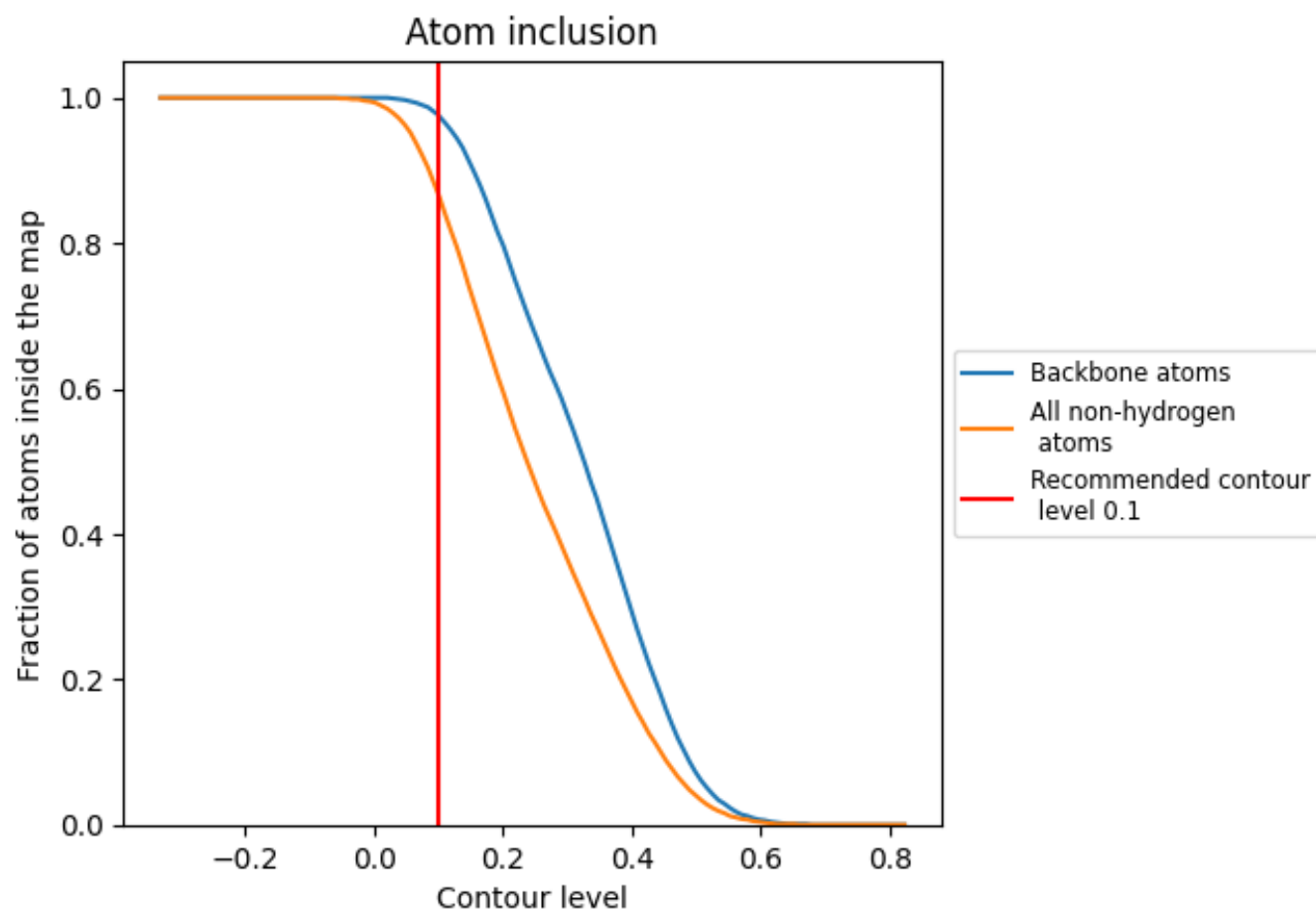
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 87% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8670	0.4410
A	0.8850	0.4650
B	0.8370	0.4050
C	0.8790	0.4520

