



Full wwPDB EM Validation Report ⓘ

May 31, 2026 – 01:40 am BST

PDB ID : 9RBO / pdb_00009rbo
EMDB ID : EMD-53900
Title : A cryo-EM structure of native C3 protein in a compact conformation.
Authors : Whittaker, J.J.; Eikrem, D.; Seisenbaeva, G.; Nilsson-Ekdahl, K.; Nilsson, B.; Sandgren, M.; Kessler, V.G.
Deposited on : 2025-05-27
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

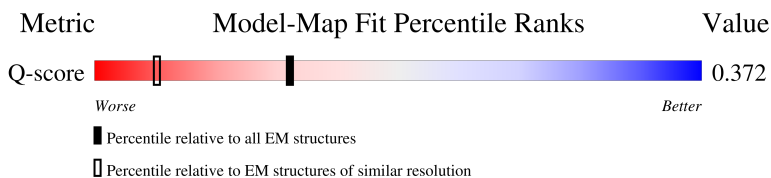
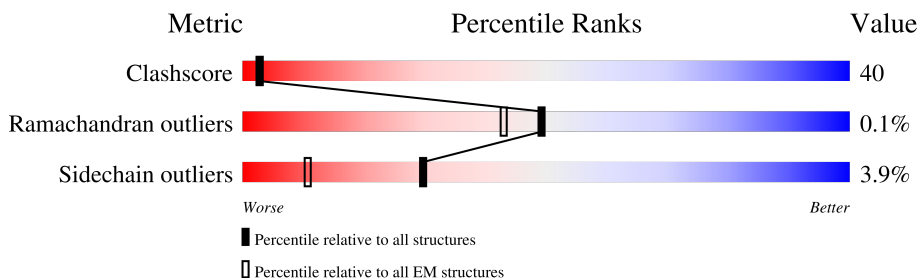
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	196	<div> <div>9%</div> <div>25%</div> <div>67%</div> <div>6%</div> <div>.</div> </div>
2	B	316	<div> <div>9%</div> <div>30%</div> <div>62%</div> <div>7%</div> <div>.</div> </div>
3	C	49	<div> <div>27%</div> <div>63%</div> <div>37%</div> </div>
4	D	902	<div> <div>.</div> <div>55%</div> <div>43%</div> <div>.</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11606 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 Complement C3 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	196	Total	C	N	O	S	0	0
			1553	994	258	297	4		

- Molecule 2 is a protein called Complement C3 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	316	Total	C	N	O	S	0	0
			2443	1541	427	466	9		

- Molecule 3 is a protein called Acylation stimulating protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	49	Total	C	N	O	S	0	0
			405	251	74	72	8		

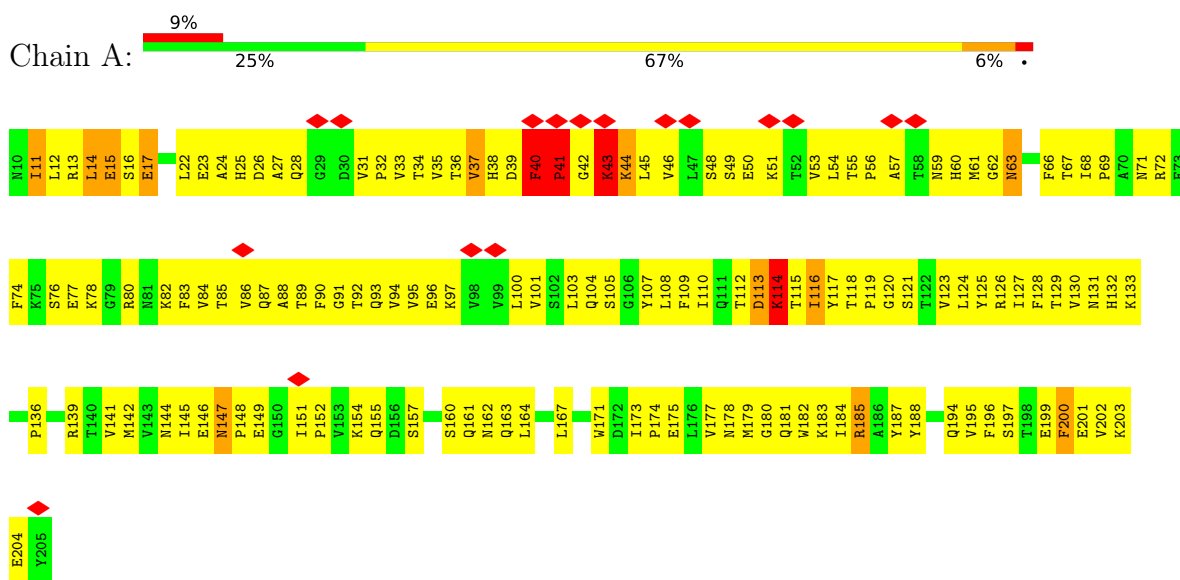
- Molecule 4 is a protein called Complement C3b alpha' chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	902	Total	C	N	O	S	0	0
			7205	4565	1216	1386	38		

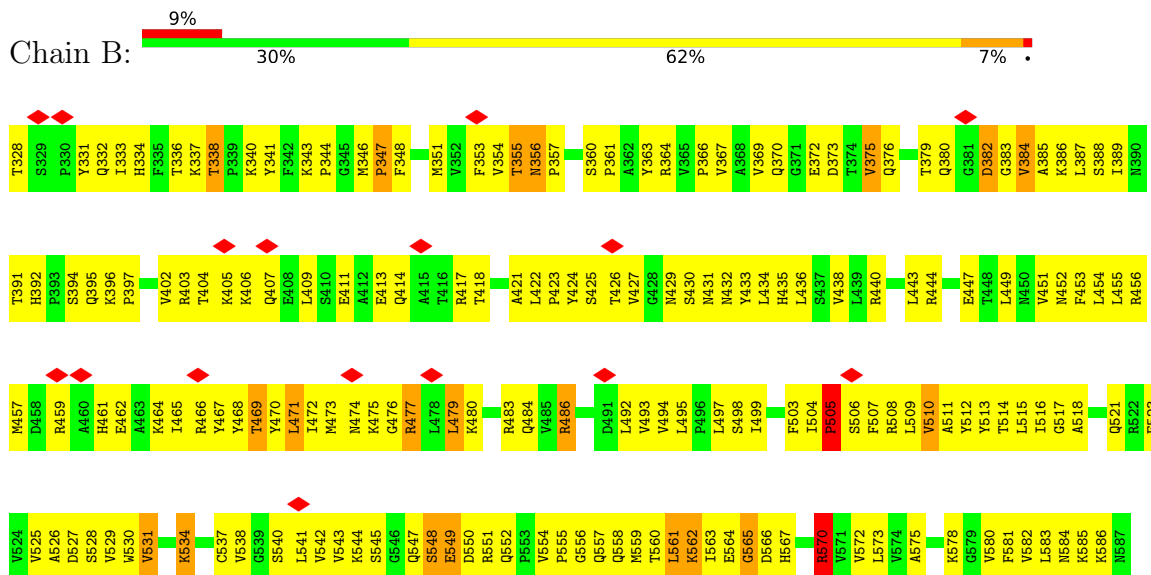
3 Residue-property plots

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: Complement C3 beta chain

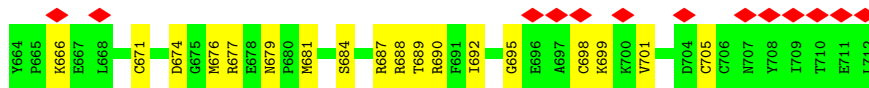


• Molecule 2: Complement C3 beta chain

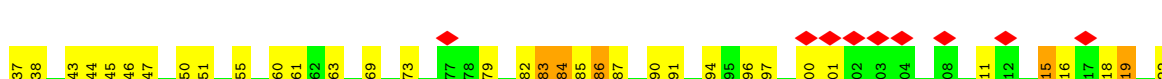
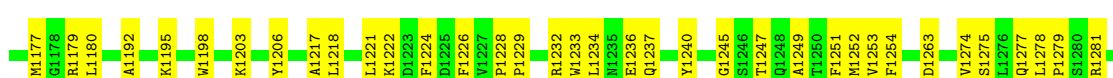
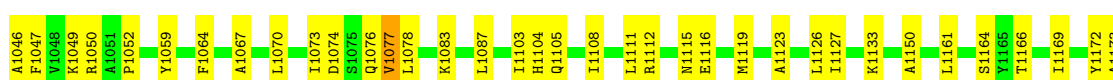
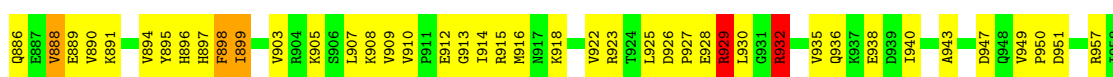
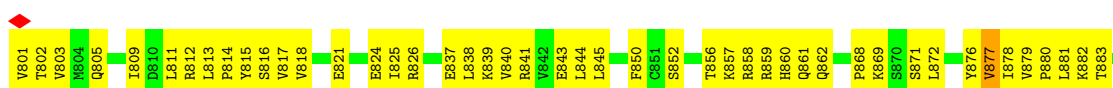


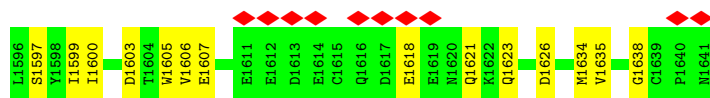


• Molecule 3: Acylation stimulating protein



• Molecule 4: Complement C3b alpha' chain





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	200000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.923	Depositor
Minimum map value	-0.347	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	259.2, 259.2, 259.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.648, 0.648, 0.648	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	0.74	3/1586 (0.2%)	1.10	10/2159 (0.5%)
2	B	0.47	0/2491	1.16	18/3381 (0.5%)
3	C	0.30	0/411	0.66	0/546
4	D	0.50	0/7351	0.74	18/9953 (0.2%)
All	All	0.53	3/11839 (0.0%)	0.90	46/16039 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
4	D	0	4
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	PHE	C-N	12.58	1.44	1.33
1	A	41	PRO	C-N	10.74	1.49	1.33
1	A	41	PRO	N-CD	6.17	1.56	1.47

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1418	ASP	N-CA-C	19.76	140.50	112.04
2	B	356	ASN	N-CA-CB	-16.25	81.44	110.37
2	B	506	SER	N-CA-CB	12.40	129.96	110.86
1	A	114	LYS	N-CA-C	-11.72	92.57	108.74
2	B	506	SER	N-CA-C	-11.43	87.78	107.20
1	A	41	PRO	N-CA-CB	-11.24	95.70	103.23
2	B	355	THR	N-CA-C	-10.55	90.93	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	355	THR	CB-CA-C	10.47	128.64	109.70
2	B	505	PRO	N-CA-C	10.23	133.54	112.47
4	D	1418	ASP	CB-CA-C	-9.97	92.32	110.56
1	A	44	LYS	N-CA-CB	-9.43	97.38	110.95
4	D	1483	LEU	CB-CA-C	-9.06	99.71	111.40
1	A	41	PRO	CA-C-N	-7.33	107.04	121.41
1	A	41	PRO	C-N-CA	-7.33	107.04	121.41
2	B	548	SER	CA-C-N	7.17	135.23	121.54
2	B	548	SER	C-N-CA	7.17	135.23	121.54
4	D	1483	LEU	N-CA-C	7.15	121.34	111.55
4	D	1419	ARG	N-CA-CB	-7.12	98.20	110.17
2	B	486	ARG	CG-CD-NE	7.12	127.65	112.00
4	D	1483	LEU	CA-CB-CG	7.03	140.91	116.30
4	D	787	MET	N-CA-C	6.97	120.69	111.28
1	A	114	LYS	N-CA-CB	6.59	122.21	111.21
4	D	1484	CYS	CA-C-N	-6.38	113.00	122.83
4	D	1484	CYS	C-N-CA	-6.38	113.00	122.83
1	A	42	GLY	N-CA-C	6.30	128.12	113.18
1	A	113	ASP	CB-CA-C	-6.21	100.22	110.72
4	D	1419	ARG	N-CA-C	-6.16	99.17	108.96
4	D	929	ARG	CB-CA-C	-6.03	100.92	110.86
1	A	43	LYS	CB-CA-C	-5.98	98.52	110.42
4	D	789	ASP	N-CA-C	5.97	119.33	111.28
2	B	562	LYS	CA-CB-CG	5.76	125.62	114.10
4	D	1483	LEU	CA-C-N	-5.72	112.78	121.53
4	D	1483	LEU	C-N-CA	-5.72	112.78	121.53
4	D	929	ARG	N-CA-C	5.54	118.39	111.24
4	D	898	PHE	N-CA-C	5.50	116.14	108.00
2	B	530	TRP	N-CA-C	-5.47	98.09	107.61
1	A	41	PRO	CA-N-CD	-5.42	104.41	112.00
2	B	565	GLY	N-CA-C	-5.41	107.13	116.01
4	D	1485	ARG	N-CA-C	-5.36	106.51	112.57
2	B	561	LEU	CA-C-N	5.33	131.73	121.54
2	B	561	LEU	C-N-CA	5.33	131.73	121.54
2	B	477	ARG	N-CA-C	-5.29	106.95	113.41
2	B	549	GLU	N-CA-C	5.23	121.94	110.80
4	D	779	THR	N-CA-C	5.20	116.95	111.28
2	B	479	LEU	CA-C-N	-5.05	114.27	122.34
2	B	479	LEU	C-N-CA	-5.05	114.27	122.34

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	570	ARG	Sidechain
4	D	1040	PRO	Peptide
4	D	1419	ARG	Sidechain
4	D	929	ARG	Sidechain
4	D	932	ARG	Sidechain

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	1553	0	1562	221	0
2	B	2443	0	2466	335	0
3	C	405	0	398	27	0
4	D	7205	0	7138	422	0
All	All	11606	0	11564	936	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 40.

All (936) 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:44:LYS:HE2	1:A:66:PHE:CD2	1.53	1.43
4:D:787:MET:CE	4:D:793:ILE:HB	1.77	1.13
1:A:44:LYS:CE	1:A:66:PHE:HD2	1.64	1.09
4:D:787:MET:HE2	4:D:793:ILE:CB	1.82	1.07
1:A:41:PRO:HB3	1:A:74:PHE:HE2	1.19	1.05
1:A:44:LYS:CE	1:A:66:PHE:CD2	2.40	1.03
2:B:462:GLU:HG2	2:B:486:ARG:HD3	1.41	1.02
2:B:562:LYS:HD2	4:D:802:THR:HG23	1.43	0.99
1:A:113:ASP:CG	2:B:544:LYS:HD2	1.86	0.98
4:D:790:LYS:HG3	4:D:794:CYS:HA	1.44	0.97
4:D:816:SER:OG	4:D:908:LYS:HG3	1.63	0.97
2:B:355:THR:HG23	2:B:361:PRO:HA	1.48	0.95
2:B:544:LYS:HB3	2:B:547:GLN:HB2	1.47	0.95
4:D:1362:MET:HE1	4:D:1473:PRO:HB3	1.48	0.94
2:B:331:TYR:CD2	2:B:332:GLN:OE1	2.23	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:ARG:HH22	2:B:376:GLN:HB3	1.35	0.92
2:B:351:MET:HE1	2:B:386:LYS:HG2	1.52	0.91
1:A:36:THR:HA	1:A:45:LEU:HG	1.52	0.91
4:D:910:VAL:HG11	4:D:1418:ASP:HB3	1.51	0.91
1:A:76:SER:HA	1:A:80:ARG:HD2	1.52	0.90
1:A:179:MET:HE3	1:A:180:GLY:H	1.36	0.90
1:A:124:LEU:HD22	2:B:544:LYS:HE3	1.55	0.89
2:B:424:TYR:HB3	2:B:612:ASP:HA	1.53	0.89
4:D:797:ASP:OD1	4:D:798:PRO:HD2	1.72	0.89
1:A:44:LYS:HE2	1:A:66:PHE:HD2	0.75	0.88
3:C:681:MET:HE1	4:D:1436:CYS:HB3	1.53	0.88
4:D:879:VAL:HG21	4:D:1483:LEU:HD11	1.53	0.88
4:D:1126:LEU:HD23	4:D:1173:ALA:HB1	1.56	0.87
4:D:1411:GLU:HG2	4:D:1413:ASP:HB2	1.56	0.86
4:D:1385:MET:HE1	4:D:1391:PRO:HD3	1.56	0.86
2:B:508:ARG:HE	2:B:510:VAL:HG22	1.40	0.86
4:D:787:MET:HE2	4:D:793:ILE:HB	0.91	0.85
1:A:41:PRO:HB3	1:A:74:PHE:CE2	2.10	0.85
2:B:567:HIS:CE1	4:D:751:TRP:H	1.93	0.85
4:D:1026:LEU:HA	4:D:1029:LYS:HE2	1.58	0.85
2:B:600:LYS:HA	2:B:638:LEU:HB3	1.57	0.84
4:D:749:TRP:CD2	4:D:773:LEU:HA	2.11	0.84
2:B:472:ILE:HD12	2:B:474:ASN:H	1.43	0.84
1:A:139:ARG:H	1:A:160:SER:HB3	1.41	0.84
1:A:13:ARG:HB2	1:A:101:VAL:HA	1.59	0.84
2:B:432:ASN:HB3	2:B:456:ARG:HE	1.41	0.83
2:B:331:TYR:HD2	2:B:332:GLN:OE1	1.58	0.83
3:C:681:MET:CE	4:D:1436:CYS:CB	2.57	0.83
2:B:425:SER:HB3	2:B:612:ASP:HB2	1.60	0.82
4:D:782:ILE:HD12	4:D:798:PRO:HG2	1.60	0.82
1:A:110:ILE:HG21	1:A:127:ILE:HD12	1.63	0.81
3:C:681:MET:HE2	4:D:1436:CYS:CB	2.10	0.81
3:C:681:MET:CE	4:D:1436:CYS:HB3	2.10	0.79
4:D:1275:SER:HB2	4:D:1284:LYS:HD2	1.64	0.79
4:D:883:THR:HA	4:D:909:VAL:HG13	1.62	0.79
1:A:38:HIS:HA	1:A:44:LYS:H	1.47	0.79
2:B:508:ARG:HH21	2:B:510:VAL:HG13	1.48	0.79
4:D:1522:VAL:HB	4:D:1548:LYS:HB3	1.63	0.78
2:B:550:ASP:HB2	4:D:797:ASP:OD2	1.84	0.78
4:D:817:VAL:HG23	4:D:909:VAL:HG23	1.63	0.78
2:B:551:ARG:HH11	2:B:561:LEU:HA	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:818:VAL:HG11	4:D:1451:GLN:HG3	1.65	0.77
1:A:71:ASN:HB2	1:A:72:ARG:CZ	2.15	0.77
1:A:113:ASP:CG	2:B:544:LYS:CD	2.57	0.77
2:B:508:ARG:NH1	2:B:528:SER:HA	2.00	0.76
1:A:31:VAL:HG13	1:A:33:VAL:HG12	1.65	0.76
2:B:438:VAL:HA	2:B:451:VAL:HA	1.66	0.76
2:B:575:ALA:HA	2:B:578:LYS:HE2	1.64	0.76
3:C:681:MET:HE2	4:D:1436:CYS:HB2	1.68	0.76
4:D:1119:MET:HE3	4:D:1161:LEU:HD21	1.66	0.76
2:B:554:VAL:HG23	2:B:585:LYS:HG3	1.67	0.75
1:A:87:GLN:HA	1:A:96:GLU:HG3	1.67	0.75
1:A:154:LYS:HD3	1:A:171:TRP:HE3	1.52	0.75
3:C:681:MET:HE2	4:D:1436:CYS:C	2.11	0.75
1:A:173:ILE:HD11	1:A:177:VAL:HG21	1.68	0.75
2:B:551:ARG:HA	4:D:800:GLU:OE2	1.86	0.75
4:D:805:GLN:HB3	4:D:899:ILE:HD13	1.68	0.75
2:B:332:GLN:HB3	2:B:357:PRO:HG3	1.69	0.74
2:B:556:GLY:HA2	2:B:582:VAL:HG22	1.69	0.74
1:A:41:PRO:HD2	1:A:82:LYS:HD2	1.70	0.74
2:B:552:GLN:NE2	2:B:555:PRO:HB3	2.02	0.74
4:D:816:SER:OG	4:D:908:LYS:CG	2.35	0.74
4:D:845:LEU:HB2	4:D:889:GLU:HG2	1.69	0.74
4:D:1277:GLN:HE21	4:D:1284:LYS:HE2	1.53	0.74
2:B:465:ILE:HG12	2:B:515:LEU:HD11	1.70	0.74
2:B:434:LEU:HD12	2:B:456:ARG:H	1.53	0.74
4:D:1108:ILE:HD12	4:D:1111:LEU:HD12	1.69	0.73
4:D:1529:LYS:HB3	4:D:1540:ILE:HD13	1.68	0.73
4:D:1025:GLU:HA	4:D:1028:LYS:HD2	1.69	0.73
4:D:1405:ARG:HH12	4:D:1408:SER:HA	1.53	0.73
2:B:560:THR:HB	2:B:564:GLU:HB3	1.70	0.73
2:B:541:LEU:HD21	4:D:791:LYS:HG3	1.71	0.73
2:B:369:VAL:HA	2:B:402:VAL:HA	1.70	0.73
2:B:457:MET:HG3	2:B:518:ALA:HA	1.72	0.72
2:B:538:VAL:HA	2:B:588:LYS:HZ2	1.52	0.72
4:D:778:THR:HG23	4:D:803:VAL:HG12	1.72	0.71
4:D:1343:VAL:HG12	4:D:1366:ILE:HD12	1.72	0.71
4:D:940:ILE:HG21	4:D:1322:VAL:HG11	1.72	0.71
4:D:992:ASN:ND2	4:D:1037:PHE:HE1	1.89	0.71
4:D:1180:LEU:HD23	4:D:1221:LEU:HD11	1.72	0.71
1:A:181:GLN:HE22	1:A:201:GLU:H	1.37	0.71
2:B:457:MET:HE1	2:B:515:LEU:HD22	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:589:LEU:HG	2:B:590:THR:H	1.56	0.71
2:B:470:TYR:HA	2:B:511:ALA:HA	1.73	0.70
4:D:1531:GLN:HE22	4:D:1540:ILE:HD11	1.56	0.70
4:D:1334:LEU:HG	4:D:1335:THR:HG23	1.74	0.70
2:B:561:LEU:C	2:B:562:LYS:HD3	2.16	0.70
2:B:477:ARG:HD2	2:B:505:PRO:HG3	1.72	0.70
4:D:747:GLU:H	4:D:774:LYS:HG2	1.56	0.70
1:A:14:LEU:HD21	1:A:104:GLN:HB3	1.72	0.69
1:A:38:HIS:O	1:A:39:ASP:OD1	2.10	0.69
1:A:149:GLU:HG3	1:A:178:ASN:HD21	1.57	0.69
4:D:787:MET:CE	4:D:793:ILE:CB	2.55	0.69
2:B:425:SER:HG	2:B:613:TYR:HD1	1.37	0.69
3:C:698:CYS:HA	3:C:701:VAL:HG12	1.74	0.69
1:A:115:THR:HG23	1:A:116:ILE:H	1.57	0.69
1:A:89:THR:HG23	1:A:93:GLN:O	1.92	0.69
1:A:127:ILE:HB	1:A:167:LEU:HB2	1.74	0.69
2:B:523:GLU:OE1	2:B:525:VAL:HG23	1.92	0.69
1:A:32:PRO:HD2	1:A:92:THR:HG22	1.74	0.69
1:A:117:TYR:C	1:A:202:VAL:HG23	2.18	0.69
4:D:813:LEU:HD23	4:D:907:LEU:HD13	1.74	0.69
2:B:508:ARG:HH12	2:B:528:SER:HA	1.57	0.69
3:C:681:MET:SD	4:D:1437:LEU:C	2.76	0.69
2:B:508:ARG:NE	2:B:510:VAL:HG22	2.08	0.68
1:A:144:ASN:HD21	1:A:152:PRO:HB2	1.59	0.68
2:B:457:MET:HE3	2:B:461:HIS:HB3	1.74	0.68
4:D:785:VAL:HB	4:D:798:PRO:HD3	1.76	0.68
1:A:44:LYS:HG2	1:A:66:PHE:CE2	2.28	0.68
2:B:608:GLY:O	2:B:619:ASP:HB3	1.94	0.68
4:D:747:GLU:HB2	4:D:774:LYS:HB3	1.75	0.68
1:A:44:LYS:HG2	1:A:66:PHE:CD2	2.28	0.68
4:D:1516:GLU:HG3	4:D:1518:GLY:H	1.59	0.68
2:B:459:ARG:HA	2:B:462:GLU:HB3	1.74	0.67
4:D:925:LEU:HD13	4:D:1312:ALA:HB2	1.75	0.67
4:D:1064:PHE:HB3	4:D:1078:LEU:HD21	1.77	0.67
4:D:1359:LYS:HD2	4:D:1446:ASN:ND2	2.10	0.67
1:A:80:ARG:HH22	1:A:82:LYS:HZ3	1.42	0.67
1:A:71:ASN:HB2	1:A:72:ARG:NE	2.10	0.67
3:C:681:MET:CE	4:D:1436:CYS:HB2	2.24	0.67
1:A:88:ALA:HB3	1:A:95:VAL:O	1.95	0.66
2:B:456:ARG:HH21	2:B:523:GLU:HB3	1.60	0.66
4:D:787:MET:CE	4:D:793:ILE:CG2	2.73	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ASP:OD1	2:B:544:LYS:HD2	1.95	0.66
4:D:1354:ARG:HH11	4:D:1360:ASN:HA	1.61	0.66
4:D:742:ARG:HH12	4:D:745:PHE:HB3	1.60	0.66
2:B:407:GLN:O	2:B:409:LEU:HD23	1.95	0.66
1:A:39:ASP:HA	1:A:85:THR:H	1.59	0.66
2:B:379:THR:HG22	2:B:385:ALA:HB2	1.78	0.66
3:C:681:MET:SD	4:D:1438:ALA:N	2.69	0.66
4:D:883:THR:HA	4:D:909:VAL:CG1	2.25	0.66
2:B:503:PHE:O	2:B:534:LYS:HG3	1.96	0.66
1:A:33:VAL:HG23	1:A:89:THR:HG22	1.77	0.66
2:B:493:VAL:O	2:B:495:LEU:HD22	1.97	0.65
1:A:105:SER:C	1:A:132:HIS:HE1	2.05	0.65
4:D:1522:VAL:HG12	4:D:1547:ILE:HB	1.78	0.65
4:D:1310:VAL:HG21	4:D:1320:LEU:HD21	1.79	0.65
2:B:473:MET:HE3	2:B:505:PRO:HB2	1.79	0.65
1:A:171:TRP:CD1	1:A:171:TRP:C	2.73	0.65
4:D:1634:MET:HE3	4:D:1638:GLY:HA2	1.79	0.65
2:B:609:SER:OG	2:B:620:ALA:HA	1.97	0.65
4:D:746:PRO:HA	4:D:774:LYS:NZ	2.12	0.65
4:D:756:LEU:HB2	4:D:767:LYS:NZ	2.12	0.65
1:A:72:ARG:HB3	1:A:74:PHE:CE2	2.32	0.65
2:B:367:VAL:HG22	2:B:404:THR:OG1	1.97	0.64
4:D:856:THR:HB	4:D:857:LYS:HE2	1.78	0.64
1:A:146:GLU:HA	1:A:152:PRO:HA	1.77	0.64
2:B:589:LEU:HG	2:B:590:THR:N	2.12	0.64
4:D:809:ILE:HG21	4:D:890:VAL:HG21	1.78	0.64
1:A:148:PRO:HD2	1:A:182:TRP:CE3	2.33	0.64
2:B:557:GLN:HA	2:B:584:ASN:HB3	1.79	0.64
4:D:1203:LYS:HB3	4:D:1206:TYR:HD2	1.63	0.64
2:B:561:LEU:O	2:B:562:LYS:HD3	1.98	0.64
1:A:51:LYS:HA	1:A:54:LEU:HG	1.80	0.64
2:B:572:VAL:HG12	2:B:573:LEU:H	1.63	0.64
4:D:838:LEU:HD11	4:D:898:PHE:CE1	2.33	0.64
4:D:1359:LYS:HD2	4:D:1446:ASN:HD22	1.63	0.64
1:A:113:ASP:OD1	2:B:544:LYS:CD	2.46	0.64
4:D:784:ALA:HA	4:D:797:ASP:OD1	1.98	0.64
1:A:112:THR:HG23	1:A:114:LYS:O	1.98	0.64
1:A:179:MET:HE1	1:A:201:GLU:OE2	1.98	0.63
4:D:1405:ARG:NH1	4:D:1408:SER:HA	2.13	0.63
1:A:147:ASN:HB2	1:A:182:TRP:CE3	2.33	0.63
1:A:44:LYS:HE2	1:A:66:PHE:CE2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ILE:HG21	1:A:127:ILE:CD1	2.28	0.63
3:C:692:ILE:HG12	3:C:699:LYS:HE2	1.80	0.63
1:A:45:LEU:HD11	1:A:48:SER:N	2.13	0.63
2:B:597:VAL:HG13	2:B:598:VAL:HG13	1.80	0.63
2:B:434:LEU:H	2:B:456:ARG:HH11	1.46	0.63
4:D:1274:VAL:HA	4:D:1311:THR:O	1.99	0.63
4:D:1112:ARG:HD3	4:D:1115:ASN:HB3	1.79	0.62
2:B:557:GLN:HA	2:B:584:ASN:CB	2.29	0.62
4:D:1022:GLY:HA2	4:D:1025:GLU:OE1	1.99	0.62
1:A:45:LEU:HD22	1:A:46:VAL:H	1.63	0.62
2:B:364:ARG:NH2	2:B:376:GLN:HB3	2.12	0.62
4:D:1563:ILE:HB	4:D:1599:ILE:HG22	1.81	0.62
1:A:162:ASN:HA	4:D:1028:LYS:NZ	2.15	0.62
2:B:616:VAL:HG23	2:B:617:PHE:H	1.64	0.62
2:B:438:VAL:HB	2:B:451:VAL:HG23	1.80	0.61
2:B:547:GLN:CD	4:D:751:TRP:HA	2.25	0.61
4:D:749:TRP:HE1	4:D:774:LYS:HG3	1.64	0.61
4:D:754:GLU:HB2	4:D:757:LYS:HD3	1.83	0.61
1:A:129:THR:HG21	1:A:160:SER:HB2	1.82	0.61
2:B:434:LEU:H	2:B:456:ARG:NH1	1.98	0.61
4:D:1348:ALA:HB3	4:D:1361:THR:HG23	1.82	0.61
2:B:356:ASN:HB2	2:B:360:SER:O	2.00	0.61
2:B:431:ASN:HD21	2:B:521:GLN:H	1.48	0.61
4:D:812:ARG:HB2	4:D:826:ARG:HG3	1.83	0.61
4:D:790:LYS:HE3	4:D:794:CYS:SG	2.40	0.61
2:B:607:PRO:HB2	2:B:611:LYS:HG3	1.81	0.61
2:B:617:PHE:O	2:B:632:THR:HA	2.01	0.61
2:B:549:GLU:HG3	4:D:800:GLU:OE2	2.00	0.61
4:D:838:LEU:HD11	4:D:898:PHE:CD1	2.35	0.61
2:B:562:LYS:HD2	4:D:802:THR:CG2	2.24	0.61
4:D:975:ALA:HB2	4:D:1026:LEU:HD11	1.82	0.61
1:A:110:ILE:HG21	1:A:127:ILE:HA	1.83	0.60
2:B:429:ASN:HB2	2:B:523:GLU:HG2	1.81	0.60
2:B:470:TYR:HD2	2:B:472:ILE:HG21	1.64	0.60
1:A:93:GLN:HG2	1:A:95:VAL:HG23	1.83	0.60
2:B:343:LYS:HE2	2:B:525:VAL:HG21	1.82	0.60
4:D:1575:GLU:OE1	4:D:1576:GLU:HG2	2.01	0.60
1:A:114:LYS:HB2	1:A:117:TYR:CZ	2.36	0.60
2:B:425:SER:HB3	2:B:612:ASP:CB	2.30	0.60
1:A:28:GLN:HE22	1:A:59:ASN:HA	1.65	0.60
4:D:1386:MET:HG2	4:D:1450:ILE:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ASP:HB3	1:A:59:ASN:O	2.01	0.60
1:A:202:VAL:HG13	1:A:203:LYS:N	2.17	0.60
4:D:1547:ILE:HD12	4:D:1547:ILE:H	1.65	0.60
2:B:542:VAL:HB	2:B:545:SER:O	2.01	0.60
4:D:1378:MET:HA	4:D:1426:LEU:O	2.02	0.60
4:D:1575:GLU:HB3	4:D:1578:LYS:NZ	2.16	0.60
2:B:411:GLU:OE2	2:B:414:GLN:HG3	2.02	0.60
2:B:468:TYR:HA	2:B:513:TYR:HD2	1.66	0.60
2:B:469:THR:HB	2:B:512:TYR:HB2	1.84	0.60
2:B:551:ARG:NH1	2:B:561:LEU:HA	2.15	0.60
2:B:575:ALA:CA	2:B:578:LYS:HE2	2.32	0.60
1:A:179:MET:HE3	1:A:180:GLY:N	2.13	0.60
4:D:1297:LEU:C	4:D:1298:ARG:HD2	2.26	0.60
1:A:38:HIS:HB2	1:A:85:THR:HB	1.84	0.59
2:B:434:LEU:HD11	2:B:453:PHE:HB2	1.83	0.59
1:A:86:VAL:HG12	1:A:88:ALA:HB2	1.83	0.59
1:A:12:LEU:CD1	1:A:14:LEU:HB2	2.32	0.59
1:A:80:ARG:HH22	1:A:82:LYS:NZ	1.99	0.59
4:D:1618:GLU:HA	4:D:1621:GLN:HE22	1.67	0.59
2:B:389:ILE:HD11	2:B:391:THR:HB	1.85	0.59
2:B:567:HIS:CE1	4:D:750:LEU:HB3	2.38	0.59
4:D:745:PHE:CE1	4:D:777:ILE:HD11	2.37	0.59
4:D:749:TRP:NE1	4:D:774:LYS:HG3	2.18	0.59
1:A:51:LYS:HA	1:A:54:LEU:HB2	1.84	0.59
4:D:993:MET:HE3	4:D:993:MET:HA	1.84	0.59
1:A:185:ARG:HB3	1:A:195:VAL:HG13	1.84	0.59
4:D:818:VAL:O	4:D:821:GLU:HG3	2.03	0.59
1:A:148:PRO:HD2	1:A:182:TRP:HE3	1.67	0.59
2:B:475:LYS:HB2	2:B:480:LYS:HB2	1.84	0.59
2:B:508:ARG:NH2	2:B:510:VAL:HG13	2.17	0.59
2:B:512:TYR:HE1	2:B:616:VAL:O	1.84	0.59
4:D:838:LEU:HD12	4:D:894:VAL:HG11	1.83	0.59
1:A:113:ASP:CG	1:A:113:ASP:O	2.43	0.59
4:D:773:LEU:HB3	4:D:783:LEU:HD11	1.84	0.59
4:D:814:PRO:HD2	4:D:907:LEU:HD21	1.85	0.58
4:D:858:ARG:HH12	4:D:860:HIS:HA	1.67	0.58
1:A:100:LEU:HB3	2:B:600:LYS:NZ	2.19	0.58
1:A:145:ILE:HG22	1:A:145:ILE:O	2.02	0.58
2:B:462:GLU:CG	2:B:486:ARG:HD3	2.27	0.58
2:B:538:VAL:HA	2:B:588:LYS:CG	2.33	0.58
2:B:334:HIS:HD2	2:B:336:THR:CG2	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:756:LEU:HB2	4:D:767:LYS:HZ2	1.68	0.58
4:D:838:LEU:HD12	4:D:894:VAL:CG1	2.33	0.58
4:D:963:THR:HG22	4:D:965:VAL:H	1.68	0.58
1:A:202:VAL:HG13	1:A:203:LYS:H	1.69	0.58
4:D:814:PRO:HG2	4:D:817:VAL:HG13	1.85	0.58
2:B:585:LYS:HB3	2:B:588:LYS:NZ	2.19	0.58
4:D:1281:ARG:HD2	4:D:1285:ILE:HD11	1.85	0.58
1:A:108:LEU:HD12	1:A:187:TYR:HA	1.84	0.58
4:D:1067:ALA:HA	4:D:1070:LEU:HD13	1.85	0.58
4:D:1195:LYS:HD3	4:D:1226:PHE:HE1	1.69	0.58
2:B:370:GLN:HB2	2:B:403:ARG:HG2	1.86	0.58
1:A:110:ILE:CG2	1:A:127:ILE:HA	2.34	0.57
1:A:126:ARG:CZ	2:B:544:LYS:HA	2.34	0.57
2:B:434:LEU:HD12	2:B:456:ARG:N	2.19	0.57
2:B:497:LEU:CD2	2:B:499:ILE:HG12	2.34	0.57
4:D:843:GLU:OE2	4:D:859:ARG:HD3	2.04	0.57
4:D:918:LYS:HD2	4:D:943:ALA:HB1	1.86	0.57
1:A:144:ASN:ND2	1:A:152:PRO:HB2	2.18	0.57
4:D:1445:PHE:O	4:D:1447:VAL:HG23	2.03	0.57
4:D:882:LYS:HE2	4:D:882:LYS:HA	1.87	0.57
2:B:462:GLU:O	2:B:486:ARG:HD2	2.04	0.57
2:B:556:GLY:O	2:B:582:VAL:HA	2.03	0.57
4:D:1515:CYS:SG	4:D:1634:MET:HE1	2.43	0.57
1:A:25:HIS:CD2	2:B:483:ARG:HD3	2.40	0.57
1:A:50:GLU:HG3	1:A:62:GLY:HA2	1.85	0.57
2:B:581:PHE:CD1	2:B:582:VAL:HG23	2.40	0.57
2:B:471:LEU:HG	2:B:510:VAL:HB	1.86	0.57
2:B:508:ARG:HD2	2:B:529:VAL:HG22	1.87	0.57
1:A:171:TRP:HZ2	1:A:174:PRO:HD2	1.70	0.57
2:B:341:TYR:CE2	2:B:607:PRO:HB3	2.39	0.57
2:B:395:GLN:CD	2:B:395:GLN:H	2.13	0.57
2:B:453:PHE:CE1	2:B:455:LEU:HD22	2.40	0.57
4:D:843:GLU:HG3	4:D:860:HIS:O	2.04	0.57
4:D:957:ARG:HH12	4:D:959:LEU:HD12	1.69	0.57
1:A:136:PRO:HG2	1:A:164:LEU:HD11	1.86	0.57
4:D:782:ILE:HG13	4:D:783:LEU:N	2.20	0.56
4:D:1524:LYS:HB2	4:D:1547:ILE:HD11	1.87	0.56
1:A:91:GLY:N	1:A:93:GLN:HE22	2.03	0.56
2:B:472:ILE:HG13	2:B:480:LYS:O	2.05	0.56
4:D:1354:ARG:CZ	4:D:1361:THR:HG22	2.36	0.56
1:A:26:ASP:CG	2:B:483:ARG:HH22	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:782:ILE:HD11	4:D:800:GLU:OE1	2.05	0.56
1:A:23:GLU:HB2	1:A:61:MET:SD	2.45	0.56
2:B:403:ARG:HH22	2:B:405:LYS:HA	1.70	0.56
2:B:561:LEU:HB2	2:B:564:GLU:OE2	2.05	0.56
4:D:898:PHE:C	4:D:899:ILE:HG13	2.31	0.56
2:B:395:GLN:O	2:B:423:PRO:HG3	2.05	0.56
2:B:452:ASN:HA	2:B:492:LEU:HD22	1.88	0.56
4:D:926:ASP:HB3	4:D:930:LEU:HD23	1.87	0.56
1:A:181:GLN:CD	1:A:199:GLU:HB3	2.30	0.56
1:A:23:GLU:CD	2:B:483:ARG:HH21	2.14	0.56
2:B:425:SER:OG	2:B:613:TYR:HD1	1.89	0.56
2:B:548:SER:HB3	2:B:558:GLN:HB3	1.87	0.56
3:C:689:THR:HA	3:C:692:ILE:HG22	1.86	0.56
4:D:1369:ARG:HH22	4:D:1371:ARG:HH22	1.54	0.56
2:B:343:LYS:HB3	2:B:346:MET:HB2	1.87	0.56
4:D:1278:LEU:HD12	4:D:1281:ARG:H	1.71	0.56
2:B:425:SER:OG	2:B:427:VAL:HG23	2.05	0.55
2:B:550:ASP:H	2:B:558:GLN:NE2	2.04	0.55
4:D:882:LYS:HD3	4:D:883:THR:N	2.22	0.55
4:D:1083:LYS:HZ3	4:D:1087:LEU:HD21	1.71	0.55
1:A:55:THR:HG22	1:A:57:ALA:H	1.71	0.55
2:B:572:VAL:HB	2:B:575:ALA:HB2	1.87	0.55
4:D:787:MET:HE3	4:D:793:ILE:CG2	2.36	0.55
4:D:1555:GLN:HB2	4:D:1558:GLN:NE2	2.21	0.55
4:D:840:VAL:HG12	4:D:894:VAL:HG13	1.87	0.55
1:A:68:ILE:O	1:A:68:ILE:HD12	2.07	0.55
1:A:126:ARG:NE	2:B:544:LYS:HA	2.22	0.55
2:B:434:LEU:N	2:B:456:ARG:HD2	2.21	0.55
2:B:508:ARG:HE	2:B:510:VAL:CG2	2.15	0.55
4:D:821:GLU:O	4:D:879:VAL:HG22	2.07	0.55
4:D:965:VAL:HG11	4:D:1254:PHE:CE1	2.42	0.55
4:D:1112:ARG:HG2	4:D:1115:ASN:HB3	1.87	0.55
1:A:90:PHE:H	1:A:93:GLN:NE2	2.05	0.55
1:A:173:ILE:HD12	1:A:174:PRO:HD2	1.89	0.55
2:B:341:TYR:CD1	2:B:422:LEU:HB2	2.42	0.55
4:D:1332:ASP:OD1	4:D:1469:ARG:HA	2.07	0.55
4:D:1376:ALA:HB3	4:D:1429:VAL:HB	1.88	0.55
4:D:1024:LEU:O	4:D:1028:LYS:HG3	2.07	0.55
1:A:131:ASN:ND2	1:A:133:LYS:H	2.05	0.55
2:B:538:VAL:O	2:B:585:LYS:HD2	2.06	0.55
2:B:630:GLN:O	2:B:630:GLN:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1112:ARG:CG	4:D:1115:ASN:HB3	2.37	0.54
4:D:1479:LYS:HE3	4:D:1570:GLU:HG2	1.88	0.54
1:A:12:LEU:HD11	1:A:14:LEU:HB2	1.87	0.54
2:B:616:VAL:HG23	2:B:617:PHE:N	2.22	0.54
4:D:1386:MET:HB3	4:D:1389:PHE:CD2	2.42	0.54
4:D:1575:GLU:HB3	4:D:1578:LYS:HZ3	1.71	0.54
1:A:34:THR:H	1:A:89:THR:HG21	1.73	0.54
2:B:457:MET:HG2	2:B:461:HIS:HB2	1.88	0.54
4:D:818:VAL:CG1	4:D:912:GLU:HA	2.37	0.54
2:B:617:PHE:CD2	2:B:624:PHE:HE1	2.26	0.54
4:D:858:ARG:HH12	4:D:860:HIS:CA	2.21	0.54
2:B:392:HIS:CE1	2:B:394:SER:HB3	2.43	0.54
2:B:434:LEU:HG	2:B:454:LEU:HG	1.89	0.54
1:A:194:GLN:OE1	1:A:196:PHE:HB2	2.08	0.54
4:D:1419:ARG:O	4:D:1420:ASN:C	2.51	0.54
2:B:334:HIS:HD2	2:B:336:THR:HG21	1.72	0.54
2:B:541:LEU:HA	4:D:789:ASP:HA	1.90	0.54
3:C:679:ASN:OD1	3:C:681:MET:HB2	2.08	0.54
4:D:1049:LYS:O	4:D:1050:ARG:HG2	2.08	0.54
1:A:139:ARG:HB2	1:A:188:TYR:CE1	2.43	0.53
2:B:540:SER:OG	4:D:790:LYS:HB2	2.08	0.53
4:D:930:LEU:HD21	4:D:1232:ARG:HG2	1.89	0.53
4:D:1414:LYS:HD3	4:D:1414:LYS:C	2.33	0.53
1:A:142:MET:HA	1:A:157:SER:HA	1.89	0.53
2:B:465:ILE:HD13	2:B:515:LEU:HD21	1.90	0.53
4:D:950:PRO:HA	4:D:1592:GLU:OE2	2.08	0.53
4:D:1479:LYS:HE2	4:D:1569:ARG:HB2	1.90	0.53
1:A:117:TYR:CE2	1:A:123:VAL:HG22	2.43	0.53
4:D:824:GLU:HA	4:D:877:VAL:HA	1.89	0.53
3:C:684:SER:O	3:C:688:ARG:HG3	2.08	0.53
4:D:1334:LEU:HD23	4:D:1334:LEU:H	1.74	0.53
2:B:424:TYR:HB3	2:B:612:ASP:CA	2.34	0.53
2:B:544:LYS:O	2:B:547:GLN:HG3	2.09	0.53
4:D:1245:GLY:HA3	4:D:1463:LEU:HD22	1.90	0.53
4:D:1585:LEU:HD22	4:D:1603:ASP:HB2	1.90	0.53
4:D:788:SER:HA	4:D:795:VAL:O	2.08	0.53
4:D:1031:TYR:CZ	4:D:1035:LEU:HD21	2.43	0.53
2:B:468:TYR:OH	2:B:486:ARG:NE	2.42	0.53
4:D:1600:ILE:HD12	4:D:1600:ILE:O	2.08	0.53
1:A:184:ILE:O	1:A:197:SER:HA	2.09	0.53
4:D:1414:LYS:NZ	4:D:1416:PHE:O	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1522:VAL:HG22	4:D:1583:TRP:HB3	1.91	0.53
1:A:124:LEU:HD22	2:B:544:LYS:CE	2.35	0.52
2:B:443:LEU:HD11	2:B:449:LEU:HD22	1.90	0.52
4:D:778:THR:HG23	4:D:803:VAL:CG1	2.38	0.52
4:D:1164:SER:HB3	4:D:1198:TRP:HB3	1.90	0.52
1:A:119:PRO:HB2	1:A:175:GLU:OE2	2.09	0.52
2:B:468:TYR:HB2	2:B:484:GLN:OE1	2.09	0.52
4:D:1229:PRO:HA	4:D:1232:ARG:HD2	1.91	0.52
4:D:1347:PRO:HA	4:D:1362:MET:HG2	1.89	0.52
4:D:1516:GLU:HG3	4:D:1518:GLY:N	2.22	0.52
1:A:22:LEU:HD12	1:A:90:PHE:HZ	1.74	0.52
2:B:549:GLU:O	2:B:550:ASP:HB2	2.09	0.52
4:D:927:PRO:O	4:D:928:GLU:HB2	2.08	0.52
1:A:26:ASP:OD2	1:A:61:MET:HE1	2.08	0.52
1:A:181:GLN:NE2	1:A:201:GLU:H	2.06	0.52
2:B:351:MET:HA	2:B:351:MET:HE2	1.91	0.52
4:D:982:ILE:HD13	4:D:1247:THR:HG22	1.91	0.52
1:A:39:ASP:OD2	1:A:72:ARG:NH2	2.42	0.52
4:D:1126:LEU:HD13	4:D:1150:ALA:HB3	1.90	0.52
1:A:40:PHE:HB3	1:A:41:PRO:HD3	1.90	0.52
1:A:171:TRP:CZ2	1:A:174:PRO:HD2	2.45	0.52
2:B:343:LYS:NZ	2:B:344:PRO:HD2	2.25	0.52
4:D:1166:THR:HA	4:D:1169:ILE:HG22	1.90	0.52
1:A:46:VAL:HG23	1:A:66:PHE:HE1	1.75	0.52
1:A:129:THR:O	1:A:136:PRO:HA	2.09	0.52
4:D:782:ILE:HG13	4:D:783:LEU:H	1.73	0.52
1:A:203:LYS:HD3	1:A:204:GLU:N	2.25	0.52
2:B:538:VAL:HA	2:B:588:LYS:HG2	1.91	0.52
4:D:1369:ARG:NH2	4:D:1371:ARG:HH12	2.07	0.52
1:A:87:GLN:HG3	1:A:89:THR:OG1	2.10	0.52
1:A:120:GLY:N	1:A:173:ILE:HG23	2.24	0.52
1:A:163:GLN:NE2	1:A:167:LEU:HD21	2.25	0.52
2:B:343:LYS:HG3	2:B:525:VAL:HG11	1.91	0.52
2:B:551:ARG:HB2	2:B:559:MET:O	2.10	0.52
2:B:580:VAL:C	2:B:583:LEU:HD23	2.34	0.52
1:A:117:TYR:O	1:A:202:VAL:HG23	2.09	0.52
2:B:567:HIS:HE2	4:D:751:TRP:H	1.58	0.52
2:B:563:ILE:O	2:B:570:ARG:HG2	2.10	0.51
1:A:24:ALA:HA	1:A:90:PHE:CD2	2.45	0.51
1:A:41:PRO:CD	1:A:82:LYS:HD2	2.39	0.51
2:B:406:LYS:HD2	2:B:409:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:432:ASN:HB3	2:B:523:GLU:O	2.10	0.51
4:D:809:ILE:O	4:D:903:VAL:HG21	2.09	0.51
4:D:1112:ARG:CD	4:D:1115:ASN:HB3	2.41	0.51
1:A:26:ASP:HB2	1:A:28:GLN:OE1	2.10	0.51
4:D:779:THR:H	4:D:803:VAL:CG1	2.23	0.51
4:D:813:LEU:HB3	4:D:907:LEU:HD13	1.92	0.51
4:D:1278:LEU:HD13	4:D:1306:GLU:OE2	2.10	0.51
1:A:126:ARG:HG2	2:B:543:VAL:O	2.10	0.51
1:A:155:GLN:N	1:A:155:GLN:OE1	2.44	0.51
2:B:565:GLY:HA3	2:B:570:ARG:HB2	1.92	0.51
4:D:992:ASN:HD22	4:D:1037:PHE:HE1	1.58	0.51
1:A:146:GLU:CG	1:A:152:PRO:HB3	2.40	0.51
2:B:443:LEU:HB2	2:B:447:GLU:OE2	2.11	0.51
4:D:1192:ALA:HB2	4:D:1198:TRP:CZ2	2.46	0.51
1:A:59:ASN:O	1:A:61:MET:HE2	2.11	0.51
1:A:77:GLU:O	1:A:80:ARG:HG3	2.11	0.51
2:B:525:VAL:HG22	2:B:613:TYR:HA	1.93	0.51
1:A:104:GLN:CD	1:A:105:SER:H	2.17	0.51
4:D:814:PRO:HB3	4:D:1445:PHE:HE2	1.75	0.51
2:B:396:LYS:CG	2:B:397:PRO:HD2	2.41	0.51
2:B:600:LYS:CA	2:B:638:LEU:HB3	2.35	0.51
4:D:749:TRP:CE3	4:D:773:LEU:HA	2.44	0.51
1:A:105:SER:C	1:A:132:HIS:CE1	2.86	0.51
2:B:332:GLN:CG	2:B:354:VAL:HG13	2.41	0.51
2:B:432:ASN:CG	2:B:517:GLY:HA2	2.35	0.51
2:B:562:LYS:HG2	4:D:744:GLU:OE2	2.11	0.51
4:D:747:GLU:HB2	4:D:774:LYS:CB	2.41	0.51
4:D:1420:ASN:N	4:D:1420:ASN:OD1	2.43	0.51
1:A:41:PRO:HD2	1:A:82:LYS:CD	2.39	0.50
2:B:495:LEU:CD2	2:B:497:LEU:HB2	2.40	0.50
2:B:624:PHE:CE1	2:B:631:GLN:HA	2.46	0.50
1:A:44:LYS:CG	1:A:66:PHE:CD2	2.94	0.50
1:A:84:VAL:HG23	1:A:84:VAL:O	2.09	0.50
1:A:148:PRO:HG3	1:A:181:GLN:N	2.26	0.50
4:D:1574:LEU:HD23	4:D:1580:TYR:CZ	2.46	0.50
2:B:582:VAL:O	2:B:586:LYS:HG2	2.11	0.50
4:D:815:TYR:OH	4:D:1414:LYS:HD2	2.12	0.50
4:D:974:ASP:HB2	4:D:977:ARG:HB2	1.94	0.50
4:D:1385:MET:HE1	4:D:1391:PRO:CD	2.35	0.50
2:B:508:ARG:HH21	2:B:510:VAL:HA	1.76	0.50
4:D:880:PRO:CB	4:D:909:VAL:HG21	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:CD2	2:B:544:LYS:HE3	2.33	0.50
4:D:776:SER:OG	4:D:777:ILE:HG13	2.11	0.50
4:D:815:TYR:CD2	4:D:1418:ASP:O	2.65	0.50
1:A:173:ILE:HD12	1:A:174:PRO:CD	2.41	0.50
2:B:338:THR:HG22	2:B:351:MET:O	2.11	0.50
2:B:343:LYS:CG	2:B:525:VAL:HG11	2.41	0.50
2:B:583:LEU:HD22	2:B:586:LYS:NZ	2.27	0.50
4:D:779:THR:H	4:D:803:VAL:HG11	1.76	0.50
4:D:779:THR:OG1	4:D:803:VAL:HG11	2.12	0.50
1:A:203:LYS:HE2	1:A:203:LYS:HA	1.94	0.50
2:B:380:GLN:CD	2:B:380:GLN:H	2.20	0.50
3:C:681:MET:SD	4:D:1437:LEU:CA	2.99	0.50
4:D:1527:LEU:HD13	4:D:1539:TYR:HB3	1.93	0.50
4:D:1605:TRP:NE1	4:D:1607:GLU:HB2	2.27	0.50
1:A:109:PHE:HA	1:A:196:PHE:CD1	2.46	0.50
1:A:72:ARG:HB3	1:A:74:PHE:CZ	2.47	0.50
1:A:100:LEU:HB3	2:B:600:LYS:HZ2	1.77	0.50
2:B:494:VAL:O	2:B:495:LEU:HB3	2.10	0.50
2:B:562:LYS:HE2	4:D:744:GLU:OE2	2.11	0.50
4:D:1218:LEU:HD11	4:D:1226:PHE:CD2	2.47	0.50
4:D:1354:ARG:NH1	4:D:1361:THR:H	2.09	0.50
4:D:1108:ILE:HD11	4:D:1116:GLU:O	2.11	0.49
4:D:1356:GLN:NE2	4:D:1357:ASP:H	2.10	0.49
2:B:429:ASN:HB3	2:B:521:GLN:HE22	1.77	0.49
2:B:443:LEU:HD12	2:B:447:GLU:CG	2.42	0.49
4:D:841:ARG:HH12	4:D:859:ARG:HH22	1.60	0.49
4:D:926:ASP:OD2	4:D:929:ARG:HB2	2.12	0.49
4:D:877:VAL:HG23	4:D:1483:LEU:HD23	1.94	0.49
1:A:46:VAL:HG23	1:A:66:PHE:CE1	2.47	0.49
2:B:499:ILE:HG23	2:B:503:PHE:CZ	2.47	0.49
1:A:28:GLN:C	1:A:56:PRO:HG3	2.38	0.49
1:A:113:ASP:OD2	2:B:544:LYS:NZ	2.44	0.49
4:D:785:VAL:CB	4:D:798:PRO:HD3	2.41	0.49
1:A:120:GLY:H	1:A:173:ILE:HG23	1.78	0.49
2:B:512:TYR:CE1	2:B:616:VAL:O	2.64	0.49
2:B:585:LYS:HB3	2:B:588:LYS:HZ1	1.78	0.49
2:B:609:SER:HA	2:B:619:ASP:C	2.37	0.49
1:A:113:ASP:CB	2:B:544:LYS:HD2	2.42	0.49
2:B:432:ASN:ND2	2:B:517:GLY:HA2	2.27	0.49
4:D:1043:ALA:HB1	4:D:1052:PRO:CB	2.42	0.49
4:D:1360:ASN:OD1	4:D:1443:GLN:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:965:VAL:HG13	4:D:968:MET:HB2	1.93	0.49
1:A:162:ASN:HA	4:D:1028:LYS:HZ3	1.76	0.49
2:B:461:HIS:NE2	2:B:516:ILE:HD11	2.28	0.49
4:D:1043:ALA:HB1	4:D:1052:PRO:HB3	1.94	0.49
1:A:49:SER:O	1:A:50:GLU:HG2	2.12	0.49
2:B:493:VAL:O	2:B:494:VAL:C	2.56	0.49
4:D:898:PHE:O	4:D:899:ILE:HG13	2.12	0.49
2:B:430:SER:O	2:B:523:GLU:HB2	2.13	0.48
4:D:880:PRO:O	4:D:881:LEU:HD23	2.13	0.48
4:D:993:MET:HG3	4:D:1059:TYR:CE2	2.47	0.48
4:D:1574:LEU:HD23	4:D:1580:TYR:CE1	2.47	0.48
2:B:555:PRO:HG2	2:B:558:GLN:HA	1.95	0.48
4:D:1074:ASP:HB3	4:D:1076:GLN:HG2	1.93	0.48
1:A:133:LYS:HG3	1:A:133:LYS:O	2.12	0.48
4:D:760:PRO:HA	4:D:767:LYS:HB3	1.96	0.48
4:D:940:ILE:HD13	4:D:1322:VAL:HG11	1.95	0.48
1:A:184:ILE:C	1:A:185:ARG:HD2	2.38	0.48
2:B:347:PRO:HB3	2:B:388:SER:OG	2.13	0.48
2:B:461:HIS:CE1	2:B:516:ILE:HD11	2.49	0.48
4:D:766:THR:HB	4:D:786:SER:OG	2.14	0.48
4:D:797:ASP:OD1	4:D:798:PRO:CD	2.54	0.48
4:D:1228:PRO:O	4:D:1232:ARG:HG3	2.13	0.48
4:D:1389:PHE:CZ	4:D:1443:GLN:HB2	2.48	0.48
1:A:145:ILE:HD12	1:A:154:LYS:HE2	1.94	0.48
2:B:372:GLU:OE2	2:B:375:VAL:HG22	2.12	0.48
2:B:538:VAL:HA	2:B:588:LYS:HG3	1.94	0.48
4:D:742:ARG:NH1	4:D:745:PHE:HB3	2.27	0.48
4:D:1041:SER:O	4:D:1042:SER:C	2.57	0.48
4:D:1487:GLU:OE1	4:D:1487:GLU:O	2.32	0.48
1:A:161:GLN:OE1	1:A:161:GLN:N	2.39	0.48
2:B:537:CYS:HB3	2:B:588:LYS:HA	1.96	0.48
4:D:755:ASP:OD1	4:D:769:MET:HE3	2.14	0.48
4:D:814:PRO:CB	4:D:1445:PHE:HE2	2.27	0.48
4:D:1031:TYR:CE1	4:D:1035:LEU:HD21	2.49	0.48
4:D:1511:LEU:O	4:D:1515:CYS:HB2	2.14	0.48
1:A:146:GLU:HG2	1:A:152:PRO:HB3	1.96	0.48
2:B:425:SER:CB	2:B:612:ASP:HB2	2.39	0.48
2:B:461:HIS:HA	2:B:464:LYS:CG	2.44	0.48
2:B:476:GLY:HA3	2:B:479:LEU:HB2	1.96	0.48
3:C:676:MET:HE2	3:C:676:MET:N	2.29	0.48
4:D:896:HIS:HB2	4:D:898:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:THR:O	1:A:69:PRO:HD3	2.14	0.48
2:B:396:LYS:HG3	2:B:397:PRO:HD2	1.96	0.48
4:D:837:GLU:C	4:D:838:LEU:HD22	2.39	0.48
4:D:922:VAL:HG11	4:D:1236:GLU:HA	1.96	0.48
2:B:566:ASP:HA	4:D:746:PRO:HB3	1.94	0.48
4:D:913:GLY:N	4:D:949:VAL:HG21	2.29	0.48
4:D:1039:GLN:HB2	4:D:1043:ALA:HB3	1.95	0.48
1:A:105:SER:HB2	1:A:139:ARG:HH22	1.78	0.48
4:D:1538:GLU:HG3	4:D:1563:ILE:HD12	1.95	0.48
1:A:38:HIS:N	1:A:85:THR:O	2.46	0.47
2:B:563:ILE:HG21	4:D:742:ARG:HG3	1.95	0.47
1:A:154:LYS:HD3	1:A:171:TRP:CE3	2.40	0.47
2:B:549:GLU:HB2	4:D:750:LEU:HD11	1.94	0.47
2:B:552:GLN:HE21	2:B:555:PRO:HB3	1.76	0.47
4:D:824:GLU:HB3	4:D:877:VAL:HG12	1.95	0.47
4:D:1074:ASP:HB3	4:D:1076:GLN:CD	2.39	0.47
4:D:1359:LYS:NZ	4:D:1446:ASN:H	2.12	0.47
4:D:1383:ILE:HG23	4:D:1455:VAL:HG22	1.95	0.47
4:D:1588:ASP:HA	4:D:1599:ILE:HD11	1.95	0.47
4:D:1332:ASP:OD1	4:D:1469:ARG:HD3	2.15	0.47
2:B:468:TYR:HA	2:B:513:TYR:CD2	2.48	0.47
2:B:514:THR:HG23	2:B:630:GLN:NE2	2.29	0.47
4:D:882:LYS:HD3	4:D:883:THR:H	1.79	0.47
4:D:915:ARG:HA	4:D:1327:HIS:HA	1.96	0.47
4:D:1074:ASP:O	4:D:1077:VAL:HG22	2.14	0.47
4:D:1378:MET:HE2	4:D:1378:MET:HB2	1.69	0.47
4:D:1385:MET:O	4:D:1419:ARG:HB3	2.14	0.47
2:B:572:VAL:HG12	2:B:573:LEU:N	2.29	0.47
2:B:624:PHE:CD2	2:B:625:THR:N	2.83	0.47
4:D:923:ARG:HH11	4:D:938:GLU:HG3	1.80	0.47
4:D:965:VAL:HG11	4:D:1254:PHE:HE1	1.79	0.47
1:A:121:SER:O	1:A:173:ILE:HG22	2.15	0.47
2:B:429:ASN:HA	2:B:521:GLN:HE22	1.80	0.47
2:B:444:ARG:HD3	2:B:444:ARG:HA	1.74	0.47
2:B:551:ARG:HA	4:D:800:GLU:CD	2.40	0.47
2:B:612:ASP:OD1	2:B:618:SER:HB2	2.14	0.47
4:D:988:CYS:HB2	4:D:1046:ALA:O	2.15	0.47
1:A:25:HIS:HA	2:B:483:ARG:CZ	2.44	0.47
1:A:26:ASP:CB	1:A:59:ASN:OD1	2.62	0.47
1:A:182:TRP:HB2	1:A:200:PHE:CE1	2.50	0.47
4:D:862:GLN:HE22	4:D:876:TYR:HE1	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1222:LYS:HD3	4:D:1224:PHE:CE2	2.49	0.47
2:B:514:THR:HG23	2:B:630:GLN:CD	2.40	0.47
4:D:940:ILE:O	4:D:1307:GLY:HA2	2.14	0.47
4:D:1593:LYS:HB2	4:D:1597:SER:HB3	1.97	0.47
1:A:123:VAL:HG12	1:A:125:TYR:HD1	1.80	0.47
2:B:337:LYS:O	2:B:337:LYS:HG3	2.15	0.47
2:B:465:ILE:CG2	2:B:486:ARG:HE	2.27	0.47
2:B:514:THR:HG23	2:B:630:GLN:CG	2.45	0.47
3:C:671:CYS:SG	4:D:1403:VAL:HG11	2.55	0.47
4:D:925:LEU:HG	4:D:1320:LEU:HB2	1.97	0.47
2:B:614:ALA:O	2:B:618:SER:HB2	2.15	0.46
4:D:982:ILE:HD12	4:D:994:ILE:HG12	1.98	0.46
4:D:1516:GLU:O	4:D:1519:VAL:HG12	2.15	0.46
2:B:334:HIS:NE2	2:B:353:PHE:O	2.48	0.46
2:B:431:ASN:ND2	2:B:517:GLY:HA3	2.30	0.46
2:B:443:LEU:HD21	2:B:449:LEU:HD21	1.98	0.46
1:A:39:ASP:CA	1:A:85:THR:H	2.26	0.46
2:B:583:LEU:HD22	2:B:586:LYS:HE3	1.97	0.46
2:B:635:ARG:C	2:B:637:GLU:H	2.21	0.46
4:D:764:ILE:HG22	4:D:765:SER:N	2.31	0.46
4:D:844:LEU:HD11	4:D:876:TYR:CG	2.50	0.46
4:D:988:CYS:HB3	4:D:1047:PHE:CE1	2.50	0.46
4:D:1104:HIS:CG	4:D:1105:GLN:H	2.34	0.46
2:B:434:LEU:HG	2:B:454:LEU:H	1.81	0.46
2:B:567:HIS:NE2	4:D:751:TRP:N	2.61	0.46
4:D:859:ARG:HH21	4:D:861:GLN:HG2	1.80	0.46
4:D:1568:CYS:HB3	4:D:1572:LEU:HD12	1.97	0.46
2:B:363:TYR:HD1	2:B:364:ARG:N	2.13	0.46
2:B:434:LEU:HB2	2:B:456:ARG:HB2	1.97	0.46
4:D:1359:LYS:HZ2	4:D:1446:ASN:H	1.63	0.46
2:B:343:LYS:HD2	2:B:346:MET:HG2	1.97	0.46
4:D:930:LEU:CD2	4:D:1232:ARG:HG2	2.45	0.46
4:D:1340:ASP:O	4:D:1368:THR:HA	2.16	0.46
1:A:27:ALA:H	1:A:60:HIS:CB	2.29	0.46
1:A:100:LEU:HB2	2:B:601:ALA:HB2	1.97	0.46
2:B:567:HIS:CE1	4:D:751:TRP:N	2.73	0.46
4:D:785:VAL:HG12	4:D:797:ASP:HA	1.98	0.46
4:D:811:LEU:HD11	4:D:890:VAL:HG13	1.98	0.46
4:D:850:PHE:CE2	4:D:878:ILE:HD11	2.51	0.46
4:D:1338:LYS:C	4:D:1371:ARG:HG3	2.41	0.46
2:B:507:PHE:CD2	2:B:531:VAL:HG13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:681:MET:HE2	4:D:1436:CYS:O	2.13	0.46
4:D:1192:ALA:HB2	4:D:1198:TRP:CE2	2.50	0.46
4:D:1407:ILE:HD12	4:D:1424:ILE:HG21	1.97	0.46
4:D:1487:GLU:O	4:D:1490:ARG:HB3	2.16	0.46
4:D:1590:TRP:HD1	4:D:1599:ILE:HG12	1.81	0.46
1:A:53:VAL:HG11	1:A:63:ASN:OD1	2.16	0.46
4:D:993:MET:HG3	4:D:1059:TYR:HE2	1.79	0.46
4:D:998:PRO:HG3	4:D:1251:PHE:CE1	2.50	0.46
1:A:78:LYS:HB2	1:A:103:LEU:HD12	1.98	0.46
2:B:600:LYS:HA	2:B:638:LEU:HD13	1.97	0.46
4:D:1045:ALA:HB2	4:D:1052:PRO:HA	1.98	0.46
2:B:331:TYR:CE2	2:B:357:PRO:HG2	2.51	0.45
4:D:973:VAL:HG21	4:D:1015:PHE:CE2	2.51	0.45
4:D:1073:ILE:HD11	4:D:1077:VAL:CG2	2.46	0.45
1:A:83:PHE:CZ	1:A:100:LEU:HD11	2.51	0.45
2:B:348:PHE:HD2	2:B:389:ILE:HG12	1.81	0.45
2:B:552:GLN:HE21	2:B:559:MET:HB3	1.81	0.45
2:B:603:ILE:HG22	2:B:603:ILE:O	2.16	0.45
4:D:742:ARG:NH2	4:D:745:PHE:HA	2.30	0.45
4:D:1234:LEU:HD23	4:D:1234:LEU:HA	1.61	0.45
1:A:45:LEU:HD22	1:A:46:VAL:N	2.29	0.45
1:A:154:LYS:CE	1:A:171:TRP:HB2	2.46	0.45
2:B:563:ILE:HD13	4:D:744:GLU:OE1	2.16	0.45
4:D:812:ARG:C	4:D:813:LEU:HD12	2.42	0.45
4:D:1418:ASP:HB2	4:D:1419:ARG:HG2	1.98	0.45
4:D:1525:THR:HB	4:D:1541:MET:HB3	1.98	0.45
4:D:1547:ILE:HG23	4:D:1635:VAL:HG23	1.99	0.45
4:D:1623:GLN:HA	4:D:1626:ASP:OD2	2.15	0.45
1:A:26:ASP:HB3	1:A:61:MET:HE2	1.99	0.45
1:A:26:ASP:HB2	1:A:59:ASN:OD1	2.16	0.45
2:B:472:ILE:HB	2:B:509:LEU:HD22	1.99	0.45
4:D:841:ARG:HH12	4:D:859:ARG:NH2	2.14	0.45
4:D:1070:LEU:HD12	4:D:1070:LEU:H	1.81	0.45
4:D:1345:ILE:HG23	4:D:1473:PRO:HA	1.99	0.45
1:A:71:ASN:OD1	1:A:72:ARG:HG2	2.17	0.45
1:A:203:LYS:CG	1:A:204:GLU:H	2.29	0.45
2:B:429:ASN:HB2	2:B:523:GLU:OE2	2.16	0.45
4:D:1074:ASP:HB3	4:D:1076:GLN:CG	2.46	0.45
1:A:89:THR:C	1:A:90:PHE:HD1	2.24	0.45
2:B:550:ASP:OD1	2:B:558:GLN:NE2	2.48	0.45
2:B:567:HIS:HE2	4:D:751:TRP:N	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:749:TRP:HZ3	4:D:771:ILE:HD11	1.82	0.45
4:D:857:LYS:HA	4:D:857:LYS:HD3	1.71	0.45
4:D:961:GLN:HG2	4:D:966:ALA:HB3	1.99	0.45
4:D:991:GLN:HG2	4:D:1460:TYR:OH	2.16	0.45
4:D:1103:ILE:HG22	4:D:1461:TYR:HE2	1.82	0.45
4:D:1482:LYS:HE3	4:D:1482:LYS:HB2	1.63	0.45
1:A:11:ILE:HG13	1:A:12:LEU:O	2.17	0.45
2:B:380:GLN:HB2	2:B:382:ASP:OD1	2.17	0.45
4:D:960:LEU:HD21	4:D:1274:VAL:HG11	1.98	0.45
4:D:1004:HIS:NE2	4:D:1070:LEU:HD11	2.31	0.45
4:D:1412:LEU:H	4:D:1422:LEU:HD12	1.82	0.45
2:B:332:GLN:HG3	2:B:354:VAL:HG13	1.99	0.45
4:D:841:ARG:HH21	4:D:891:LYS:NZ	2.14	0.45
4:D:973:VAL:HG11	4:D:1015:PHE:CE2	2.52	0.45
1:A:25:HIS:HA	2:B:483:ARG:NH2	2.31	0.45
2:B:611:LYS:HB3	2:B:618:SER:OG	2.16	0.45
3:C:681:MET:CE	4:D:1436:CYS:C	2.87	0.45
4:D:879:VAL:CG2	4:D:1483:LEU:HD11	2.37	0.45
4:D:1240:TYR:CD1	4:D:1463:LEU:HD23	2.51	0.45
2:B:343:LYS:HZ3	2:B:344:PRO:HD2	1.80	0.45
2:B:433:TYR:C	2:B:456:ARG:HD2	2.42	0.45
2:B:457:MET:SD	2:B:516:ILE:O	2.74	0.45
2:B:600:LYS:O	2:B:638:LEU:HD22	2.17	0.45
4:D:761:LYS:HE2	4:D:761:LYS:HB2	1.69	0.45
4:D:801:VAL:HG22	4:D:803:VAL:H	1.82	0.45
4:D:809:ILE:HG21	4:D:890:VAL:CG2	2.45	0.45
4:D:839:LYS:HG2	4:D:895:TYR:CD2	2.52	0.45
1:A:51:LYS:HA	1:A:54:LEU:CG	2.46	0.44
1:A:181:GLN:HG3	1:A:199:GLU:OE1	2.18	0.44
2:B:364:ARG:NH2	2:B:366:PRO:HA	2.31	0.44
4:D:749:TRP:CZ3	4:D:750:LEU:HG	2.52	0.44
4:D:888:VAL:HG12	4:D:905:LYS:O	2.17	0.44
4:D:1386:MET:O	4:D:1389:PHE:HB2	2.17	0.44
4:D:1526:ARG:HB2	4:D:1579:HIS:CD2	2.52	0.44
2:B:461:HIS:O	2:B:465:ILE:HG22	2.17	0.44
4:D:1426:LEU:HD23	4:D:1426:LEU:HA	1.70	0.44
2:B:333:ILE:CD1	2:B:417:ARG:HB3	2.48	0.44
2:B:459:ARG:O	2:B:462:GLU:HB3	2.18	0.44
2:B:517:GLY:HA3	2:B:521:GLN:O	2.16	0.44
4:D:1572:LEU:HD23	4:D:1606:VAL:HG11	1.98	0.44
1:A:41:PRO:HD2	1:A:82:LYS:CG	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ARG:HH12	1:A:82:LYS:HZ2	1.66	0.44
2:B:453:PHE:O	2:B:453:PHE:CD1	2.71	0.44
4:D:750:LEU:HA	4:D:750:LEU:HD23	1.85	0.44
4:D:1496:CYS:SG	4:D:1497:PHE:HD1	2.41	0.44
1:A:139:ARG:HB2	1:A:188:TYR:HE1	1.83	0.44
2:B:386:LYS:O	2:B:387:LEU:HD13	2.18	0.44
1:A:148:PRO:HD3	1:A:181:GLN:O	2.17	0.44
1:A:162:ASN:HB3	4:D:1028:LYS:HD3	1.99	0.44
2:B:403:ARG:O	2:B:403:ARG:NH1	2.51	0.44
2:B:461:HIS:HD2	2:B:464:LYS:HG2	1.82	0.44
2:B:465:ILE:HD12	2:B:466:ARG:H	1.83	0.44
2:B:470:TYR:HE1	2:B:483:ARG:N	2.16	0.44
2:B:547:GLN:HB3	2:B:567:HIS:ND1	2.32	0.44
4:D:1531:GLN:N	4:D:1531:GLN:OE1	2.51	0.44
2:B:363:TYR:CD1	2:B:363:TYR:C	2.95	0.44
2:B:570:ARG:HA	2:B:570:ARG:HD2	1.31	0.44
4:D:758:GLU:N	4:D:759:PRO:HD2	2.33	0.44
1:A:37:VAL:HG22	1:A:44:LYS:HB3	2.00	0.44
2:B:461:HIS:HA	2:B:464:LYS:HG3	1.99	0.44
2:B:503:PHE:HB2	2:B:534:LYS:CG	2.47	0.44
2:B:508:ARG:HD2	2:B:509:LEU:H	1.83	0.44
4:D:749:TRP:CZ3	4:D:771:ILE:HD11	2.53	0.44
4:D:947:ASP:O	4:D:1329:LYS:HG3	2.17	0.44
1:A:43:LYS:HB3	1:A:43:LYS:HE3	1.83	0.44
2:B:459:ARG:CA	2:B:462:GLU:HB3	2.47	0.44
3:C:681:MET:SD	4:D:1437:LEU:HA	2.58	0.44
4:D:1198:TRP:HH2	4:D:1226:PHE:HE2	1.64	0.44
2:B:353:PHE:CZ	2:B:384:VAL:HG12	2.53	0.43
2:B:403:ARG:HH12	2:B:405:LYS:CA	2.31	0.43
2:B:406:LYS:HD3	2:B:409:LEU:HD21	2.00	0.43
2:B:580:VAL:HA	2:B:583:LEU:HD23	2.00	0.43
4:D:985:PRO:HB2	4:D:1425:TYR:OH	2.18	0.43
1:A:109:PHE:HD1	1:A:109:PHE:O	2.01	0.43
1:A:182:TRP:HE1	1:A:202:VAL:CG1	2.31	0.43
2:B:435:HIS:H	2:B:454:LEU:CD2	2.31	0.43
2:B:497:LEU:HD23	2:B:498:SER:N	2.33	0.43
4:D:982:ILE:HD11	4:D:1247:THR:HA	1.99	0.43
4:D:1049:LYS:HA	4:D:1049:LYS:HD2	1.74	0.43
4:D:1500:LYS:HG2	4:D:1605:TRP:CH2	2.53	0.43
1:A:164:LEU:HD22	1:A:164:LEU:HA	1.82	0.43
2:B:457:MET:CE	2:B:461:HIS:HB3	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:526:ALA:O	2:B:615:GLY:HA3	2.18	0.43
4:D:778:THR:CG2	4:D:801:VAL:HG13	2.48	0.43
4:D:1341:LEU:O	4:D:1342:LYS:HD2	2.18	0.43
4:D:1409:LYS:HG3	4:D:1425:TYR:HD2	1.83	0.43
4:D:1411:GLU:CG	4:D:1413:ASP:HB2	2.38	0.43
1:A:97:LYS:HA	2:B:622:LEU:HD22	2.00	0.43
1:A:113:ASP:OD1	2:B:544:LYS:HD3	2.16	0.43
2:B:343:LYS:HD3	2:B:343:LYS:C	2.43	0.43
2:B:557:GLN:O	2:B:558:GLN:HG2	2.19	0.43
3:C:676:MET:HE3	3:C:705:CYS:SG	2.58	0.43
1:A:164:LEU:HD13	1:A:164:LEU:C	2.44	0.43
2:B:465:ILE:HD11	2:B:467:TYR:CD2	2.54	0.43
2:B:493:VAL:O	2:B:495:LEU:CD2	2.64	0.43
1:A:37:VAL:HG22	1:A:37:VAL:O	2.17	0.43
1:A:83:PHE:HZ	2:B:636:ALA:O	2.02	0.43
2:B:340:LYS:O	2:B:421:ALA:HA	2.18	0.43
2:B:540:SER:H	4:D:790:LYS:CB	2.32	0.43
2:B:635:ARG:C	2:B:637:GLU:N	2.77	0.43
4:D:1004:HIS:O	4:D:1008:GLU:HG2	2.19	0.43
4:D:1014:LYS:HD3	4:D:1292:GLU:HA	2.01	0.43
4:D:1222:LYS:HD3	4:D:1224:PHE:HE2	1.83	0.43
4:D:1568:CYS:O	4:D:1572:LEU:HD12	2.18	0.43
4:D:1172:TYR:HA	4:D:1217:ALA:HB2	2.01	0.43
4:D:1395:ASP:HA	4:D:1398:GLN:HB3	2.01	0.43
1:A:15:GLU:O	1:A:17:GLU:OE1	2.36	0.43
2:B:434:LEU:HA	2:B:454:LEU:HG	2.01	0.43
3:C:681:MET:SD	4:D:1438:ALA:CB	3.07	0.43
4:D:1031:TYR:OH	4:D:1073:ILE:HG13	2.18	0.43
4:D:1358:ALA:HA	4:D:1444:TYR:CE1	2.54	0.43
2:B:624:PHE:CZ	2:B:626:SER:HB3	2.54	0.43
4:D:747:GLU:H	4:D:774:LYS:HZ2	1.67	0.43
2:B:443:LEU:HD12	2:B:447:GLU:HG2	2.01	0.43
4:D:779:THR:O	4:D:780:TRP:CE3	2.72	0.43
4:D:1484:CYS:C	4:D:1486:ASP:H	2.26	0.43
1:A:107:TYR:HA	1:A:194:GLN:HG2	2.01	0.42
1:A:142:MET:C	1:A:142:MET:SD	3.02	0.42
4:D:871:SER:O	4:D:872:LEU:HD22	2.19	0.42
4:D:1026:LEU:CA	4:D:1029:LYS:HE2	2.40	0.42
4:D:1491:CYS:HA	4:D:1494:GLU:OE2	2.18	0.42
1:A:13:ARG:NH2	2:B:601:ALA:HB1	2.34	0.42
1:A:25:HIS:NE2	2:B:467:TYR:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:403:ARG:HH12	2:B:405:LYS:N	2.17	0.42
2:B:425:SER:OG	2:B:613:TYR:CD1	2.65	0.42
2:B:470:TYR:CE1	2:B:483:ARG:N	2.87	0.42
2:B:583:LEU:HD22	2:B:586:LYS:CE	2.50	0.42
4:D:882:LYS:O	4:D:909:VAL:HG11	2.20	0.42
4:D:1302:THR:HG22	4:D:1304:GLU:H	1.82	0.42
4:D:1540:ILE:N	4:D:1540:ILE:HD12	2.34	0.42
1:A:55:THR:HG22	1:A:57:ALA:N	2.34	0.42
1:A:196:PHE:HD2	1:A:196:PHE:O	2.02	0.42
2:B:417:ARG:HD3	2:B:418:THR:N	2.34	0.42
2:B:550:ASP:N	2:B:558:GLN:HE22	2.18	0.42
3:C:687:ARG:NH1	3:C:690:ARG:HD3	2.34	0.42
4:D:868:PRO:O	4:D:869:LYS:HG2	2.19	0.42
4:D:1554:VAL:HG13	4:D:1560:ARG:NH2	2.34	0.42
2:B:624:PHE:CD1	2:B:631:GLN:HA	2.54	0.42
4:D:785:VAL:H	4:D:798:PRO:HD3	1.83	0.42
4:D:1203:LYS:H	4:D:1203:LYS:HG2	1.71	0.42
2:B:472:ILE:HB	2:B:509:LEU:CD2	2.49	0.42
4:D:964:PRO:HD3	4:D:1317:GLN:O	2.19	0.42
1:A:94:VAL:HG23	1:A:94:VAL:O	2.20	0.42
2:B:495:LEU:HD21	2:B:497:LEU:HB2	2.01	0.42
2:B:605:CYS:HB2	2:B:640:CYS:HB2	1.52	0.42
4:D:852:SER:HB2	4:D:878:ILE:HG13	2.02	0.42
4:D:897:HIS:ND1	4:D:897:HIS:N	2.68	0.42
4:D:1331:LYS:H	4:D:1331:LYS:HG3	1.70	0.42
4:D:1397:LYS:O	4:D:1401:ASN:HB3	2.19	0.42
1:A:51:LYS:HA	1:A:54:LEU:CB	2.48	0.42
1:A:128:PHE:HB3	4:D:791:LYS:HE2	2.00	0.42
2:B:504:ILE:O	2:B:504:ILE:HG22	2.20	0.42
4:D:818:VAL:N	4:D:821:GLU:OE2	2.53	0.42
4:D:961:GLN:O	4:D:1318:GLY:HA3	2.18	0.42
4:D:1407:ILE:HD12	4:D:1424:ILE:CG2	2.50	0.42
1:A:51:LYS:HG2	1:A:54:LEU:HB2	2.02	0.42
1:A:82:LYS:HZ3	1:A:84:VAL:HG12	1.84	0.42
2:B:363:TYR:HD1	2:B:363:TYR:C	2.27	0.42
2:B:369:VAL:CG1	2:B:372:GLU:HG2	2.49	0.42
4:D:1369:ARG:CZ	4:D:1371:ARG:HH12	2.32	0.42
4:D:932:ARG:HA	4:D:932:ARG:HD3	1.28	0.42
4:D:1414:LYS:HE3	4:D:1420:ASN:HA	2.01	0.42
1:A:35:VAL:O	1:A:48:SER:HA	2.20	0.41
4:D:749:TRP:CE2	4:D:773:LEU:HA	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:850:PHE:HB3	4:D:880:PRO:HA	2.02	0.41
4:D:1369:ARG:HG3	4:D:1430:SER:O	2.20	0.41
4:D:1409:LYS:HG3	4:D:1425:TYR:CD2	2.55	0.41
4:D:1585:LEU:HD23	4:D:1585:LEU:H	1.84	0.41
2:B:413:GLU:O	2:B:413:GLU:HG2	2.20	0.41
2:B:434:LEU:HA	2:B:454:LEU:CD1	2.50	0.41
2:B:642:GLN:HA	2:B:643:PRO:HD3	1.90	0.41
3:C:674:ASP:OD2	4:D:1403:VAL:HG23	2.20	0.41
4:D:825:ILE:O	4:D:825:ILE:HD12	2.19	0.41
4:D:1406:TYR:O	4:D:1407:ILE:HD13	2.20	0.41
2:B:386:LYS:NZ	2:B:440:ARG:HB3	2.36	0.41
2:B:551:ARG:HD3	2:B:561:LEU:CD2	2.50	0.41
3:C:666:LYS:HB3	3:C:666:LYS:HE3	1.87	0.41
4:D:960:LEU:HB3	4:D:1289:ILE:HD11	2.02	0.41
4:D:1252:MET:HA	4:D:1252:MET:HE3	2.02	0.41
4:D:1279:PRO:HG2	4:D:1306:GLU:OE1	2.19	0.41
4:D:1287:HIS:ND1	4:D:1298:ARG:HG2	2.35	0.41
4:D:1564:SER:HB3	4:D:1600:ILE:HD11	2.02	0.41
1:A:68:ILE:HD13	1:A:71:ASN:HB3	2.01	0.41
2:B:346:MET:CE	2:B:433:TYR:HD1	2.33	0.41
2:B:515:LEU:HA	2:B:515:LEU:HD23	1.27	0.41
2:B:624:PHE:HB3	2:B:632:THR:HG23	2.02	0.41
4:D:771:ILE:HD13	4:D:771:ILE:HG21	1.86	0.41
4:D:1240:TYR:CE1	4:D:1463:LEU:HB3	2.55	0.41
1:A:114:LYS:HD2	1:A:114:LYS:HA	1.57	0.41
2:B:435:HIS:CE1	2:B:436:LEU:HD12	2.55	0.41
2:B:551:ARG:HH11	2:B:561:LEU:HD23	1.84	0.41
4:D:1123:ALA:O	4:D:1127:ILE:HG13	2.21	0.41
4:D:1177:MET:HB2	4:D:1179:ARG:HG3	2.03	0.41
1:A:16:SER:C	1:A:17:GLU:OE1	2.63	0.41
1:A:39:ASP:HA	1:A:85:THR:N	2.29	0.41
2:B:328:THR:HG21	2:B:417:ARG:HH21	1.85	0.41
2:B:406:LYS:O	2:B:407:GLN:C	2.64	0.41
2:B:600:LYS:HG2	2:B:638:LEU:HD13	2.03	0.41
4:D:811:LEU:O	4:D:813:LEU:HD13	2.21	0.41
4:D:850:PHE:HE1	4:D:886:GLN:HB3	1.86	0.41
4:D:1103:ILE:HG23	4:D:1378:MET:HG2	2.01	0.41
1:A:31:VAL:HG23	1:A:92:THR:HG22	2.01	0.41
1:A:144:ASN:OD1	1:A:152:PRO:HB2	2.21	0.41
2:B:548:SER:HB3	2:B:558:GLN:CB	2.51	0.41
2:B:556:GLY:O	2:B:584:ASN:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:677:ARG:HH12	4:D:1398:GLN:HA	1.86	0.41
4:D:785:VAL:HG22	4:D:786:SER:H	1.85	0.41
2:B:353:PHE:HA	2:B:383:GLY:O	2.20	0.41
4:D:896:HIS:HB2	4:D:897:HIS:H	1.59	0.41
4:D:1233:TRP:O	4:D:1237:GLN:HG2	2.20	0.41
4:D:1249:ALA:O	4:D:1253:VAL:HG12	2.21	0.41
4:D:1511:LEU:HD12	4:D:1511:LEU:HA	1.86	0.41
4:D:1522:VAL:CG1	4:D:1547:ILE:HB	2.48	0.41
1:A:39:ASP:HA	1:A:84:VAL:HA	2.02	0.41
2:B:369:VAL:HA	2:B:402:VAL:HG23	2.03	0.41
2:B:435:HIS:CE1	2:B:527:ASP:HB2	2.56	0.41
2:B:495:LEU:HD23	2:B:497:LEU:HB2	2.03	0.41
2:B:564:GLU:HG2	2:B:566:ASP:H	1.85	0.41
2:B:596:ASP:HB3	2:B:605:CYS:SG	2.61	0.41
4:D:973:VAL:HG11	4:D:1015:PHE:HE2	1.85	0.41
4:D:992:ASN:ND2	4:D:1037:PHE:CE1	2.79	0.41
4:D:1035:LEU:HD13	4:D:1035:LEU:HA	1.81	0.41
1:A:91:GLY:H	1:A:93:GLN:HE22	1.67	0.41
1:A:116:ILE:HG23	1:A:201:GLU:O	2.21	0.41
2:B:514:THR:HG22	2:B:514:THR:O	2.21	0.41
4:D:759:PRO:HA	4:D:760:PRO:HD3	1.92	0.41
4:D:800:GLU:OE1	4:D:800:GLU:N	2.54	0.41
4:D:1031:TYR:O	4:D:1035:LEU:HD22	2.21	0.41
4:D:1133:LYS:HE2	4:D:1133:LYS:HB3	1.77	0.41
4:D:1359:LYS:HE3	4:D:1359:LYS:HB2	1.77	0.41
1:A:110:ILE:O	1:A:110:ILE:HD12	2.21	0.40
1:A:154:LYS:HD3	1:A:171:TRP:HB2	2.02	0.40
1:A:167:LEU:HD23	1:A:167:LEU:HA	1.59	0.40
2:B:353:PHE:CE1	2:B:384:VAL:HG12	2.56	0.40
2:B:426:THR:O	2:B:426:THR:HG22	2.21	0.40
2:B:498:SER:O	2:B:499:ILE:C	2.63	0.40
4:D:787:MET:HE3	4:D:793:ILE:HG21	2.03	0.40
4:D:982:ILE:CG2	4:D:984:THR:H	2.34	0.40
4:D:1354:ARG:HB2	4:D:1358:ALA:HB3	2.04	0.40
1:A:39:ASP:HB3	1:A:82:LYS:HE2	2.03	0.40
1:A:84:VAL:O	1:A:86:VAL:HG23	2.22	0.40
1:A:147:ASN:ND2	1:A:151:ILE:H	2.20	0.40
2:B:366:PRO:HB3	2:B:376:GLN:NE2	2.36	0.40
4:D:1358:ALA:HA	4:D:1444:TYR:CD1	2.56	0.40
1:A:187:TYR:CD2	1:A:188:TYR:O	2.75	0.40
2:B:346:MET:HE2	2:B:433:TYR:HD1	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:429:ASN:CA	2:B:521:GLN:HE22	2.35	0.40
2:B:474:ASN:ND2	2:B:503:PHE:CZ	2.89	0.40
2:B:585:LYS:O	2:B:588:LYS:HD2	2.22	0.40
3:C:695:GLY:O	3:C:699:LYS:HG2	2.21	0.40
4:D:877:VAL:CG2	4:D:1483:LEU:HD23	2.52	0.40
4:D:1047:PHE:HB2	4:D:1050:ARG:HG3	2.03	0.40
4:D:1354:ARG:HB2	4:D:1358:ALA:CB	2.51	0.40
4:D:1414:LYS:HA	4:D:1414:LYS:HE2	2.02	0.40
1:A:109:PHE:CZ	1:A:130:VAL:HG11	2.55	0.40
1:A:196:PHE:C	1:A:196:PHE:CD2	3.00	0.40
1:A:200:PHE:O	1:A:201:GLU:C	2.65	0.40
2:B:454:LEU:O	2:B:454:LEU:HD12	2.22	0.40
2:B:464:LYS:NZ	2:B:516:ILE:HG23	2.36	0.40
4:D:746:PRO:HA	4:D:774:LYS:HZ1	1.84	0.40
4:D:935:VAL:O	4:D:936:GLN:C	2.64	0.40
1:A:183:LYS:HG2	1:A:197:SER:HB3	2.04	0.40
2:B:372:GLU:OE1	2:B:373:ASP:O	2.40	0.40
2:B:406:LYS:CD	2:B:409:LEU:HD21	2.52	0.40
4:D:758:GLU:N	4:D:759:PRO:CD	2.84	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	194/196 (99%)	152 (78%)	42 (22%)	0	100	100
2	B	314/316 (99%)	219 (70%)	94 (30%)	1 (0%)	36	70
3	C	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
4	D	900/902 (100%)	819 (91%)	81 (9%)	0	100	100
All	All	1455/1463 (100%)	1235 (85%)	219 (15%)	1 (0%)	49	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	505	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	179/179 (100%)	163 (91%)	16 (9%)	9	34
2	B	273/273 (100%)	260 (95%)	13 (5%)	23	57
3	C	46/46 (100%)	46 (100%)	0	100	100
4	D	798/798 (100%)	777 (97%)	21 (3%)	40	72
All	All	1296/1296 (100%)	1246 (96%)	50 (4%)	30	62

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	14	LEU
1	A	15	GLU
1	A	17	GLU
1	A	37	VAL
1	A	40	PHE
1	A	41	PRO
1	A	43	LYS
1	A	63	ASN
1	A	114	LYS
1	A	116	ILE
1	A	118	THR
1	A	141	VAL
1	A	147	ASN
1	A	185	ARG
1	A	200	PHE
2	B	338	THR
2	B	347	PRO
2	B	375	VAL

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Mol	Chain	Res	Type
2	B	382	ASP
2	B	384	VAL
2	B	469	THR
2	B	471	LEU
2	B	510	VAL
2	B	531	VAL
2	B	534	LYS
2	B	570	ARG
2	B	589	LEU
2	B	617	PHE
4	D	753	VAL
4	D	783	LEU
4	D	877	VAL
4	D	888	VAL
4	D	899	ILE
4	D	914	ILE
4	D	916	MET
4	D	932	ARG
4	D	951	ASP
4	D	1077	VAL
4	D	1263	ASP
4	D	1322	VAL
4	D	1325	MET
4	D	1386	MET
4	D	1414	LYS
4	D	1418	ASP
4	D	1486	ASP
4	D	1501	SER
4	D	1515	CYS
4	D	1519	VAL
4	D	1545	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	93	GLN
1	A	132	HIS
1	A	163	GLN
1	A	178	ASN
2	B	334	HIS
2	B	376	GLN

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Mol	Chain	Res	Type
2	B	431	ASN
2	B	435	HIS
2	B	461	HIS
2	B	552	GLN
2	B	557	GLN
2	B	558	GLN
2	B	642	GLN
4	D	820	ASN
4	D	1162	GLN
4	D	1176	GLN
4	D	1204	GLN
4	D	1277	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

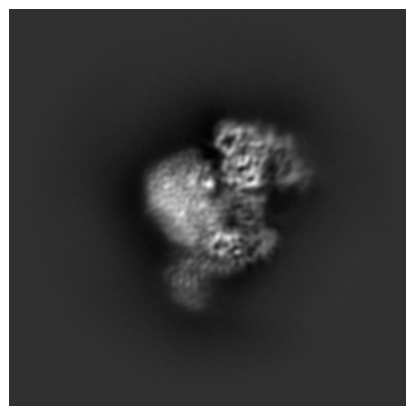
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53900. These allow visual inspection of the internal detail of the map and identification of artifacts.

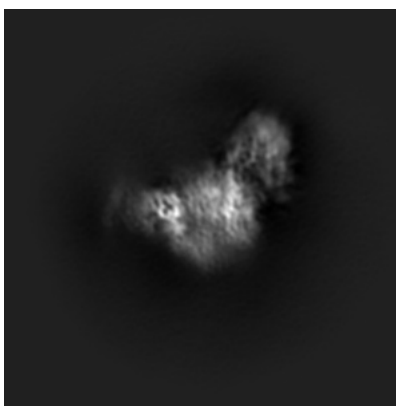
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

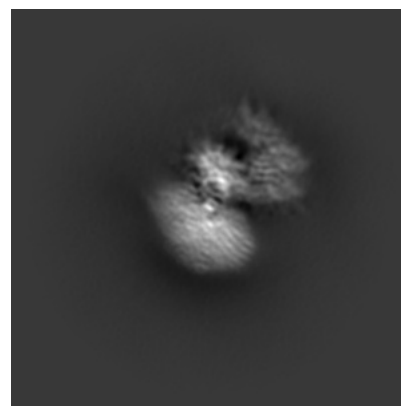
6.1.1 Primary map



X

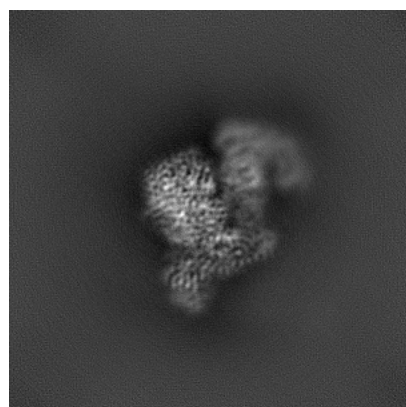


Y

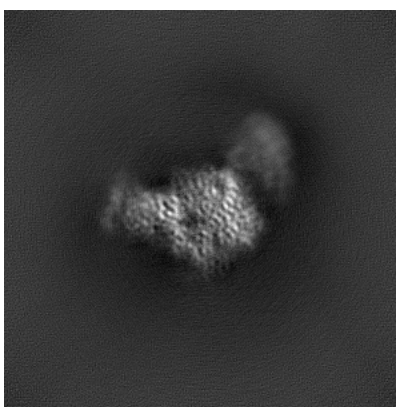


Z

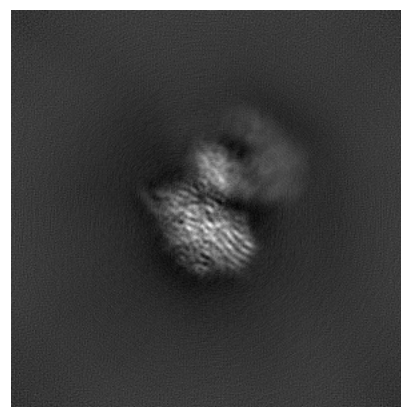
6.1.2 Raw map



X



Y

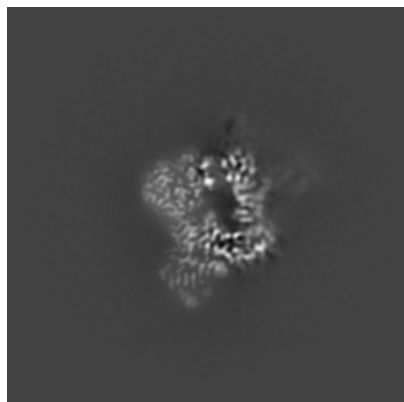


Z

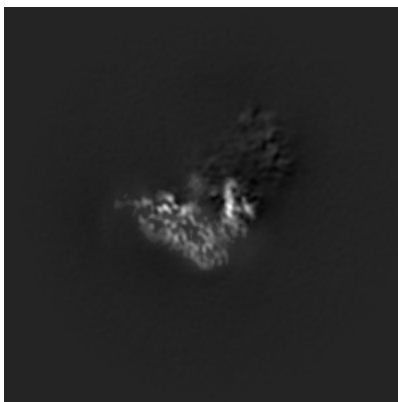
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

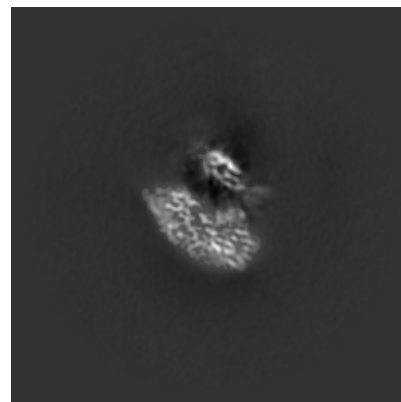
6.2.1 Primary map



X Index: 200

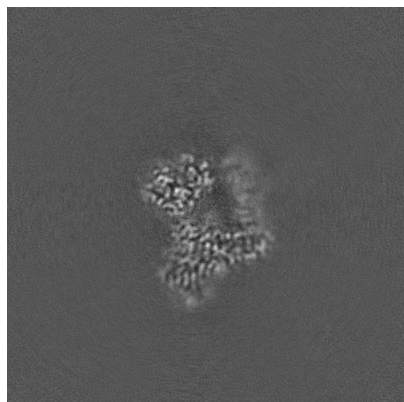


Y Index: 200

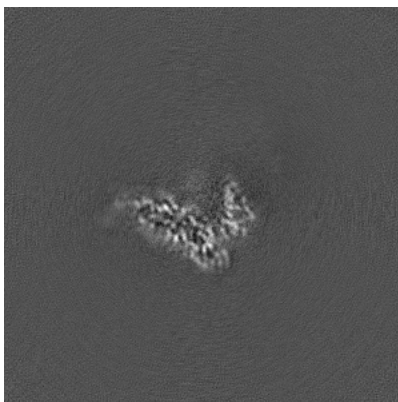


Z Index: 200

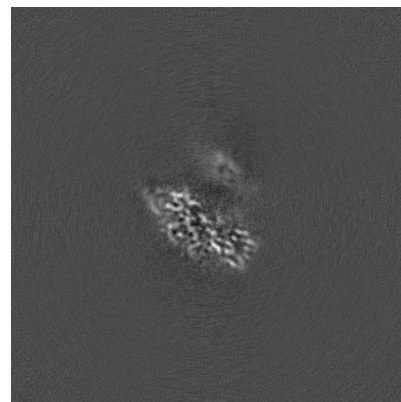
6.2.2 Raw map



X Index: 200



Y Index: 200

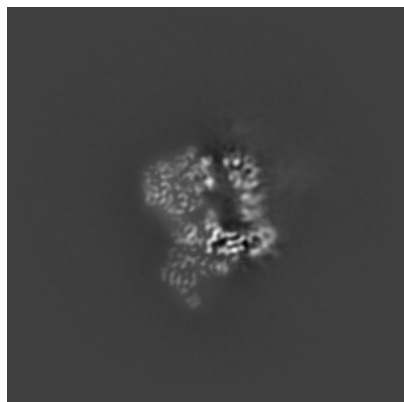


Z Index: 200

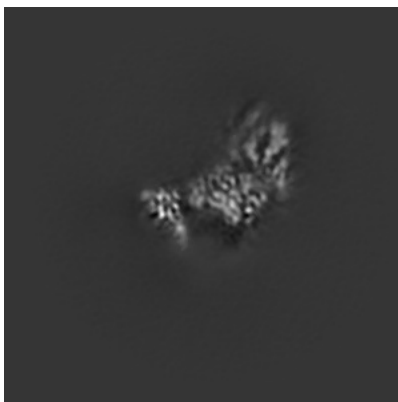
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

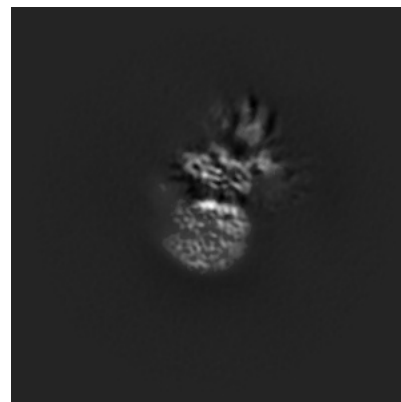
6.3.1 Primary map



X Index: 196

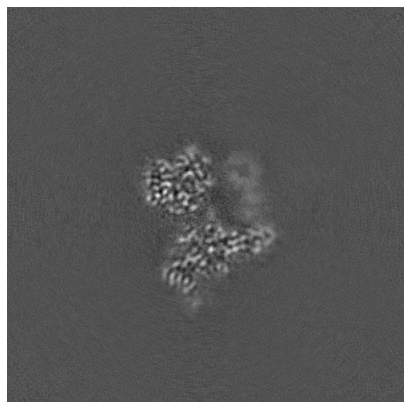


Y Index: 229

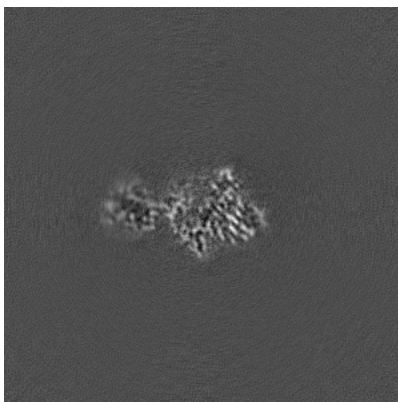


Z Index: 225

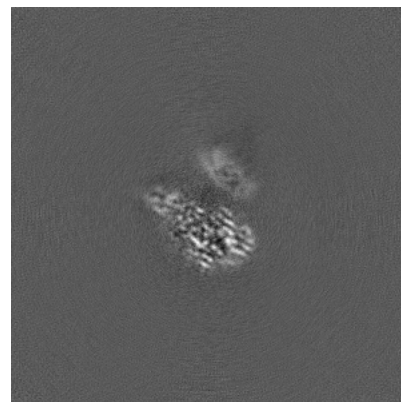
6.3.2 Raw map



X Index: 194



Y Index: 182

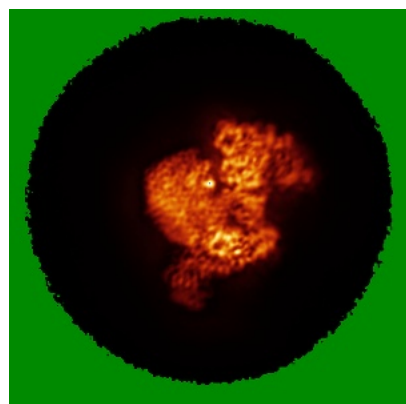


Z Index: 209

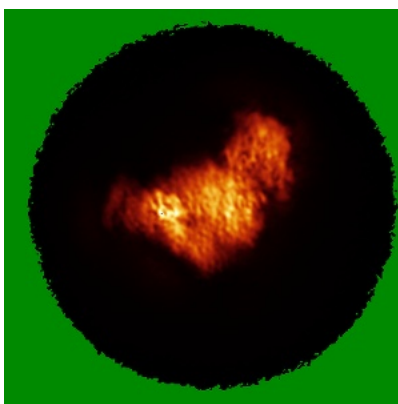
The images above show the largest variance slices of the map in three orthogonal directions.

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

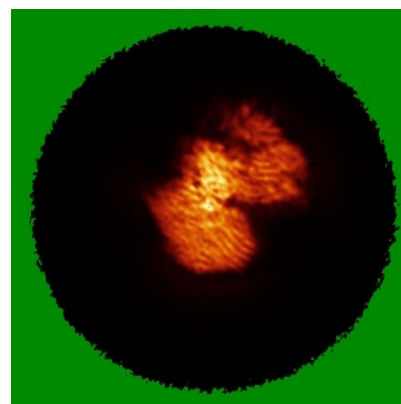
6.4.1 Primary map



X

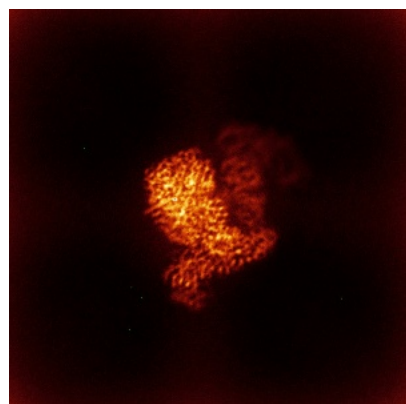


Y

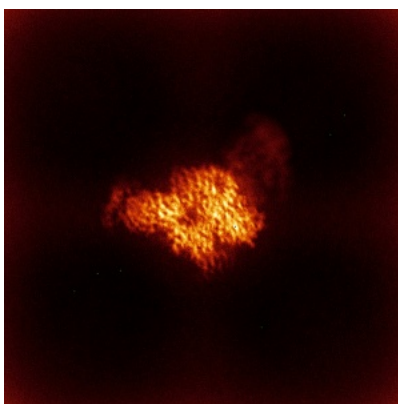


Z

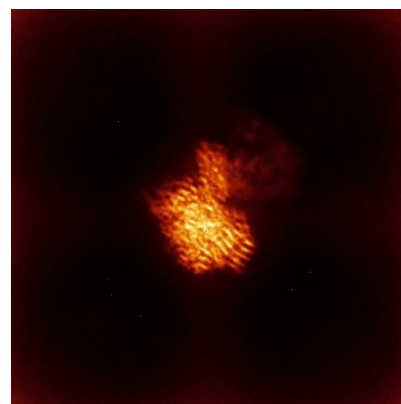
6.4.2 Raw map



X



Y

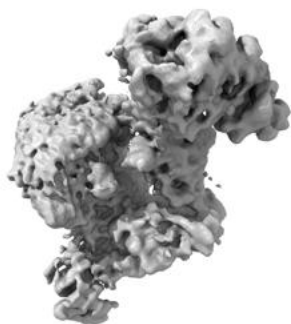


Z

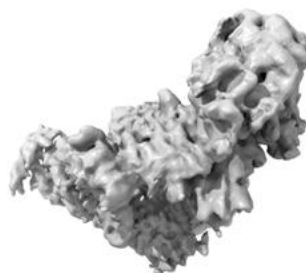
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

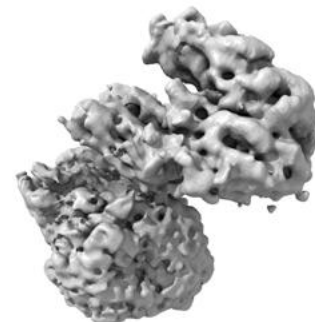
6.5.1 Primary map



X



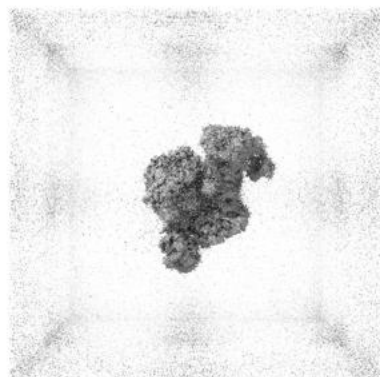
Y



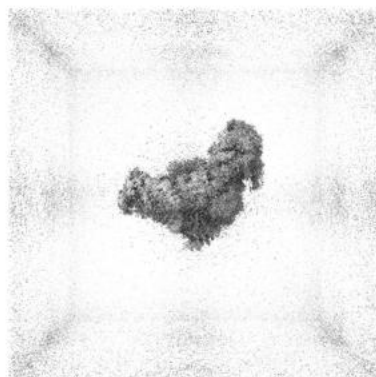
Z

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

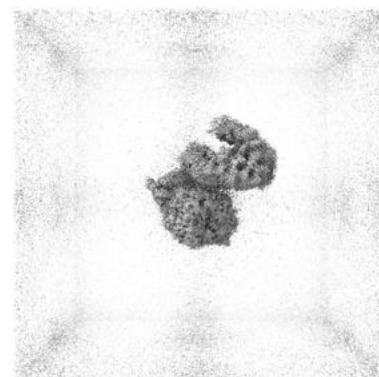
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

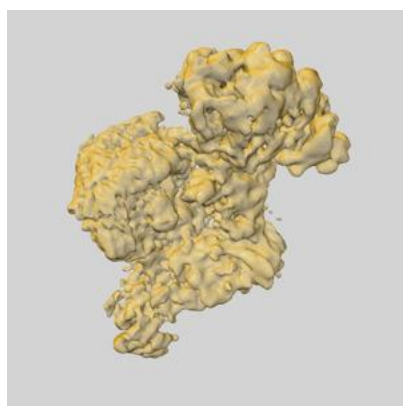
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

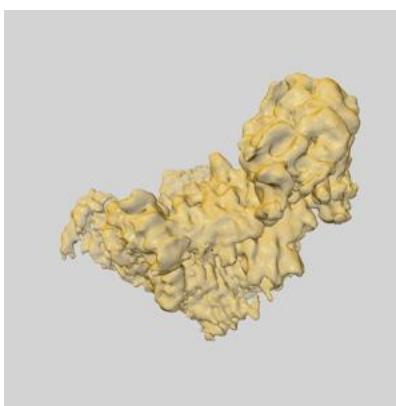
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

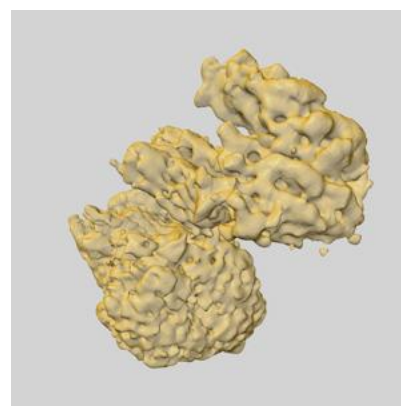
6.6.1 emd_53900_msk_1.map [i](#)



X



Y

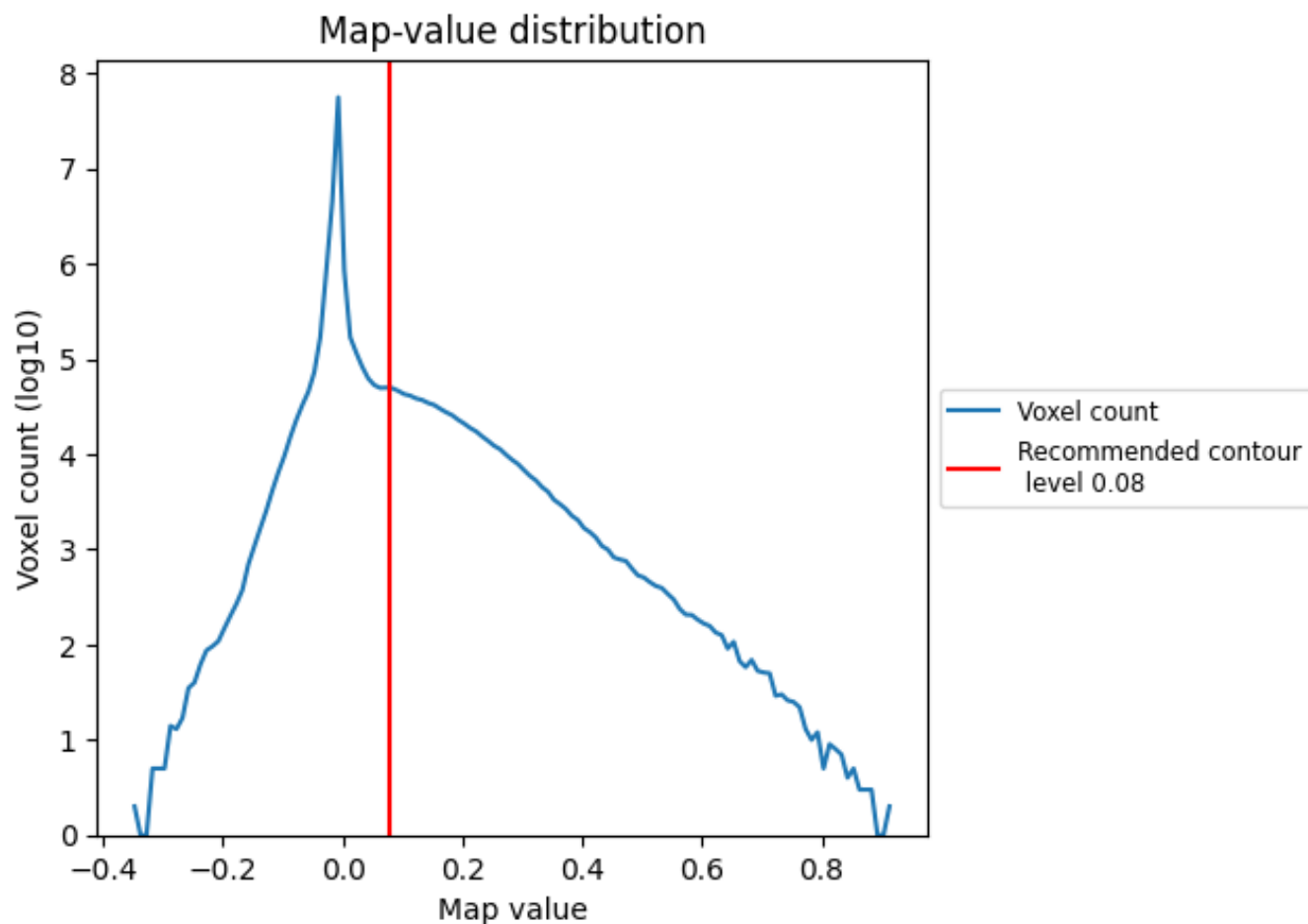


Z

7 Map analysis [i](#)

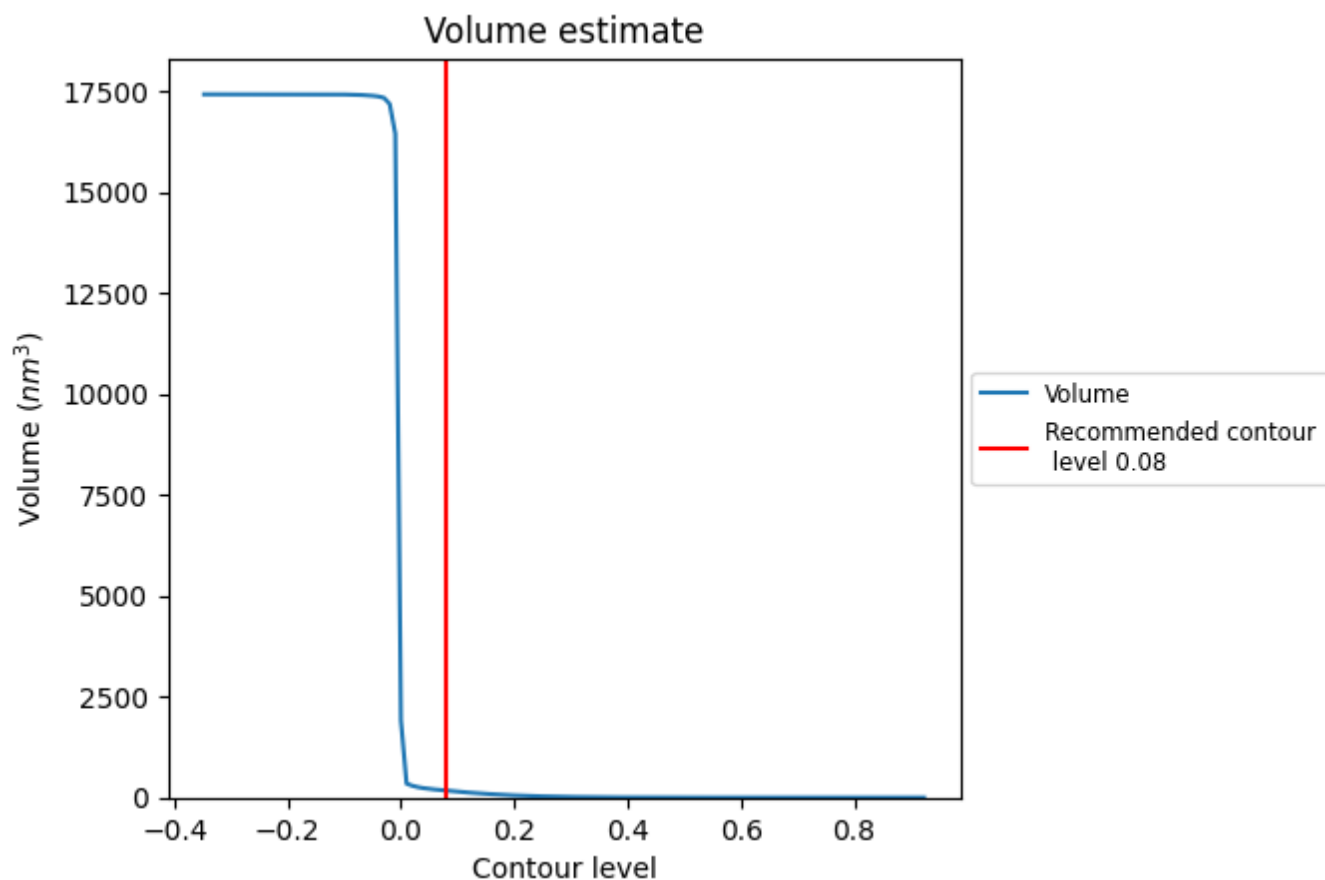
This section contains the results of statistical analysis of the map.

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.

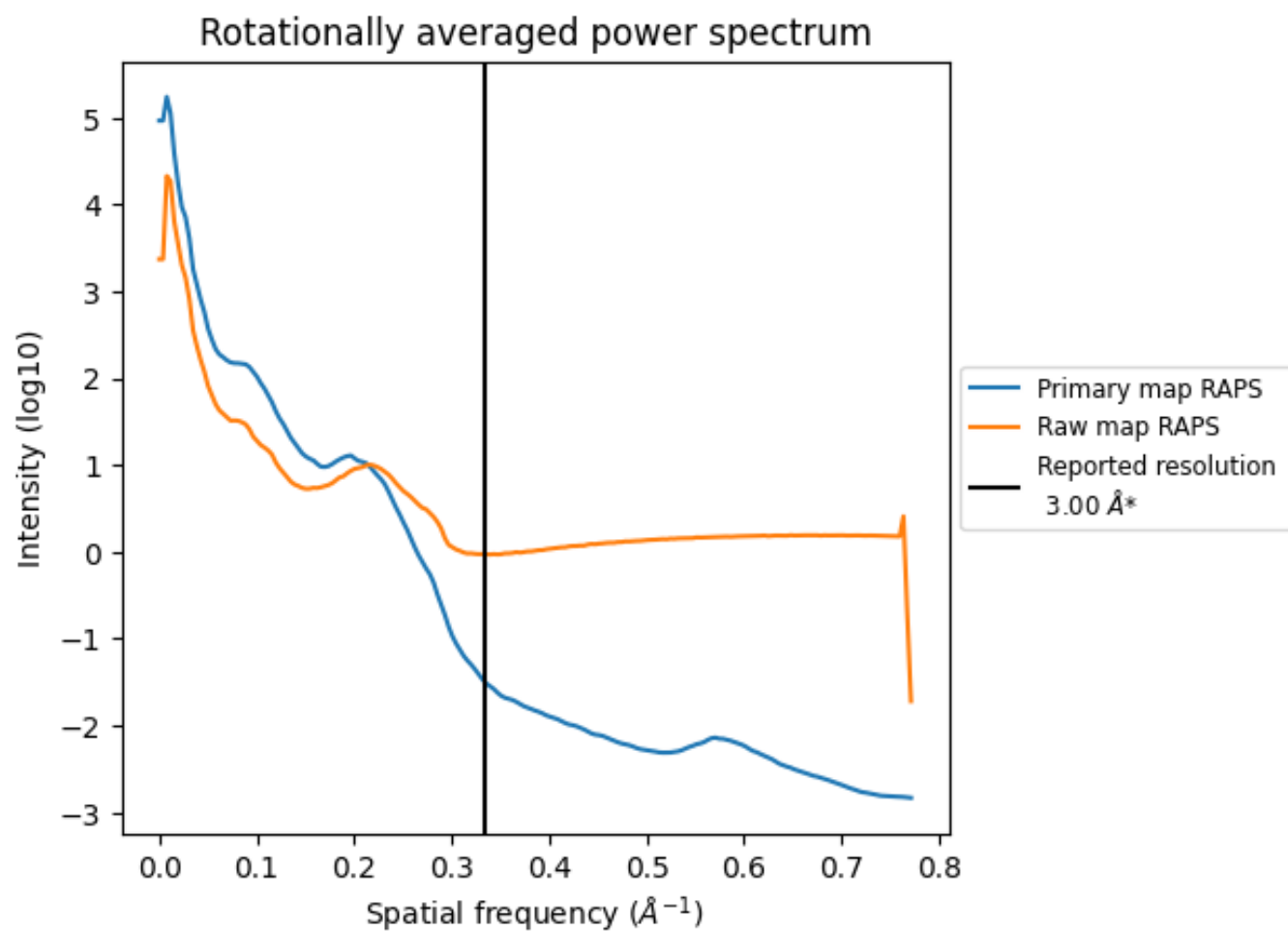
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 173 nm³; this corresponds to an approximate mass of 156 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 ⓘ

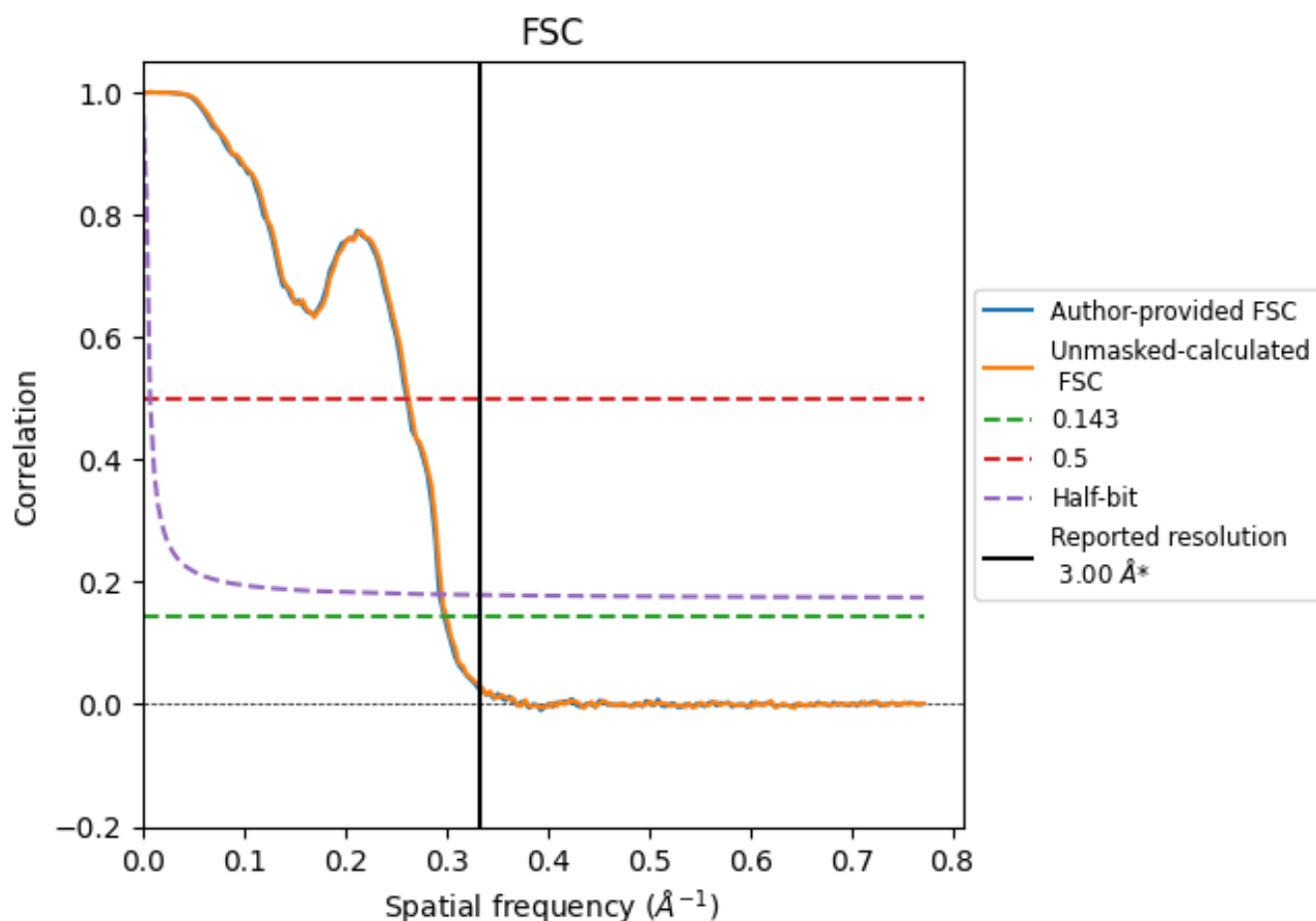


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

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 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.35	3.83	3.41
Unmasked-calculated*	3.33	3.81	3.38

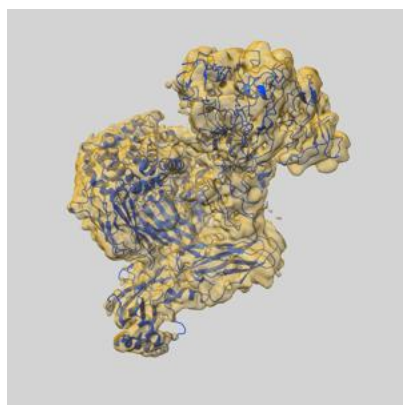
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.35 differs from the reported value 3.0 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.33 differs from the reported value 3.0 by more than 10 %

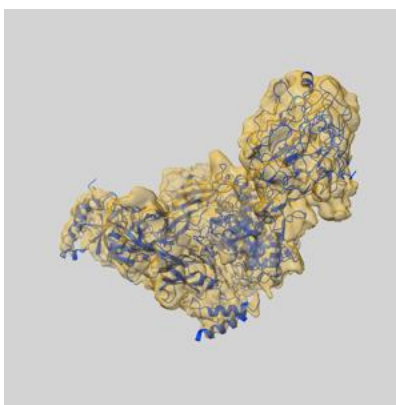
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53900 and PDB model 9RBO. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

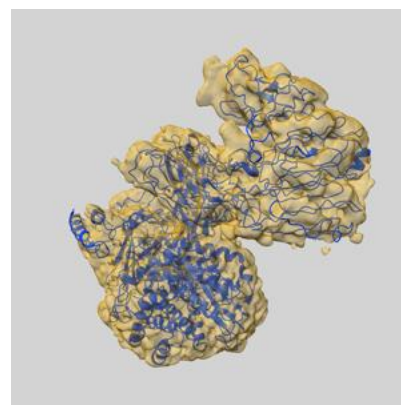
9.1 Map-model overlay [i](#)



X



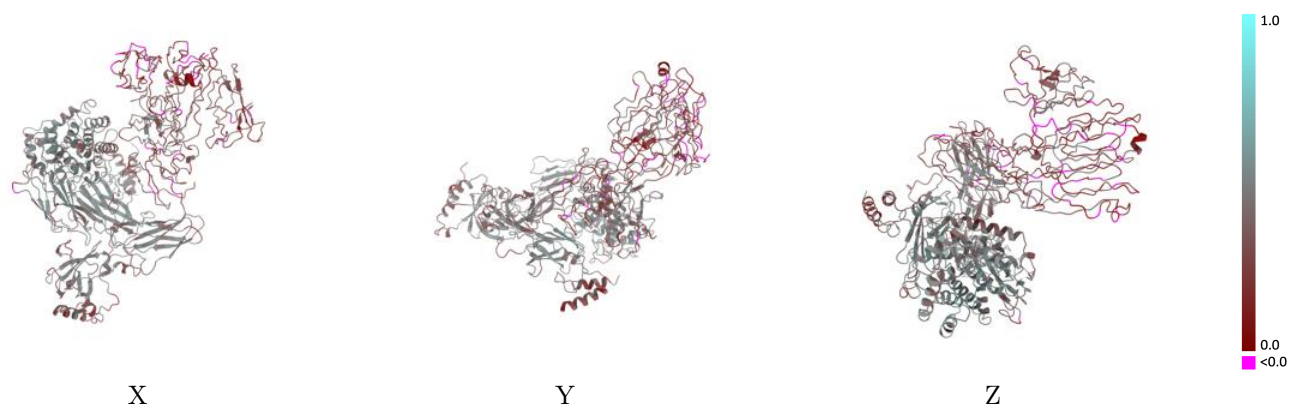
Y



Z

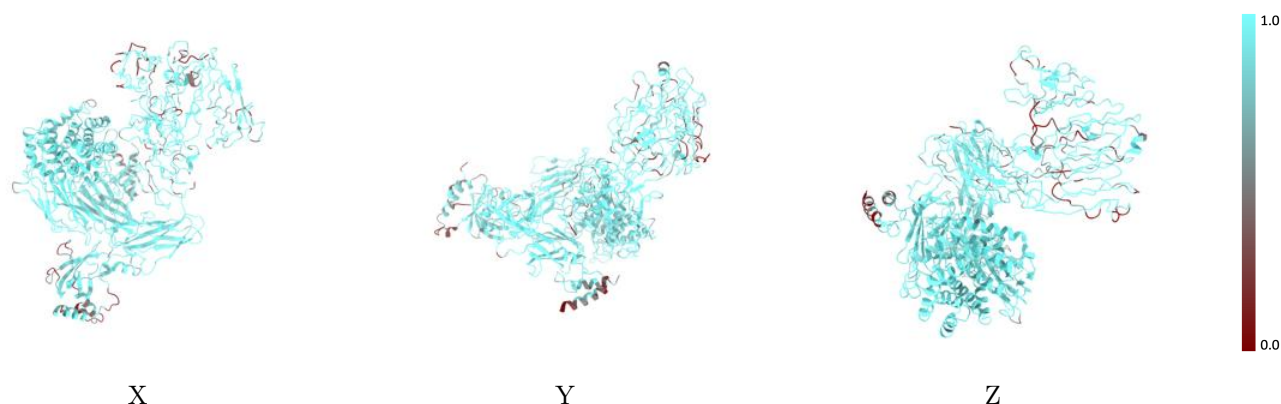
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



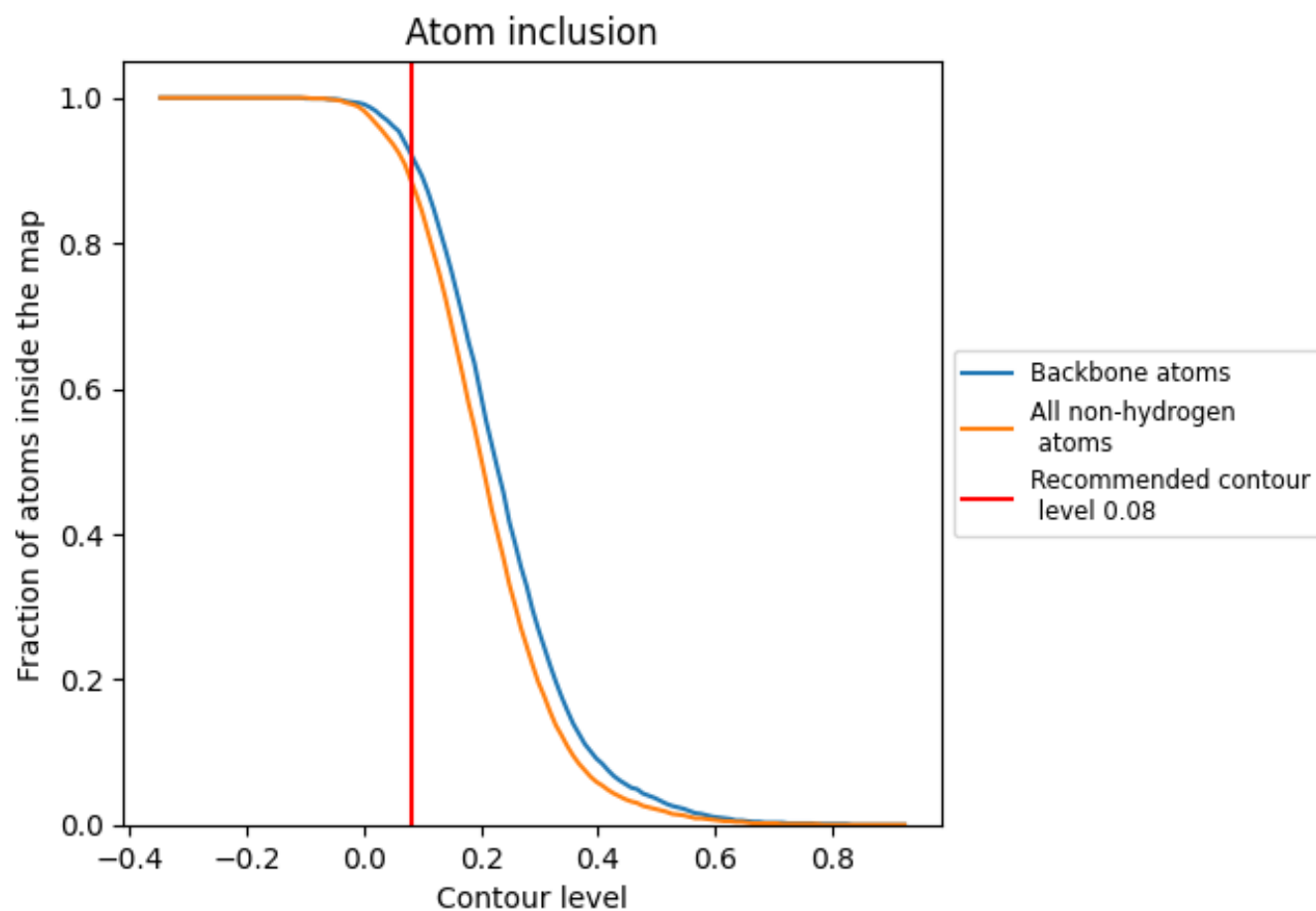
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8870	<div></div> 0.3720
A	<div></div> 0.8520	<div></div> 0.2930
B	<div></div> 0.8340	<div></div> 0.2510
C	<div></div> 0.6700	<div></div> 0.3430
D	<div></div> 0.9250	<div></div> 0.4310

