



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:30 PM UTC

PDB ID : 9KHF / pdb_00009khf
EMDB ID : EMD-62338
Title : AtGORK Full length 1
Authors : Chen, Y.H.; Li, Q.Y.; Zhang, C.R.; Tang, L.H.
Deposited on : 2024-11-10
Resolution : 3.40 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

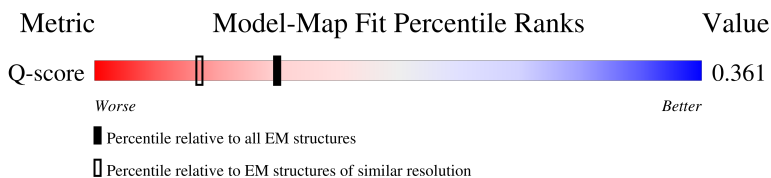
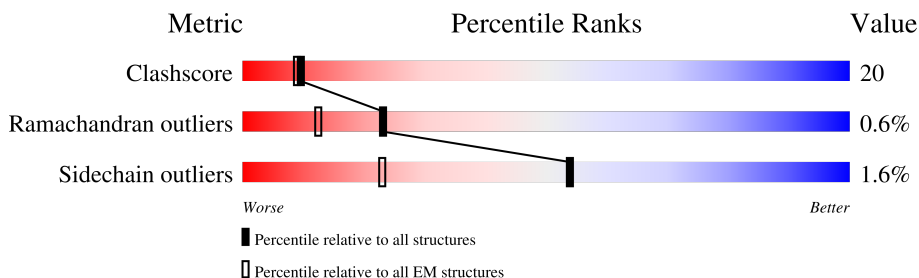
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	763	12% 55% 31% • 13%
1	B	763	13% 53% 31% • 13%
1	C	763	11% 56% 30% • 13%
1	D	763	13% 52% 34% • 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21610 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Potassium channel GORK.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	667	Total	C	N	O	S	0	0
			5408	3508	901	974	25		
1	B	666	Total	C	N	O	S	0	0
			5396	3499	900	972	25		
1	C	667	Total	C	N	O	S	0	0
			5408	3508	901	974	25		
1	D	666	Total	C	N	O	S	0	0
			5396	3499	900	972	25		

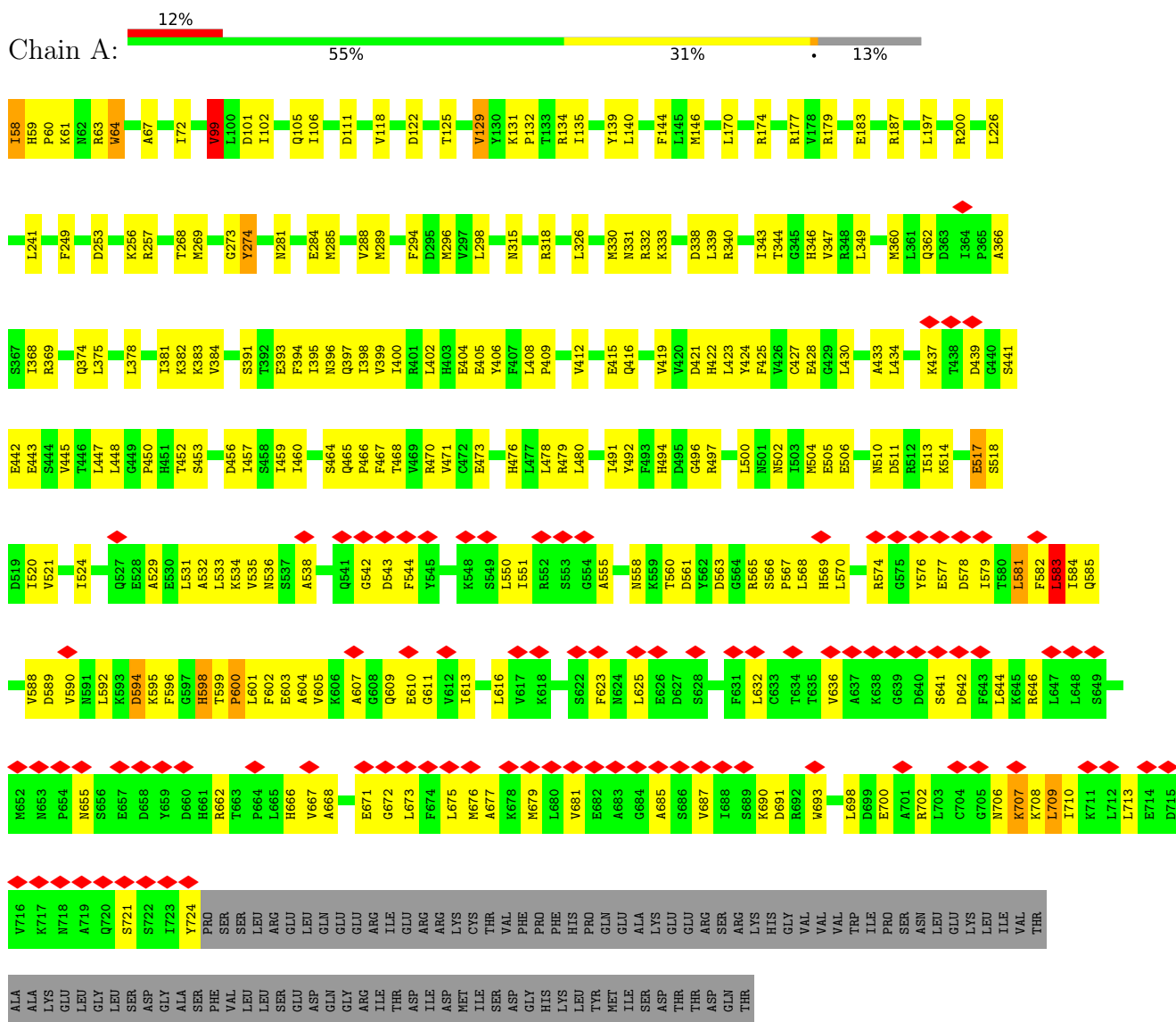
- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	K	0
			1	1	
2	C	1	Total	K	0
			1	1	

3 Residue-property plots

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

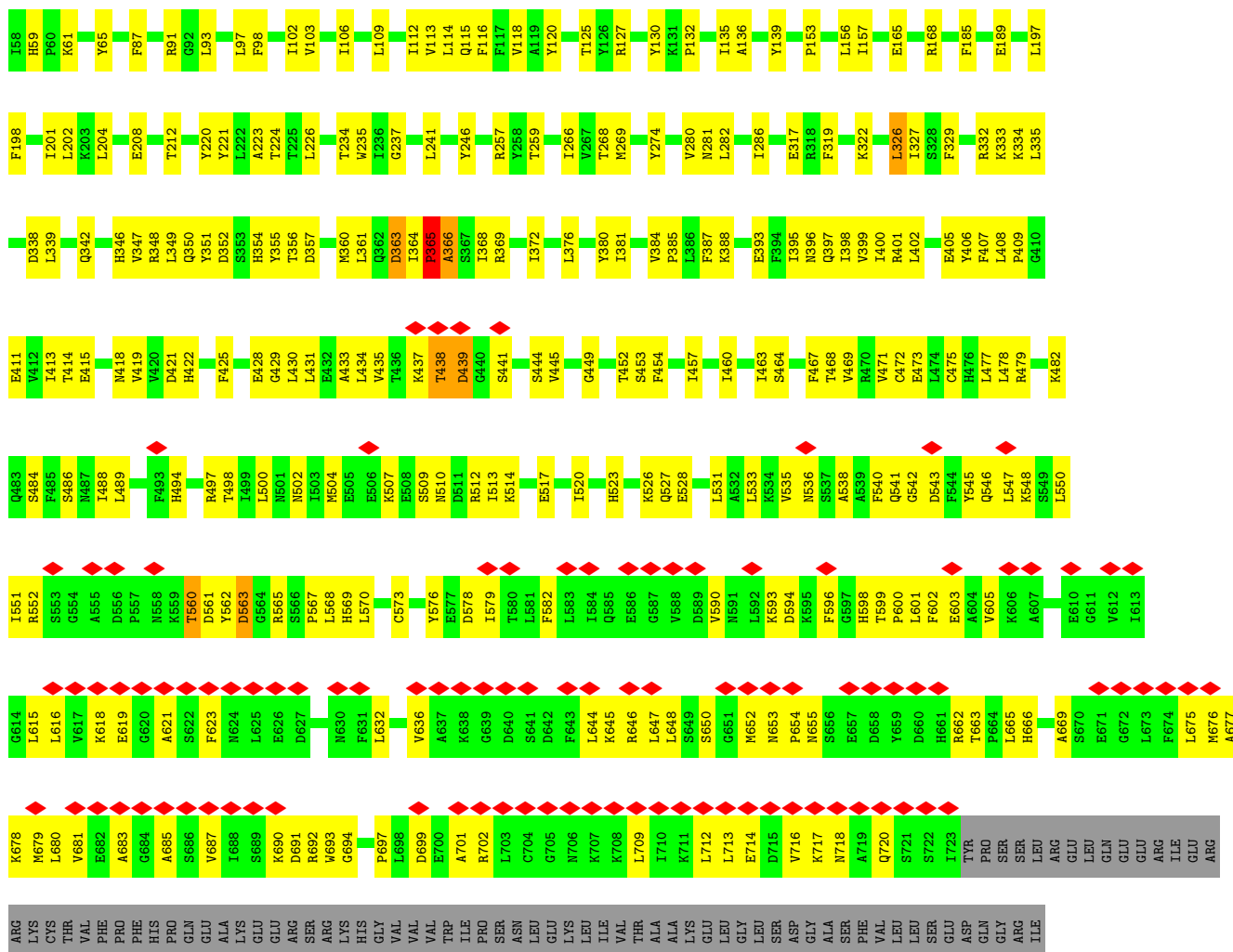
• Molecule 1: Potassium channel GORK



• Molecule 1: Potassium channel GORK



- Molecule 1: Potassium channel GORK



THR
ASP
ILE
ASP
MET
ILE
SER
ASP
GLY
HIS
LYS
LEU
TYR
MET
ILE
SER
ASP
THR
THR
ASP
GLN
THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	156313	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.859	Depositor
Minimum map value	-1.195	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.0966	Depositor
Map size (Å)	305.27997, 305.27997, 305.27997	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.23	0/5533	0.54	13/7484 (0.2%)
1	B	0.33	2/5520 (0.0%)	0.55	11/7466 (0.1%)
1	C	0.23	0/5533	0.50	4/7484 (0.1%)
1	D	0.22	0/5520	0.47	5/7466 (0.1%)
All	All	0.25	2/22106 (0.0%)	0.52	33/29900 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	355	TYR	C-O	6.42	1.32	1.24
1	B	386	LEU	CA-C	5.82	1.60	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	596	PHE	N-CA-C	8.42	122.97	112.87
1	B	340	ARG	N-CA-C	-7.92	101.60	111.11
1	A	709	LEU	N-CA-C	7.58	120.21	111.11
1	A	63	ARG	N-CA-C	7.54	120.22	111.02
1	A	64	TRP	N-CA-C	7.39	121.54	112.23
1	A	707	LYS	N-CA-C	-7.18	104.66	113.50
1	D	563	ASP	N-CA-C	7.09	119.87	111.71
1	B	387	PHE	N-CA-C	7.04	121.95	111.81
1	B	254	LEU	N-CA-C	6.67	120.28	111.75
1	A	581	LEU	N-CA-C	6.61	118.14	111.07
1	D	439	ASP	N-CA-C	6.40	122.14	107.48
1	A	583	LEU	N-CA-C	-6.35	103.62	112.45
1	A	274	TYR	N-CA-C	-6.31	104.33	111.14
1	C	274	TYR	N-CA-C	-6.23	104.41	111.14
1	B	646	ARG	N-CA-C	-6.21	104.43	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	583	LEU	N-CA-CB	6.20	119.85	110.30
1	B	386	LEU	N-CA-C	6.19	119.67	111.75
1	A	583	LEU	N-CA-CB	6.17	119.46	110.26
1	C	581	LEU	N-CA-C	6.10	117.60	111.07
1	C	583	LEU	N-CA-C	-6.10	104.55	112.23
1	D	365	PRO	CB-CA-C	-5.84	101.92	111.56
1	B	252	ILE	N-CA-C	-5.84	102.03	109.80
1	B	356	THR	N-CA-C	-5.75	104.39	111.75
1	B	386	LEU	CA-C-O	5.71	126.59	120.20
1	B	387	PHE	N-CA-CB	-5.67	101.74	110.25
1	D	438	THR	N-CA-C	-5.61	105.78	113.30
1	A	64	TRP	N-CA-CB	-5.60	101.68	110.30
1	A	99	VAL	N-CA-C	5.42	117.83	111.05
1	B	365	PRO	N-CA-CB	-5.35	97.63	103.25
1	A	594	ASP	N-CA-C	5.31	118.07	109.79
1	D	675	LEU	N-CA-C	5.23	116.67	111.07
1	B	644	LEU	N-CA-C	5.20	117.86	111.82
1	A	600	PRO	N-CA-C	-5.08	106.46	113.53

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	5408	0	5433	218	0
1	B	5396	0	5424	242	0
1	C	5408	0	5433	214	0
1	D	5396	0	5424	239	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
All	All	21610	0	21714	864	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 20.

All (864) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ARG:NH1	1:B:352:ASP:HB3	1.69	1.05
1:A:504:MET:HE2	1:A:520:ILE:HG23	1.39	1.02
1:B:348:ARG:HH12	1:B:352:ASP:HB3	0.86	1.02
1:B:349:LEU:HD12	1:B:408:LEU:HD21	1.45	0.98
1:B:348:ARG:HH12	1:B:352:ASP:CB	1.78	0.97
1:B:349:LEU:CD1	1:B:408:LEU:HD21	1.97	0.93
1:D:533:LEU:HD11	1:D:562:TYR:HB3	1.48	0.93
1:D:504:MET:HE1	1:D:507:LYS:HZ1	1.37	0.86
1:C:63:ARG:HG3	1:C:64:TRP:HD1	1.39	0.86
1:A:362:GLN:HA	1:A:369:ARG:HH22	1.38	0.85
1:B:354:HIS:HB3	1:B:406:TYR:CE2	2.11	0.84
1:C:672:GLY:HA2	1:C:709:LEU:HD11	1.57	0.84
1:A:672:GLY:HA2	1:A:709:LEU:HD11	1.60	0.84
1:D:115:GLN:HG2	1:D:139:TYR:CZ	2.14	0.83
1:A:568:LEU:HD22	1:A:600:PRO:HB3	1.62	0.81
1:B:644:LEU:HD22	1:B:676:MET:HE3	1.61	0.81
1:A:58:ILE:HG21	1:A:118:VAL:HG22	1.64	0.80
1:D:387:PHE:HE2	1:D:398:ILE:HG13	1.47	0.80
1:D:411:GLU:H	1:D:471:VAL:HG12	1.47	0.80
1:B:319:PHE:HE2	1:B:348:ARG:HA	1.45	0.80
1:A:434:LEU:HD21	1:A:442:GLU:HB2	1.62	0.79
1:D:623:PHE:CD1	1:D:652:MET:HE3	2.18	0.79
1:C:362:GLN:HA	1:C:369:ARG:HH22	1.48	0.79
1:A:707:LYS:HA	1:A:710:ILE:HD12	1.65	0.79
1:B:369:ARG:HA	1:B:372:ILE:HD12	1.65	0.78
1:D:662:ARG:HD2	1:D:691:ASP:HB2	1.66	0.77
1:C:707:LYS:HA	1:C:710:ILE:HD12	1.66	0.77
1:B:662:ARG:HD2	1:B:691:ASP:HB2	1.65	0.77
1:A:578:ASP:O	1:A:582:PHE:CD2	2.39	0.76
1:C:409:PRO:HG3	1:C:473:GLU:HA	1.67	0.76
1:B:438:THR:O	1:B:439:ASP:OD1	2.04	0.76
1:B:360:MET:O	1:B:361:LEU:C	2.29	0.75
1:A:600:PRO:HB2	1:A:616:LEU:HD11	1.69	0.74
1:D:497:ARG:HH12	1:D:500:LEU:HD22	1.51	0.74
1:A:428:GLU:HB2	1:A:476:HIS:HB3	1.68	0.74
1:A:409:PRO:HG3	1:A:473:GLU:HA	1.68	0.74
1:D:319:PHE:HE1	1:D:348:ARG:HA	1.49	0.74
1:A:595:LYS:NZ	1:D:573:CYS:SG	2.59	0.74
1:C:416:GLN:HA	1:C:465:GLN:HB2	1.68	0.74
1:D:648:LEU:HD21	1:D:654:PRO:HB3	1.69	0.74
1:A:494:HIS:HA	1:A:497:ARG:HE	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:VAL:HG21	1:C:467:PHE:CE1	2.23	0.74
1:C:428:GLU:HB2	1:C:476:HIS:HB3	1.68	0.74
1:A:551:ILE:HA	1:A:555:ALA:HB3	1.70	0.73
1:B:565:ARG:HH12	1:B:603:GLU:HG3	1.53	0.73
1:A:416:GLN:HA	1:A:465:GLN:HB2	1.69	0.73
1:D:498:THR:O	1:D:502:ASN:ND2	2.22	0.73
1:B:360:MET:HE2	1:C:325:ASP:HB3	1.71	0.73
1:C:674:PHE:HB3	1:C:708:LYS:HZ3	1.52	0.73
1:B:463:ILE:O	1:B:464:SER:HB3	1.88	0.72
1:C:421:ASP:OD1	1:C:422:HIS:ND1	2.21	0.72
1:C:489:LEU:HD22	1:C:496:GLY:HA3	1.72	0.71
1:A:607:ALA:HB3	1:A:609:GLN:HE22	1.55	0.71
1:B:405:GLU:OE2	1:B:479:ARG:NH1	2.23	0.71
1:C:578:ASP:O	1:C:582:PHE:CD2	2.43	0.71
1:D:413:ILE:HD11	1:D:471:VAL:HB	1.71	0.71
1:C:362:GLN:HA	1:C:369:ARG:NH2	2.05	0.71
1:D:369:ARG:HA	1:D:372:ILE:HD12	1.72	0.71
1:D:348:ARG:NH1	1:D:348:ARG:O	2.24	0.71
1:B:335:LEU:HB3	1:B:339:LEU:HD11	1.72	0.70
1:B:371:LYS:HA	1:B:374:GLN:HG2	1.71	0.70
1:D:439:ASP:OD1	1:D:439:ASP:O	2.10	0.70
1:B:497:ARG:HH12	1:B:500:LEU:HD22	1.55	0.70
1:C:445:VAL:HG11	1:C:467:PHE:HE1	1.55	0.70
1:D:517:GLU:HA	1:D:520:ILE:HD12	1.72	0.70
1:C:607:ALA:HB3	1:C:609:GLN:HE22	1.55	0.70
1:A:544:PHE:HD1	1:A:582:PHE:CZ	2.10	0.70
1:D:366:ALA:HA	1:D:369:ARG:NH1	2.07	0.70
1:A:655:ASN:HB3	1:A:685:ALA:HA	1.74	0.69
1:C:655:ASN:HB3	1:C:685:ALA:HA	1.75	0.69
1:B:654:PRO:HB2	1:B:680:LEU:HD23	1.73	0.69
1:B:530:GLU:HA	1:B:533:LEU:HD13	1.74	0.69
1:B:547:LEU:HD11	1:B:579:ILE:HG23	1.75	0.69
1:A:605:VAL:HA	1:A:646:ARG:HH11	1.57	0.69
1:A:601:LEU:HD22	1:A:616:LEU:HD22	1.75	0.69
1:B:690:LYS:HD3	1:B:694:GLY:HA2	1.75	0.69
1:D:429:GLY:HA3	1:D:475:CYS:HB3	1.74	0.69
1:B:498:THR:O	1:B:502:ASN:ND2	2.24	0.68
1:B:517:GLU:HA	1:B:520:ILE:HD12	1.75	0.68
1:D:113:VAL:HA	1:D:116:PHE:CD1	2.29	0.68
1:D:690:LYS:HD3	1:D:694:GLY:HA2	1.74	0.68
1:B:353:SER:O	1:B:354:HIS:C	2.34	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:THR:O	1:B:361:LEU:HB3	1.94	0.68
1:C:605:VAL:HA	1:C:646:ARG:HH11	1.58	0.68
1:D:349:LEU:HB2	1:D:408:LEU:HD11	1.76	0.67
1:A:421:ASP:OD1	1:A:422:HIS:ND1	2.24	0.67
1:B:363:ASP:O	1:B:364:ILE:C	2.36	0.67
1:B:397:GLN:HE22	1:C:419:VAL:H	1.42	0.67
1:B:339:LEU:HA	1:B:342:GLN:HG2	1.76	0.67
1:B:357:ASP:CG	1:C:329:PHE:HB2	2.20	0.67
1:C:146:MET:HE3	1:C:146:MET:HA	1.77	0.67
1:C:349:LEU:HD11	1:C:474:LEU:HD12	1.75	0.67
1:A:338:ASP:OD2	1:A:339:LEU:N	2.28	0.66
1:C:581:LEU:O	1:C:584:ILE:HG22	1.95	0.66
1:C:610:GLU:OE2	1:C:646:ARG:NH2	2.25	0.66
1:D:568:LEU:HD13	1:D:590:VAL:HA	1.76	0.66
1:C:338:ASP:OD2	1:C:339:LEU:N	2.28	0.66
1:C:445:VAL:HG11	1:C:467:PHE:CE1	2.29	0.66
1:B:529:ALA:O	1:B:533:LEU:HD12	1.95	0.66
1:C:398:ILE:HG13	1:C:480:LEU:HD22	1.78	0.66
1:A:504:MET:HE2	1:A:520:ILE:CG2	2.21	0.66
1:D:477:LEU:HD12	1:D:477:LEU:H	1.61	0.66
1:A:296:MET:HE1	1:B:269:MET:HE3	1.77	0.65
1:B:349:LEU:HG	1:B:408:LEU:HD11	1.78	0.65
1:A:641:SER:H	1:C:641:SER:HB2	1.62	0.65
1:B:396:ASN:HA	1:B:399:VAL:HG22	1.79	0.65
1:A:641:SER:HB2	1:C:641:SER:H	1.61	0.65
1:C:544:PHE:HD1	1:C:582:PHE:CZ	2.14	0.65
1:A:581:LEU:O	1:A:584:ILE:HG22	1.97	0.65
1:A:362:GLN:HA	1:A:369:ARG:NH2	2.11	0.65
1:C:513:ILE:HG22	1:C:514:LYS:HD2	1.78	0.65
1:A:285:MET:O	1:A:289:MET:HG3	1.97	0.65
1:B:437:LYS:HG3	1:B:438:THR:H	1.60	0.65
1:A:513:ILE:HG22	1:A:514:LYS:HD2	1.78	0.64
1:C:551:ILE:HA	1:C:555:ALA:HB3	1.78	0.64
1:D:605:VAL:HG22	1:D:646:ARG:HB3	1.79	0.64
1:D:593:LYS:NZ	1:D:594:ASP:O	2.30	0.64
1:D:644:LEU:HD22	1:D:676:MET:SD	2.38	0.64
1:B:430:LEU:H	1:B:473:GLU:HB2	1.63	0.64
1:A:599:THR:HG22	1:A:601:LEU:H	1.62	0.64
1:B:360:MET:SD	1:B:361:LEU:N	2.70	0.64
1:B:435:VAL:HG13	1:B:445:VAL:HG21	1.80	0.64
1:A:415:GLU:HA	1:A:468:THR:HG23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:LYS:H	1:B:441:SER:HA	1.63	0.63
1:B:636:VAL:HG22	1:B:676:MET:HE2	1.79	0.63
1:C:674:PHE:HB3	1:C:708:LYS:NZ	2.12	0.63
1:C:599:THR:HB	1:C:602:PHE:HB2	1.78	0.63
1:D:335:LEU:HB3	1:D:339:LEU:HD11	1.79	0.63
1:D:357:ASP:HA	1:D:360:MET:SD	2.39	0.63
1:D:560:THR:HA	1:D:567:PRO:HD3	1.81	0.63
1:A:601:LEU:HD13	1:A:616:LEU:HD13	1.81	0.63
1:A:398:ILE:HG13	1:A:480:LEU:HD22	1.81	0.63
1:C:558:ASN:HA	1:C:588:VAL:HG23	1.81	0.63
1:D:654:PRO:HB2	1:D:680:LEU:HD12	1.81	0.62
1:B:568:LEU:HD13	1:B:590:VAL:HA	1.80	0.62
1:A:610:GLU:OE2	1:A:646:ARG:NH2	2.25	0.62
1:C:496:GLY:HA2	1:C:499:ILE:HB	1.80	0.62
1:B:357:ASP:OD2	1:C:332:ARG:NH1	2.32	0.62
1:D:596:PHE:HB2	1:D:598:HIS:CE1	2.35	0.62
1:A:708:LYS:HE2	1:C:705:GLY:HA3	1.80	0.62
1:B:593:LYS:NZ	1:B:594:ASP:O	2.33	0.62
1:C:579:ILE:HA	1:C:582:PHE:CE2	2.35	0.62
1:B:687:VAL:HB	1:B:717:LYS:HD3	1.81	0.62
1:C:296:MET:HE1	1:D:269:MET:HE3	1.81	0.62
1:D:354:HIS:HB3	1:D:406:TYR:HE2	1.62	0.62
1:C:268:THR:HG1	1:D:274:TYR:HH	1.47	0.62
1:A:200:ARG:NH1	1:B:317:GLU:OE2	2.32	0.62
1:C:200:ARG:NH1	1:D:317:GLU:OE2	2.33	0.62
1:C:434:LEU:HD13	1:C:442:GLU:HB2	1.82	0.62
1:D:435:VAL:HG13	1:D:445:VAL:HG21	1.81	0.62
1:D:632:LEU:HD13	1:D:644:LEU:HD11	1.82	0.62
1:A:558:ASN:HA	1:A:588:VAL:HG23	1.81	0.62
1:B:354:HIS:HB3	1:B:406:TYR:HE2	1.62	0.61
1:D:565:ARG:HH12	1:D:603:GLU:HG3	1.65	0.61
1:A:567:PRO:HB2	1:A:583:LEU:HD21	1.82	0.61
1:C:369:ARG:HA	1:C:372:ILE:HD12	1.82	0.61
1:B:357:ASP:OD2	1:C:332:ARG:NH2	2.33	0.61
1:C:706:ASN:HB3	1:C:709:LEU:HD12	1.83	0.61
1:D:431:LEU:HB3	1:D:471:VAL:HG23	1.81	0.61
1:B:114:LEU:HA	1:B:117:PHE:CE2	2.36	0.61
1:D:115:GLN:CG	1:D:139:TYR:CZ	2.84	0.61
1:D:714:GLU:O	1:D:718:ASN:ND2	2.34	0.61
1:A:58:ILE:HG22	1:A:118:VAL:HA	1.83	0.60
1:C:352:ASP:O	1:C:352:ASP:OD1	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:LEU:HD22	1:C:600:PRO:HB3	1.81	0.60
1:B:601:LEU:HG	1:B:616:LEU:HD13	1.84	0.60
1:C:581:LEU:O	1:C:585:GLN:HG2	2.01	0.60
1:A:326:LEU:O	1:A:330:MET:HG3	2.01	0.60
1:A:706:ASN:HB3	1:A:709:LEU:HD12	1.83	0.60
1:D:435:VAL:HG12	1:D:467:PHE:HA	1.84	0.60
1:C:102:ILE:O	1:C:106:ILE:HG23	2.02	0.60
1:B:636:VAL:HG21	1:B:664:PRO:HB3	1.83	0.60
1:D:687:VAL:HB	1:D:717:LYS:HD3	1.82	0.60
1:B:435:VAL:HG12	1:B:467:PHE:HA	1.84	0.60
1:D:430:LEU:H	1:D:473:GLU:HB2	1.67	0.60
1:A:102:ILE:O	1:A:106:ILE:HG23	2.02	0.60
1:B:382:LYS:HG2	1:B:395:ILE:HG21	1.83	0.60
1:D:415:GLU:HB3	1:D:468:THR:HG23	1.83	0.60
1:A:560:THR:HB	1:A:566:SER:HA	1.84	0.59
1:D:594:ASP:HB2	1:D:598:HIS:H	1.65	0.59
1:B:533:LEU:HG	1:B:562:TYR:HD2	1.67	0.59
1:C:448:LEU:H	1:C:448:LEU:HD23	1.66	0.59
1:B:87:PHE:O	1:B:168:ARG:NH2	2.32	0.59
1:B:714:GLU:O	1:B:718:ASN:ND2	2.36	0.59
1:A:346:HIS:CE1	1:D:365:PRO:HG3	2.38	0.59
1:D:93:LEU:HD22	1:D:97:LEU:HD12	1.84	0.59
1:B:394:PHE:O	1:B:398:ILE:HG12	2.03	0.59
1:C:98:PHE:HE1	1:C:156:LEU:HD11	1.68	0.59
1:B:153:PRO:O	1:B:157:ILE:HG12	2.02	0.58
1:B:411:GLU:H	1:B:471:VAL:HG12	1.67	0.58
1:C:63:ARG:HG3	1:C:64:TRP:CD1	2.30	0.58
1:C:427:CYS:SG	1:C:476:HIS:O	2.53	0.58
1:D:381:ILE:HG21	1:D:399:VAL:HG12	1.83	0.58
1:B:605:VAL:HG22	1:B:646:ARG:HB3	1.85	0.58
1:D:599:THR:HG21	1:D:623:PHE:HA	1.84	0.58
1:D:541:GLN:O	1:D:541:GLN:NE2	2.37	0.58
1:D:366:ALA:HA	1:D:369:ARG:HH12	1.67	0.58
1:A:579:ILE:HA	1:A:582:PHE:CE2	2.39	0.58
1:C:434:LEU:HD22	1:C:442:GLU:HG3	1.85	0.58
1:D:223:ALA:HB2	1:D:235:TRP:NE1	2.19	0.58
1:B:223:ALA:HB2	1:B:235:TRP:NE1	2.19	0.58
1:A:59:HIS:O	1:A:61:LYS:N	2.37	0.57
1:B:636:VAL:HG11	1:B:667:VAL:HG13	1.85	0.57
1:D:433:ALA:HA	1:D:469:VAL:HG22	1.86	0.57
1:B:424:TYR:CE1	1:B:479:ARG:HD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:ALA:O	1:C:374:GLN:HG2	2.04	0.57
1:D:87:PHE:O	1:D:168:ARG:NH2	2.32	0.57
1:A:430:LEU:HD11	1:A:447:LEU:HB3	1.86	0.57
1:B:599:THR:HG23	1:B:602:PHE:H	1.68	0.57
1:B:663:THR:HB	1:B:666:HIS:CD2	2.39	0.57
1:C:326:LEU:O	1:C:330:MET:HG3	2.04	0.57
1:B:364:ILE:O	1:B:365:PRO:C	2.46	0.57
1:B:692:ARG:NH1	1:C:659:TYR:OH	2.37	0.57
1:A:146:MET:HA	1:A:146:MET:HE3	1.85	0.57
1:A:349:LEU:HD22	1:A:408:LEU:HG	1.86	0.57
1:B:114:LEU:HG	1:B:117:PHE:CZ	2.40	0.57
1:B:590:VAL:HG22	1:B:621:ALA:HB2	1.86	0.57
1:D:560:THR:HB	1:D:565:ARG:C	2.30	0.57
1:B:543:ASP:HB3	1:B:546:GLN:HB2	1.86	0.57
1:B:645:LYS:N	1:B:679:MET:HE1	2.19	0.57
1:C:268:THR:OG1	1:D:274:TYR:OH	2.20	0.57
1:D:644:LEU:HD12	1:D:647:LEU:HD12	1.86	0.57
1:B:431:LEU:HB3	1:B:471:VAL:HG23	1.86	0.57
1:D:599:THR:HG23	1:D:602:PHE:H	1.69	0.57
1:D:701:ALA:HB2	1:D:713:LEU:HD12	1.87	0.57
1:B:59:HIS:CG	1:B:130:TYR:HH	2.23	0.56
1:D:453:SER:OG	1:D:512:ARG:NH1	2.37	0.56
1:A:578:ASP:O	1:A:582:PHE:CE2	2.58	0.56
1:C:576:TYR:HB3	1:C:579:ILE:HB	1.87	0.56
1:C:600:PRO:HB2	1:C:616:LEU:HD11	1.87	0.56
1:D:547:LEU:HD11	1:D:579:ILE:HG23	1.86	0.56
1:D:347:VAL:HA	1:D:350:GLN:OE1	2.06	0.56
1:D:125:THR:HG23	1:D:127:ARG:H	1.71	0.56
1:B:339:LEU:HA	1:B:342:GLN:CG	2.36	0.56
1:B:663:THR:HB	1:B:666:HIS:HD2	1.71	0.56
1:C:702:ARG:HB3	1:C:710:ILE:HD11	1.88	0.56
1:B:103:VAL:HA	1:B:106:ILE:HG12	1.86	0.56
1:B:415:GLU:HB3	1:B:468:THR:HG23	1.86	0.56
1:B:653:ASN:ND2	1:B:655:ASN:OD1	2.35	0.56
1:A:673:LEU:HD11	1:A:676:MET:HB3	1.87	0.56
1:D:408:LEU:O	1:D:411:GLU:HG2	2.06	0.56
1:A:466:PRO:HB2	1:A:467:PHE:CD1	2.40	0.56
1:C:445:VAL:HG21	1:C:467:PHE:CD1	2.40	0.56
1:D:113:VAL:O	1:D:114:LEU:C	2.47	0.56
1:D:504:MET:HE1	1:D:507:LYS:NZ	2.16	0.56
1:A:346:HIS:NE2	1:D:365:PRO:HD3	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:GLN:HA	1:C:378:LEU:HD13	1.88	0.55
1:C:426:VAL:HG21	1:C:431:LEU:HD21	1.86	0.55
1:A:427:CYS:SG	1:A:476:HIS:O	2.51	0.55
1:B:548:LYS:HA	1:B:551:ILE:HG22	1.88	0.55
1:A:511:ASP:OD1	1:A:511:ASP:N	2.39	0.55
1:B:369:ARG:O	1:B:372:ILE:N	2.39	0.55
1:B:433:ALA:HA	1:B:469:VAL:HG22	1.88	0.55
1:A:434:LEU:O	1:A:468:THR:N	2.39	0.55
1:B:357:ASP:CG	1:C:332:ARG:HH22	2.14	0.55
1:B:507:LYS:HG3	1:B:514:LYS:HA	1.89	0.55
1:D:419:VAL:HA	1:D:464:SER:HA	1.87	0.55
1:C:560:THR:HB	1:C:566:SER:HA	1.88	0.55
1:B:422:HIS:CE1	1:B:479:ARG:HH21	2.25	0.55
1:D:319:PHE:CE1	1:D:348:ARG:HA	2.38	0.55
1:D:654:PRO:HB2	1:D:680:LEU:CD1	2.36	0.55
1:A:241:LEU:HB3	1:D:280:VAL:HG23	1.89	0.55
1:B:220:TYR:OH	1:B:257:ARG:NH1	2.39	0.55
1:B:343:ILE:O	1:B:347:VAL:HG13	2.07	0.55
1:D:59:HIS:CD2	1:D:61:LYS:HE3	2.41	0.55
1:A:544:PHE:CD1	1:A:582:PHE:CZ	2.94	0.54
1:B:685:ALA:O	1:B:720:GLN:NE2	2.40	0.54
1:C:501:ASN:O	1:C:504:MET:HG3	2.07	0.54
1:A:268:THR:OG1	1:B:274:TYR:OH	2.21	0.54
1:D:59:HIS:HD2	1:D:61:LYS:HG2	1.72	0.54
1:D:399:VAL:HA	1:D:402:LEU:HD12	1.90	0.54
1:D:605:VAL:O	1:D:646:ARG:NH1	2.40	0.54
1:D:590:VAL:HG22	1:D:621:ALA:HB2	1.89	0.54
1:C:601:LEU:O	1:C:605:VAL:HG13	2.07	0.54
1:A:393:GLU:O	1:A:397:GLN:NE2	2.41	0.54
1:A:601:LEU:O	1:A:605:VAL:HG13	2.07	0.54
1:A:500:LEU:HD23	1:A:500:LEU:H	1.73	0.54
1:C:179:ARG:O	1:C:183:GLU:HG3	2.08	0.54
1:C:494:HIS:O	1:C:497:ARG:HB3	2.07	0.54
1:C:391:SER:OG	1:C:393:GLU:OE1	2.25	0.54
1:D:548:LYS:HA	1:D:551:ILE:HG22	1.90	0.54
1:D:590:VAL:HG21	1:D:619:GLU:HG2	1.90	0.54
1:A:58:ILE:CG2	1:A:118:VAL:HG22	2.36	0.54
1:A:466:PRO:HB2	1:A:467:PHE:CE1	2.43	0.54
1:C:63:ARG:HG3	1:C:64:TRP:N	2.23	0.54
1:C:381:ILE:HG21	1:C:395:ILE:HG23	1.89	0.54
1:D:437:LYS:H	1:D:441:SER:HA	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:HIS:CD2	1:B:61:LYS:HE3	2.43	0.54
1:B:65:TYR:CZ	1:B:118:VAL:HG21	2.42	0.54
1:B:99:VAL:O	1:B:103:VAL:HG13	2.08	0.54
1:B:599:THR:HG21	1:B:623:PHE:HA	1.90	0.54
1:D:663:THR:HB	1:D:666:HIS:HD2	1.73	0.54
1:D:384:VAL:HG22	1:D:385:PRO:HD2	1.88	0.54
1:B:359:VAL:O	1:B:362:GLN:HB2	2.08	0.53
1:D:387:PHE:CE2	1:D:398:ILE:HG13	2.36	0.53
1:D:687:VAL:HA	1:D:697:PRO:HG2	1.89	0.53
1:B:647:LEU:O	1:B:650:SER:OG	2.23	0.53
1:B:701:ALA:HB2	1:B:713:LEU:HD12	1.91	0.53
1:B:369:ARG:O	1:B:370:ALA:C	2.51	0.53
1:B:415:GLU:HA	1:B:468:THR:HA	1.90	0.53
1:D:407:PHE:HE2	1:D:477:LEU:HD22	1.73	0.53
1:A:256:LYS:HE3	1:D:282:LEU:HD13	1.91	0.53
1:D:346:HIS:ND1	1:D:408:LEU:HD13	2.23	0.53
1:D:364:ILE:O	1:D:365:PRO:C	2.52	0.53
1:D:601:LEU:HG	1:D:616:LEU:HD13	1.90	0.53
1:A:268:THR:HG1	1:B:274:TYR:HH	1.56	0.53
1:A:448:LEU:HD23	1:A:452:THR:HG21	1.90	0.53
1:A:567:PRO:HB2	1:A:583:LEU:CD2	2.38	0.53
1:B:662:ARG:HH12	1:B:666:HIS:HB2	1.73	0.53
1:B:687:VAL:HA	1:B:697:PRO:HG2	1.91	0.53
1:C:442:GLU:O	1:C:443:GLU:HG3	2.08	0.53
1:D:103:VAL:HA	1:D:106:ILE:HG12	1.90	0.53
1:D:669:ALA:HA	1:D:709:LEU:HD21	1.91	0.53
1:A:644:LEU:HD13	1:A:676:MET:HG3	1.89	0.53
1:C:456:ASP:O	1:C:460:ILE:HG13	2.08	0.53
1:C:698:LEU:O	1:C:702:ARG:HG2	2.09	0.53
1:A:179:ARG:O	1:A:183:GLU:HG3	2.08	0.53
1:B:504:MET:CE	1:B:507:LYS:HD2	2.38	0.53
1:C:502:ASN:O	1:C:505:GLU:HG2	2.09	0.53
1:D:380:TYR:OH	1:D:428:GLU:OE2	2.27	0.53
1:B:109:LEU:O	1:B:112:ILE:HG22	2.10	0.52
1:C:393:GLU:O	1:C:397:GLN:NE2	2.41	0.52
1:D:413:ILE:HD13	1:D:469:VAL:HG12	1.91	0.52
1:A:456:ASP:O	1:A:460:ILE:HG13	2.09	0.52
1:A:698:LEU:O	1:A:702:ARG:HG2	2.09	0.52
1:C:510:ASN:HB2	1:C:513:ILE:HG12	1.91	0.52
1:D:132:PRO:HA	1:D:135:ILE:HG12	1.90	0.52
1:A:673:LEU:HB3	1:C:673:LEU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:ARG:HB3	1:A:710:ILE:HD11	1.90	0.52
1:A:636:VAL:HG12	1:A:671:GLU:HG3	1.92	0.52
1:B:456:ASP:O	1:B:460:ILE:HG12	2.10	0.52
1:D:364:ILE:HG23	1:D:365:PRO:HD2	1.91	0.52
1:B:263:TYR:O	1:B:267:VAL:HG22	2.08	0.52
1:B:366:ALA:O	1:B:367:SER:C	2.52	0.52
1:C:315:ASN:HA	1:C:318:ARG:HE	1.75	0.52
1:A:416:GLN:O	1:A:464:SER:OG	2.26	0.52
1:A:576:TYR:HB3	1:A:579:ILE:HB	1.92	0.52
1:C:349:LEU:HD12	1:C:408:LEU:HG	1.92	0.52
1:C:534:LYS:HG3	1:C:550:LEU:HD11	1.90	0.52
1:C:641:SER:HA	1:C:644:LEU:HD12	1.92	0.52
1:D:685:ALA:O	1:D:720:GLN:NE2	2.43	0.52
1:A:330:MET:HE1	1:A:340:ARG:HA	1.92	0.52
1:C:285:MET:O	1:C:289:MET:HG3	2.10	0.52
1:D:507:LYS:HB2	1:D:513:ILE:HB	1.91	0.52
1:A:315:ASN:HA	1:A:318:ARG:HE	1.76	0.51
1:A:394:PHE:O	1:A:398:ILE:HG22	2.10	0.51
1:A:590:VAL:O	1:A:600:PRO:HG2	2.10	0.51
1:B:365:PRO:HG2	1:C:346:HIS:CE1	2.45	0.51
1:D:112:ILE:HG23	1:D:116:PHE:CE1	2.45	0.51
1:D:338:ASP:O	1:D:342:GLN:HG2	2.11	0.51
1:B:125:THR:HG23	1:B:127:ARG:H	1.74	0.51
1:B:362:GLN:O	1:B:363:ASP:C	2.52	0.51
1:B:132:PRO:HA	1:B:135:ILE:HG12	1.93	0.51
1:C:538:ALA:O	1:C:542:GLY:N	2.44	0.51
1:D:454:PHE:CE1	1:D:469:VAL:HG21	2.45	0.51
1:D:504:MET:SD	1:D:507:LYS:HD2	2.51	0.51
1:D:220:TYR:OH	1:D:257:ARG:NH1	2.41	0.51
1:D:437:LYS:HG3	1:D:438:THR:H	1.74	0.51
1:B:223:ALA:HB2	1:B:235:TRP:CD1	2.45	0.51
1:C:365:PRO:HG3	1:C:369:ARG:HH21	1.75	0.51
1:D:645:LYS:HB3	1:D:679:MET:HE1	1.91	0.51
1:A:368:ILE:HD12	1:A:368:ILE:H	1.75	0.51
1:B:59:HIS:HD2	1:B:61:LYS:HG2	1.76	0.51
1:B:669:ALA:HA	1:B:709:LEU:HD21	1.93	0.51
1:C:131:LYS:HE3	1:C:134:ARG:HG3	1.93	0.51
1:A:502:ASN:O	1:A:506:GLU:HG2	2.10	0.51
1:C:415:GLU:HA	1:C:468:THR:HG23	1.91	0.51
1:C:416:GLN:O	1:C:464:SER:OG	2.27	0.51
1:D:663:THR:HB	1:D:666:HIS:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:VAL:HG23	1:C:241:LEU:HB3	1.91	0.51
1:C:511:ASP:N	1:C:511:ASP:OD1	2.40	0.51
1:A:131:LYS:HE3	1:A:134:ARG:HG3	1.92	0.51
1:A:445:VAL:HG21	1:A:467:PHE:CD2	2.46	0.51
1:B:91:ARG:HH12	1:B:221:TYR:HE1	1.59	0.51
1:B:349:LEU:HD23	1:B:349:LEU:N	2.24	0.51
1:B:449:GLY:O	1:B:452:THR:OG1	2.25	0.51
1:B:349:LEU:CG	1:B:408:LEU:HD21	2.39	0.51
1:C:381:ILE:HG13	1:C:399:VAL:HG22	1.93	0.51
1:C:698:LEU:HD12	1:C:713:LEU:HD23	1.92	0.51
1:C:529:ALA:O	1:C:533:LEU:HG	2.10	0.50
1:A:456:ASP:O	1:A:459:ILE:HG22	2.12	0.50
1:A:579:ILE:HA	1:A:582:PHE:CZ	2.46	0.50
1:D:548:LYS:HG3	1:D:552:ARG:HH21	1.77	0.50
1:B:527:GLN:NE2	1:B:528:GLU:OE1	2.44	0.50
1:D:109:LEU:O	1:D:112:ILE:HG22	2.11	0.50
1:D:185:PHE:O	1:D:189:GLU:HG2	2.12	0.50
1:D:356:THR:HG23	1:D:360:MET:HE1	1.92	0.50
1:A:504:MET:HE1	1:A:524:ILE:HD12	1.92	0.50
1:B:115:GLN:HG2	1:B:139:TYR:CZ	2.46	0.50
1:B:344:THR:O	1:B:347:VAL:HG22	2.11	0.50
1:C:331:ASN:OD1	1:C:332:ARG:N	2.44	0.50
1:C:406:TYR:HE1	1:C:476:HIS:CD2	2.29	0.50
1:A:437:LYS:HG2	1:A:439:ASP:H	1.76	0.50
1:A:668:ALA:HB1	1:A:677:ALA:HA	1.93	0.50
1:B:349:LEU:HD12	1:B:408:LEU:CD2	2.29	0.50
1:B:590:VAL:HG21	1:B:619:GLU:HG2	1.93	0.50
1:C:601:LEU:HB3	1:C:623:PHE:HB2	1.91	0.50
1:D:562:TYR:CE1	1:D:563:ASP:OD1	2.64	0.50
1:A:391:SER:OG	1:A:393:GLU:OE1	2.30	0.50
1:A:544:PHE:HD1	1:A:582:PHE:CE1	2.28	0.50
1:A:406:TYR:HE1	1:A:476:HIS:CD2	2.30	0.50
1:A:442:GLU:O	1:A:443:GLU:HG3	2.11	0.50
1:B:114:LEU:HG	1:B:117:PHE:HZ	1.77	0.50
1:D:223:ALA:HB2	1:D:235:TRP:CD1	2.46	0.50
1:A:599:THR:HG22	1:A:600:PRO:N	2.27	0.50
1:A:601:LEU:HD23	1:A:623:PHE:H	1.76	0.50
1:B:507:LYS:HB2	1:B:513:ILE:HB	1.93	0.50
1:C:437:LYS:HG2	1:C:439:ASP:H	1.75	0.50
1:C:456:ASP:O	1:C:459:ILE:HG22	2.11	0.50
1:D:369:ARG:HH11	1:D:369:ARG:HB2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:ARG:CZ	1:B:497:ARG:HA	2.42	0.50
1:C:404:GLU:OE1	1:C:476:HIS:NE2	2.43	0.50
1:A:599:THR:HB	1:A:602:PHE:HB2	1.92	0.49
1:A:641:SER:HA	1:A:644:LEU:HD12	1.93	0.49
1:B:185:PHE:O	1:B:189:GLU:HG2	2.11	0.49
1:A:510:ASN:HB2	1:A:513:ILE:HG12	1.95	0.49
1:A:567:PRO:HB3	1:A:583:LEU:HD11	1.93	0.49
1:A:581:LEU:O	1:A:585:GLN:HG2	2.12	0.49
1:C:579:ILE:HA	1:C:582:PHE:CZ	2.46	0.49
1:A:381:ILE:HG21	1:A:395:ILE:HG23	1.93	0.49
1:C:174:ARG:HD2	1:C:177:ARG:HH12	1.78	0.49
1:A:568:LEU:HD22	1:A:600:PRO:CB	2.38	0.49
1:B:393:GLU:HA	1:B:396:ASN:ND2	2.27	0.49
1:C:454:PHE:CD2	1:C:469:VAL:HG21	2.47	0.49
1:D:98:PHE:HZ	1:D:156:LEU:HD21	1.78	0.49
1:A:457:ILE:HG21	1:A:514:LYS:HG2	1.95	0.49
1:D:497:ARG:CZ	1:D:497:ARG:HA	2.43	0.49
1:A:599:THR:HB	1:A:602:PHE:H	1.77	0.49
1:A:698:LEU:HD12	1:A:713:LEU:HD23	1.94	0.49
1:B:665:LEU:HD22	1:B:685:ALA:HB1	1.94	0.49
1:D:120:TYR:CE1	1:D:135:ILE:HG22	2.48	0.49
1:D:507:LYS:HG3	1:D:514:LYS:HA	1.94	0.49
1:B:361:LEU:O	1:B:362:GLN:C	2.55	0.49
1:C:423:LEU:HD23	1:C:423:LEU:H	1.78	0.49
1:D:538:ALA:O	1:D:542:GLY:N	2.46	0.49
1:B:357:ASP:OD2	1:C:329:PHE:HB2	2.13	0.49
1:A:226:LEU:HD12	1:A:281:ASN:HD21	1.78	0.48
1:B:484:SER:O	1:B:488:ILE:HG13	2.13	0.48
1:C:226:LEU:HD12	1:C:281:ASN:HD21	1.77	0.48
1:D:91:ARG:HH12	1:D:221:TYR:HE1	1.59	0.48
1:A:381:ILE:HG13	1:A:399:VAL:HG22	1.95	0.48
1:A:419:VAL:HG12	1:D:397:GLN:NE2	2.28	0.48
1:B:330:MET:HB3	1:B:340:ARG:NH1	2.28	0.48
1:B:483:GLN:O	1:B:483:GLN:NE2	2.44	0.48
1:C:578:ASP:O	1:C:582:PHE:CE2	2.66	0.48
1:A:583:LEU:O	1:A:583:LEU:HD23	2.13	0.48
1:B:93:LEU:HD22	1:B:97:LEU:HD12	1.95	0.48
1:B:397:GLN:HE22	1:C:419:VAL:N	2.10	0.48
1:B:576:TYR:HB3	1:B:579:ILE:HG12	1.95	0.48
1:C:633:CYS:HB2	1:C:667:VAL:HG21	1.96	0.48
1:D:153:PRO:O	1:D:157:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ARG:HD2	1:A:177:ARG:HH12	1.77	0.48
1:A:332:ARG:HB3	1:A:333:LYS:HE2	1.93	0.48
1:A:502:ASN:HA	1:A:505:GLU:HG2	1.96	0.48
1:B:594:ASP:HB2	1:B:598:HIS:H	1.79	0.48
1:C:365:PRO:O	1:D:346:HIS:NE2	2.46	0.48
1:D:91:ARG:NH2	1:D:165:GLU:OE2	2.47	0.48
1:D:354:HIS:HB3	1:D:406:TYR:CE2	2.46	0.48
1:C:330:MET:HE1	1:C:340:ARG:HA	1.96	0.48
1:C:544:PHE:CD1	1:C:582:PHE:CZ	3.00	0.48
1:C:601:LEU:HD22	1:C:616:LEU:HD22	1.96	0.48
1:D:543:ASP:OD2	1:D:546:GLN:NE2	2.47	0.48
1:D:665:LEU:HD22	1:D:685:ALA:HB1	1.96	0.48
1:A:434:LEU:CD2	1:A:442:GLU:HB2	2.40	0.48
1:B:607:ALA:HB1	1:B:609:GLN:HE21	1.79	0.48
1:C:387:PHE:HE1	1:C:394:PHE:CE2	2.32	0.48
1:C:498:THR:HA	1:C:501:ASN:ND2	2.28	0.48
1:A:315:ASN:OD1	1:A:318:ARG:NH2	2.46	0.48
1:D:415:GLU:HA	1:D:468:THR:HA	1.96	0.48
1:D:665:LEU:HG	1:D:697:PRO:HB3	1.96	0.48
1:B:572:ALA:O	1:B:609:GLN:HG3	2.14	0.48
1:C:413:ILE:HD11	1:C:471:VAL:HG12	1.95	0.48
1:C:534:LYS:HD2	1:C:534:LYS:O	2.13	0.48
1:D:402:LEU:HD22	1:D:478:LEU:HB3	1.95	0.48
1:D:413:ILE:HG22	1:D:414:THR:HG23	1.94	0.48
1:A:399:VAL:HA	1:A:402:LEU:HD12	1.96	0.47
1:B:531:LEU:O	1:B:535:VAL:HG13	2.14	0.47
1:B:648:LEU:HD21	1:B:654:PRO:HB3	1.95	0.47
1:C:434:LEU:O	1:C:468:THR:N	2.47	0.47
1:A:362:GLN:CA	1:A:369:ARG:HH22	2.17	0.47
1:C:315:ASN:OD1	1:C:318:ARG:NH2	2.47	0.47
1:C:604:ALA:HA	1:C:609:GLN:NE2	2.28	0.47
1:A:594:ASP:OD1	1:A:598:HIS:N	2.45	0.47
1:D:414:THR:HB	1:D:418:ASN:HD21	1.79	0.47
1:A:374:GLN:HA	1:A:378:LEU:HD13	1.96	0.47
1:A:422:HIS:HB3	1:A:479:ARG:HG3	1.97	0.47
1:B:504:MET:HE1	1:B:507:LYS:HD2	1.96	0.47
1:C:582:PHE:O	1:C:586:GLU:HG2	2.14	0.47
1:D:405:GLU:OE2	1:D:479:ARG:NE	2.37	0.47
1:A:437:LYS:NZ	1:A:441:SER:HB2	2.30	0.47
1:B:336:GLY:O	1:B:340:ARG:HG3	2.14	0.47
1:B:477:LEU:HD12	1:B:477:LEU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:687:VAL:HG13	1:D:697:PRO:HB2	1.95	0.47
1:A:404:GLU:OE1	1:A:476:HIS:NE2	2.44	0.47
1:B:357:ASP:OD2	1:C:332:ARG:CZ	2.63	0.47
1:B:456:ASP:OD1	1:B:456:ASP:N	2.44	0.47
1:B:712:LEU:O	1:B:716:VAL:HG23	2.15	0.47
1:C:397:GLN:O	1:C:400:ILE:HG12	2.15	0.47
1:A:673:LEU:HD23	1:A:673:LEU:H	1.78	0.47
1:B:453:SER:OG	1:B:512:ARG:NH1	2.45	0.47
1:C:497:ARG:O	1:C:500:LEU:HG	2.15	0.47
1:D:457:ILE:HA	1:D:460:ILE:HB	1.97	0.47
1:D:569:HIS:CD2	1:D:600:PRO:HD3	2.50	0.47
1:C:721:SER:HA	1:C:724:TYR:HB2	1.97	0.47
1:D:562:TYR:CE1	1:D:563:ASP:CG	2.93	0.47
1:A:59:HIS:C	1:A:61:LYS:H	2.23	0.46
1:A:604:ALA:HA	1:A:609:GLN:NE2	2.30	0.46
1:A:642:ASP:HB2	1:C:642:ASP:HB2	1.97	0.46
1:B:339:LEU:O	1:B:340:ARG:C	2.57	0.46
1:A:64:TRP:CD1	1:A:64:TRP:N	2.80	0.46
1:D:98:PHE:CZ	1:D:156:LEU:HD21	2.50	0.46
1:D:531:LEU:O	1:D:535:VAL:HG13	2.15	0.46
1:C:601:LEU:HD23	1:C:623:PHE:H	1.80	0.46
1:D:120:TYR:HE1	1:D:135:ILE:HG22	1.80	0.46
1:D:527:GLN:NE2	1:D:528:GLU:OE1	2.48	0.46
1:D:678:LYS:HB3	1:D:678:LYS:HE2	1.75	0.46
1:A:565:ARG:HH21	1:A:569:HIS:HB3	1.81	0.46
1:D:212:THR:HG21	1:D:266:ILE:HG13	1.96	0.46
1:C:609:GLN:O	1:C:613:ILE:HG12	2.16	0.46
1:D:65:TYR:CE1	1:D:118:VAL:HG21	2.50	0.46
1:D:565:ARG:HH22	1:D:603:GLU:CD	2.24	0.46
1:B:632:LEU:HA	1:B:632:LEU:HD12	1.73	0.46
1:D:65:TYR:CZ	1:D:118:VAL:HG21	2.51	0.46
1:B:547:LEU:O	1:B:550:LEU:HG	2.16	0.46
1:C:507:LYS:HG3	1:C:515:LYS:HE3	1.97	0.46
1:D:547:LEU:O	1:D:550:LEU:HG	2.15	0.46
1:D:653:ASN:ND2	1:D:655:ASN:OD1	2.43	0.46
1:B:632:LEU:O	1:B:636:VAL:HG23	2.16	0.46
1:D:560:THR:HB	1:D:565:ARG:O	2.16	0.46
1:D:636:VAL:HA	1:D:676:MET:HE3	1.98	0.46
1:D:662:ARG:HD3	1:D:692:ARG:HG2	1.97	0.46
1:A:129:VAL:HG23	1:A:131:LYS:H	1.81	0.46
1:A:366:ALA:HB3	1:B:346:HIS:NE2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:LYS:HE2	1:B:190:LYS:HB2	1.60	0.46
1:D:654:PRO:HG3	1:D:683:ALA:HB3	1.98	0.46
1:A:423:LEU:HD23	1:A:423:LEU:H	1.81	0.45
1:B:399:VAL:HA	1:B:402:LEU:HD12	1.99	0.45
1:D:714:GLU:HG3	1:D:718:ASN:HD21	1.80	0.45
1:B:91:ARG:NH2	1:B:165:GLU:OE2	2.49	0.45
1:B:98:PHE:HZ	1:B:156:LEU:HD21	1.80	0.45
1:B:226:LEU:HD11	1:B:281:ASN:ND2	2.32	0.45
1:C:489:LEU:O	1:C:493:PHE:HA	2.16	0.45
1:D:221:TYR:HA	1:D:224:THR:HG22	1.98	0.45
1:D:365:PRO:HB2	1:D:366:ALA:H	1.48	0.45
1:A:122:ASP:OD2	1:A:125:THR:OG1	2.27	0.45
1:A:174:ARG:HD2	1:A:177:ARG:NH1	2.31	0.45
1:A:666:HIS:CE1	1:D:693:TRP:HH2	2.35	0.45
1:B:643:PHE:O	1:B:647:LEU:HG	2.16	0.45
1:A:170:LEU:HD23	1:A:170:LEU:O	2.16	0.45
1:A:681:VAL:HG11	1:A:687:VAL:HG13	1.97	0.45
1:B:98:PHE:CZ	1:B:156:LEU:HD21	2.50	0.45
1:B:430:LEU:HB3	1:B:473:GLU:HG3	1.98	0.45
1:C:132:PRO:O	1:C:135:ILE:HG12	2.17	0.45
1:D:135:ILE:HG13	1:D:136:ALA:N	2.31	0.45
1:A:529:ALA:O	1:A:533:LEU:HG	2.17	0.45
1:A:721:SER:HA	1:A:724:TYR:HB2	1.99	0.45
1:B:212:THR:HG21	1:B:266:ILE:HG13	1.99	0.45
1:B:362:GLN:HB3	1:B:363:ASP:H	1.46	0.45
1:C:394:PHE:O	1:C:398:ILE:HG22	2.16	0.45
1:D:372:ILE:O	1:D:376:LEU:HD13	2.17	0.45
1:D:400:ILE:HG23	1:D:401:ARG:HG3	1.99	0.45
1:D:596:PHE:HB2	1:D:598:HIS:HE1	1.82	0.45
1:A:691:ASP:OD2	1:A:693:TRP:HB2	2.16	0.45
1:D:115:GLN:CG	1:D:139:TYR:CE1	2.99	0.45
1:D:388:LYS:HD2	1:D:388:LYS:HA	1.59	0.45
1:B:338:ASP:O	1:B:342:GLN:HG2	2.17	0.45
1:C:170:LEU:HD23	1:C:170:LEU:O	2.16	0.45
1:C:378:LEU:HD12	1:C:399:VAL:HG21	1.99	0.45
1:C:457:ILE:HG21	1:C:514:LYS:HG2	1.99	0.45
1:C:681:VAL:HG11	1:C:687:VAL:HG13	1.99	0.45
1:D:407:PHE:CE2	1:D:477:LEU:HD13	2.51	0.45
1:D:431:LEU:HD23	1:D:431:LEU:H	1.82	0.45
1:D:650:SER:HB2	1:D:652:MET:HE2	1.99	0.45
1:B:102:ILE:O	1:B:106:ILE:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:HIS:C	1:A:61:LYS:N	2.75	0.45
1:A:101:ASP:O	1:A:105:GLN:HG2	2.17	0.45
1:B:397:GLN:NE2	1:C:419:VAL:H	2.13	0.45
1:C:422:HIS:HB3	1:C:479:ARG:HG3	1.99	0.45
1:D:655:ASN:HD22	1:D:685:ALA:HA	1.81	0.45
1:A:139:TYR:HE2	1:A:144:PHE:HD1	1.65	0.45
1:A:601:LEU:HB3	1:A:623:PHE:HB2	1.99	0.45
1:B:135:ILE:HG13	1:B:136:ALA:N	2.32	0.45
1:B:438:THR:O	1:B:438:THR:HG22	2.17	0.45
1:B:474:LEU:HD23	1:B:474:LEU:HA	1.63	0.45
1:B:695:ASN:HD22	1:B:700:GLU:HG2	1.81	0.45
1:A:609:GLN:O	1:A:613:ILE:HG12	2.17	0.44
1:B:319:PHE:CE2	1:B:348:ARG:HA	2.35	0.44
1:B:498:THR:HG22	1:B:502:ASN:HD21	1.83	0.44
1:C:604:ALA:HA	1:C:609:GLN:HE21	1.82	0.44
1:D:504:MET:HE2	1:D:504:MET:HA	1.98	0.44
1:D:527:GLN:O	1:D:531:LEU:HG	2.17	0.44
1:D:712:LEU:O	1:D:716:VAL:HG23	2.17	0.44
1:B:314:SER:C	1:B:318:ARG:HH21	2.25	0.44
1:B:423:LEU:HD21	1:B:459:ILE:HG21	1.99	0.44
1:C:282:LEU:HD12	1:C:282:LEU:HA	1.62	0.44
1:C:333:LYS:HA	1:C:333:LYS:HD3	1.72	0.44
1:C:565:ARG:HH21	1:C:569:HIS:HB3	1.82	0.44
1:A:561:ASP:HB2	1:D:562:TYR:OH	2.18	0.44
1:B:334:LYS:HB2	1:B:334:LYS:HE2	1.77	0.44
1:B:533:LEU:HG	1:B:562:TYR:CD2	2.50	0.44
1:B:687:VAL:HG13	1:B:697:PRO:HB2	2.00	0.44
1:D:282:LEU:O	1:D:286:ILE:HG13	2.16	0.44
1:B:354:HIS:HA	1:C:332:ARG:HH21	1.81	0.44
1:B:363:ASP:O	1:B:365:PRO:N	2.49	0.44
1:B:407:PHE:O	1:B:474:LEU:HD23	2.17	0.44
1:C:174:ARG:HD2	1:C:177:ARG:NH1	2.31	0.44
1:C:396:ASN:O	1:C:400:ILE:HG23	2.17	0.44
1:C:594:ASP:OD1	1:C:598:HIS:N	2.34	0.44
1:D:409:PRO:HB3	1:D:472:CYS:O	2.17	0.44
1:A:543:ASP:OD1	1:A:543:ASP:N	2.45	0.44
1:B:407:PHE:HE1	1:B:413:ILE:HG23	1.81	0.44
1:C:381:ILE:O	1:C:384:VAL:HG12	2.17	0.44
1:C:569:HIS:HA	1:C:603:GLU:OE1	2.18	0.44
1:D:393:GLU:HA	1:D:396:ASN:ND2	2.32	0.44
1:B:677:ALA:O	1:B:681:VAL:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:HIS:HD2	1:D:61:LYS:HE3	1.83	0.44
1:D:397:GLN:HG3	1:D:401:ARG:HH12	1.83	0.44
1:B:221:TYR:HA	1:B:224:THR:HG22	1.99	0.44
1:B:454:PHE:CE1	1:B:469:VAL:HG21	2.52	0.44
1:B:594:ASP:HB2	1:B:598:HIS:HB2	2.00	0.44
1:B:678:LYS:HB3	1:B:678:LYS:HE2	1.73	0.44
1:C:437:LYS:N	1:C:441:SER:O	2.48	0.44
1:C:492:TYR:HB3	1:C:495:ASP:OD2	2.18	0.44
1:C:636:VAL:HG12	1:C:671:GLU:HG3	2.00	0.44
1:D:421:ASP:HA	1:D:482:LYS:NZ	2.33	0.44
1:D:599:THR:OG1	1:D:600:PRO:HD2	2.17	0.44
1:D:647:LEU:O	1:D:652:MET:HG2	2.16	0.44
1:D:687:VAL:H	1:D:720:GLN:HE22	1.65	0.44
1:A:132:PRO:O	1:A:135:ILE:HG12	2.17	0.44
1:A:690:LYS:HB2	1:A:690:LYS:HE2	1.81	0.44
1:C:408:LEU:O	1:C:471:VAL:HG21	2.17	0.44
1:C:503:ILE:HD12	1:C:503:ILE:HA	1.70	0.44
1:D:198:PHE:CZ	1:D:202:LEU:HD11	2.53	0.44
1:D:535:VAL:HG12	1:D:550:LEU:HD22	1.99	0.44
1:C:61:LYS:HE3	1:C:61:LYS:HB3	1.81	0.44
1:C:331:ASN:OD1	1:C:331:ASN:C	2.60	0.44
1:A:445:VAL:HG21	1:A:467:PHE:CE2	2.53	0.43
1:D:102:ILE:O	1:D:106:ILE:HG23	2.18	0.43
1:A:563:ASP:O	1:A:595:LYS:HB2	2.18	0.43
1:B:431:LEU:CB	1:B:471:VAL:HG23	2.48	0.43
1:C:101:ASP:O	1:C:105:GLN:HG2	2.17	0.43
1:D:615:LEU:HA	1:D:618:LYS:HG2	1.99	0.43
1:A:497:ARG:HA	1:A:500:LEU:HD21	2.00	0.43
1:B:212:THR:OG1	1:B:269:MET:SD	2.73	0.43
1:C:602:PHE:CE2	1:C:625:LEU:HD11	2.54	0.43
1:D:322:LYS:HG2	1:D:351:TYR:CE2	2.53	0.43
1:D:368:ILE:HG22	1:D:372:ILE:HD11	2.00	0.43
1:D:449:GLY:O	1:D:452:THR:OG1	2.27	0.43
1:A:382:LYS:HD2	1:A:383:LYS:HZ1	1.83	0.43
1:B:226:LEU:HD11	1:B:281:ASN:HD21	1.83	0.43
1:B:237:GLY:HA2	1:B:246:TYR:O	2.18	0.43
1:B:486:SER:O	1:B:489:LEU:HG	2.19	0.43
1:C:574:ARG:HD2	1:C:574:ARG:HA	1.75	0.43
1:C:673:LEU:HD23	1:C:673:LEU:H	1.83	0.43
1:D:241:LEU:HD23	1:D:241:LEU:HA	1.81	0.43
1:D:699:ASP:HA	1:D:702:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:NE	1:A:134:ARG:HA	2.34	0.43
1:A:589:ASP:HB3	1:A:592:LEU:HG	2.01	0.43
1:B:357:ASP:HA	1:B:360:MET:CE	2.48	0.43
1:C:405:GLU:OE2	1:C:405:GLU:HA	2.17	0.43
1:C:495:ASP:OD1	1:C:495:ASP:N	2.51	0.43
1:C:666:HIS:CE1	1:C:691:ASP:HB3	2.54	0.43
1:D:677:ALA:O	1:D:681:VAL:HG13	2.18	0.43
1:A:381:ILE:O	1:A:384:VAL:HG12	2.19	0.43
1:B:644:LEU:HD12	1:B:647:LEU:HD12	2.00	0.43
1:C:536:ASN:HA	1:C:570:LEU:HD13	2.00	0.43
1:D:326:LEU:O	1:D:327:ILE:C	2.61	0.43
1:D:350:GLN:HA	1:D:355:TYR:CD2	2.53	0.43
1:D:498:THR:HG22	1:D:502:ASN:HD21	1.83	0.43
1:D:576:TYR:HB3	1:D:579:ILE:HG12	1.99	0.43
1:B:540:PHE:N	1:B:570:LEU:HD21	2.34	0.43
1:A:569:HIS:HA	1:A:603:GLU:OE1	2.18	0.43
1:B:326:LEU:HD12	1:B:326:LEU:HA	1.81	0.43
1:C:426:VAL:HG22	1:C:477:LEU:HD22	2.00	0.43
1:A:491:ILE:HG23	1:A:492:TYR:CD1	2.54	0.43
1:A:574:ARG:HD2	1:A:574:ARG:HA	1.76	0.43
1:B:280:VAL:HG21	1:C:242:GLY:HA3	2.01	0.43
1:C:532:ALA:O	1:C:535:VAL:HG12	2.19	0.43
1:D:363:ASP:OD2	1:D:363:ASP:N	2.51	0.43
1:A:333:LYS:HD3	1:A:333:LYS:HA	1.72	0.43
1:A:424:TYR:CD2	1:A:479:ARG:HB2	2.54	0.43
1:B:126:TYR:HB2	1:C:474:LEU:HD13	2.01	0.43
1:B:362:GLN:O	1:B:364:ILE:N	2.52	0.43
1:B:560:THR:HA	1:B:567:PRO:HD3	2.01	0.43
1:C:139:TYR:HE2	1:C:144:PHE:HD1	1.66	0.43
1:C:681:VAL:HA	1:C:685:ALA:H	1.84	0.43
1:D:237:GLY:HA2	1:D:246:TYR:O	2.19	0.43
1:D:395:ILE:O	1:D:399:VAL:HG13	2.18	0.43
1:D:433:ALA:O	1:D:434:LEU:HD23	2.18	0.43
1:D:644:LEU:O	1:D:648:LEU:HG	2.19	0.43
1:A:405:GLU:OE2	1:A:405:GLU:HA	2.18	0.42
1:A:536:ASN:ND2	1:D:562:TYR:OH	2.51	0.42
1:B:690:LYS:HG2	1:B:691:ASP:H	1.84	0.42
1:C:507:LYS:HG2	1:C:508:GLU:N	2.34	0.42
1:D:396:ASN:HA	1:D:399:VAL:HG22	2.00	0.42
1:A:494:HIS:HA	1:A:497:ARG:NE	2.29	0.42
1:B:509:SER:OG	1:B:510:ASN:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ARG:HA	1:C:134:ARG:NE	2.34	0.42
1:C:284:GLU:O	1:C:288:VAL:HG23	2.19	0.42
1:C:601:LEU:HD13	1:C:616:LEU:HD13	2.01	0.42
1:C:662:ARG:HH22	1:C:670:SER:HB2	1.83	0.42
1:D:486:SER:O	1:D:489:LEU:HG	2.19	0.42
1:D:605:VAL:HG13	1:D:646:ARG:HD2	2.01	0.42
1:B:355:TYR:C	1:B:357:ASP:N	2.75	0.42
1:B:578:ASP:OD1	1:B:578:ASP:N	2.53	0.42
1:C:662:ARG:HD2	1:C:662:ARG:HA	1.74	0.42
1:A:274:TYR:OH	1:D:268:THR:OG1	2.30	0.42
1:A:274:TYR:HH	1:D:268:THR:HG1	1.56	0.42
1:A:681:VAL:HA	1:A:685:ALA:H	1.83	0.42
1:B:59:HIS:HD2	1:B:61:LYS:HE3	1.82	0.42
1:D:361:LEU:HG	1:D:369:ARG:HD3	2.00	0.42
1:D:509:SER:OG	1:D:510:ASN:N	2.52	0.42
1:D:665:LEU:HD11	1:D:713:LEU:HD21	2.01	0.42
1:A:532:ALA:O	1:A:535:VAL:HG12	2.20	0.42
1:B:349:LEU:HA	1:B:352:ASP:OD2	2.19	0.42
1:B:353:SER:O	1:B:357:ASP:HB2	2.19	0.42
1:B:388:LYS:HD2	1:B:388:LYS:HA	1.60	0.42
1:C:197:LEU:HD23	1:C:197:LEU:HA	1.71	0.42
1:C:226:LEU:CD1	1:C:281:ASN:HD21	2.32	0.42
1:C:488:ILE:HA	1:C:491:ILE:HG22	2.00	0.42
1:C:708:LYS:HD3	1:C:708:LYS:C	2.44	0.42
1:D:197:LEU:O	1:D:201:ILE:HG12	2.19	0.42
1:D:226:LEU:HD11	1:D:281:ASN:ND2	2.35	0.42
1:D:460:ILE:HD13	1:D:460:ILE:HA	1.91	0.42
1:D:578:ASP:OD1	1:D:578:ASP:N	2.52	0.42
1:A:567:PRO:HA	1:A:570:LEU:HD12	2.00	0.42
1:A:667:VAL:O	1:A:671:GLU:HG2	2.20	0.42
1:B:347:VAL:O	1:B:350:GLN:HG2	2.20	0.42
1:B:371:LYS:HA	1:B:374:GLN:CG	2.44	0.42
1:B:422:HIS:CG	1:B:479:ARG:HE	2.38	0.42
1:C:281:ASN:HB2	1:C:284:GLU:OE2	2.19	0.42
1:A:99:VAL:H	1:A:99:VAL:HG13	1.60	0.42
1:A:375:LEU:HD12	1:A:375:LEU:O	2.19	0.42
1:A:641:SER:HB2	1:C:641:SER:HB2	2.02	0.42
1:C:415:GLU:HG3	1:C:417:GLY:H	1.85	0.42
1:D:599:THR:HG21	1:D:623:PHE:CD1	2.54	0.42
1:C:430:LEU:HD11	1:C:447:LEU:HB3	2.02	0.42
1:D:407:PHE:CD2	1:D:477:LEU:HD13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:434:LEU:HD22	1:D:444:SER:H	1.83	0.42
1:C:372:ILE:H	1:C:372:ILE:HG13	1.61	0.42
1:D:685:ALA:HB3	1:D:716:VAL:HG11	2.02	0.42
1:B:381:ILE:O	1:B:384:VAL:HG12	2.20	0.42
1:B:437:LYS:HG3	1:B:438:THR:N	2.33	0.42
1:B:599:THR:OG1	1:B:600:PRO:HD2	2.19	0.42
1:C:504:MET:HA	1:C:507:LYS:HD3	2.02	0.42
1:A:281:ASN:HB2	1:A:284:GLU:OE2	2.19	0.41
1:A:517:GLU:HB3	1:A:518:SER:H	1.64	0.41
1:B:559:LYS:HD2	1:B:559:LYS:HA	1.78	0.41
1:C:602:PHE:O	1:C:605:VAL:HG22	2.20	0.41
1:C:668:ALA:HB1	1:C:677:ALA:HA	2.02	0.41
1:A:577:GLU:CG	1:A:611:GLY:HA3	2.50	0.41
1:A:666:HIS:CE1	1:A:691:ASP:HB3	2.56	0.41
1:C:84:PRO:HD3	1:C:175:LEU:HD11	2.02	0.41
1:C:566:SER:O	1:C:570:LEU:HG	2.20	0.41
1:C:601:LEU:HD12	1:C:601:LEU:HA	1.69	0.41
1:D:430:LEU:HB3	1:D:473:GLU:HG3	2.01	0.41
1:D:484:SER:O	1:D:488:ILE:HG13	2.19	0.41
1:D:545:TYR:CE1	1:D:546:GLN:NE2	2.85	0.41
1:A:344:THR:HA	1:A:347:VAL:HG12	2.02	0.41
1:A:492:TYR:O	1:A:496:GLY:N	2.53	0.41
1:B:652:MET:HE3	1:B:652:MET:HB3	1.94	0.41
1:A:433:ALA:HB2	1:A:448:LEU:HD11	2.02	0.41
1:A:566:SER:O	1:A:569:HIS:HB2	2.21	0.41
1:A:604:ALA:HA	1:A:609:GLN:HE21	1.85	0.41
1:B:114:LEU:HA	1:B:117:PHE:CZ	2.55	0.41
1:B:375:LEU:HD23	1:B:376:LEU:HD23	2.02	0.41
1:B:547:LEU:HD13	1:B:582:PHE:CD2	2.55	0.41
1:B:605:VAL:HG21	1:B:647:LEU:HD23	2.02	0.41
1:B:636:VAL:HG22	1:B:676:MET:CE	2.46	0.41
1:B:644:LEU:HB3	1:B:679:MET:SD	2.60	0.41
1:B:714:GLU:HG3	1:B:718:ASN:HD21	1.84	0.41
1:C:282:LEU:HD11	1:D:259:THR:CG2	2.50	0.41
1:C:492:TYR:HB3	1:C:495:ASP:CG	2.45	0.41
1:C:577:GLU:CG	1:C:611:GLY:HA3	2.50	0.41
1:D:425:PHE:HB2	1:D:478:LEU:HB2	2.02	0.41
1:D:526:LYS:HA	1:D:526:LYS:HD2	1.77	0.41
1:D:536:ASN:CG	1:D:561:ASP:HB3	2.46	0.41
1:A:538:ALA:O	1:A:542:GLY:N	2.52	0.41
1:A:602:PHE:CE2	1:A:625:LEU:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:HIS:CD2	1:B:600:PRO:HD3	2.55	0.41
1:A:64:TRP:O	1:A:67:ALA:N	2.53	0.41
1:A:131:LYS:O	1:A:135:ILE:HG23	2.20	0.41
1:A:445:VAL:HG11	1:A:467:PHE:CE2	2.55	0.41
1:B:197:LEU:O	1:B:201:ILE:HG12	2.20	0.41
1:B:389:GLY:HA2	1:B:498:THR:HG21	2.03	0.41
1:B:504:MET:HE3	1:B:504:MET:HA	2.01	0.41
1:C:183:GLU:O	1:C:187:ARG:HG2	2.20	0.41
1:C:360:MET:SD	1:C:360:MET:C	3.04	0.41
1:D:348:ARG:HH12	1:D:352:ASP:HB3	1.84	0.41
1:A:183:GLU:O	1:A:187:ARG:HG2	2.20	0.41
1:A:346:HIS:CE1	1:D:365:PRO:CG	3.04	0.41
1:A:360:MET:SD	1:A:360:MET:C	3.03	0.41
1:B:340:ARG:O	1:B:344:THR:HG23	2.21	0.41
1:B:353:SER:HB2	1:C:332:ARG:NH1	2.36	0.41
1:C:294:PHE:CZ	1:C:298:LEU:HD22	2.56	0.41
1:C:344:THR:HA	1:C:347:VAL:HG12	2.03	0.41
1:D:422:HIS:CE1	1:D:479:ARG:HH11	2.39	0.41
1:D:463:ILE:O	1:D:464:SER:HB3	2.21	0.41
1:A:294:PHE:CZ	1:A:298:LEU:HD22	2.56	0.41
1:A:632:LEU:O	1:A:636:VAL:HG23	2.21	0.41
1:A:72:ILE:HG21	1:A:111:ASP:OD2	2.21	0.41
1:A:197:LEU:HA	1:A:197:LEU:HD23	1.71	0.41
1:A:284:GLU:O	1:A:288:VAL:HG23	2.20	0.41
1:A:378:LEU:HD12	1:A:399:VAL:HG11	2.02	0.41
1:A:427:CYS:SG	1:A:478:LEU:HD21	2.61	0.41
1:A:584:ILE:HD12	1:A:588:VAL:HG13	2.03	0.41
1:A:595:LYS:CE	1:D:573:CYS:SG	3.09	0.41
1:B:354:HIS:CB	1:B:406:TYR:HE2	2.33	0.41
1:B:457:ILE:H	1:B:457:ILE:HG12	1.67	0.41
1:B:532:ALA:HA	1:B:535:VAL:HG22	2.02	0.41
1:B:687:VAL:H	1:B:720:GLN:HE22	1.69	0.41
1:C:409:PRO:HA	1:C:471:VAL:HG23	2.03	0.41
1:D:332:ARG:HG2	1:D:333:LYS:HD3	2.01	0.41
1:D:439:ASP:O	1:D:439:ASP:CG	2.64	0.41
1:A:425:PHE:CD1	1:A:453:SER:HB2	2.56	0.41
1:A:494:HIS:HA	1:A:497:ARG:HH21	1.86	0.41
1:A:550:LEU:HA	1:A:550:LEU:HD23	1.81	0.41
1:B:241:LEU:HD23	1:B:241:LEU:HA	1.76	0.41
1:B:367:SER:HB3	1:C:412:VAL:O	2.21	0.41
1:B:408:LEU:CD2	1:B:474:LEU:HD21	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:564:GLY:HA3	1:C:594:ASP:HA	2.03	0.41
1:D:204:LEU:O	1:D:208:GLU:HG3	2.21	0.41
1:A:331:ASN:OD1	1:A:331:ASN:C	2.63	0.40
1:A:343:ILE:HG12	1:D:368:ILE:HG21	2.02	0.40
1:A:531:LEU:HD21	1:A:555:ALA:HB2	2.03	0.40
1:B:85:MET:HE2	1:B:85:MET:HB2	1.93	0.40
1:B:355:TYR:O	1:B:359:VAL:HG23	2.21	0.40
1:B:517:GLU:H	1:B:517:GLU:HG2	1.73	0.40
1:B:636:VAL:HA	1:B:676:MET:HE1	2.03	0.40
1:C:666:HIS:CD2	1:C:697:PRO:HA	2.55	0.40
1:D:334:LYS:HE2	1:D:334:LYS:HB2	1.77	0.40
1:D:497:ARG:NH1	1:D:500:LEU:HD22	2.28	0.40
1:D:540:PHE:N	1:D:570:LEU:HD21	2.37	0.40
1:A:298:LEU:HD12	1:A:298:LEU:HA	1.81	0.40
1:A:412:VAL:HA	1:A:470:ARG:HA	2.03	0.40
1:A:534:LYS:HG3	1:A:550:LEU:HD11	2.03	0.40
1:A:662:ARG:NH2	1:A:700:GLU:HG3	2.36	0.40
1:B:413:ILE:HD11	1:B:471:VAL:HB	2.03	0.40
1:C:131:LYS:O	1:C:135:ILE:HG23	2.20	0.40
1:C:166:LEU:HA	1:C:166:LEU:HD13	1.87	0.40
1:C:384:VAL:HA	1:C:451:HIS:O	2.21	0.40
1:D:59:HIS:CG	1:D:130:TYR:HH	2.33	0.40
1:D:326:LEU:O	1:D:329:PHE:N	2.54	0.40
1:A:249:PHE:O	1:A:257:ARG:HD3	2.22	0.40
1:A:504:MET:SD	1:A:521:VAL:HG22	2.61	0.40
1:A:531:LEU:HA	1:A:534:LYS:HE2	2.03	0.40
1:B:642:ASP:OD2	1:B:646:ARG:NH2	2.34	0.40
1:C:335:LEU:HD12	1:C:335:LEU:H	1.86	0.40
1:C:382:LYS:HD2	1:C:383:LYS:HZ1	1.86	0.40
1:A:396:ASN:O	1:A:400:ILE:HG23	2.21	0.40
1:A:542:GLY:HA3	1:A:576:TYR:CE1	2.55	0.40
1:A:607:ALA:HB3	1:A:609:GLN:NE2	2.31	0.40
1:C:667:VAL:O	1:C:671:GLU:HG2	2.21	0.40
1:D:433:ALA:O	1:D:445:VAL:HB	2.22	0.40
1:D:547:LEU:HD13	1:D:582:PHE:CD2	2.57	0.40
1:A:397:GLN:O	1:A:400:ILE:HG12	2.22	0.40
1:A:408:LEU:O	1:A:471:VAL:HG21	2.21	0.40
1:A:675:LEU:O	1:A:679:MET:HG2	2.22	0.40
1:B:226:LEU:HD23	1:B:226:LEU:HA	1.96	0.40
1:C:381:ILE:HD13	1:C:381:ILE:HA	1.92	0.40
1:C:422:HIS:CD2	1:C:479:ARG:HH11	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:LEU:HD12	1:C:468:THR:HB	2.03	0.40
1:D:361:LEU:HD12	1:D:361:LEU:HA	1.82	0.40
1:D:500:LEU:HD21	1:D:523:HIS:NE2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	665/763 (87%)	621 (93%)	40 (6%)	4 (1%)	21	50
1	B	664/763 (87%)	616 (93%)	40 (6%)	8 (1%)	10	35
1	C	665/763 (87%)	624 (94%)	38 (6%)	3 (0%)	24	54
1	D	664/763 (87%)	626 (94%)	36 (5%)	2 (0%)	36	65
All	All	2658/3052 (87%)	2487 (94%)	154 (6%)	17 (1%)	23	50

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	362	GLN
1	B	363	ASP
1	B	365	PRO
1	D	366	ALA
1	B	361	LEU
1	B	366	ALA
1	C	517	GLU
1	A	517	GLU
1	B	464	SER
1	A	60	PRO
1	B	357	ASP
1	A	450	PRO

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Mol	Chain	Res	Type
1	C	450	PRO
1	D	365	PRO
1	B	364	ILE
1	A	273	GLY
1	C	273	GLY

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	589/676 (87%)	581 (99%)	8 (1%)	59	70
1	B	588/676 (87%)	575 (98%)	13 (2%)	45	63
1	C	589/676 (87%)	577 (98%)	12 (2%)	48	65
1	D	588/676 (87%)	583 (99%)	5 (1%)	70	76
All	All	2354/2704 (87%)	2316 (98%)	38 (2%)	54	68

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ILE
1	A	99	VAL
1	A	129	VAL
1	A	140	LEU
1	A	253	ASP
1	A	269	MET
1	A	583	LEU
1	A	598	HIS
1	B	118	VAL
1	B	343	ILE
1	B	346	HIS
1	B	349	LEU
1	B	350	GLN
1	B	358	THR
1	B	360	MET
1	B	362	GLN

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Mol	Chain	Res	Type
1	B	363	ASP
1	B	365	PRO
1	B	367	SER
1	B	368	ILE
1	B	679	MET
1	C	253	ASP
1	C	269	MET
1	C	494	HIS
1	C	495	ASP
1	C	498	THR
1	C	499	ILE
1	C	500	LEU
1	C	503	ILE
1	C	506	GLU
1	C	507	LYS
1	C	508	GLU
1	C	517	GLU
1	D	234	THR
1	D	326	LEU
1	D	363	ASP
1	D	494	HIS
1	D	560	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	ASN
1	A	483	GLN
1	A	609	GLN
1	A	655	ASN
1	A	666	HIS
1	B	62	ASN
1	B	124	GLN
1	B	278	HIS
1	B	305	ASN
1	B	362	GLN
1	B	462	ASN
1	B	536	ASN
1	B	591	ASN
1	B	666	HIS
1	B	695	ASN
1	B	718	ASN

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Mol	Chain	Res	Type
1	C	230	ASN
1	C	281	ASN
1	C	350	GLN
1	C	483	GLN
1	C	501	ASN
1	C	541	GLN
1	C	546	GLN
1	C	598	HIS
1	C	609	GLN
1	C	655	ASN
1	C	695	ASN
1	D	62	ASN
1	D	278	HIS
1	D	305	ASN
1	D	462	ASN
1	D	483	GLN
1	D	591	ASN
1	D	609	GLN
1	D	630	ASN
1	D	666	HIS
1	D	718	ASN

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

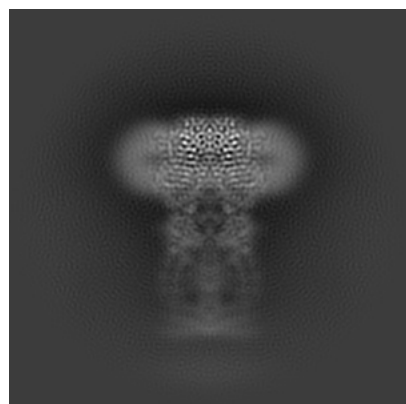
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62338. These allow visual inspection of the internal detail of the map and identification of artifacts.

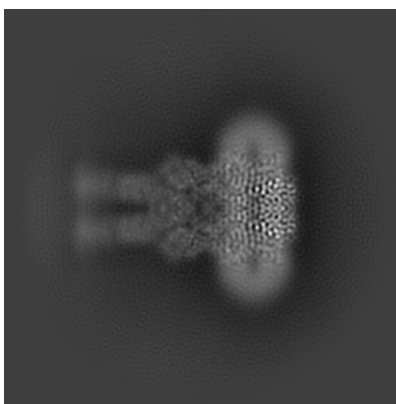
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

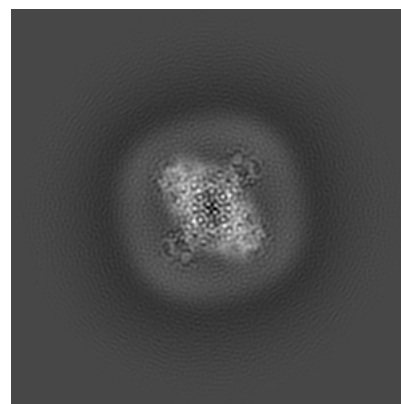
6.1.1 Primary map



X

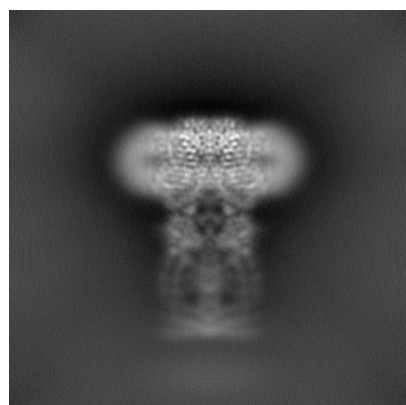


Y

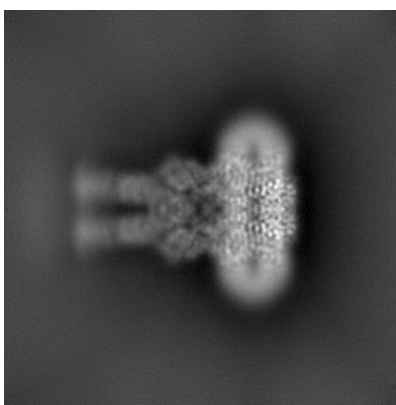


Z

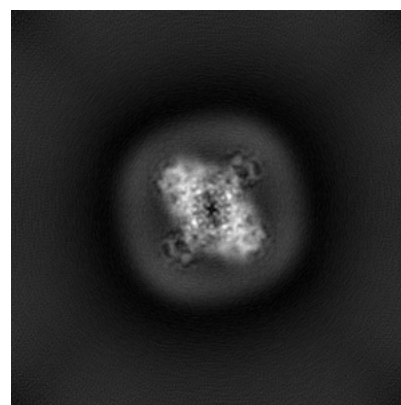
6.1.2 Raw map



X



Y

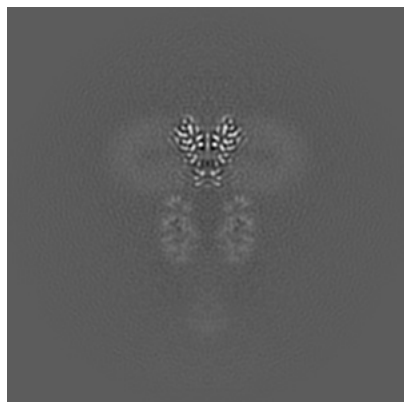


Z

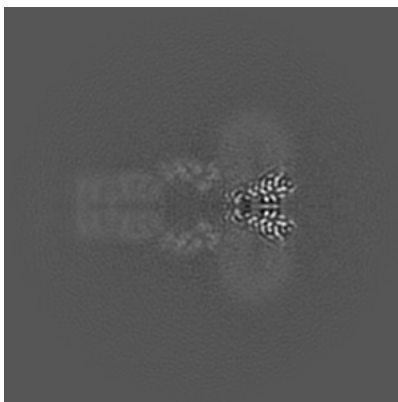
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

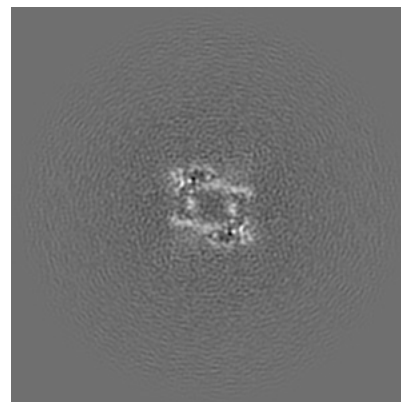
6.2.1 Primary map



X Index: 144

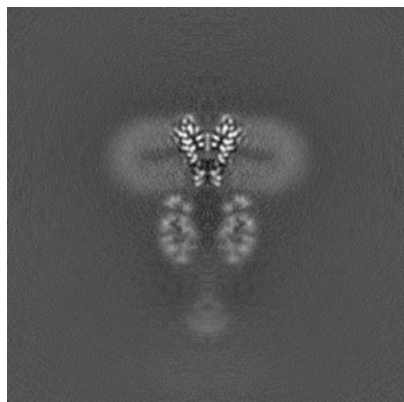


Y Index: 144

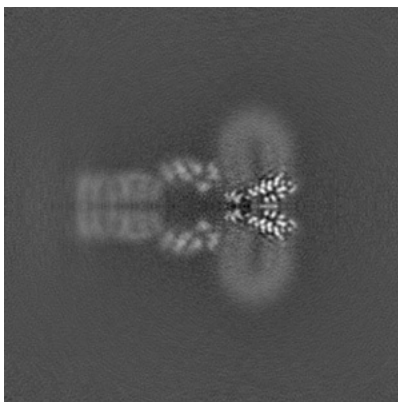


Z Index: 144

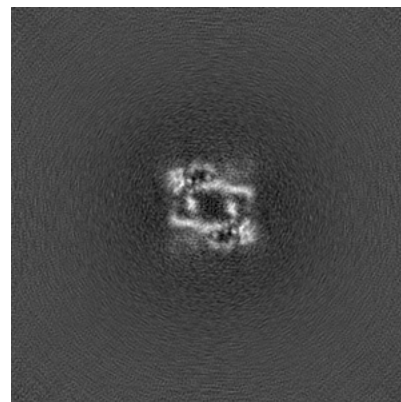
6.2.2 Raw map



X Index: 144



Y Index: 144

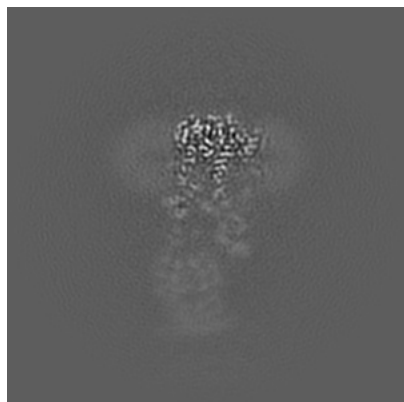


Z Index: 144

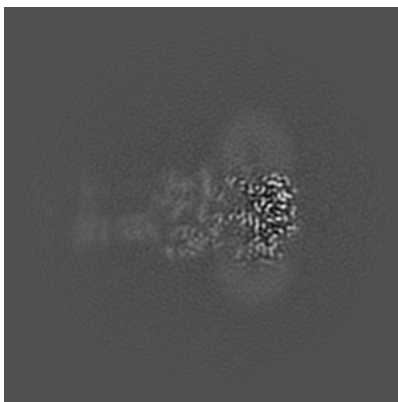
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

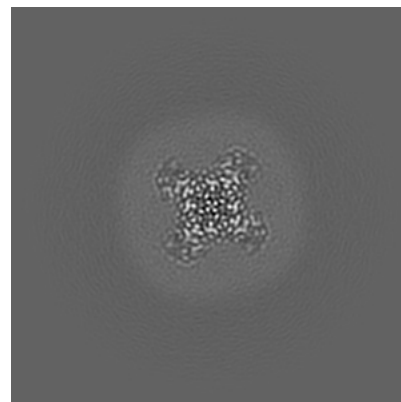
6.3.1 Primary map



X Index: 157

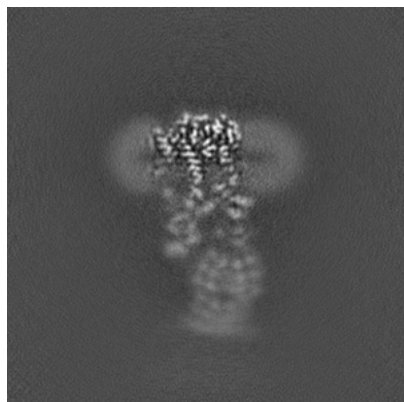


Y Index: 157

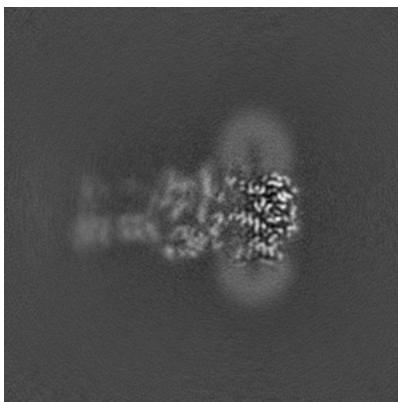


Z Index: 191

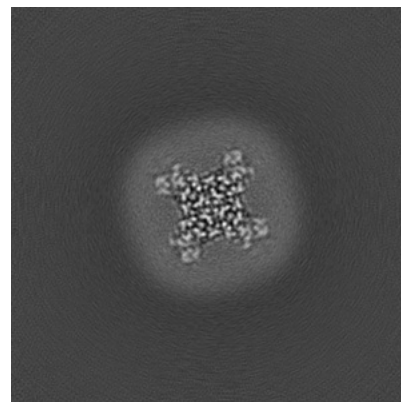
6.3.2 Raw map



X Index: 131



Y Index: 157

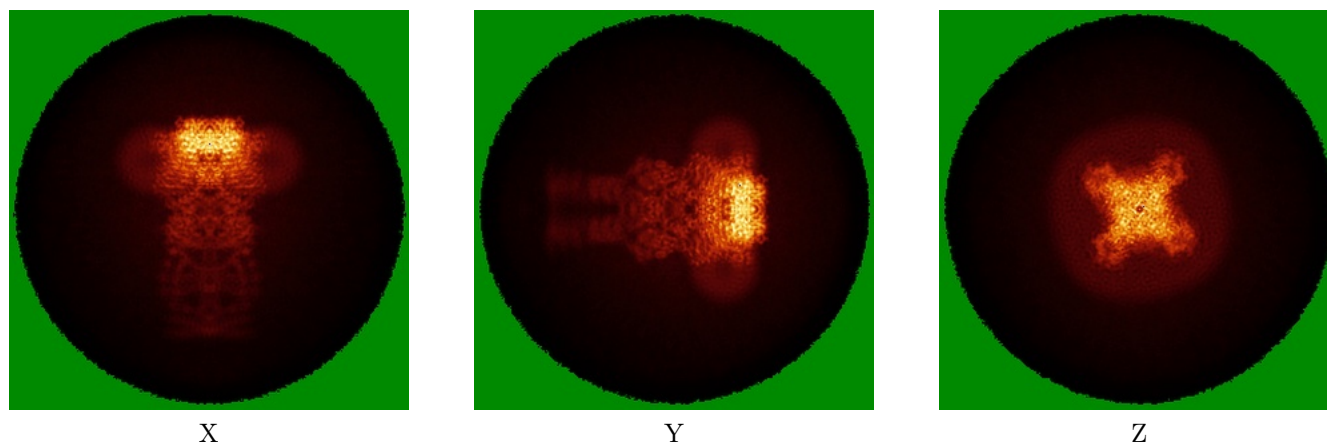


Z Index: 197

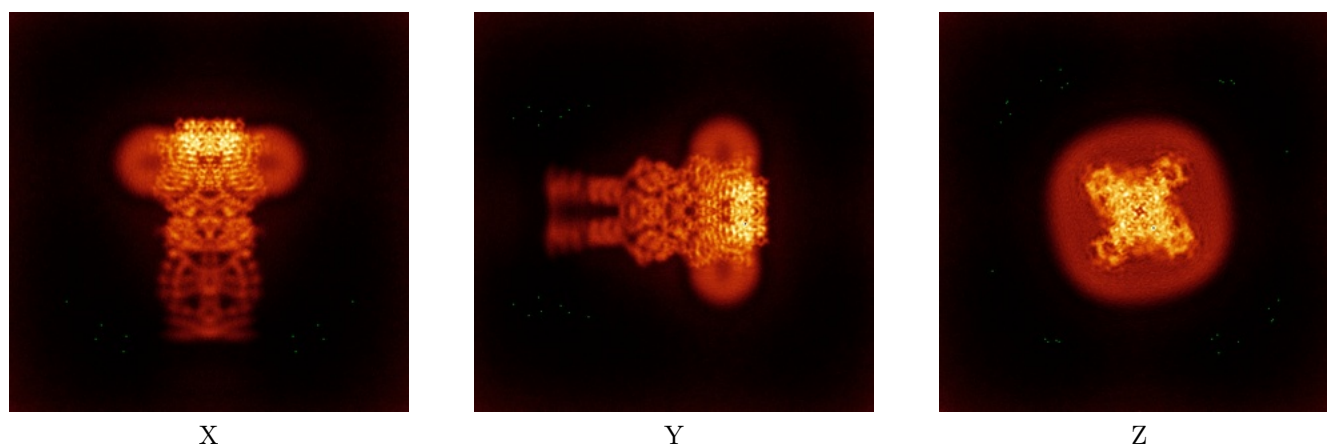
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

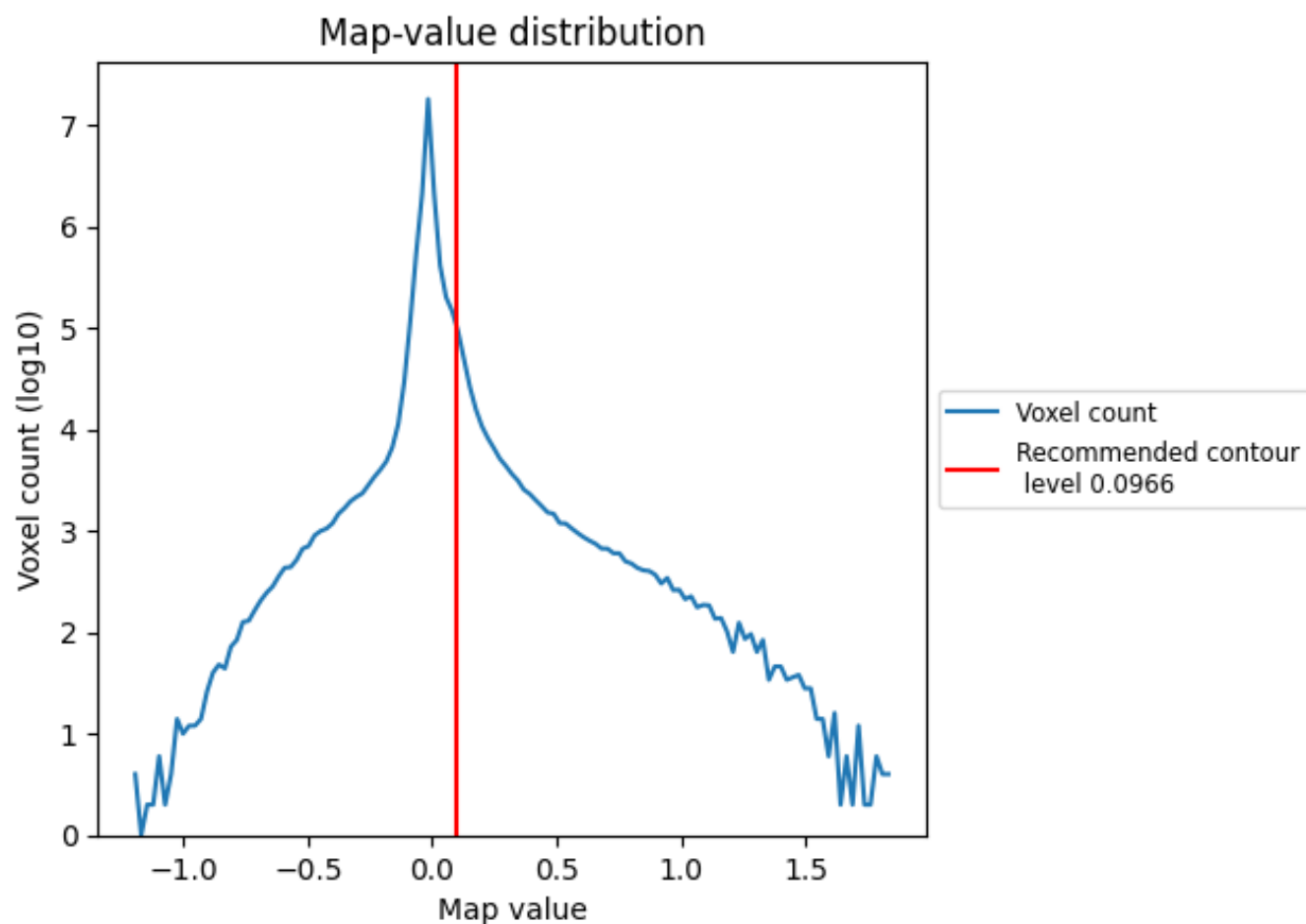
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

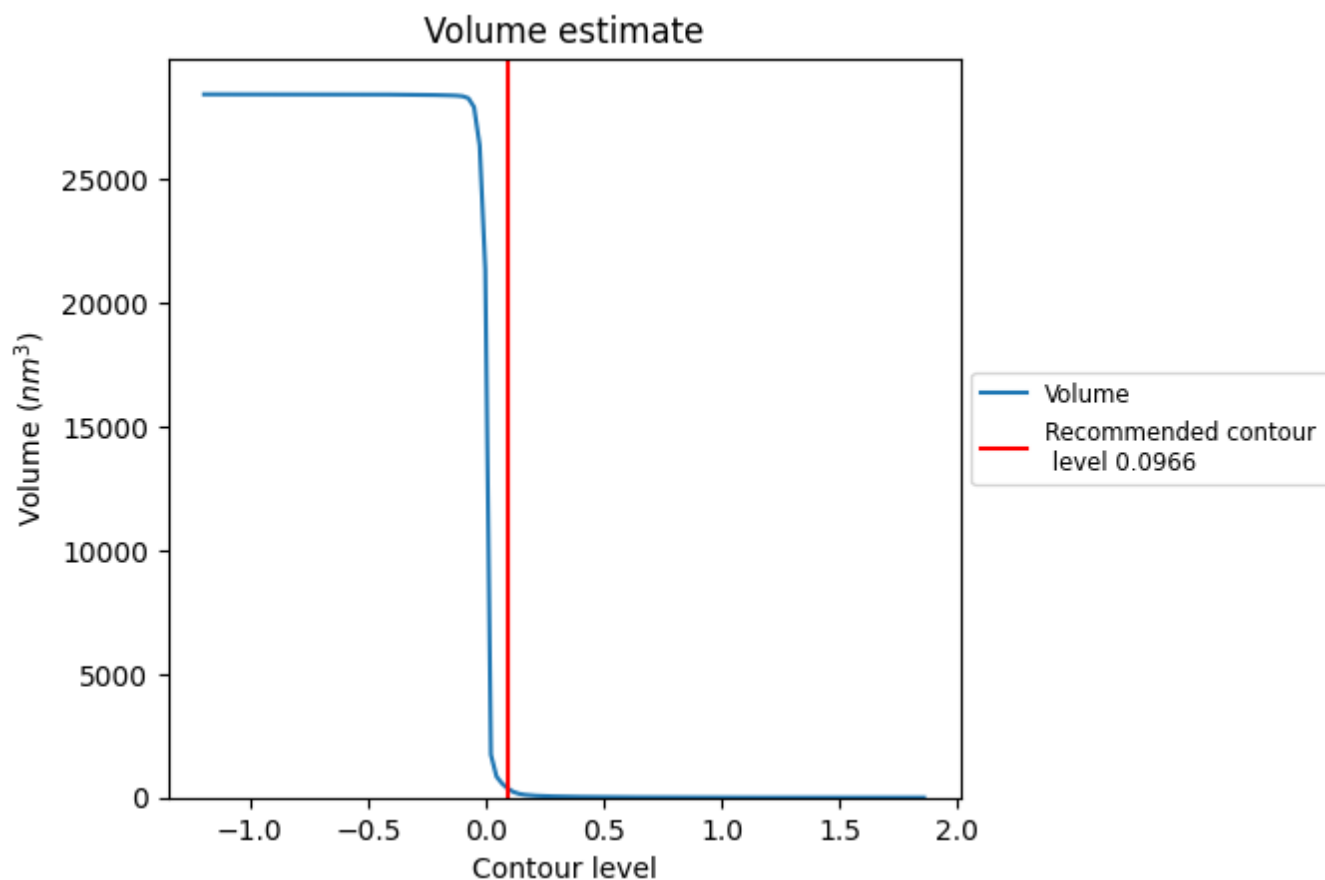
This section contains the results of statistical analysis of the map.

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.

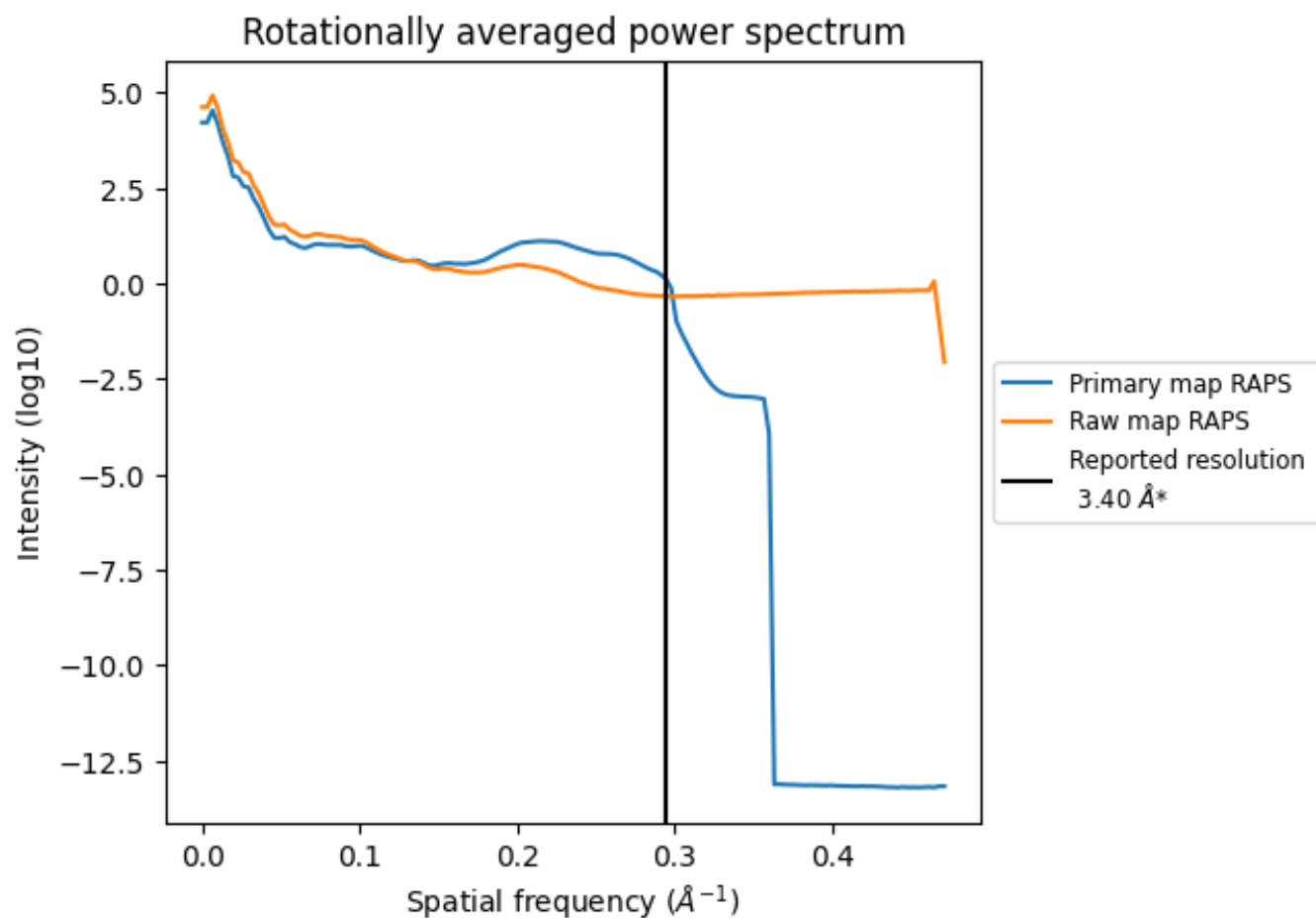
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 347 nm³; this corresponds to an approximate mass of 313 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 ⓘ

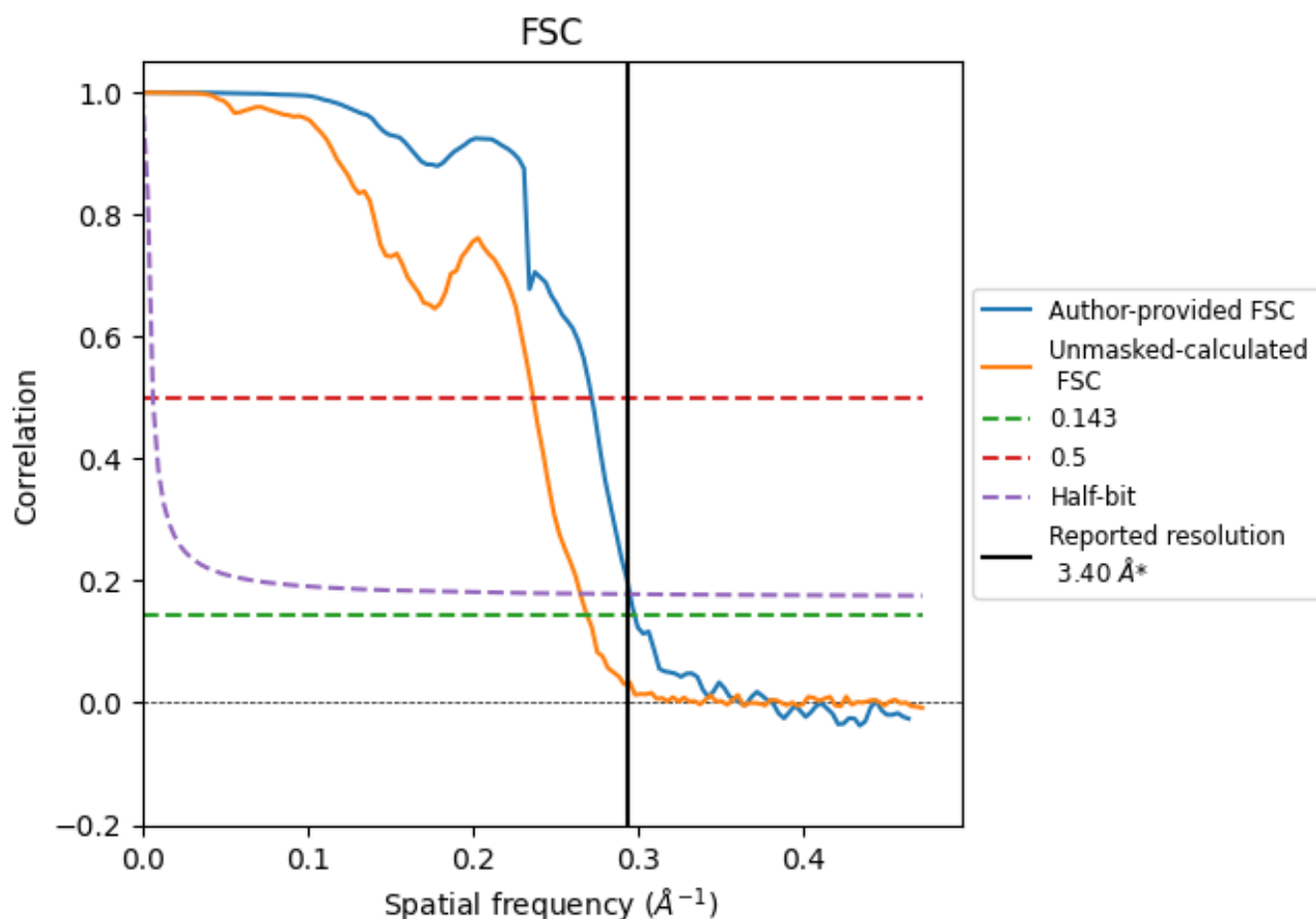


*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.36	3.68	3.39
Unmasked-calculated*	3.72	4.23	3.77

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

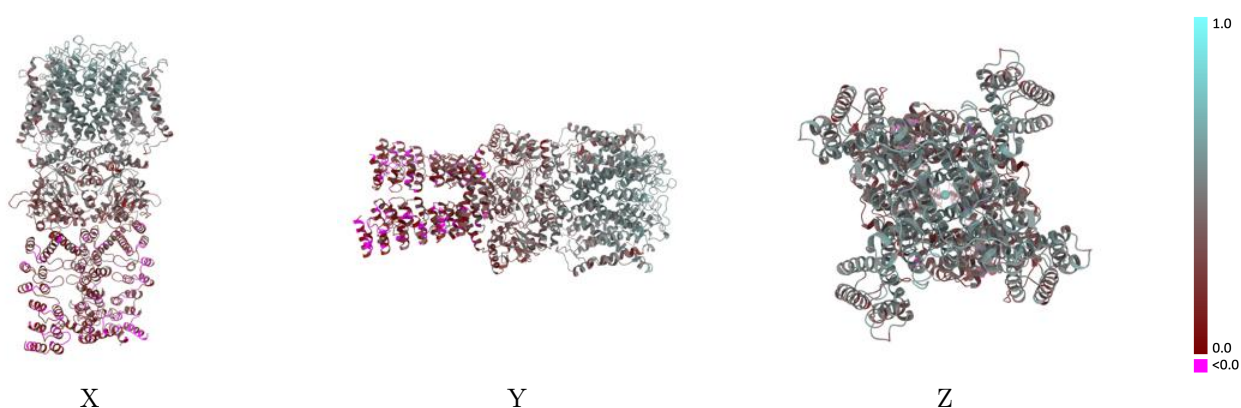
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62338 and PDB model 9KHF. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

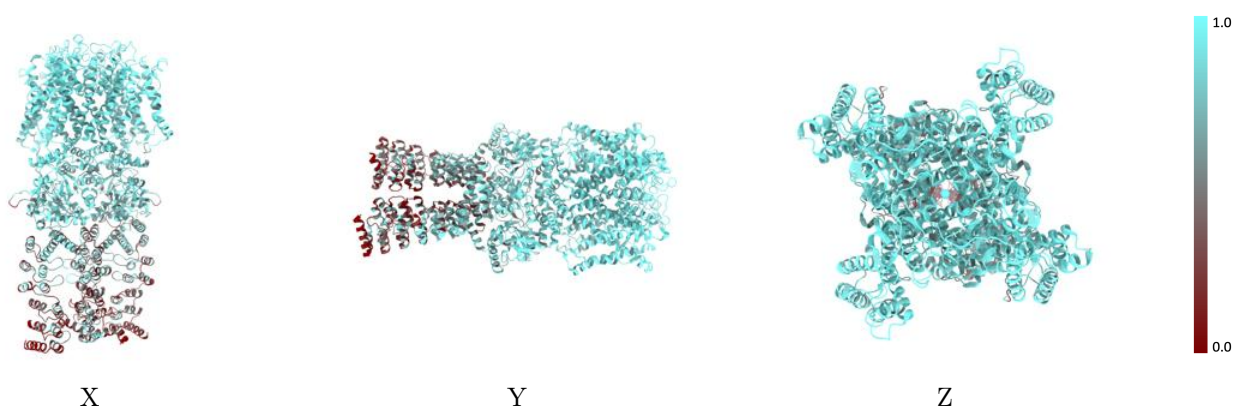
This section was not generated.

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



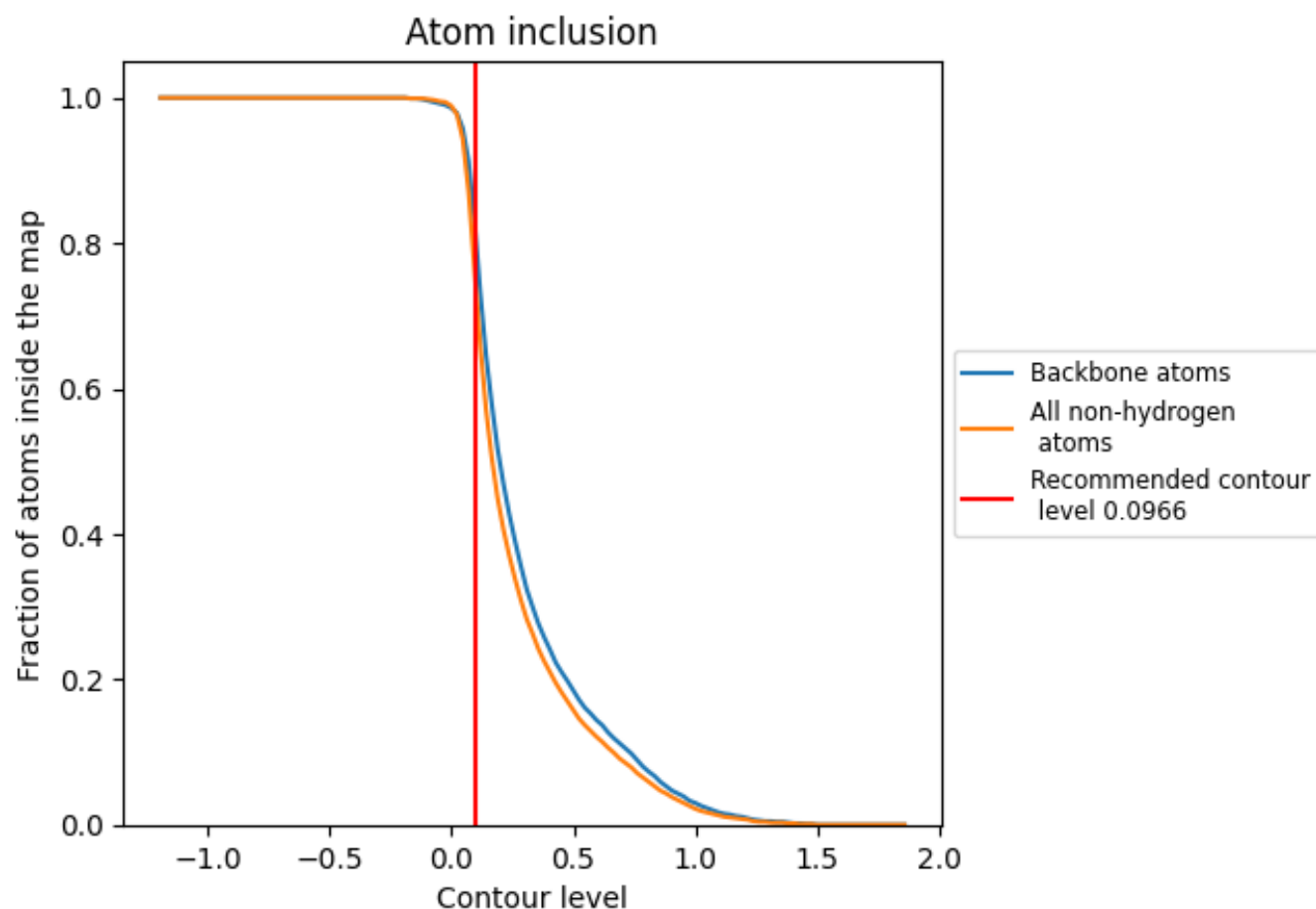
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0966).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% 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 (0.0966) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7490	0.3610
A	0.7580	0.3790
B	0.7420	0.3520
C	0.7620	0.3750
D	0.7360	0.3400

