



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:25 PM UTC

PDB ID : 9KWC / pdb_00009kwc
EMDB ID : EMD-62607
Title : Cas12a-PCPS-light
Authors : Zhang, M.F.
Deposited on : 2024-12-05
Resolution : 2.90 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

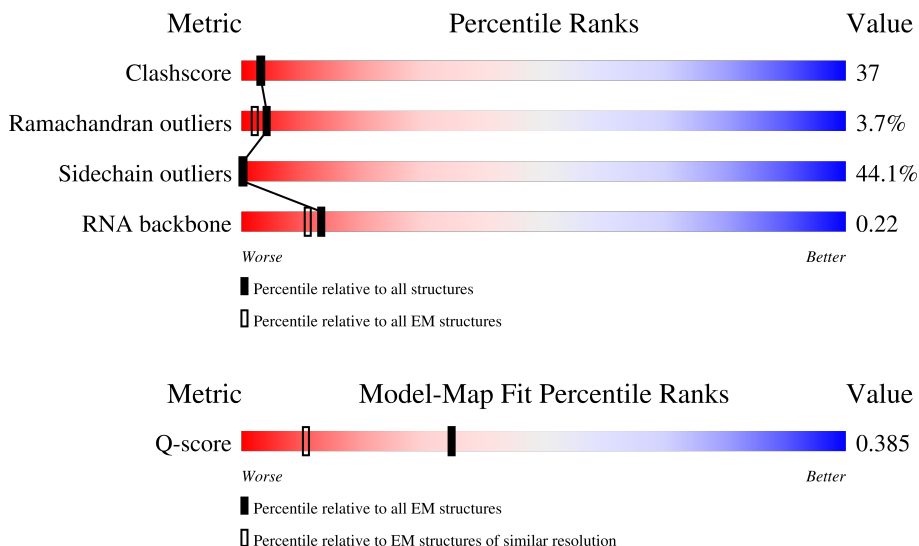
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	1225	
2	G	25	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9614 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 LbCas12a.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1121	Total	C	N	O	S	2	0
			9079	5835	1485	1735	24		

- Molecule 2 is a RNA chain called RNA (25-MER).

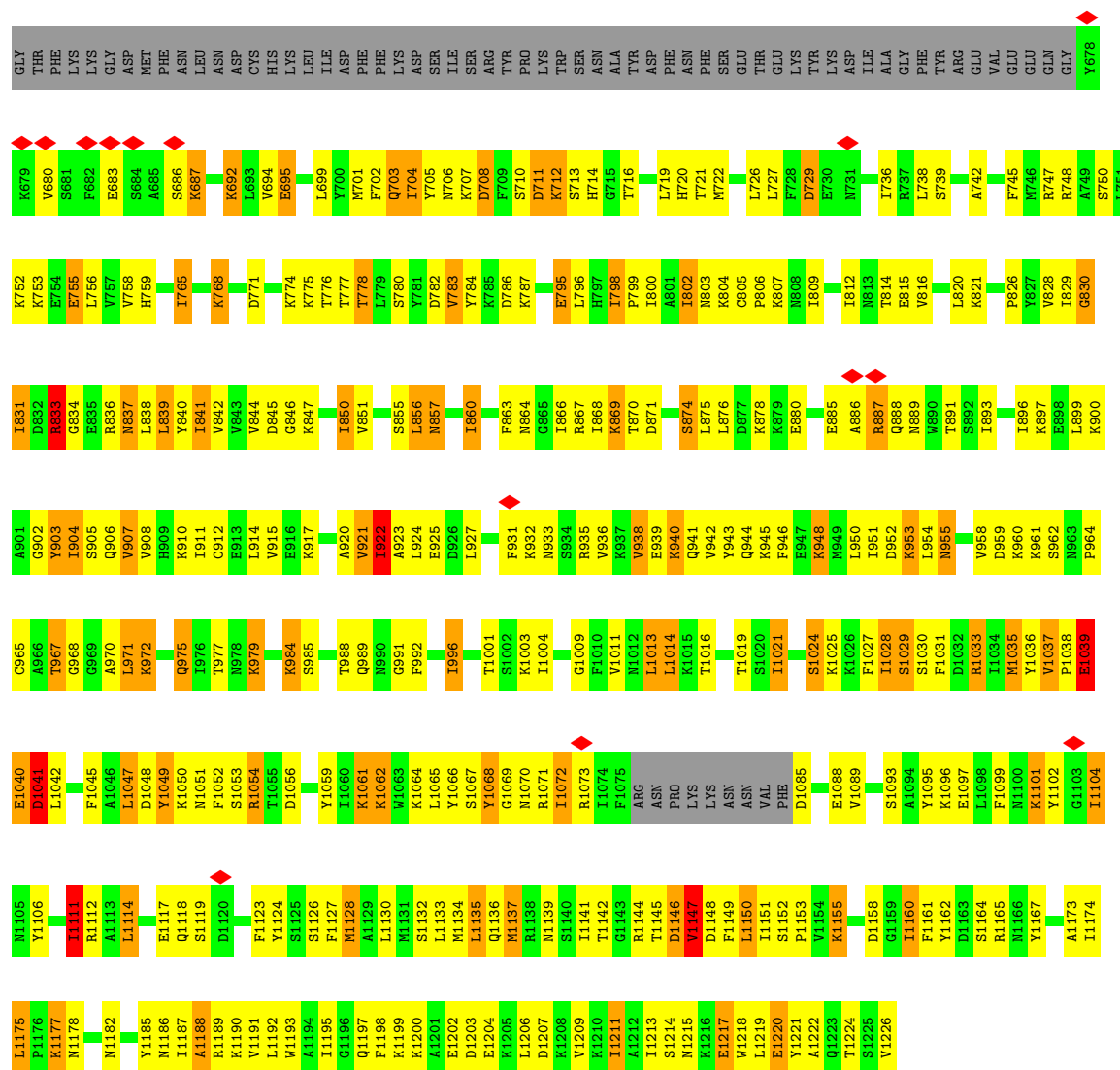
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	25	Total	C	N	O	P	0	0
			535	239	94	177	25		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: LbCas12a





• Molecule 2: RNA (25-MER)

Chain G:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	84400	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI MORGAGNI	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.478	Depositor
Minimum map value	-0.341	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	291.84, 291.84, 291.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.57, 0.57, 0.57	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.67	8/9270 (0.1%)	1.05	72/12499 (0.6%)
2	G	0.36	0/598	0.72	1/930 (0.1%)
All	All	0.66	8/9868 (0.1%)	1.03	73/13429 (0.5%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1070[A]	ASN	C-O	11.95	1.38	1.24
1	A	1070[B]	ASN	C-O	11.95	1.38	1.24
1	A	714[A]	HIS	C-O	11.01	1.38	1.24
1	A	714[B]	HIS	C-O	11.01	1.38	1.24
1	A	1070[A]	ASN	CA-C	8.02	1.62	1.52
1	A	1070[B]	ASN	CA-C	8.02	1.62	1.52
1	A	714[A]	HIS	CA-C	7.09	1.62	1.52
1	A	714[B]	HIS	CA-C	7.09	1.62	1.52

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1070[A]	ASN	CA-C-O	14.41	136.08	120.38
1	A	1070[B]	ASN	CA-C-O	14.41	136.08	120.38
1	A	1220	GLU	N-CA-C	-13.77	81.47	110.80
1	A	714[A]	HIS	CA-C-O	13.26	135.75	119.31
1	A	714[B]	HIS	CA-C-O	13.26	135.75	119.31
1	A	212	SER	N-CA-C	-11.07	99.29	111.36
1	A	714[A]	HIS	N-CA-C	11.05	126.59	112.89
1	A	714[B]	HIS	N-CA-C	11.05	126.59	112.89
1	A	1218	TRP	N-CA-C	-10.80	94.48	110.46
1	A	1070[A]	ASN	N-CA-C	10.00	125.17	109.07
1	A	1070[B]	ASN	N-CA-C	10.00	125.17	109.07
1	A	77	TYR	N-CA-C	-10.00	98.11	110.61
1	A	1070[A]	ASN	O-C-N	-9.19	112.45	123.29
1	A	1070[B]	ASN	O-C-N	-9.19	112.45	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	498	LEU	N-CA-C	-9.17	102.10	113.38
1	A	952	ASP	N-CA-C	-9.05	101.81	113.12
1	A	1217	GLU	N-CA-C	-8.90	102.43	113.38
1	A	315	PHE	N-CA-C	-8.82	101.74	111.36
1	A	256	ASN	N-CA-C	-8.45	102.56	113.12
1	A	232	GLU	N-CA-C	-8.26	93.22	110.80
1	A	227	PHE	N-CA-C	8.18	120.79	109.18
1	A	485	SER	N-CA-C	-7.76	103.94	113.41
1	A	100	ASN	N-CA-C	-7.64	103.22	112.54
1	A	714[A]	HIS	O-C-N	-7.44	112.19	122.46
1	A	714[B]	HIS	O-C-N	-7.44	112.19	122.46
1	A	1211	ILE	N-CA-C	-7.43	105.48	112.83
2	G	14	A	C2'-C3'-O3'	7.31	120.47	109.50
1	A	903	TYR	N-CA-C	-7.18	103.39	111.14
1	A	115	TYR	N-CA-C	-6.58	104.04	111.14
1	A	1050	LYS	N-CA-C	-6.53	105.35	113.38
1	A	1187	ILE	N-CA-C	-6.43	102.83	111.44
1	A	1193	TRP	N-CA-C	-6.31	104.32	111.07
1	A	953	LYS	N-CA-C	-6.29	104.35	111.14
1	A	233	GLY	N-CA-C	-6.23	98.42	113.18
1	A	231	GLN	N-CA-C	6.22	118.58	108.26
1	A	931	PHE	N-CA-C	6.21	118.53	108.34
1	A	1190	LYS	N-CA-C	-6.21	104.59	111.36
1	A	979	LYS	N-CA-C	-6.16	97.68	110.80
1	A	255	LEU	N-CA-C	-6.06	107.71	114.62
1	A	143	SER	N-CA-C	-6.00	105.45	112.89
1	A	727	LEU	N-CA-C	-5.87	104.88	111.28
1	A	711	ASP	N-CA-C	-5.77	106.07	113.23
1	A	240	ILE	N-CA-C	-5.73	107.23	112.96
1	A	706	ASN	N-CA-C	-5.71	101.08	109.81
1	A	61	PHE	N-CA-C	-5.67	105.01	111.07
1	A	73	ASN	N-CA-C	5.63	122.80	110.80
1	A	968	GLY	N-CA-C	-5.63	107.60	114.92
1	A	944	GLN	N-CA-C	-5.60	105.25	111.36
1	A	323	LYS	N-CA-C	-5.60	106.45	113.28
1	A	1111	ILE	N-CA-C	-5.55	106.89	112.17
1	A	920	ALA	N-CA-C	5.53	117.91	108.90
1	A	328	PHE	N-CA-C	-5.46	106.62	113.28
1	A	1001	THR	N-CA-C	-5.46	106.63	113.72
1	A	922	ILE	N-CA-C	-5.45	104.05	110.21
1	A	958	VAL	N-CA-C	5.38	115.64	108.11
1	A	1188	ALA	N-CA-C	-5.35	106.53	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	THR	N-CA-C	-5.29	106.88	113.38
1	A	1027	PHE	N-CA-C	-5.25	105.20	111.03
1	A	948	LYS	N-CA-C	-5.25	105.47	111.14
1	A	955	ASN	N-CA-C	-5.25	104.48	112.04
1	A	1070[A]	ASN	CA-C-N	-5.17	114.54	122.87
1	A	1070[A]	ASN	C-N-CA	-5.17	114.54	122.87
1	A	1070[B]	ASN	CA-C-N	-5.17	114.54	122.87
1	A	1070[B]	ASN	C-N-CA	-5.17	114.54	122.87
1	A	985	SER	N-CA-C	-5.15	106.99	113.28
1	A	560	LYS	N-CA-C	5.12	121.71	110.80
1	A	857	ASN	N-CA-C	-5.12	106.89	113.23
1	A	267	LYS	N-CA-C	5.10	121.67	110.80
1	A	524	TYR	N-CA-C	-5.10	107.23	113.50
1	A	174	ARG	N-CA-C	-5.06	106.32	113.20
1	A	40	ASP	N-CA-C	-5.05	105.86	111.36
1	A	1013	LEU	N-CA-C	-5.02	106.75	112.92
1	A	305	ARG	N-CA-C	-5.01	100.12	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9079	0	8819	698	0
2	G	535	0	267	6	0
All	All	9614	0	9086	698	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 37.

All (698) 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:190:PHE:HA	1:A:221:GLU:CA	1.19	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:PHE:CA	1:A:221:GLU:HA	1.21	1.61
1:A:193:VAL:HG21	1:A:273:PHE:CE2	1.32	1.60
1:A:190:PHE:CE1	1:A:220:PHE:HB2	1.34	1.60
1:A:922:ILE:CG2	1:A:924:LEU:HD12	1.12	1.59
1:A:171:ILE:CG2	1:A:230:THR:CG2	1.82	1.57
1:A:922:ILE:HG21	1:A:924:LEU:CD1	1.08	1.55
1:A:259:ILE:CG2	1:A:270:LEU:CD1	1.81	1.54
1:A:193:VAL:CG2	1:A:273:PHE:CE2	1.90	1.49
1:A:171:ILE:CG2	1:A:230:THR:HG21	1.34	1.47
1:A:240:ILE:CA	1:A:254:GLY:CA	1.86	1.44
1:A:190:PHE:CE1	1:A:220:PHE:CB	1.98	1.42
1:A:837:ASN:CG	1:A:840:TYR:HD2	1.28	1.41
1:A:922:ILE:CG2	1:A:924:LEU:CD1	1.75	1.41
1:A:996:ILE:HD12	1:A:1191:VAL:CG2	1.52	1.40
1:A:240:ILE:HA	1:A:254:GLY:CA	1.08	1.40
1:A:190:PHE:HE1	1:A:220:PHE:CA	1.29	1.38
1:A:240:ILE:CA	1:A:254:GLY:HA2	1.38	1.38
1:A:259:ILE:CG2	1:A:270:LEU:HD12	0.91	1.37
1:A:259:ILE:HG23	1:A:270:LEU:CD1	1.44	1.36
1:A:15:LYS:CD	1:A:802:ILE:HD11	1.55	1.34
1:A:837:ASN:HB3	1:A:855:SER:OG	1.21	1.33
1:A:837:ASN:ND2	1:A:840:TYR:HB2	1.38	1.33
1:A:193:VAL:CG2	1:A:273:PHE:HE2	1.26	1.32
1:A:996:ILE:CD1	1:A:1191:VAL:CG2	2.11	1.29
1:A:1024:SER:O	1:A:1028:ILE:HG13	1.31	1.29
1:A:837:ASN:CB	1:A:855:SER:OG	1.79	1.28
1:A:190:PHE:HE1	1:A:220:PHE:CB	1.36	1.27
1:A:911:ILE:CD1	1:A:946:PHE:HZ	1.45	1.27
1:A:303:VAL:HA	1:A:307:THR:C	1.39	1.27
1:A:259:ILE:O	1:A:261:LEU:N	1.68	1.26
1:A:954:LEU:CD2	1:A:977:THR:CG2	2.14	1.26
1:A:1041:ASP:OD2	1:A:1096:LYS:HE2	1.35	1.25
1:A:240:ILE:O	1:A:255:LEU:N	1.68	1.25
1:A:1221:TYR:H	1:A:1224:THR:CG2	1.51	1.22
1:A:837:ASN:CG	1:A:840:TYR:CD2	2.19	1.21
1:A:476:GLU:CG	1:A:479:GLU:OE1	1.89	1.19
1:A:190:PHE:CE1	1:A:220:PHE:CA	2.17	1.19
1:A:377:VAL:CG2	1:A:1054:ARG:HD3	1.72	1.18
1:A:476:GLU:HG3	1:A:479:GLU:OE1	1.36	1.17
1:A:1025:LYS:O	1:A:1029:SER:OG	1.59	1.17
1:A:871:ASP:OD2	1:A:874:SER:HB3	1.41	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1041:ASP:OD2	1:A:1096:LYS:CE	1.91	1.16
1:A:395:PHE:O	1:A:396:SER:O	1.64	1.16
1:A:15:LYS:HD2	1:A:802:ILE:HD11	1.25	1.16
1:A:954:LEU:HD23	1:A:977:THR:HG23	1.24	1.16
1:A:1040:GLU:HG3	1:A:1042:LEU:CD1	1.76	1.16
1:A:1040:GLU:CG	1:A:1042:LEU:HD12	1.74	1.16
1:A:303:VAL:HB	1:A:308:LEU:HG	1.26	1.15
1:A:11:TYR:CE2	1:A:975:GLN:NE2	2.14	1.14
1:A:1038:PRO:HD2	1:A:1039:GLU:OE1	1.42	1.14
1:A:15:LYS:HD3	1:A:802:ILE:HD11	1.27	1.14
1:A:1149:PHE:CA	1:A:1164:SER:OG	1.96	1.13
1:A:837:ASN:OD1	1:A:840:TYR:HD2	1.27	1.13
1:A:922:ILE:HG21	1:A:924:LEU:HD13	1.25	1.13
1:A:954:LEU:CD2	1:A:977:THR:HG23	1.76	1.13
1:A:922:ILE:HG21	1:A:924:LEU:HD11	1.19	1.12
1:A:98:GLU:O	1:A:101:LEU:HB2	1.48	1.12
1:A:259:ILE:HG22	1:A:270:LEU:HD12	1.23	1.11
1:A:171:ILE:CG2	1:A:230:THR:HG23	1.65	1.11
1:A:15:LYS:CG	1:A:800:ILE:HD11	1.80	1.10
1:A:171:ILE:HG22	1:A:230:THR:HG23	1.26	1.10
1:A:377:VAL:HG23	1:A:1054:ARG:HD3	1.13	1.10
1:A:240:ILE:O	1:A:254:GLY:HA3	1.51	1.09
1:A:837:ASN:OD1	1:A:840:TYR:CD2	2.05	1.09
1:A:240:ILE:C	1:A:255:LEU:N	2.09	1.09
1:A:15:LYS:HG3	1:A:800:ILE:HD11	1.12	1.08
1:A:193:VAL:HG21	1:A:273:PHE:CD2	1.88	1.08
1:A:911:ILE:CD1	1:A:946:PHE:CZ	2.36	1.08
1:A:1040:GLU:HG3	1:A:1042:LEU:HD12	1.21	1.08
1:A:171:ILE:HG23	1:A:230:THR:CG2	1.77	1.07
1:A:922:ILE:HG22	1:A:924:LEU:HD12	1.15	1.07
1:A:240:ILE:C	1:A:254:GLY:CA	2.28	1.07
1:A:303:VAL:HG12	1:A:308:LEU:HA	1.35	1.06
1:A:996:ILE:CD1	1:A:1191:VAL:HG23	1.80	1.06
1:A:305:ARG:NE	1:A:429:TYR:CD1	2.23	1.06
1:A:259:ILE:HG21	1:A:270:LEU:CD1	1.84	1.05
1:A:303:VAL:CA	1:A:307:THR:C	2.26	1.05
1:A:1221:TYR:H	1:A:1224:THR:HG22	1.11	1.05
1:A:351:ILE:HD11	1:A:414:LEU:HG	1.39	1.05
1:A:190:PHE:N	1:A:221:GLU:HB2	1.70	1.05
1:A:996:ILE:HD12	1:A:1191:VAL:HG23	1.12	1.05
1:A:1149:PHE:HB2	1:A:1164:SER:HG	1.21	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ILE:HG21	1:A:270:LEU:CB	1.87	1.05
1:A:303:VAL:HA	1:A:308:LEU:N	1.72	1.04
1:A:922:ILE:HG23	1:A:924:LEU:HD12	1.38	1.04
1:A:1150:LEU:HB3	1:A:1162:TYR:HE2	1.17	1.04
1:A:240:ILE:C	1:A:254:GLY:HA3	1.82	1.03
1:A:259:ILE:HG21	1:A:270:LEU:HD12	1.36	1.03
1:A:1150:LEU:N	1:A:1164:SER:OG	1.89	1.03
1:A:954:LEU:HD22	1:A:977:THR:CG2	1.85	1.03
1:A:259:ILE:O	1:A:262:TYR:N	1.92	1.02
1:A:193:VAL:CB	1:A:273:PHE:CE2	2.43	1.02
1:A:11:TYR:CD2	1:A:975:GLN:NE2	2.28	1.01
1:A:429:TYR:CD2	1:A:459:LEU:HD11	1.95	1.01
1:A:240:ILE:C	1:A:255:LEU:H	1.65	1.01
1:A:414:LEU:HA	1:A:417:ILE:HD12	1.39	1.01
1:A:996:ILE:HD12	1:A:1191:VAL:HG22	1.38	1.01
1:A:15:LYS:HD2	1:A:802:ILE:CD1	1.90	1.00
1:A:954:LEU:HD23	1:A:977:THR:CG2	1.83	1.00
1:A:1038:PRO:HD2	1:A:1039:GLU:CD	1.87	1.00
1:A:954:LEU:HB3	1:A:977:THR:HG23	1.43	1.00
1:A:954:LEU:HB3	1:A:977:THR:CG2	1.93	0.99
1:A:1149:PHE:HA	1:A:1164:SER:OG	1.62	0.99
1:A:193:VAL:CB	1:A:273:PHE:HE2	1.74	0.99
1:A:171:ILE:HG21	1:A:230:THR:CG2	1.62	0.99
1:A:1221:TYR:N	1:A:1224:THR:HG22	1.77	0.99
1:A:190:PHE:CG	1:A:221:GLU:HB3	1.97	0.98
1:A:305:ARG:NE	1:A:429:TYR:CE1	2.32	0.98
1:A:816:VAL:HB	1:A:989:GLN:HE22	1.26	0.98
1:A:188:ASP:H	1:A:221:GLU:HG3	1.23	0.98
1:A:871:ASP:OD2	1:A:874:SER:N	1.97	0.98
1:A:996:ILE:CD1	1:A:1191:VAL:HG22	1.91	0.98
1:A:186:ASN:C	1:A:221:GLU:HG2	1.88	0.98
1:A:1068:TYR:CD1	1:A:1068:TYR:C	2.43	0.97
1:A:871:ASP:OD2	1:A:874:SER:CB	2.12	0.97
1:A:472:ALA:O	1:A:474:PHE:N	1.97	0.97
1:A:837:ASN:ND2	1:A:840:TYR:CB	2.27	0.97
1:A:1149:PHE:HB2	1:A:1164:SER:OG	1.65	0.97
1:A:954:LEU:CB	1:A:977:THR:CG2	2.43	0.96
1:A:308:LEU:CD1	1:A:503:ILE:HG21	1.96	0.96
1:A:1149:PHE:CB	1:A:1164:SER:OG	2.14	0.95
1:A:190:PHE:CE1	1:A:220:PHE:N	2.35	0.95
1:A:305:ARG:HD2	1:A:429:TYR:CD1	2.02	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:911:ILE:HD13	1:A:946:PHE:HZ	1.29	0.94
1:A:190:PHE:HE1	1:A:220:PHE:N	1.65	0.94
1:A:98:GLU:HA	1:A:101:LEU:HD22	1.46	0.94
1:A:303:VAL:HB	1:A:308:LEU:CG	1.86	0.94
1:A:193:VAL:HG11	1:A:220:PHE:HB3	1.50	0.94
1:A:186:ASN:O	1:A:221:GLU:HG2	1.67	0.93
1:A:510:TYR:O	1:A:513:GLN:HB2	1.67	0.93
1:A:837:ASN:HB2	1:A:855:SER:OG	1.69	0.93
1:A:1221:TYR:N	1:A:1224:THR:CG2	2.31	0.93
1:A:377:VAL:HG23	1:A:1054:ARG:CD	1.98	0.93
1:A:240:ILE:HG21	1:A:255:LEU:HG	1.50	0.92
1:A:954:LEU:HD22	1:A:977:THR:HG21	1.47	0.92
1:A:305:ARG:CD	1:A:429:TYR:CD1	2.52	0.92
1:A:193:VAL:HG23	1:A:273:PHE:HE2	1.30	0.91
1:A:240:ILE:HB	1:A:255:LEU:HB2	1.52	0.91
1:A:1149:PHE:CB	1:A:1165:ARG:HG3	2.01	0.91
1:A:303:VAL:HG12	1:A:308:LEU:CA	1.98	0.91
1:A:240:ILE:O	1:A:254:GLY:CA	2.17	0.91
1:A:21:ALA:HA	1:A:703:GLN:O	1.69	0.91
1:A:418:ILE:CD1	1:A:466:PHE:HE1	1.85	0.90
1:A:950:LEU:O	1:A:954:LEU:HD13	1.71	0.89
1:A:171:ILE:HG22	1:A:230:THR:CG2	1.87	0.89
1:A:172:ALA:CA	1:A:175:CYS:HB3	2.00	0.89
1:A:190:PHE:CA	1:A:221:GLU:CB	2.50	0.89
1:A:508:ARG:O	1:A:512:THR:HG22	1.72	0.89
1:A:259:ILE:CG2	1:A:270:LEU:CG	2.51	0.89
1:A:190:PHE:H	1:A:221:GLU:HB2	1.31	0.89
1:A:1036:TYR:CE2	1:A:1038:PRO:HB3	2.08	0.89
1:A:1150:LEU:HB3	1:A:1162:TYR:CE2	2.06	0.88
1:A:837:ASN:HD22	1:A:840:TYR:HB2	1.37	0.88
1:A:1040:GLU:O	1:A:1042:LEU:HG	1.73	0.88
1:A:190:PHE:CA	1:A:221:GLU:CA	2.03	0.88
1:A:305:ARG:CD	1:A:429:TYR:CE1	2.57	0.88
1:A:1145:THR:O	1:A:1146:ASP:HB3	1.70	0.88
1:A:476:GLU:HG2	1:A:479:GLU:OE1	1.70	0.87
1:A:190:PHE:N	1:A:221:GLU:CB	2.37	0.87
1:A:950:LEU:O	1:A:954:LEU:HB2	1.74	0.87
1:A:473:PHE:H	1:A:473:PHE:HD2	1.21	0.87
1:A:1066:TYR:CD1	1:A:1155:LYS:HE2	2.09	0.87
1:A:186:ASN:C	1:A:221:GLU:CG	2.47	0.86
1:A:259:ILE:HG21	1:A:270:LEU:HB3	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1150:LEU:H	1:A:1164:SER:CB	1.87	0.86
1:A:413:LYS:O	1:A:417:ILE:CD1	2.24	0.86
1:A:219:PHE:CE1	1:A:240:ILE:HG12	2.10	0.86
1:A:259:ILE:C	1:A:261:LEU:N	2.34	0.85
1:A:1024:SER:O	1:A:1028:ILE:CG1	2.22	0.85
1:A:414:LEU:HD22	1:A:473:PHE:CZ	2.10	0.85
1:A:15:LYS:CG	1:A:800:ILE:CD1	2.54	0.85
1:A:414:LEU:CA	1:A:417:ILE:HD12	2.07	0.85
1:A:15:LYS:HG3	1:A:800:ILE:CD1	2.03	0.85
1:A:186:ASN:O	1:A:221:GLU:CD	2.19	0.84
1:A:193:VAL:HB	1:A:273:PHE:CE2	2.12	0.84
1:A:240:ILE:C	1:A:254:GLY:C	2.42	0.84
1:A:186:ASN:O	1:A:221:GLU:CG	2.25	0.84
1:A:11:TYR:CE2	1:A:975:GLN:HB3	2.13	0.84
1:A:305:ARG:HD2	1:A:429:TYR:CE1	2.13	0.83
1:A:259:ILE:HG21	1:A:270:LEU:CG	2.09	0.83
1:A:954:LEU:CB	1:A:977:THR:HG23	2.04	0.83
1:A:429:TYR:CE2	1:A:459:LEU:HD11	2.12	0.83
1:A:15:LYS:CD	1:A:802:ILE:CD1	2.46	0.82
1:A:547:LEU:HB2	1:A:554:TYR:HB2	1.61	0.82
1:A:837:ASN:HD21	1:A:840:TYR:HB2	1.35	0.82
1:A:239:ALA:C	1:A:240:ILE:HD13	2.05	0.82
1:A:11:TYR:CZ	1:A:975:GLN:HB3	2.14	0.82
1:A:240:ILE:O	1:A:254:GLY:C	2.22	0.81
1:A:190:PHE:CD1	1:A:220:PHE:HB2	2.15	0.81
1:A:193:VAL:HG23	1:A:273:PHE:CE2	2.06	0.81
1:A:305:ARG:HB2	1:A:429:TYR:HE1	1.44	0.81
1:A:172:ALA:HA	1:A:175:CYS:HB3	1.63	0.80
1:A:308:LEU:HD12	1:A:503:ILE:HG21	1.61	0.80
1:A:1149:PHE:C	1:A:1164:SER:OG	2.24	0.80
1:A:351:ILE:CD1	1:A:414:LEU:HG	2.11	0.80
1:A:308:LEU:HD11	1:A:503:ILE:HG21	1.64	0.79
1:A:314:ILE:HD12	1:A:496:ILE:HB	1.65	0.79
1:A:1028:ILE:HD11	1:A:1124:TYR:CD1	2.18	0.79
1:A:472:ALA:C	1:A:474:PHE:H	1.91	0.79
1:A:172:ALA:CB	1:A:176:ILE:HD11	2.12	0.79
1:A:1041:ASP:OD2	1:A:1096:LYS:HE3	1.83	0.79
1:A:418:ILE:HD11	1:A:466:PHE:CE1	2.18	0.78
1:A:837:ASN:ND2	1:A:840:TYR:CD2	2.51	0.78
1:A:240:ILE:HG21	1:A:255:LEU:CG	2.14	0.78
1:A:172:ALA:HB1	1:A:176:ILE:HD11	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ILE:C	1:A:261:LEU:H	1.87	0.78
1:A:377:VAL:CG2	1:A:1054:ARG:CD	2.58	0.78
1:A:1066:TYR:CE1	1:A:1155:LYS:CD	2.66	0.77
1:A:1149:PHE:HB3	1:A:1165:ARG:HG3	1.64	0.77
1:A:1040:GLU:O	1:A:1041:ASP:C	2.28	0.77
1:A:171:ILE:HG21	1:A:230:THR:HG21	0.77	0.77
1:A:1149:PHE:CD1	1:A:1165:ARG:HD3	2.18	0.77
1:A:816:VAL:HB	1:A:989:GLN:NE2	2.00	0.77
1:A:414:LEU:HA	1:A:417:ILE:CD1	2.12	0.77
1:A:1066:TYR:CE1	1:A:1155:LYS:HD2	2.19	0.77
1:A:1042:LEU:CD2	1:A:1068:TYR:HB2	2.16	0.76
1:A:837:ASN:ND2	1:A:840:TYR:HD2	1.84	0.76
1:A:902:GLY:O	1:A:906:GLN:HG2	1.85	0.76
1:A:197:PHE:CE2	1:A:220:PHE:CD1	2.74	0.76
1:A:20:LYS:HE2	1:A:22:ILE:HG12	1.66	0.75
1:A:911:ILE:HD12	1:A:946:PHE:CZ	2.21	0.75
1:A:219:PHE:HB3	1:A:255:LEU:HD12	1.69	0.75
1:A:351:ILE:HG23	1:A:413:LYS:HB3	1.69	0.75
1:A:395:PHE:O	1:A:396:SER:C	2.27	0.75
1:A:996:ILE:HD11	1:A:1191:VAL:CG2	2.16	0.75
1:A:66:LEU:CD2	1:A:109:PHE:CE1	2.70	0.75
1:A:1040:GLU:HG2	1:A:1042:LEU:HD12	1.64	0.74
1:A:1149:PHE:HB3	1:A:1165:ARG:CG	2.17	0.74
1:A:954:LEU:CB	1:A:977:THR:HG21	2.18	0.74
1:A:1028:ILE:HD12	1:A:1124:TYR:HE1	1.52	0.74
1:A:418:ILE:HD13	1:A:466:PHE:HE1	1.52	0.74
1:A:520:LYS:HB3	1:A:745:PHE:HB3	1.68	0.74
1:A:259:ILE:O	1:A:260:ASN:C	2.31	0.73
1:A:1040:GLU:HG3	1:A:1042:LEU:HD11	1.68	0.73
1:A:1068:TYR:C	1:A:1068:TYR:HD1	1.91	0.73
1:A:950:LEU:O	1:A:954:LEU:CD1	2.37	0.73
1:A:193:VAL:CG1	1:A:220:PHE:HB3	2.19	0.73
1:A:418:ILE:HG12	1:A:469:TYR:HD2	1.52	0.73
1:A:197:PHE:CE2	1:A:220:PHE:CG	2.76	0.73
1:A:399:GLN:HE22	1:A:402:GLU:CD	1.97	0.73
1:A:15:LYS:HD2	1:A:802:ILE:CG1	2.19	0.72
1:A:856:LEU:O	1:A:903:TYR:OH	2.05	0.72
1:A:66:LEU:HD21	1:A:109:PHE:CZ	2.25	0.72
1:A:418:ILE:HD11	1:A:466:PHE:HE1	1.52	0.72
1:A:12:SER:CB	1:A:803:ASN:O	2.38	0.72
1:A:305:ARG:HD2	1:A:429:TYR:HD1	1.51	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:CD2	1:A:109:PHE:CZ	2.72	0.72
1:A:188:ASP:N	1:A:221:GLU:HG3	2.01	0.72
1:A:240:ILE:HD13	1:A:240:ILE:N	2.03	0.72
1:A:256:ASN:C	1:A:258:TYR:H	1.96	0.72
1:A:188:ASP:H	1:A:221:GLU:CG	2.01	0.71
1:A:240:ILE:CG2	1:A:255:LEU:HG	2.20	0.70
1:A:190:PHE:CD1	1:A:220:PHE:CB	2.65	0.70
1:A:1028:ILE:CD1	1:A:1124:TYR:CE1	2.75	0.70
1:A:1038:PRO:CD	1:A:1039:GLU:CD	2.64	0.70
1:A:219:PHE:CZ	1:A:240:ILE:HG12	2.27	0.70
1:A:87:THR:O	1:A:88:GLU:CB	2.40	0.70
1:A:1041:ASP:CG	1:A:1096:LYS:CE	2.64	0.70
1:A:15:LYS:HG2	1:A:800:ILE:CD1	2.23	0.69
1:A:911:ILE:HD13	1:A:946:PHE:CZ	2.16	0.69
1:A:210:LEU:N	1:A:210:LEU:HD12	2.07	0.69
1:A:256:ASN:C	1:A:258:TYR:N	2.47	0.69
1:A:1066:TYR:CZ	1:A:1155:LYS:HD2	2.27	0.69
1:A:1068:TYR:CD1	1:A:1069:GLY:N	2.60	0.69
1:A:1155:LYS:NZ	1:A:1155:LYS:HB3	2.08	0.69
1:A:954:LEU:CG	1:A:977:THR:HG23	2.22	0.69
1:A:1149:PHE:CG	1:A:1165:ARG:HD3	2.28	0.69
1:A:244:PHE:CG	1:A:244:PHE:O	2.46	0.68
1:A:17:LEU:O	1:A:798:ILE:HD12	1.93	0.68
1:A:193:VAL:CG2	1:A:273:PHE:CD2	2.61	0.68
1:A:1038:PRO:CD	1:A:1039:GLU:OE2	2.42	0.68
1:A:11:TYR:HE2	1:A:975:GLN:HE21	1.27	0.68
1:A:98:GLU:O	1:A:101:LEU:CB	2.34	0.68
1:A:240:ILE:HB	1:A:255:LEU:CB	2.23	0.68
1:A:399:GLN:NE2	1:A:402:GLU:CD	2.52	0.68
1:A:726:LEU:HA	1:A:729:ASP:HB2	1.75	0.68
1:A:1028:ILE:CD1	1:A:1124:TYR:HE1	2.06	0.68
1:A:190:PHE:CZ	1:A:220:PHE:HB2	2.18	0.68
1:A:418:ILE:CD1	1:A:466:PHE:CE1	2.71	0.68
1:A:1041:ASP:CG	1:A:1096:LYS:HE3	2.18	0.68
1:A:312:SER:HA	1:A:315:PHE:CE2	2.29	0.67
1:A:190:PHE:N	1:A:221:GLU:CA	2.58	0.67
1:A:1028:ILE:HD11	1:A:1124:TYR:HD1	1.58	0.67
1:A:197:PHE:HZ	1:A:220:PHE:CD2	2.13	0.67
1:A:78:ILE:HG22	1:A:81:PHE:HB2	1.76	0.66
1:A:418:ILE:HG12	1:A:469:TYR:CD2	2.30	0.66
1:A:1149:PHE:HB2	1:A:1165:ARG:HG3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:LEU:HB2	1:A:977:THR:HG21	1.77	0.66
1:A:1036:TYR:CZ	1:A:1038:PRO:HA	2.29	0.66
1:A:911:ILE:HD11	1:A:946:PHE:HZ	1.54	0.66
1:A:496:ILE:C	1:A:498:LEU:H	2.01	0.66
1:A:473:PHE:N	1:A:473:PHE:CD2	2.64	0.66
1:A:351:ILE:HD11	1:A:414:LEU:CG	2.21	0.66
1:A:259:ILE:HG23	1:A:270:LEU:HD12	0.66	0.65
1:A:1066:TYR:CE1	1:A:1155:LYS:HE2	2.31	0.65
1:A:954:LEU:HB3	1:A:977:THR:OG1	1.96	0.65
1:A:188:ASP:N	1:A:221:GLU:CD	2.53	0.65
1:A:197:PHE:HE2	1:A:220:PHE:CG	2.15	0.65
1:A:193:VAL:HB	1:A:273:PHE:CZ	2.31	0.65
1:A:12:SER:HB2	1:A:803:ASN:O	1.97	0.64
1:A:21:ALA:HB1	1:A:702:PHE:HB3	1.79	0.64
1:A:1114:LEU:HA	1:A:1117:GLU:HB2	1.79	0.64
1:A:395:PHE:C	1:A:396:SER:O	2.37	0.64
1:A:496:ILE:O	1:A:499:LYS:N	2.18	0.64
1:A:837:ASN:HB3	1:A:855:SER:CB	2.26	0.64
1:A:413:LYS:O	1:A:417:ILE:HD12	1.97	0.64
1:A:379:GLU:O	1:A:382:GLU:HG3	1.98	0.64
1:A:1189:ARG:HA	1:A:1192:LEU:HB2	1.79	0.64
1:A:950:LEU:O	1:A:954:LEU:CB	2.45	0.63
1:A:927:LEU:HD13	1:A:940:LYS:HG2	1.80	0.63
1:A:871:ASP:OD2	1:A:874:SER:CA	2.46	0.63
1:A:816:VAL:CB	1:A:989:GLN:HE22	2.05	0.63
1:A:1066:TYR:HB2	1:A:1161:PHE:CZ	2.34	0.63
1:A:190:PHE:CG	1:A:221:GLU:CB	2.70	0.63
1:A:954:LEU:CD2	1:A:977:THR:HG21	2.05	0.63
1:A:12:SER:OG	1:A:803:ASN:O	2.17	0.62
1:A:193:VAL:CB	1:A:273:PHE:CZ	2.82	0.62
1:A:871:ASP:CG	1:A:874:SER:HB3	2.23	0.62
1:A:189:ILE:O	1:A:190:PHE:C	2.42	0.62
1:A:922:ILE:HG23	1:A:924:LEU:CD1	2.09	0.62
1:A:186:ASN:O	1:A:221:GLU:OE2	2.07	0.62
1:A:886:ALA:HB1	1:A:889:ASN:ND2	2.15	0.62
1:A:240:ILE:CG2	1:A:255:LEU:CG	2.77	0.62
1:A:399:GLN:NE2	1:A:402:GLU:OE2	2.32	0.62
1:A:816:VAL:CB	1:A:989:GLN:NE2	2.62	0.61
1:A:418:ILE:HB	1:A:469:TYR:HE2	1.64	0.61
1:A:470:ILE:O	1:A:470:ILE:HG13	2.01	0.61
1:A:1149:PHE:CB	1:A:1165:ARG:CG	2.76	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1182:ASN:O	1:A:1185:TYR:HB3	1.99	0.61
1:A:1186:ASN:HA	1:A:1189:ARG:HB2	1.81	0.60
1:A:188:ASP:N	1:A:221:GLU:CG	2.63	0.60
1:A:256:ASN:HA	1:A:259:ILE:CG1	2.31	0.60
1:A:549:TYR:HB2	1:A:554:TYR:HE1	1.65	0.60
1:A:1028:ILE:HD11	1:A:1124:TYR:CE1	2.36	0.60
1:A:954:LEU:HB3	1:A:977:THR:CB	2.31	0.60
1:A:305:ARG:CD	1:A:429:TYR:HD1	2.09	0.60
1:A:1038:PRO:CG	1:A:1039:GLU:OE2	2.50	0.60
1:A:66:LEU:HD23	1:A:109:PHE:CE1	2.34	0.60
1:A:420:GLN:HA	1:A:423:ASP:OD2	2.02	0.60
1:A:197:PHE:CZ	1:A:220:PHE:CG	2.90	0.59
1:A:871:ASP:CG	1:A:874:SER:H	2.11	0.59
1:A:1045:PHE:HB2	1:A:1065:LEU:HB2	1.84	0.59
1:A:185:SER:O	1:A:220:PHE:O	2.20	0.59
1:A:328:PHE:HA	1:A:331:TYR:HB2	1.85	0.59
1:A:954:LEU:CG	1:A:977:THR:CG2	2.78	0.59
1:A:488:GLY:H	1:A:491:VAL:HG13	1.66	0.59
1:A:704:ILE:HD13	1:A:796:LEU:HD23	1.85	0.59
1:A:1038:PRO:O	1:A:1039:GLU:C	2.45	0.59
1:A:1134:MET:HG2	1:A:1153:PRO:HB3	1.84	0.59
1:A:303:VAL:CG1	1:A:308:LEU:CA	2.76	0.59
1:A:259:ILE:HG22	1:A:270:LEU:CD1	1.98	0.58
1:A:303:VAL:CG1	1:A:308:LEU:HA	2.23	0.58
1:A:496:ILE:O	1:A:498:LEU:N	2.36	0.58
1:A:1066:TYR:CE1	1:A:1155:LYS:CG	2.86	0.58
1:A:148:THR:C	1:A:150:ALA:H	2.10	0.58
1:A:1014:LEU:HD21	1:A:1052:PHE:HB3	1.86	0.58
1:A:954:LEU:CB	1:A:977:THR:OG1	2.52	0.58
1:A:1040:GLU:CG	1:A:1042:LEU:CD1	2.54	0.58
1:A:186:ASN:HA	1:A:220:PHE:O	2.03	0.58
1:A:239:ALA:O	1:A:254:GLY:HA2	2.02	0.58
1:A:197:PHE:HZ	1:A:220:PHE:CE2	2.21	0.58
1:A:1066:TYR:CE1	1:A:1155:LYS:CE	2.86	0.58
1:A:1068:TYR:HD1	1:A:1068:TYR:O	1.87	0.57
1:A:911:ILE:HD11	1:A:946:PHE:CZ	2.32	0.57
1:A:413:LYS:O	1:A:417:ILE:HG13	2.04	0.57
1:A:1038:PRO:O	1:A:1039:GLU:O	2.22	0.57
1:A:418:ILE:CG1	1:A:469:TYR:CD2	2.87	0.56
1:A:1024:SER:HB3	1:A:1128:MET:SD	2.45	0.56
1:A:17:LEU:HG	1:A:800:ILE:HG12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:VAL:HG11	1:A:273:PHE:CZ	2.39	0.56
1:A:577:ASN:H	1:A:687:LYS:HB2	1.70	0.56
1:A:197:PHE:CZ	1:A:220:PHE:CD2	2.93	0.56
1:A:268:GLN:HA	1:A:331:TYR:OH	2.05	0.56
1:A:1038:PRO:CD	1:A:1039:GLU:OE1	2.35	0.56
1:A:1066:TYR:HB2	1:A:1161:PHE:HZ	1.69	0.56
1:A:1124:TYR:HA	1:A:1127:PHE:HB3	1.87	0.56
1:A:1101:LYS:HE3	1:A:1102:TYR:CE1	2.41	0.56
1:A:382:GLU:HB2	1:A:386:ARG:NH2	2.21	0.56
1:A:1037:VAL:HG12	1:A:1039:GLU:HG2	1.88	0.56
1:A:1150:LEU:H	1:A:1164:SER:HB3	1.69	0.55
1:A:1186:ASN:HD21	1:A:1189:ARG:HH21	1.54	0.55
1:A:1221:TYR:HA	1:A:1224:THR:HG23	1.89	0.55
1:A:1066:TYR:CE1	1:A:1155:LYS:HG2	2.41	0.55
1:A:190:PHE:HA	1:A:221:GLU:C	2.18	0.55
1:A:413:LYS:O	1:A:417:ILE:CG1	2.55	0.55
1:A:922:ILE:CG2	1:A:924:LEU:HD13	2.01	0.55
1:A:726:LEU:HD22	1:A:971:LEU:HD21	1.89	0.55
1:A:1038:PRO:HG2	1:A:1039:GLU:OE2	2.06	0.55
1:A:190:PHE:CB	1:A:221:GLU:CB	2.85	0.55
1:A:800:ILE:C	1:A:800:ILE:HD12	2.32	0.55
1:A:837:ASN:ND2	1:A:840:TYR:CG	2.75	0.55
1:A:171:ILE:HG22	1:A:175:CYS:HB2	1.89	0.55
1:A:1041:ASP:OD1	1:A:1096:LYS:HE3	2.05	0.55
1:A:1148:ASP:OD2	1:A:1178:ASN:HB2	2.06	0.55
1:A:1198:PHE:HA	1:A:1206:LEU:HD21	1.89	0.55
1:A:148:THR:C	1:A:150:ALA:N	2.63	0.54
1:A:240:ILE:N	1:A:254:GLY:HA2	2.17	0.54
1:A:240:ILE:CG2	1:A:255:LEU:CB	2.84	0.54
1:A:580:LYS:HB3	1:A:683:GLU:HG3	1.88	0.54
1:A:922:ILE:CG2	1:A:923:ALA:N	2.70	0.54
1:A:351:ILE:HA	1:A:413:LYS:HG2	1.89	0.54
1:A:518:LYS:HA	1:A:747:ARG:HD2	1.88	0.54
1:A:1041:ASP:CG	1:A:1096:LYS:HE2	2.23	0.54
1:A:259:ILE:O	1:A:261:LEU:CA	2.54	0.54
1:A:418:ILE:CG1	1:A:469:TYR:HD2	2.19	0.54
1:A:922:ILE:HG22	1:A:923:ALA:N	2.22	0.54
1:A:509:ASN:HA	1:A:512:THR:CG2	2.38	0.54
1:A:98:GLU:HA	1:A:101:LEU:CD2	2.30	0.54
1:A:572:ASP:HB3	1:A:575:ASN:HB2	1.87	0.54
1:A:198:ASP:H	1:A:201:GLU:HB2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ILE:HA	1:A:127:ILE:HG13	1.89	0.54
1:A:362:TRP:HH2	1:A:388:SER:HB2	1.72	0.54
1:A:496:ILE:C	1:A:498:LEU:N	2.63	0.54
1:A:259:ILE:HG23	1:A:270:LEU:HD13	1.74	0.54
1:A:305:ARG:CD	1:A:429:TYR:HE1	2.20	0.53
1:A:786:ASP:H	2:G:4:A:H5'	1.72	0.53
1:A:369:ILE:HG13	1:A:370:HIS:HD2	1.72	0.53
1:A:190:PHE:CB	1:A:221:GLU:HB3	2.38	0.53
1:A:85:THR:HA	1:A:93:GLU:HG3	1.90	0.53
1:A:532:GLY:H	1:A:542:TYR:HB3	1.74	0.53
1:A:582:ASN:HB2	1:A:683:GLU:HG2	1.91	0.53
1:A:837:ASN:OD1	1:A:840:TYR:CE2	2.60	0.53
1:A:92:LYS:O	1:A:93:GLU:C	2.51	0.52
1:A:256:ASN:O	1:A:258:TYR:N	2.42	0.52
1:A:833:ARG:HD2	1:A:938:VAL:HG13	1.90	0.52
1:A:172:ALA:O	1:A:176:ILE:HG12	2.09	0.52
1:A:311:ASN:HB3	1:A:315:PHE:CZ	2.45	0.52
1:A:1141:ILE:HD12	1:A:1147:VAL:HG21	1.91	0.52
1:A:162:PHE:HB3	1:A:284:ARG:HD3	1.91	0.52
1:A:429:TYR:CD2	1:A:459:LEU:CD1	2.81	0.52
1:A:783:VAL:HG22	1:A:783:VAL:O	2.09	0.52
1:A:1149:PHE:HA	1:A:1164:SER:CB	2.37	0.52
1:A:509:ASN:HA	1:A:512:THR:HG22	1.92	0.52
1:A:839:LEU:HD11	1:A:943:TYR:HE1	1.73	0.52
1:A:210:LEU:O	1:A:210:LEU:CD1	2.58	0.52
1:A:1040:GLU:O	1:A:1042:LEU:CG	2.52	0.52
1:A:828:VAL:HG12	1:A:923:ALA:HB2	1.91	0.52
1:A:303:VAL:CB	1:A:308:LEU:HG	2.18	0.51
1:A:413:LYS:C	1:A:417:ILE:CD1	2.82	0.51
1:A:712:LYS:HZ3	2:G:16:U:H2'	1.75	0.51
1:A:256:ASN:HA	1:A:259:ILE:HG13	1.90	0.51
1:A:413:LYS:C	1:A:417:ILE:HD11	2.36	0.51
1:A:1145:THR:O	1:A:1146:ASP:CB	2.47	0.51
1:A:9:ASN:HD22	1:A:806:PRO:HA	1.74	0.51
1:A:124:ILE:HG22	1:A:141:VAL:HG13	1.92	0.51
1:A:828:VAL:CG1	1:A:923:ALA:HB2	2.40	0.51
1:A:305:ARG:CZ	1:A:429:TYR:CD1	2.92	0.51
1:A:185:SER:C	1:A:220:PHE:O	2.53	0.51
1:A:922:ILE:CG2	1:A:924:LEU:HD11	1.97	0.51
1:A:1099:PHE:HA	1:A:1104:ILE:HG13	1.93	0.51
1:A:197:PHE:CZ	1:A:220:PHE:CD1	2.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLU:HG3	1:A:403:TYR:HE1	1.76	0.51
1:A:828:VAL:HB	1:A:1188:ALA:HB1	1.92	0.51
1:A:174:ARG:HG3	1:A:278:LYS:O	2.11	0.51
1:A:549:TYR:HB2	1:A:554:TYR:CE1	2.44	0.51
1:A:1049:TYR:HB2	1:A:1061:LYS:HA	1.93	0.51
1:A:837:ASN:HB3	1:A:855:SER:HG	1.61	0.50
1:A:94:LEU:O	1:A:95:GLU:C	2.54	0.50
1:A:172:ALA:C	1:A:175:CYS:HB3	2.36	0.50
1:A:400:LEU:HB3	1:A:410:VAL:HG11	1.93	0.50
1:A:820:LEU:HD11	1:A:921:VAL:HG11	1.92	0.50
1:A:86:ARG:H	1:A:93:GLU:HG3	1.77	0.50
1:A:413:LYS:O	1:A:417:ILE:HD11	2.07	0.50
1:A:996:ILE:HD13	1:A:1191:VAL:HG22	1.87	0.50
1:A:205:ILE:HD12	1:A:240:ILE:CG2	2.42	0.50
1:A:1072:ILE:HG13	1:A:1139:ASN:HB3	1.92	0.50
1:A:15:LYS:HD2	1:A:802:ILE:HG13	1.94	0.49
1:A:240:ILE:HG21	1:A:255:LEU:CD2	2.41	0.49
1:A:15:LYS:HG2	1:A:800:ILE:HD12	1.92	0.49
1:A:472:ALA:C	1:A:474:PHE:N	2.55	0.49
1:A:954:LEU:CD2	1:A:977:THR:HG22	2.30	0.49
1:A:708:ASP:HB2	1:A:721:THR:HG21	1.93	0.49
1:A:816:VAL:CG1	1:A:989:GLN:NE2	2.76	0.49
1:A:173:PHE:C	1:A:175:CYS:H	2.21	0.49
1:A:1221:TYR:H	1:A:1224:THR:HG21	1.63	0.49
1:A:26:LYS:HB2	1:A:695:GLU:HA	1.95	0.49
1:A:742:ALA:HA	1:A:799:PRO:HD3	1.95	0.49
1:A:359:ARG:HH22	1:A:386:ARG:HA	1.78	0.49
1:A:543:ARG:HH12	1:A:560:LYS:HD3	1.78	0.49
1:A:399:GLN:NE2	1:A:399:GLN:O	2.40	0.48
1:A:239:ALA:C	1:A:254:GLY:HA2	2.38	0.48
1:A:471:LYS:HE3	1:A:471:LYS:HB2	1.64	0.48
1:A:534:TRP:H	1:A:587:PRO:HG3	1.77	0.48
1:A:280:VAL:HG23	1:A:284:ARG:HA	1.95	0.48
1:A:1009:GLY:HA3	1:A:1222:ALA:O	2.12	0.48
1:A:172:ALA:HA	1:A:176:ILE:CD1	2.43	0.48
1:A:210:LEU:O	1:A:210:LEU:HD13	2.13	0.48
1:A:259:ILE:HG22	1:A:270:LEU:CG	2.37	0.48
1:A:1036:TYR:HE2	1:A:1038:PRO:HB3	1.67	0.48
1:A:382:GLU:HA	1:A:385:ARG:HH11	1.78	0.48
1:A:816:VAL:HG11	1:A:989:GLN:NE2	2.29	0.48
1:A:1137:MET:HE2	1:A:1137:MET:HB3	1.63	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ASP:HB3	1:A:217:GLU:HG3	1.96	0.48
1:A:418:ILE:CB	1:A:469:TYR:HE2	2.26	0.48
1:A:964:PRO:HA	1:A:970:ALA:H	1.78	0.48
1:A:240:ILE:HA	1:A:254:GLY:HA2	0.48	0.48
1:A:765:ILE:H	1:A:778:THR:H	1.62	0.48
1:A:127:ILE:H	1:A:127:ILE:HG12	1.33	0.48
1:A:221:GLU:HG3	1:A:222:GLY:H	1.79	0.48
1:A:20:LYS:HG2	1:A:705:TYR:O	2.14	0.48
1:A:172:ALA:HA	1:A:176:ILE:HD13	1.96	0.47
1:A:352:PHE:CE1	1:A:410:VAL:CG2	2.98	0.47
1:A:337:PHE:HB3	1:A:394:SER:HB2	1.96	0.47
1:A:190:PHE:H	1:A:221:GLU:CB	2.09	0.47
1:A:303:VAL:HA	1:A:307:THR:CA	2.33	0.47
1:A:418:ILE:HD12	1:A:470:ILE:HD13	1.96	0.47
1:A:1177:LYS:HE3	1:A:1177:LYS:HB3	1.49	0.47
1:A:79:SER:HA	1:A:224:PHE:HB2	1.97	0.47
1:A:1035:MET:HE2	1:A:1035:MET:HB2	1.63	0.47
1:A:1040:GLU:O	1:A:1040:GLU:HG2	2.14	0.47
1:A:1102:TYR:CE2	1:A:1123:PHE:HA	2.50	0.47
1:A:259:ILE:O	1:A:261:LEU:C	2.56	0.47
1:A:308:LEU:HD13	1:A:311:ASN:OD1	2.15	0.47
1:A:833:ARG:HB2	1:A:834:GLY:H	1.57	0.47
1:A:72:LYS:HB2	1:A:77:TYR:HA	1.95	0.47
1:A:831:ILE:HG23	1:A:841:ILE:HG12	1.96	0.47
1:A:897:LYS:HB2	1:A:897:LYS:HE2	1.56	0.47
1:A:193:VAL:CG1	1:A:273:PHE:CZ	2.98	0.47
1:A:20:LYS:HB3	2:G:6:U:H4'	1.97	0.47
1:A:157:ASN:HD22	1:A:157:ASN:HA	1.51	0.46
1:A:270:LEU:HA	1:A:271:PRO:HD2	1.74	0.46
1:A:837:ASN:CB	1:A:855:SER:HG	2.14	0.46
1:A:1066:TYR:HE1	1:A:1155:LYS:CG	2.26	0.46
1:A:185:SER:HA	1:A:222:GLY:HA2	1.97	0.46
1:A:305:ARG:HB2	1:A:429:TYR:CE1	2.36	0.46
1:A:219:PHE:HB3	1:A:255:LEU:CD1	2.43	0.46
1:A:948:LYS:HB3	1:A:948:LYS:HE2	1.59	0.46
1:A:886:ALA:HB1	1:A:889:ASN:HD21	1.81	0.46
1:A:15:LYS:HE2	1:A:15:LYS:HB3	1.30	0.46
1:A:826:PRO:HG3	1:A:1195:ILE:HG21	1.97	0.46
1:A:75:ASN:O	1:A:76:ASN:C	2.58	0.46
1:A:1042:LEU:HD21	1:A:1068:TYR:HB2	1.93	0.46
1:A:1149:PHE:HB3	1:A:1165:ARG:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:HD23	1:A:109:PHE:CZ	2.47	0.46
1:A:274:LYS:HA	1:A:274:LYS:HD3	1.50	0.46
1:A:460:LEU:HD22	1:A:504:TYR:HA	1.98	0.46
1:A:30:ASN:OD1	1:A:694:VAL:O	2.33	0.45
1:A:240:ILE:CB	1:A:255:LEU:CB	2.93	0.45
1:A:833:ARG:HH22	1:A:927:LEU:HD21	1.80	0.45
1:A:692:LYS:HB3	1:A:692:LYS:HE3	1.38	0.45
1:A:954:LEU:HD23	1:A:977:THR:HG22	1.90	0.45
1:A:518:LYS:HE3	1:A:518:LYS:HB2	1.64	0.45
1:A:1021:ILE:H	1:A:1021:ILE:HG12	1.27	0.45
1:A:1028:ILE:HD12	1:A:1124:TYR:CE1	2.38	0.45
1:A:168:SER:HB2	1:A:169:THR:H	1.58	0.45
1:A:245:VAL:HG22	1:A:251:LYS:NZ	2.32	0.45
1:A:339:LYS:HB3	1:A:339:LYS:HE3	1.33	0.45
1:A:414:LEU:HD22	1:A:473:PHE:CE1	2.52	0.45
1:A:569:ILE:H	1:A:569:ILE:HG13	1.49	0.45
1:A:571:LYS:HD2	1:A:571:LYS:HA	1.37	0.45
1:A:206:LYS:HE3	1:A:206:LYS:HB3	1.73	0.45
1:A:1059:TYR:CE2	1:A:1224:THR:HB	2.51	0.45
1:A:361:LYS:HD2	1:A:361:LYS:HA	1.73	0.45
1:A:1042:LEU:HD22	1:A:1068:TYR:HB2	1.97	0.45
1:A:305:ARG:CB	1:A:429:TYR:HE1	2.23	0.45
1:A:816:VAL:HG21	1:A:991:GLY:C	2.42	0.45
1:A:1160:ILE:H	1:A:1160:ILE:HG13	1.52	0.45
1:A:259:ILE:CG2	1:A:270:LEU:CB	2.73	0.45
1:A:1014:LEU:HA	1:A:1014:LEU:HD22	1.80	0.45
1:A:98:GLU:C	1:A:101:LEU:HB2	2.33	0.44
1:A:268:GLN:CA	1:A:331:TYR:OH	2.65	0.44
1:A:1186:ASN:ND2	1:A:1189:ARG:HH21	2.15	0.44
1:A:26:LYS:HB3	1:A:26:LYS:HE3	1.53	0.44
1:A:86:ARG:HB3	1:A:87:THR:H	1.62	0.44
1:A:302:GLU:HB2	1:A:436:PHE:HE1	1.82	0.44
1:A:856:LEU:HD13	1:A:856:LEU:HA	1.61	0.44
1:A:197:PHE:HE2	1:A:220:PHE:CB	2.31	0.44
1:A:256:ASN:O	1:A:259:ILE:HG13	2.18	0.44
1:A:975:GLN:HB3	1:A:975:GLN:HE21	1.53	0.44
1:A:1036:TYR:CZ	1:A:1038:PRO:CA	3.00	0.44
1:A:456:MET:HE2	1:A:456:MET:HB2	1.70	0.44
1:A:869:LYS:H	1:A:869:LYS:HG3	1.53	0.44
1:A:996:ILE:CD1	1:A:1191:VAL:HG21	2.32	0.44
1:A:498:LEU:HD23	1:A:498:LEU:HA	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:927:LEU:HA	1:A:927:LEU:HD23	1.64	0.44
1:A:1065:LEU:HD13	1:A:1135:LEU:HD11	1.98	0.44
1:A:1221:TYR:CA	1:A:1224:THR:CG2	2.96	0.44
1:A:163:SER:HB2	1:A:164:GLU:H	1.57	0.44
1:A:167:LYS:HE2	1:A:167:LYS:HB2	1.25	0.44
1:A:240:ILE:CB	1:A:255:LEU:HG	2.48	0.44
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.75	0.44
1:A:520:LYS:HB2	1:A:520:LYS:HE3	1.58	0.44
1:A:860:ILE:H	1:A:860:ILE:HG12	1.43	0.44
1:A:878:LYS:HB2	1:A:878:LYS:HE2	1.72	0.44
1:A:1062:LYS:HE2	1:A:1062:LYS:HB2	1.72	0.44
1:A:759:HIS:HB2	1:A:783:VAL:HG13	2.00	0.44
1:A:193:VAL:HB	1:A:273:PHE:HE2	1.54	0.44
1:A:4:LEU:HD21	1:A:915:VAL:HG12	1.99	0.43
1:A:70:LYS:HB3	1:A:70:LYS:HE3	1.45	0.43
1:A:259:ILE:HB	1:A:263:ASN:HB2	2.00	0.43
1:A:109:PHE:O	1:A:110:LYS:C	2.61	0.43
1:A:124:ILE:H	1:A:124:ILE:HG12	1.32	0.43
1:A:172:ALA:O	1:A:176:ILE:N	2.25	0.43
1:A:460:LEU:HB3	1:A:504:TYR:HD1	1.82	0.43
1:A:548:ARG:HB3	1:A:579:GLU:HB2	2.01	0.43
1:A:558:MET:HG3	1:A:699:LEU:HD12	2.01	0.43
1:A:967:THR:HG23	1:A:972:LYS:HZ2	1.82	0.43
1:A:1066:TYR:CB	1:A:1161:PHE:HZ	2.31	0.43
1:A:385:ARG:HE	1:A:385:ARG:HB2	1.60	0.43
1:A:1054:ARG:HD2	1:A:1054:ARG:HA	1.38	0.43
1:A:756:LEU:HB2	1:A:784:TYR:HD2	1.83	0.43
1:A:171:ILE:HG23	1:A:230:THR:HG23	1.68	0.43
1:A:704:ILE:HD13	1:A:796:LEU:CD2	2.48	0.43
1:A:712:LYS:HB2	2:G:16:U:H3'	2.00	0.43
1:A:954:LEU:HB2	1:A:977:THR:CG2	2.33	0.43
1:A:303:VAL:CA	1:A:308:LEU:N	2.41	0.43
1:A:400:LEU:HD12	1:A:400:LEU:HA	1.67	0.43
1:A:570:ASP:HB2	1:A:571:LYS:H	1.56	0.43
1:A:768:LYS:HG3	2:G:12:U:OP2	2.18	0.43
1:A:89:LYS:HE3	1:A:89:LYS:HB3	1.71	0.43
1:A:272:LYS:HE3	1:A:272:LYS:HB3	1.14	0.43
1:A:378:THR:O	1:A:382:GLU:CG	2.66	0.43
1:A:783:VAL:O	1:A:783:VAL:CG2	2.65	0.43
1:A:11:TYR:HE2	1:A:975:GLN:NE2	1.96	0.43
1:A:145:ASN:HB3	1:A:146:GLY:H	1.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:GLU:O	1:A:1042:LEU:N	2.52	0.43
1:A:1221:TYR:CA	1:A:1224:THR:HG23	2.48	0.43
1:A:220:PHE:O	1:A:221:GLU:C	2.62	0.42
1:A:133:ASP:OD2	1:A:133:ASP:N	2.53	0.42
1:A:189:ILE:H	1:A:189:ILE:HG13	1.47	0.42
1:A:258:TYR:O	1:A:259:ILE:C	2.62	0.42
1:A:281:LEU:HB3	1:A:282:SER:H	1.57	0.42
1:A:922:ILE:HG22	1:A:924:LEU:CD1	1.95	0.42
1:A:196:ILE:HD11	1:A:259:ILE:HA	2.01	0.42
1:A:1167:TYR:HB3	1:A:1173:ALA:HB1	2.00	0.42
1:A:240:ILE:N	1:A:240:ILE:CD1	2.70	0.42
1:A:329:ASP:HA	1:A:333:SER:HB2	2.00	0.42
1:A:1152:SER:O	1:A:1161:PHE:HD2	2.03	0.42
1:A:255:LEU:HD23	1:A:255:LEU:HA	1.73	0.42
1:A:344:ILE:HA	1:A:344:ILE:HD12	1.72	0.42
1:A:322:GLU:OE2	1:A:418:ILE:HD12	2.19	0.42
1:A:395:PHE:HD1	1:A:395:PHE:HA	1.68	0.42
1:A:174:ARG:HD3	1:A:278:LYS:O	2.19	0.42
1:A:197:PHE:CZ	1:A:220:PHE:CE2	3.05	0.42
1:A:229:LEU:HD23	1:A:229:LEU:HA	1.80	0.42
1:A:950:LEU:C	1:A:954:LEU:HD13	2.43	0.42
1:A:205:ILE:HD12	1:A:240:ILE:HG21	2.02	0.42
1:A:401:GLN:HG2	1:A:410:VAL:HB	2.00	0.42
1:A:950:LEU:HD12	1:A:950:LEU:HA	1.90	0.42
1:A:996:ILE:HD11	1:A:1191:VAL:HG23	1.82	0.42
1:A:1198:PHE:N	1:A:1198:PHE:CD1	2.87	0.42
1:A:418:ILE:CD1	1:A:470:ILE:HD13	2.50	0.42
1:A:755:GLU:H	1:A:755:GLU:HG3	1.69	0.42
1:A:795:GLU:H	1:A:795:GLU:HG2	1.50	0.42
1:A:903:TYR:O	1:A:906:GLN:N	2.52	0.42
1:A:1048:ASP:HB3	1:A:1051:ASN:HB2	2.01	0.42
1:A:172:ALA:CB	1:A:176:ILE:CD1	2.92	0.42
1:A:172:ALA:O	1:A:173:PHE:C	2.63	0.42
1:A:447:LYS:H	1:A:447:LYS:HG2	1.38	0.42
1:A:1071:ARG:HG3	1:A:1133:LEU:HB3	2.01	0.42
1:A:51:LYS:HG3	1:A:151:PHE:HE1	1.84	0.41
1:A:457:LYS:HE3	1:A:457:LYS:HB3	1.35	0.41
1:A:473:PHE:HD2	1:A:473:PHE:N	1.97	0.41
1:A:1175:LEU:HD12	1:A:1175:LEU:HA	1.93	0.41
1:A:303:VAL:CB	1:A:308:LEU:CA	2.91	0.41
1:A:580:LYS:HB2	1:A:580:LYS:HE2	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:HIS:CE1	2:G:22:U:H2'	2.55	0.41
1:A:837:ASN:HA	1:A:857:ASN:HD22	1.85	0.41
1:A:833:ARG:H	1:A:833:ARG:HG2	1.51	0.41
1:A:1036:TYR:CE2	1:A:1038:PRO:CB	2.93	0.41
1:A:1106:TYR:HA	1:A:1111:ILE:HD12	2.01	0.41
1:A:118:LEU:HD22	1:A:118:LEU:HA	1.88	0.41
1:A:161:MET:HE3	1:A:161:MET:HB3	1.69	0.41
1:A:1031:PHE:CD1	1:A:1047:LEU:HB2	2.55	0.41
1:A:842:VAL:HG13	1:A:850:ILE:HG23	2.02	0.41
1:A:3:LYS:HB2	1:A:3:LYS:HE2	1.84	0.41
1:A:279:GLN:H	1:A:279:GLN:HG2	1.52	0.41
1:A:428:VAL:HG11	1:A:458:ASP:HB3	2.03	0.41
1:A:184:ILE:HD13	1:A:184:ILE:HA	1.67	0.41
1:A:911:ILE:HD12	1:A:946:PHE:CE1	2.55	0.41
1:A:311:ASN:HA	1:A:314:ILE:HD13	2.02	0.41
1:A:352:PHE:CE1	1:A:410:VAL:HG22	2.55	0.41
1:A:845:ASP:HB2	1:A:846:GLY:H	1.72	0.41
1:A:545:THR:HG23	1:A:556:ALA:HB3	2.02	0.41
1:A:51:LYS:HB2	1:A:51:LYS:HE2	1.74	0.41
1:A:102:ARG:H	1:A:102:ARG:HG3	1.56	0.41
1:A:308:LEU:CD1	1:A:311:ASN:OD1	2.69	0.41
1:A:414:LEU:CD2	1:A:473:PHE:CZ	2.94	0.41
1:A:826:PRO:HB2	1:A:1195:ILE:HD13	2.03	0.41
1:A:945:LYS:HB2	1:A:945:LYS:HE2	1.75	0.41
1:A:529:GLN:H	1:A:529:GLN:HG3	1.69	0.40
1:A:722:MET:HE3	1:A:722:MET:HB2	1.94	0.40
1:A:984:LYS:H	1:A:984:LYS:HG2	1.54	0.40
1:A:1040:GLU:CG	1:A:1040:GLU:O	2.67	0.40
1:A:11:TYR:HD2	1:A:975:GLN:HE22	1.63	0.40
1:A:167:LYS:O	1:A:168:SER:C	2.64	0.40
1:A:830:GLY:HA2	1:A:923:ALA:HB3	2.03	0.40
1:A:953:LYS:C	1:A:955:ASN:H	2.28	0.40
1:A:1066:TYR:HE1	1:A:1155:LYS:HG2	1.85	0.40
1:A:904:ILE:HA	1:A:907:VAL:HG23	2.03	0.40
1:A:1155:LYS:HG2	1:A:1155:LYS:H	1.61	0.40
1:A:954:LEU:CG	1:A:977:THR:HG21	2.50	0.40
1:A:3:LYS:HB3	1:A:992:PHE:HZ	1.87	0.40
1:A:210:LEU:N	1:A:210:LEU:CD1	2.77	0.40
1:A:216:VAL:O	1:A:217:GLU:C	2.65	0.40
1:A:568:LYS:HE2	1:A:568:LYS:HB2	1.31	0.40
1:A:1033:ARG:HE	1:A:1033:ARG:HB3	1.64	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	1115/1225 (91%)	892 (80%)	182 (16%)	41 (4%)	2 11

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	76	ASN
1	A	109	PHE
1	A	146	GLY
1	A	260	ASN
1	A	271	PRO
1	A	285	GLU
1	A	396	SER
1	A	473	PHE
1	A	497	LEU
1	A	1039	GLU
1	A	1041	ASP
1	A	1146	ASP
1	A	74	LEU
1	A	110	LYS
1	A	173	PHE
1	A	221	GLU
1	A	223	GLU
1	A	268	GLN
1	A	560	LYS
1	A	63	ASN
1	A	88	GLU
1	A	90	GLU
1	A	95	GLU
1	A	217	GLU

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Mol	Chain	Res	Type
1	A	302	GLU
1	A	833	ARG
1	A	887	ARG
1	A	1207	ASP
1	A	267	LYS
1	A	300	VAL
1	A	577	ASN
1	A	272	LYS
1	A	305	ARG
1	A	821	LYS
1	A	196	ILE
1	A	573	ASP
1	A	830	GLY
1	A	23	PRO
1	A	1147	VAL
1	A	270	LEU

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	974/1112 (88%)	545 (56%)	429 (44%)	0 0

All (429) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	6	LYS
1	A	8	THR
1	A	9	ASN
1	A	11	TYR
1	A	13	LEU
1	A	15	LYS
1	A	16	THR
1	A	22	ILE
1	A	24	VAL

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Mol	Chain	Res	Type
1	A	26	LYS
1	A	29	GLU
1	A	34	LYS
1	A	35	ARG
1	A	36	LEU
1	A	37	LEU
1	A	38	VAL
1	A	48	LYS
1	A	51	LYS
1	A	54	LEU
1	A	56	ARG
1	A	57	TYR
1	A	59	LEU
1	A	61	PHE
1	A	66	LEU
1	A	70	LYS
1	A	71	LEU
1	A	72	LYS
1	A	73	ASN
1	A	74	LEU
1	A	80	LEU
1	A	82	ARG
1	A	83	LYS
1	A	84	LYS
1	A	85	THR
1	A	87	THR
1	A	89	LYS
1	A	94	LEU
1	A	97	LEU
1	A	101	LEU
1	A	102	ARG
1	A	103	LYS
1	A	105	ILE
1	A	110	LYS
1	A	116	LYS
1	A	118	LEU
1	A	120	LYS
1	A	121	LYS
1	A	122	ASP
1	A	124	ILE
1	A	125	GLU
1	A	126	THR

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Mol	Chain	Res	Type
1	A	127	ILE
1	A	130	GLU
1	A	133	ASP
1	A	137	GLU
1	A	140	LEU
1	A	141	VAL
1	A	144	PHE
1	A	148	THR
1	A	152	THR
1	A	157	ASN
1	A	158	ARG
1	A	161	MET
1	A	163	SER
1	A	164	GLU
1	A	165	GLU
1	A	167	LYS
1	A	168	SER
1	A	169	THR
1	A	170	SER
1	A	171	ILE
1	A	174	ARG
1	A	176	ILE
1	A	178	GLU
1	A	182	ARG
1	A	183	TYR
1	A	184	ILE
1	A	185	SER
1	A	186	ASN
1	A	187	MET
1	A	189	ILE
1	A	190	PHE
1	A	191	GLU
1	A	196	ILE
1	A	198	ASP
1	A	202	VAL
1	A	203	GLN
1	A	204	GLU
1	A	205	ILE
1	A	206	LYS
1	A	207	GLU
1	A	208	LYS
1	A	210	LEU

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Mol	Chain	Res	Type
1	A	214	TYR
1	A	215	ASP
1	A	216	VAL
1	A	217	GLU
1	A	219	PHE
1	A	226	ASN
1	A	229	LEU
1	A	230	THR
1	A	234	ILE
1	A	235	ASP
1	A	240	ILE
1	A	241	ILE
1	A	244	PHE
1	A	246	THR
1	A	251	LYS
1	A	253	LYS
1	A	256	ASN
1	A	257	GLU
1	A	258	TYR
1	A	259	ILE
1	A	262	TYR
1	A	263	ASN
1	A	265	LYS
1	A	266	THR
1	A	267	LYS
1	A	268	GLN
1	A	270	LEU
1	A	272	LYS
1	A	274	LYS
1	A	276	LEU
1	A	278	LYS
1	A	279	GLN
1	A	280	VAL
1	A	281	LEU
1	A	282	SER
1	A	283	ASP
1	A	284	ARG
1	A	285	GLU
1	A	286	SER
1	A	287	LEU
1	A	288	SER
1	A	290	TYR

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Mol	Chain	Res	Type
1	A	296	SER
1	A	298	GLU
1	A	301	LEU
1	A	303	VAL
1	A	304	PHE
1	A	306	ASN
1	A	307	THR
1	A	308	LEU
1	A	309	ASN
1	A	310	LYS
1	A	314	ILE
1	A	316	SER
1	A	318	ILE
1	A	324	LEU
1	A	325	PHE
1	A	339	LYS
1	A	344	ILE
1	A	345	SER
1	A	346	THR
1	A	347	ILE
1	A	349	LYS
1	A	354	GLU
1	A	356	ASN
1	A	361	LYS
1	A	367	ASP
1	A	380	LYS
1	A	383	ASP
1	A	385	ARG
1	A	386	ARG
1	A	390	LYS
1	A	391	LYS
1	A	392	ILE
1	A	395	PHE
1	A	396	SER
1	A	397	LEU
1	A	398	GLU
1	A	399	GLN
1	A	400	LEU
1	A	401	GLN
1	A	402	GLU
1	A	408	LEU
1	A	413	LYS

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Mol	Chain	Res	Type
1	A	416	GLU
1	A	417	ILE
1	A	418	ILE
1	A	419	ILE
1	A	421	LYS
1	A	422	VAL
1	A	424	GLU
1	A	428	VAL
1	A	431	SER
1	A	433	GLU
1	A	434	LYS
1	A	435	LEU
1	A	437	ASP
1	A	441	VAL
1	A	446	LEU
1	A	447	LYS
1	A	449	ASN
1	A	456	MET
1	A	457	LYS
1	A	464	LYS
1	A	470	ILE
1	A	473	PHE
1	A	474	PHE
1	A	480	THR
1	A	485	SER
1	A	491	VAL
1	A	492	LEU
1	A	496	ILE
1	A	497	LEU
1	A	500	VAL
1	A	503	ILE
1	A	505	ASP
1	A	513	GLN
1	A	514	LYS
1	A	518	LYS
1	A	519	ASP
1	A	520	LYS
1	A	522	LYS
1	A	529	GLN
1	A	530	PHE
1	A	531	MET
1	A	537	ASP

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Mol	Chain	Res	Type
1	A	539	GLU
1	A	542	TYR
1	A	545	THR
1	A	549	TYR
1	A	552	LYS
1	A	557	ILE
1	A	558	MET
1	A	559	ASP
1	A	562	TYR
1	A	564	LYS
1	A	566	LEU
1	A	568	LYS
1	A	569	ILE
1	A	570	ASP
1	A	571	LYS
1	A	574	VAL
1	A	580	LYS
1	A	585	LEU
1	A	680	VAL
1	A	686	SER
1	A	687	LYS
1	A	692	LYS
1	A	695	GLU
1	A	701	MET
1	A	703	GLN
1	A	704	ILE
1	A	707	LYS
1	A	708	ASP
1	A	710	SER
1	A	711	ASP
1	A	712	LYS
1	A	713	SER
1	A	716	THR
1	A	719	LEU
1	A	729	ASP
1	A	736	ILE
1	A	738	LEU
1	A	739	SER
1	A	748	ARG
1	A	750	SER
1	A	752	LYS
1	A	753	LYS

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Mol	Chain	Res	Type
1	A	755	GLU
1	A	758	VAL
1	A	765	ILE
1	A	768	LYS
1	A	771	ASP
1	A	774	LYS
1	A	775	LYS
1	A	776	THR
1	A	777	THR
1	A	778	THR
1	A	780	SER
1	A	782	ASP
1	A	783	VAL
1	A	787	LYS
1	A	795	GLU
1	A	798	ILE
1	A	802	ILE
1	A	804	LYS
1	A	805	CYS
1	A	807	LYS
1	A	809	ILE
1	A	812	ILE
1	A	814	THR
1	A	815	GLU
1	A	829	ILE
1	A	831	ILE
1	A	833	ARG
1	A	836	ARG
1	A	837	ASN
1	A	838	LEU
1	A	839	LEU
1	A	841	ILE
1	A	844	VAL
1	A	847	LYS
1	A	850	ILE
1	A	851	VAL
1	A	856	LEU
1	A	860	ILE
1	A	863	PHE
1	A	864	ASN
1	A	866	ILE
1	A	867	ARG

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Mol	Chain	Res	Type
1	A	868	ILE
1	A	869	LYS
1	A	870	THR
1	A	874	SER
1	A	875	LEU
1	A	876	LEU
1	A	880	GLU
1	A	885	GLU
1	A	887	ARG
1	A	888	GLN
1	A	891	THR
1	A	893	ILE
1	A	896	ILE
1	A	899	LEU
1	A	900	LYS
1	A	904	ILE
1	A	905	SER
1	A	907	VAL
1	A	908	VAL
1	A	910	LYS
1	A	912	CYS
1	A	914	LEU
1	A	917	LYS
1	A	921	VAL
1	A	922	ILE
1	A	925	GLU
1	A	932	LYS
1	A	933	ASN
1	A	935	ARG
1	A	936	VAL
1	A	938	VAL
1	A	939	GLU
1	A	940	LYS
1	A	941	GLN
1	A	942	VAL
1	A	951	ILE
1	A	959	ASP
1	A	960	LYS
1	A	961	LYS
1	A	962	SER
1	A	965	CYS
1	A	967	THR

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Mol	Chain	Res	Type
1	A	971	LEU
1	A	972	LYS
1	A	975	GLN
1	A	979	LYS
1	A	984	LYS
1	A	988	THR
1	A	996	ILE
1	A	1003	LYS
1	A	1004	ILE
1	A	1011	VAL
1	A	1013	LEU
1	A	1014	LEU
1	A	1016	THR
1	A	1019	THR
1	A	1021	ILE
1	A	1024	SER
1	A	1028	ILE
1	A	1029	SER
1	A	1030	SER
1	A	1033	ARG
1	A	1035	MET
1	A	1037	VAL
1	A	1039	GLU
1	A	1040	GLU
1	A	1041	ASP
1	A	1047	LEU
1	A	1049	TYR
1	A	1053	SER
1	A	1054	ARG
1	A	1056	ASP
1	A	1061	LYS
1	A	1062	LYS
1	A	1064	LYS
1	A	1067	SER
1	A	1068	TYR
1	A	1072	ILE
1	A	1073	ARG
1	A	1085	ASP
1	A	1088	GLU
1	A	1089	VAL
1	A	1093	SER
1	A	1095	TYR

Continued on next page...

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Mol	Chain	Res	Type
1	A	1097	GLU
1	A	1101	LYS
1	A	1104	ILE
1	A	1111	ILE
1	A	1112	ARG
1	A	1114	LEU
1	A	1118	GLN
1	A	1119	SER
1	A	1126	SER
1	A	1128	MET
1	A	1130	LEU
1	A	1132	SER
1	A	1135	LEU
1	A	1136	GLN
1	A	1137	MET
1	A	1142	THR
1	A	1144	ARG
1	A	1147	VAL
1	A	1150	LEU
1	A	1151	ILE
1	A	1155	LYS
1	A	1158	ASP
1	A	1160	ILE
1	A	1174	ILE
1	A	1175	LEU
1	A	1177	LYS
1	A	1197	GLN
1	A	1199	LYS
1	A	1200	LYS
1	A	1202	GLU
1	A	1203	ASP
1	A	1204	GLU
1	A	1209	VAL
1	A	1211	ILE
1	A	1213	ILE
1	A	1214	SER
1	A	1215	ASN
1	A	1217	GLU
1	A	1219	LEU
1	A	1220	GLU
1	A	1226	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	30	ASN
1	A	33	ASN
1	A	142	ASN
1	A	145	ASN
1	A	157	ASN
1	A	200	HIS
1	A	211	ASN
1	A	226	ASN
1	A	306	ASN
1	A	309	ASN
1	A	327	ASN
1	A	356	ASN
1	A	370	HIS
1	A	399	GLN
1	A	449	ASN
1	A	513	GLN
1	A	703	GLN
1	A	706	ASN
1	A	720	HIS
1	A	762	ASN
1	A	767	ASN
1	A	772	ASN
1	A	793	GLN
1	A	797	HIS
1	A	803	ASN
1	A	813	ASN
1	A	873	HIS
1	A	889	ASN
1	A	895	ASN
1	A	909	HIS
1	A	955	ASN
1	A	975	GLN
1	A	989	GLN
1	A	990	ASN
1	A	1012	ASN
1	A	1051	ASN
1	A	1100	ASN
1	A	1170	GLN
1	A	1186	ASN
1	A	1197	GLN
1	A	1215	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	24/25 (96%)	10 (41%)	2 (8%)

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	4	A
2	G	14	A
2	G	15	G
2	G	16	U
2	G	17	G
2	G	18	U
2	G	20	G
2	G	24	G
2	G	25	G
2	G	27	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	G	14	A
2	G	16	U

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 ⓘ

There are no chain breaks in this entry.

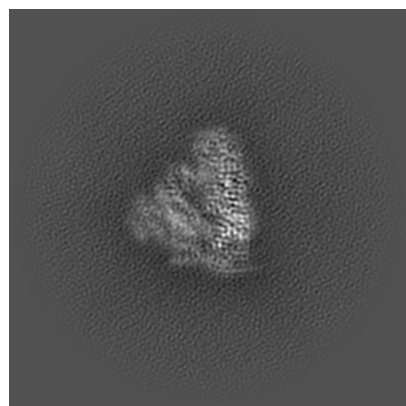
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62607. These allow visual inspection of the internal detail of the map and identification of artifacts.

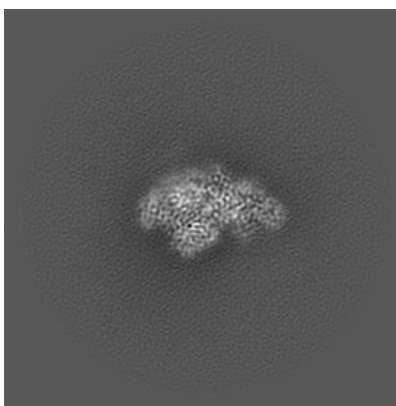
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

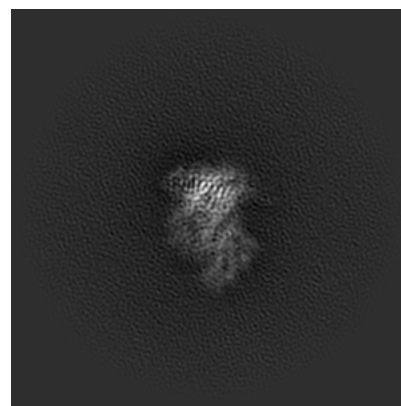
6.1.1 Primary map



X

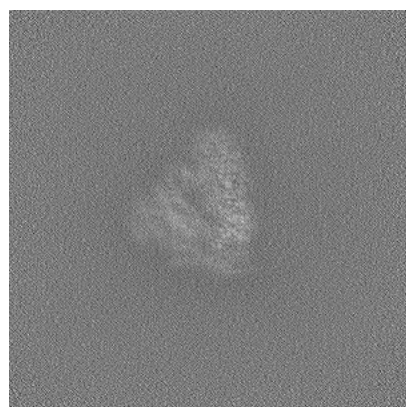


Y

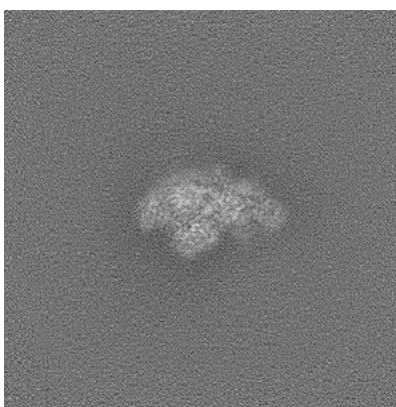


Z

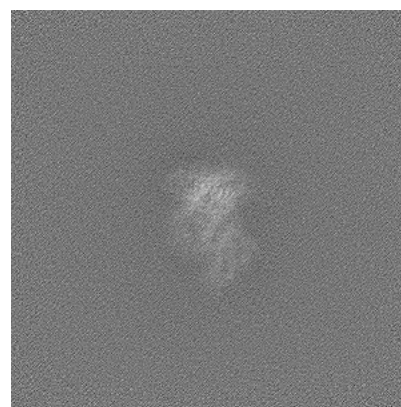
6.1.2 Raw map



X



Y

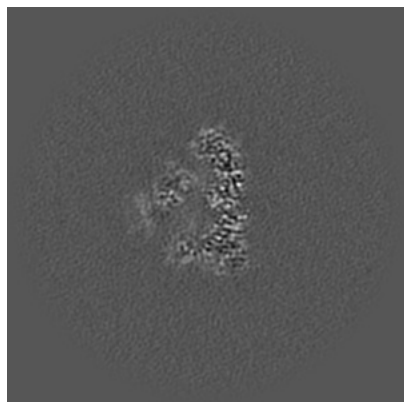


Z

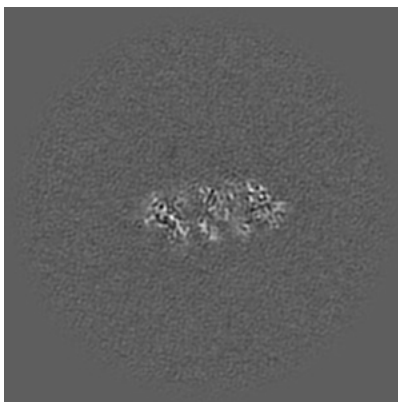
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

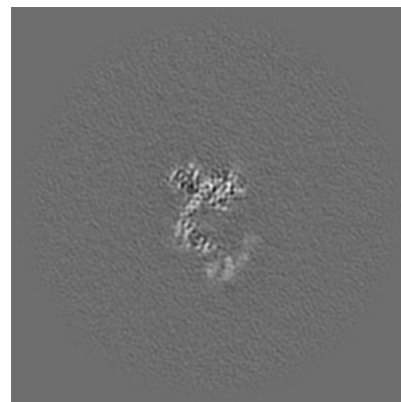
6.2.1 Primary map



X Index: 256

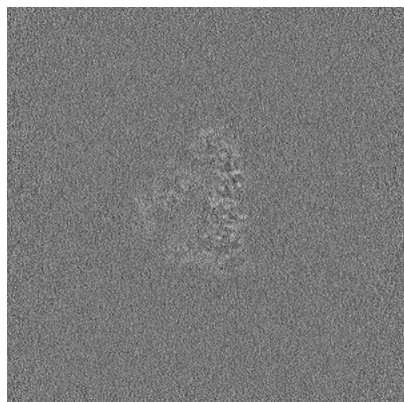


Y Index: 256

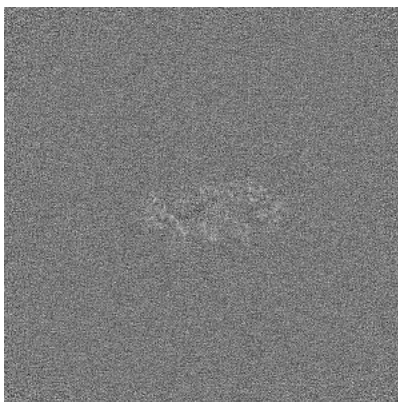


Z Index: 256

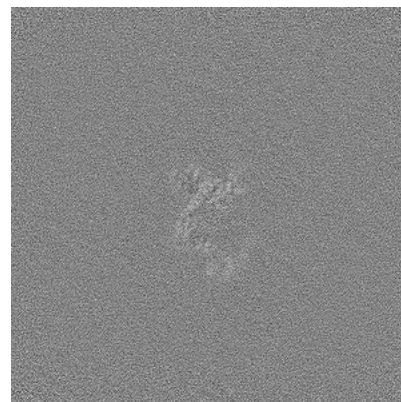
6.2.2 Raw map



X Index: 256



Y Index: 256

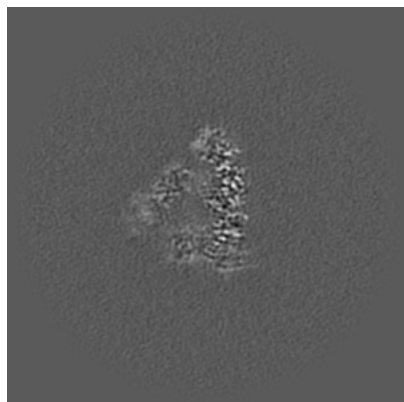


Z Index: 256

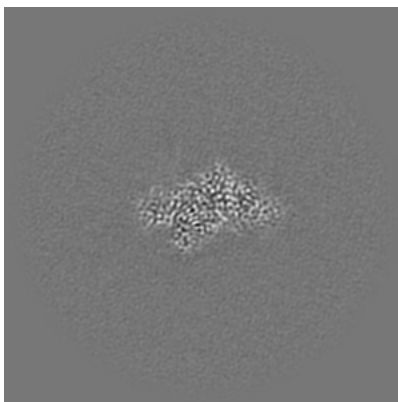
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

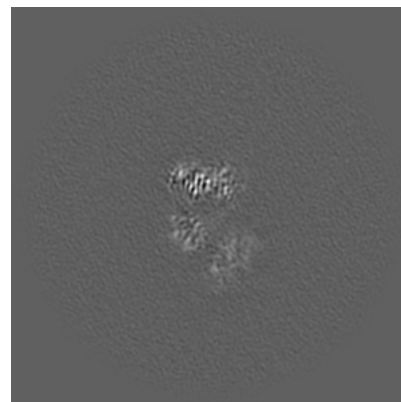
6.3.1 Primary map



X Index: 260

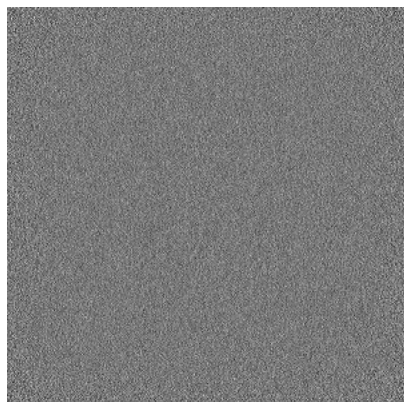


Y Index: 278

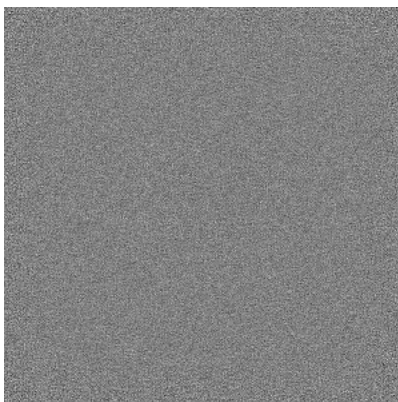


Z Index: 246

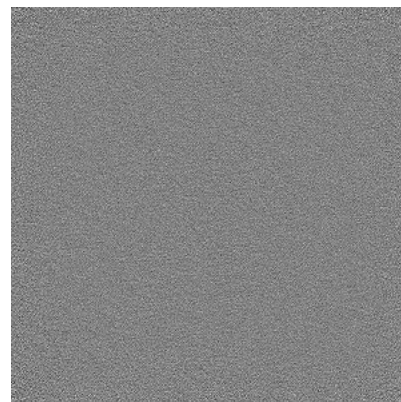
6.3.2 Raw map



X Index: 0



Y Index: 0

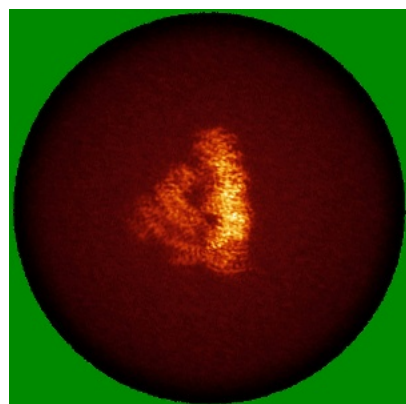


Z Index: 0

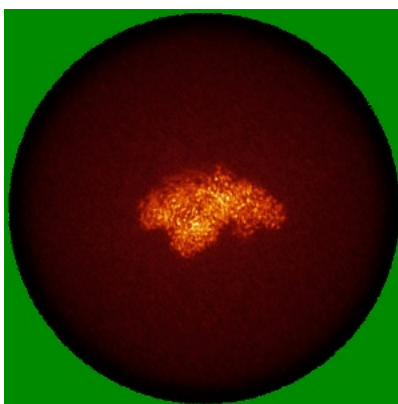
The images above show the largest variance slices of the map in three orthogonal directions.

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

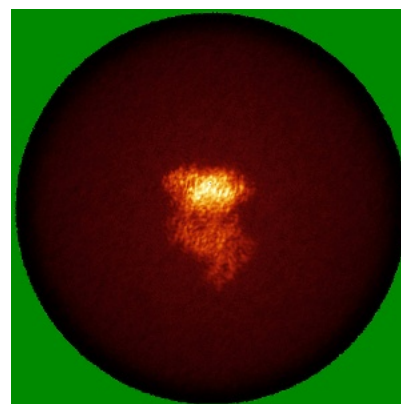
6.4.1 Primary map



X

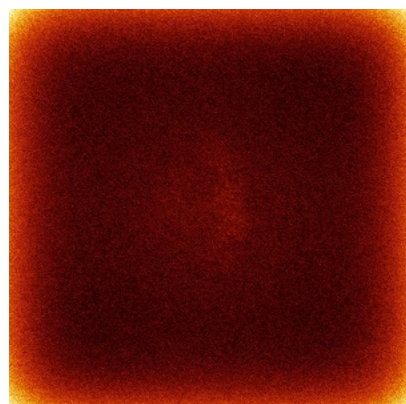


Y

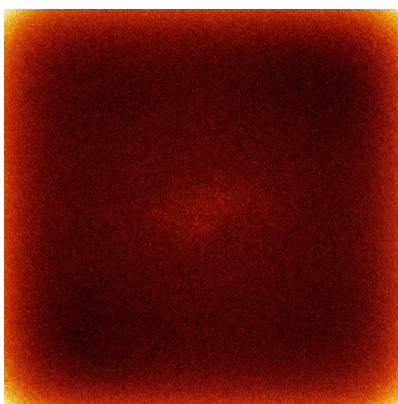


Z

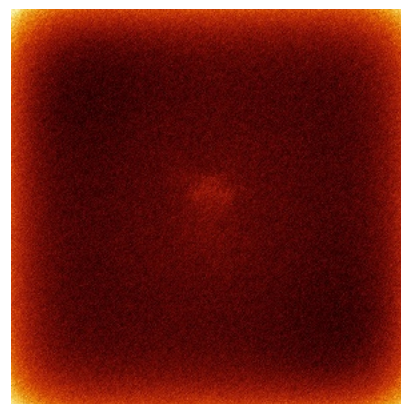
6.4.2 Raw map



X



Y

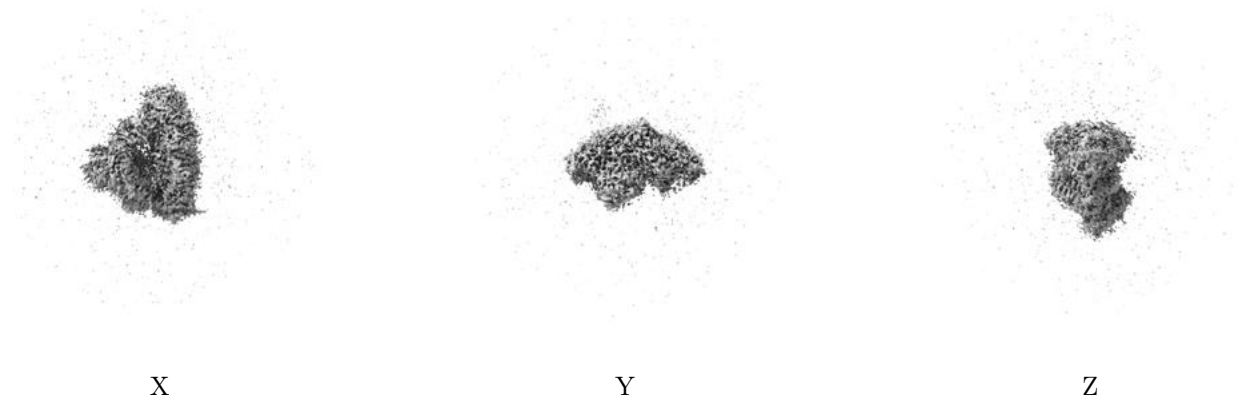


Z

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.

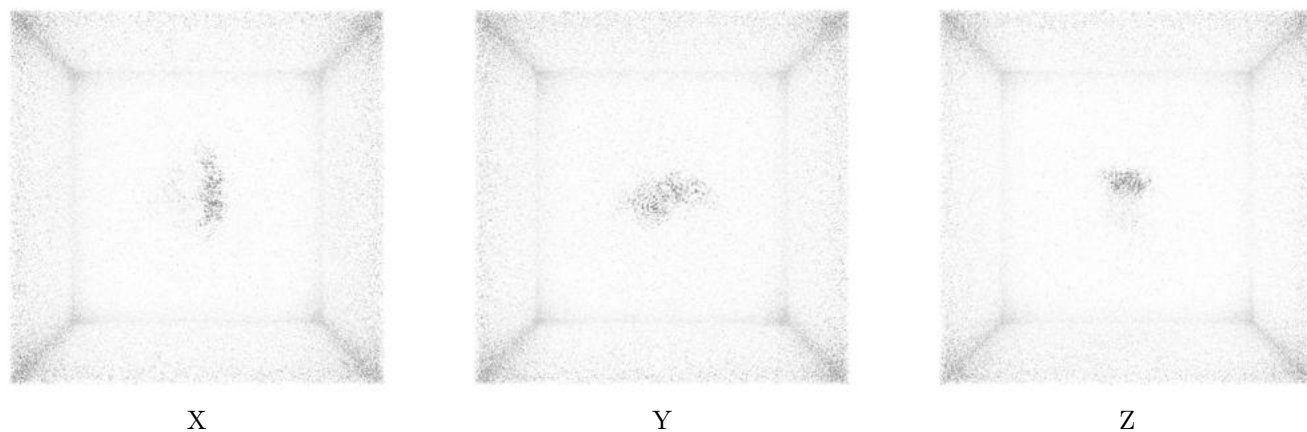
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

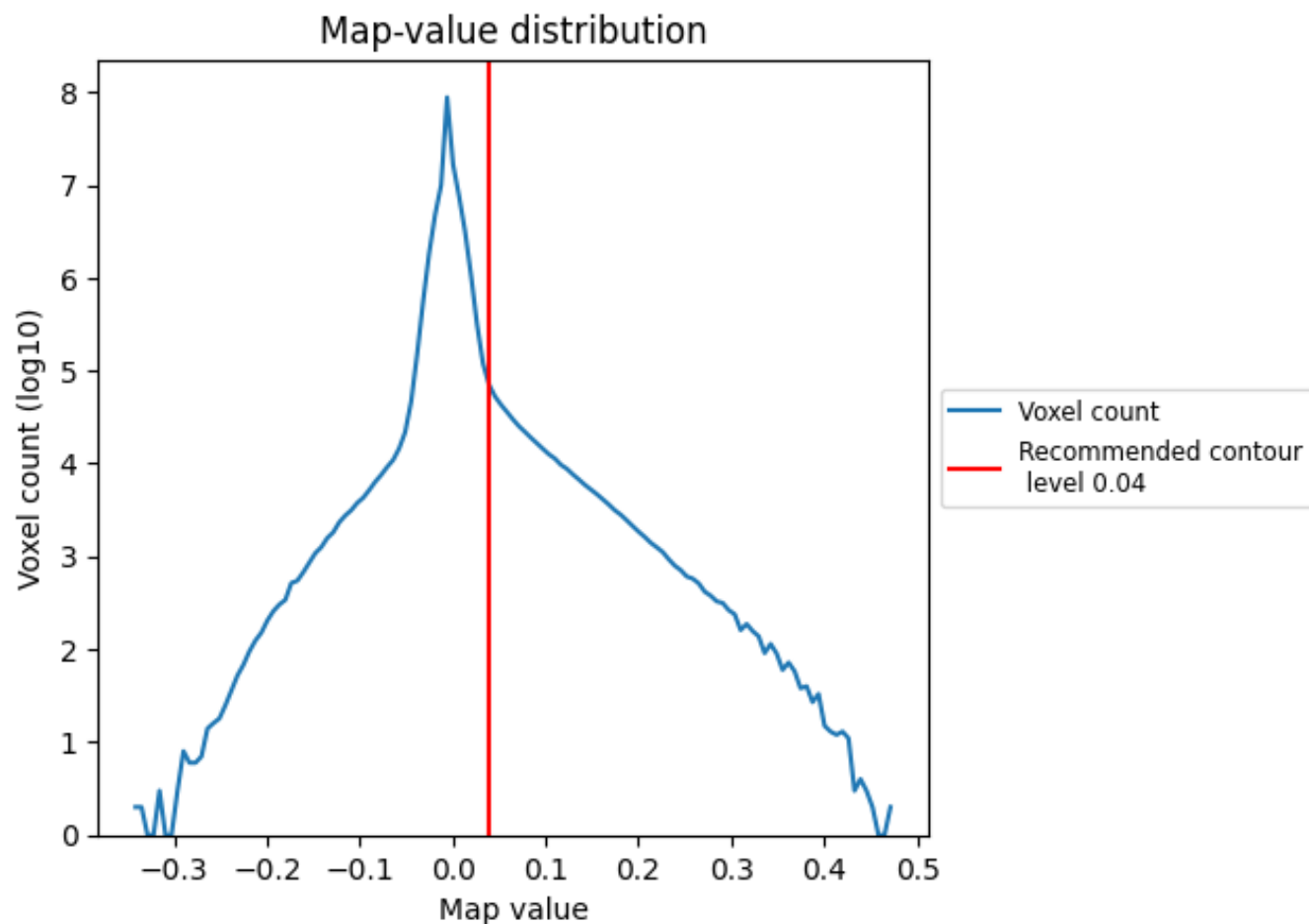
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

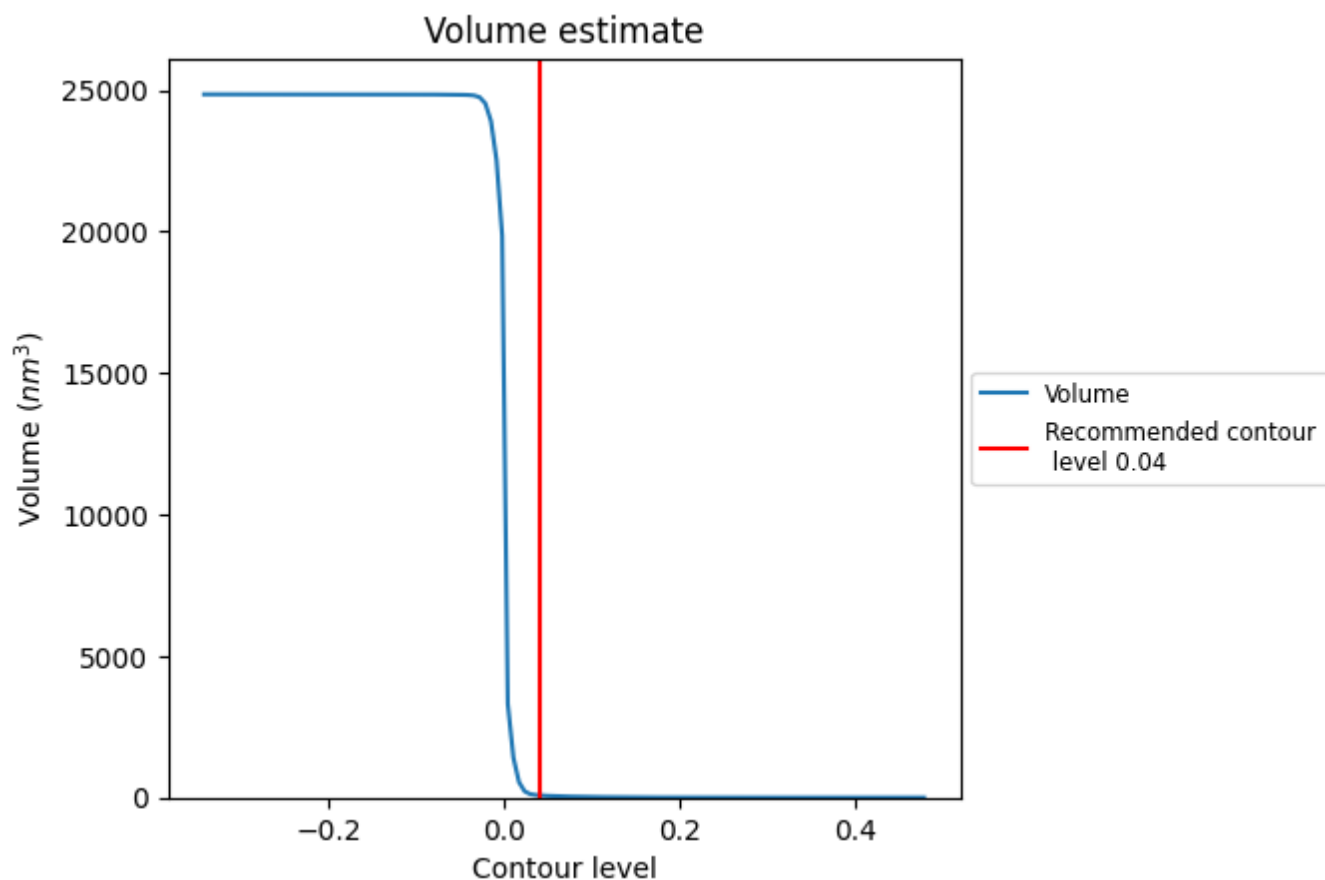
This section contains the results of statistical analysis of the map.

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.

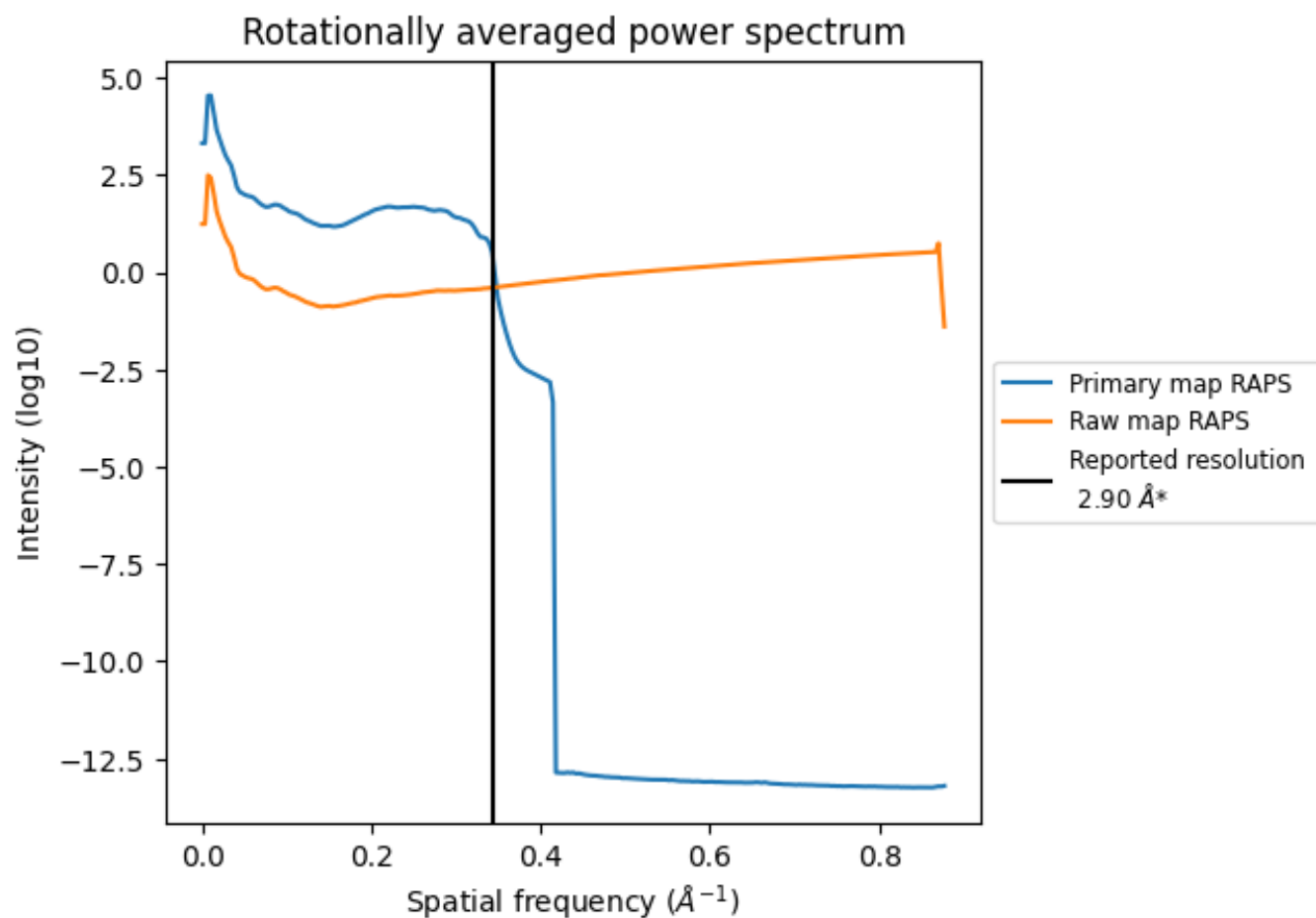
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 80 nm³; this corresponds to an approximate mass of 72 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 ⓘ

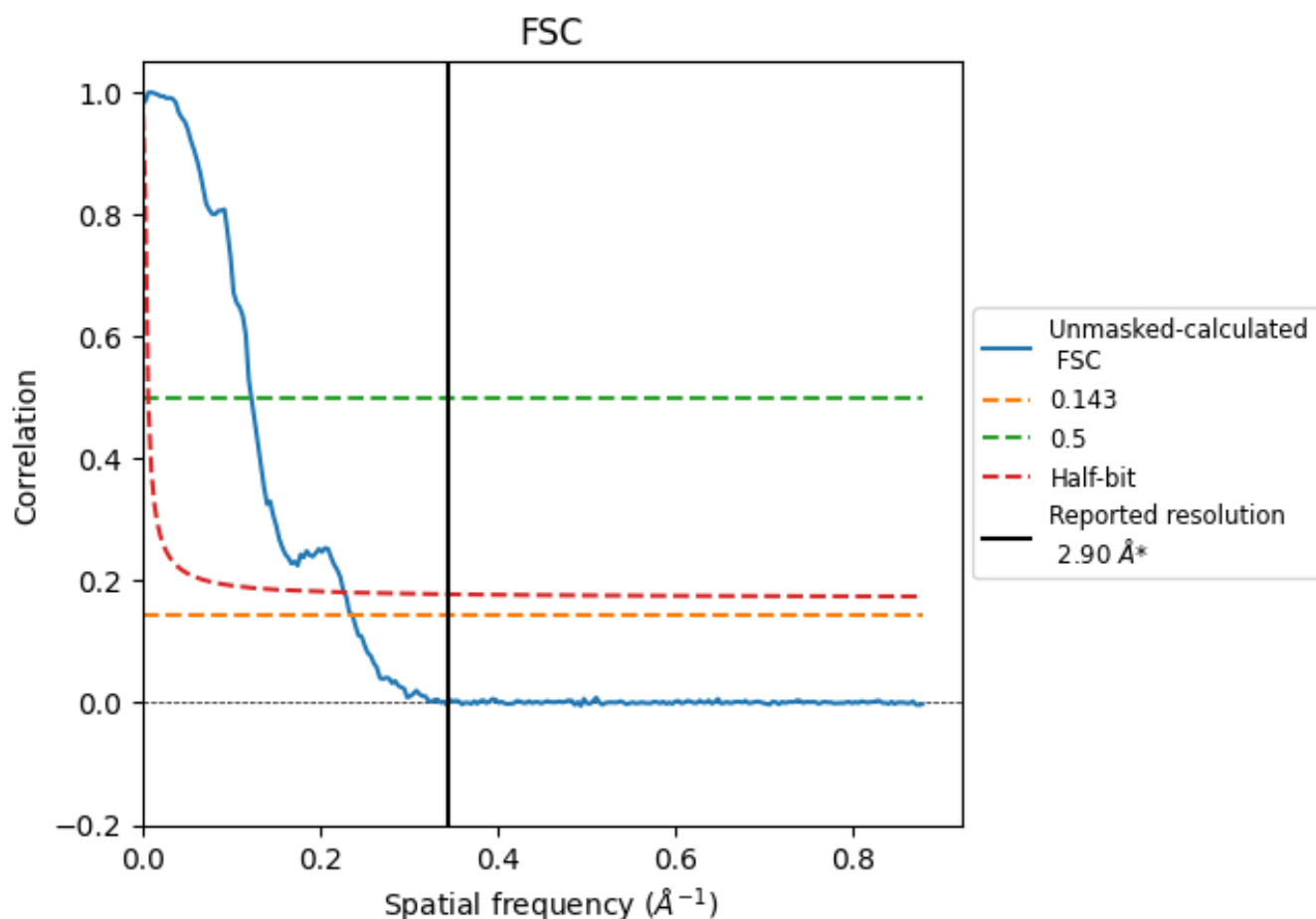


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

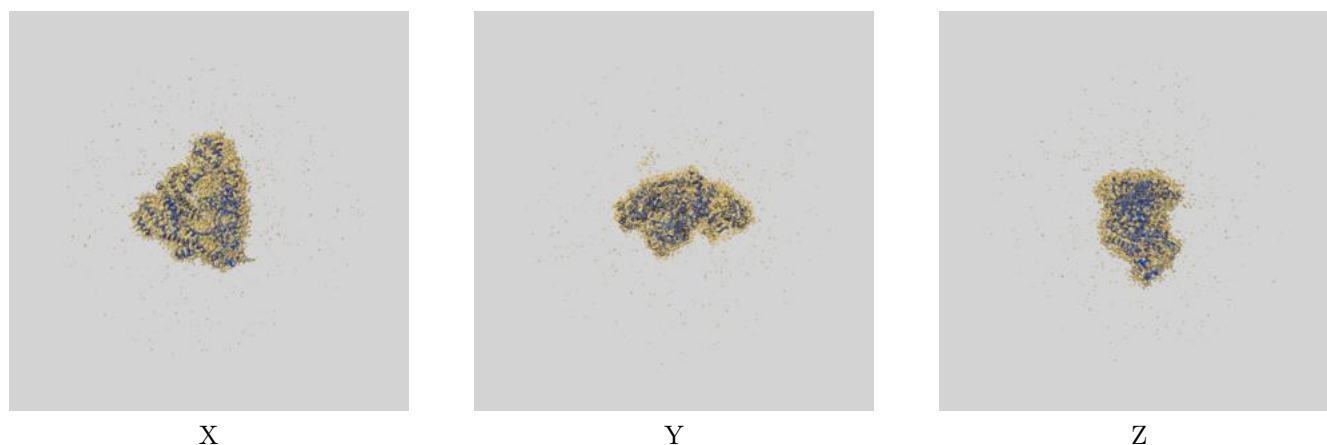
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.23	8.16	4.40

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.23 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62607 and PDB model 9KWC. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



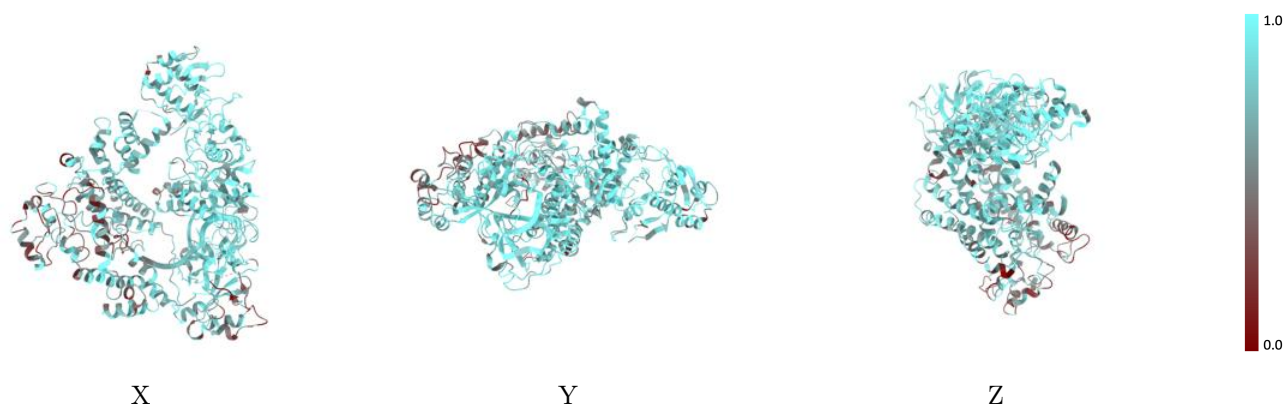
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



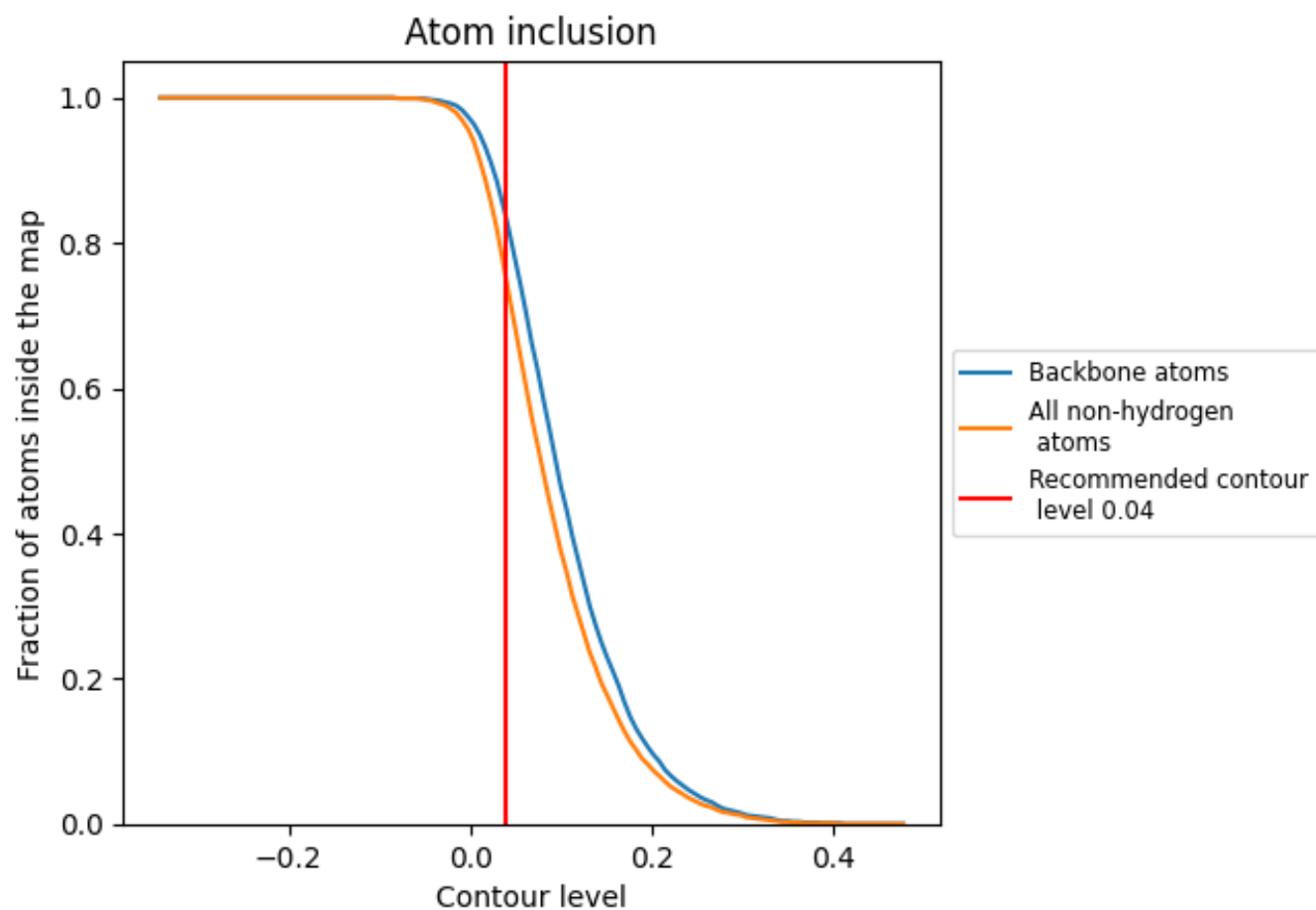
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 75% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7510	0.3850
A	0.7440	0.3810
G	0.8800	0.4540

