



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 04:42 PM UTC

PDB ID : 9NJU / pdb_00009nju
EMDB ID : EMD-49491
Title : Structure of native homodimer of D. discoideum polyketide synthase Pks16
Authors : Hoogerbrugge, G.; Keatinge-Clay, A.T.; Marcotte, E.M.
Deposited on : 2025-02-27
Resolution : 3.94 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

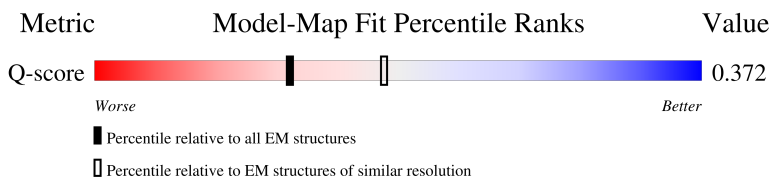
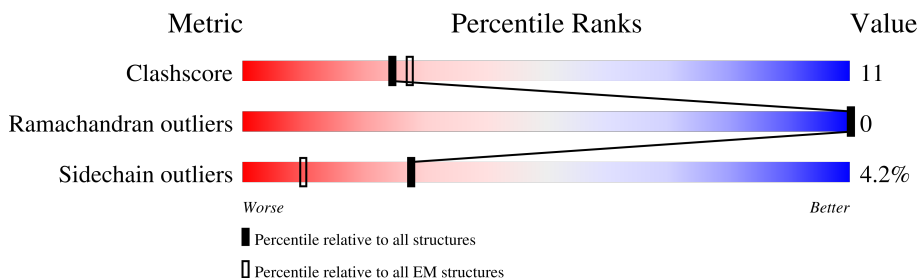
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.94 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	7757 (3.44 - 4.43)

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	2603	 5% 66% 24% • 9%
1	B	2603	 5% 66% 24% • 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 37504 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.

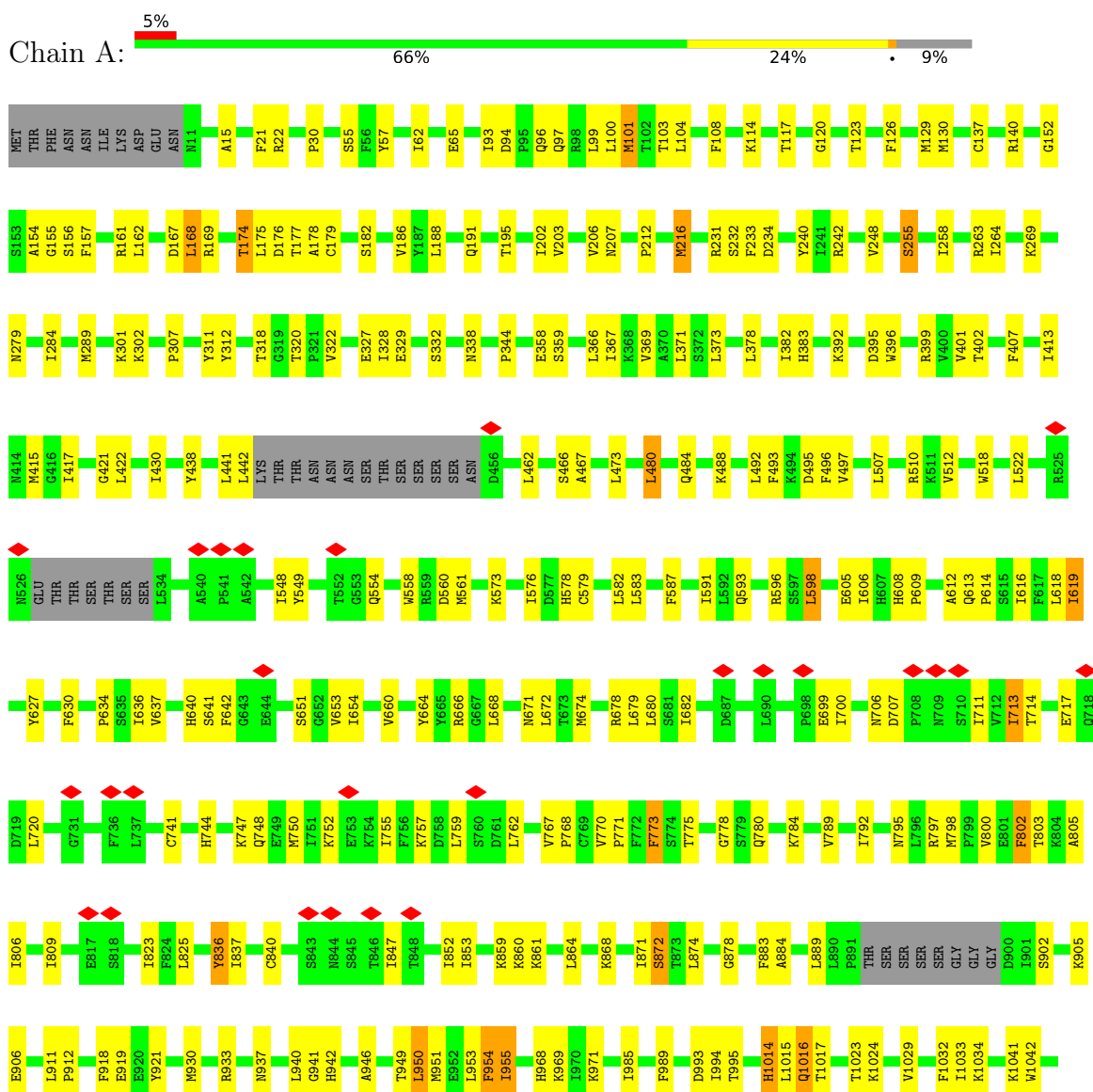
- Molecule 1 is a protein called Probable polyketide synthase 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2371	Total	C	N	O	S	0	0
			18752	11964	3092	3632	64		
1	B	2371	Total	C	N	O	S	0	0
			18752	11964	3092	3632	64		

3 Residue-property plots

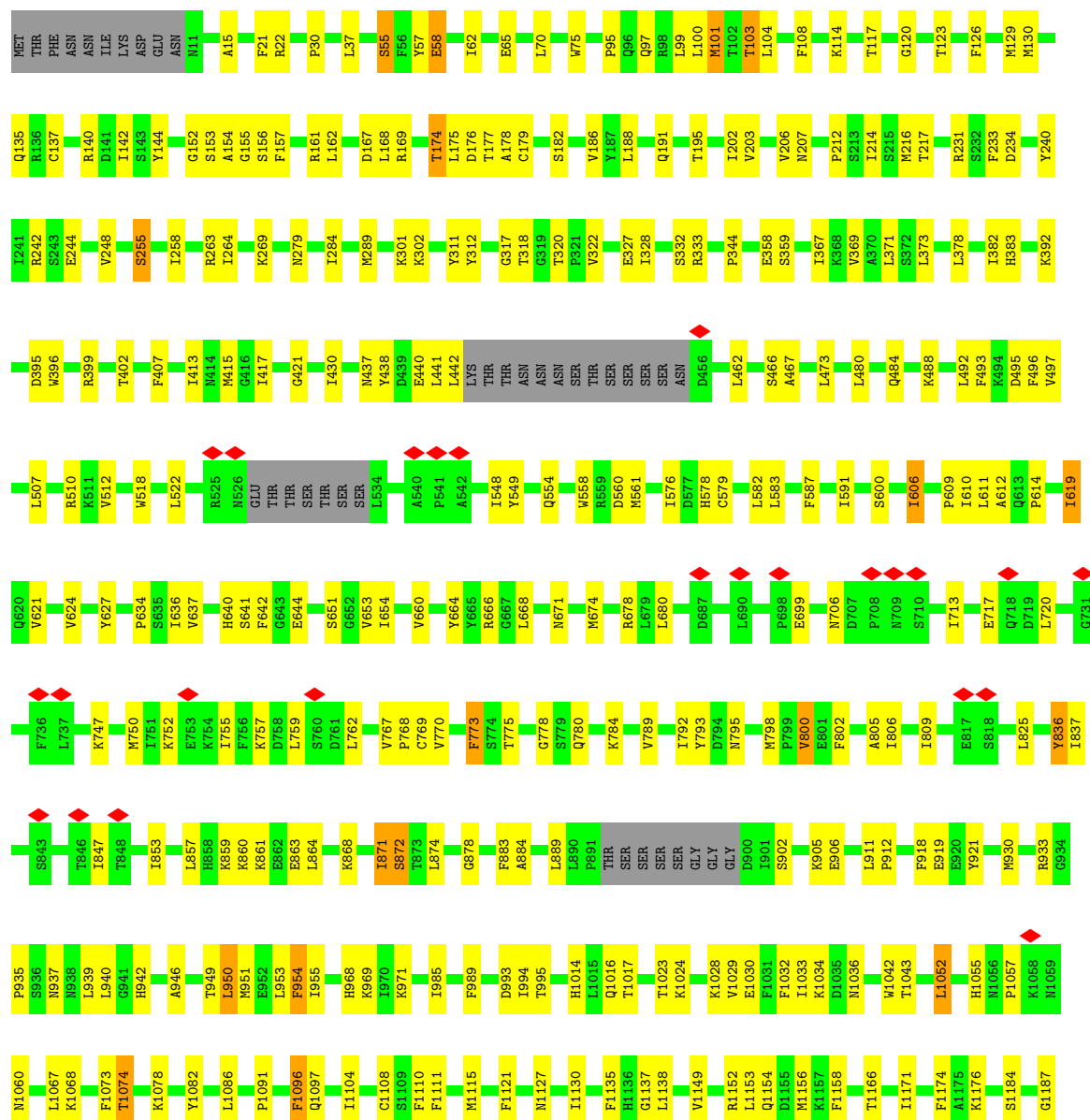
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

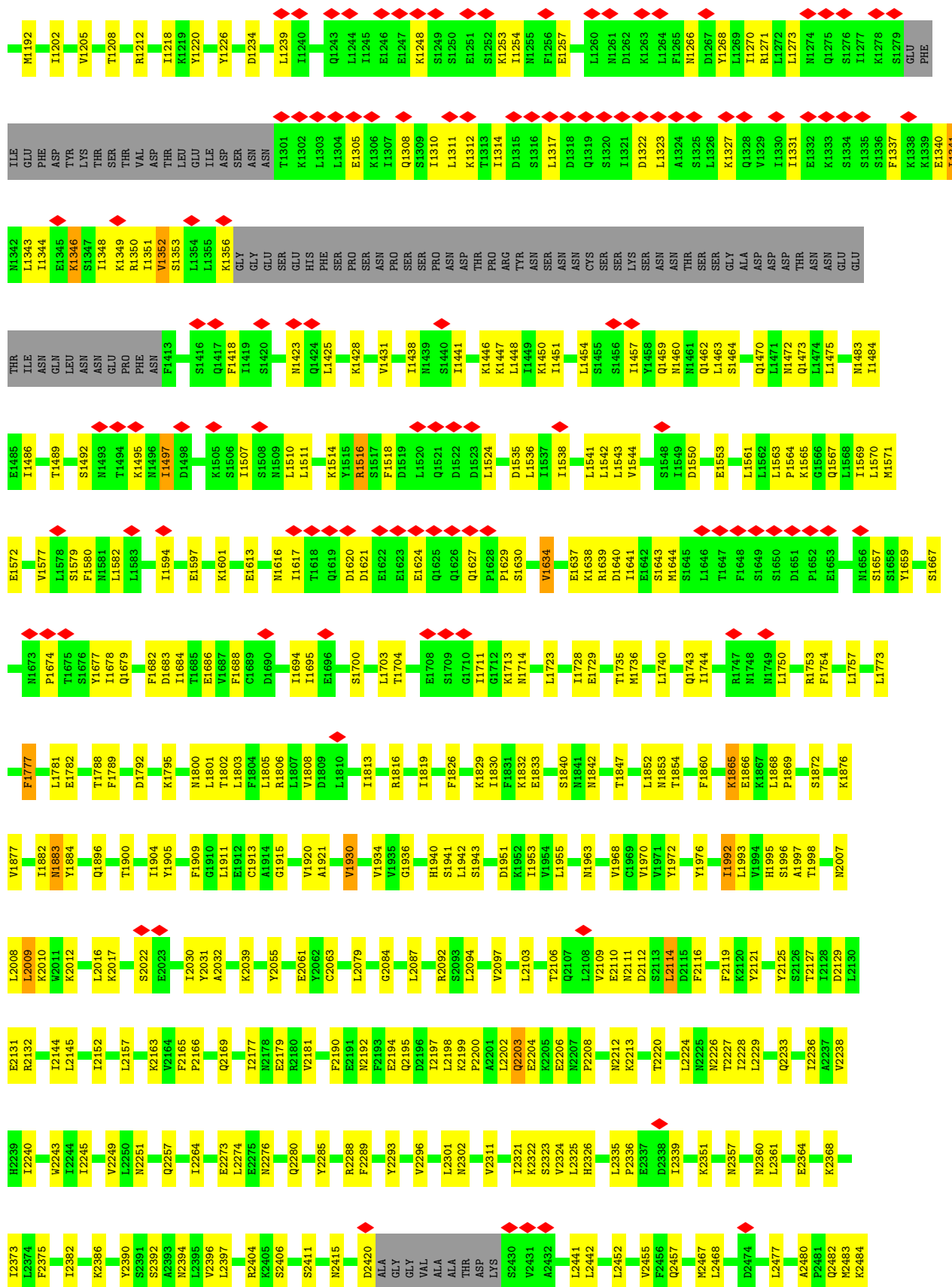
- Molecule 1: Probable polyketide synthase 16





- Molecule 1: Probable polyketide synthase 16





THR	VAL	GLN	LEU	LYS	ASN	TRP	ILE	ASP	LYS	GLU	PHE	THR	LYS	ASN	LEU	PHE	THR	HIS	LEU	GLN	LEU	SER	SER	SER	SER	ILE	ASN	SER	SER	ILE	ILE	GLN	ARG	ILE	ILE	SER	SER	LYS	SER	THR	SER	THR	THR	THR	THR	THR	THR	ALA	THR	THR	LYS	THR
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5611	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.444	Depositor
Minimum map value	-0.713	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.239	Depositor
Map size ($\text{\AA}$)	447.8464, 447.8464, 447.8464	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.7494, 1.7494, 1.7494	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.11	0/19117	0.29	0/25850
1	B	0.10	0/19117	0.30	0/25850
All	All	0.11	0/38234	0.29	0/51700

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
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	144	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	18752	0	18752	404	0
1	B	18752	0	18752	415	0
All	All	37504	0	37504	798	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 11.

All (798) 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:1270:ILE:HG12	1:A:1314:ILE:HG23	1.52	0.90
1:B:179:CYS:HB3	1:B:421:GLY:HA2	1.61	0.82
1:A:179:CYS:HB3	1:A:421:GLY:HA2	1.63	0.80
1:A:1516:ARG:HG2	1:A:2494:TYR:HB3	1.62	0.80
1:B:2382:ILE:HG13	1:B:2483:MET:HE3	1.65	0.77
1:B:129:MET:HE1	1:B:155:GLY:HA2	1.67	0.77
1:B:2238:VAL:HG11	1:B:2273:GLU:HG3	1.67	0.77
1:A:2238:VAL:HG11	1:A:2273:GLU:HG3	1.66	0.76
1:A:953:LEU:HD21	1:A:955:ILE:HG12	1.66	0.76
1:B:289:MET:HE2	1:B:333:ARG:HH21	1.52	0.74
1:B:1331:ILE:HG12	1:B:1337:PHE:H	1.53	0.74
1:A:1644:MET:H	1:A:1806:ARG:HD3	1.52	0.73
1:A:104:LEU:HD11	1:A:202:ILE:HD13	1.71	0.72
1:A:1331:ILE:HG12	1:A:1337:PHE:H	1.54	0.72
1:B:104:LEU:HD11	1:B:202:ILE:HD13	1.70	0.72
1:A:1472:ASN:HB2	1:A:1507:ILE:HG23	1.72	0.71
1:A:1448:LEU:HD21	1:A:1450:LYS:HE2	1.73	0.71
1:B:1152:ARG:HH12	1:B:2110:GLU:HG3	1.55	0.71
1:A:1152:ARG:HH12	1:A:2110:GLU:HG3	1.55	0.71
1:A:1311:LEU:HD23	1:A:1314:ILE:HD12	1.72	0.71
1:A:1679:GLN:HG3	1:A:1684:ILE:HG23	1.71	0.71
1:B:637:VAL:HG21	1:B:651:SER:HB3	1.70	0.71
1:A:637:VAL:HG21	1:A:651:SER:HB3	1.72	0.71
1:A:1543:LEU:HG	1:A:1572:GLU:HG3	1.73	0.70
1:B:930:MET:HE2	1:B:930:MET:HA	1.72	0.70
1:B:1543:LEU:HG	1:B:1572:GLU:HG3	1.73	0.70
1:A:1852:LEU:HG	1:A:2197:ILE:HD13	1.71	0.70
1:B:747:LYS:HA	1:B:750:MET:HE1	1.73	0.70
1:B:1472:ASN:HB2	1:B:1507:ILE:HG23	1.74	0.69
1:A:930:MET:HE2	1:A:930:MET:HA	1.73	0.69
1:B:2109:VAL:HG23	1:B:2112:ASP:HB3	1.75	0.69
1:B:2394:ASN:HA	1:B:2397:LEU:HD12	1.74	0.69
1:A:2233:GLN:HB2	1:A:2274:LEU:HD22	1.75	0.69
1:B:1641:ILE:HD12	1:B:1644:MET:HE1	1.75	0.68
1:A:2394:ASN:HA	1:A:2397:LEU:HD12	1.74	0.68
1:B:1679:GLN:HG3	1:B:1684:ILE:HG23	1.74	0.68
1:A:591:ILE:HG21	1:A:614:PRO:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:PHE:HA	1:B:666:ARG:HH12	1.58	0.68
1:A:642:PHE:HA	1:A:666:ARG:HH12	1.58	0.68
1:A:1489:THR:HG22	1:A:1514:LYS:HB2	1.76	0.67
1:B:2087:LEU:HD21	1:B:2114:LEU:HD23	1.74	0.67
1:B:2198:LEU:HD23	1:B:2202:LEU:HD12	1.77	0.67
1:A:2227:THR:HB	1:A:2321:ILE:HA	1.76	0.66
1:A:484:GLN:HE21	1:A:518:TRP:HB3	1.59	0.66
1:A:2404:ARG:HH11	1:A:2411:SER:HB3	1.61	0.66
1:B:484:GLN:HE21	1:B:518:TRP:HB3	1.60	0.66
1:B:1565:LYS:H	1:B:1638:LYS:HB3	1.61	0.66
1:B:1441:ILE:HD12	1:B:1447:LYS:HZ2	1.60	0.66
1:A:1853:ASN:HA	1:A:1943:SER:HB2	1.78	0.66
1:A:2249:VAL:HA	1:A:2288:ARG:HH21	1.60	0.66
1:B:123:THR:HB	1:B:168:LEU:HG	1.76	0.66
1:B:1270:ILE:HG12	1:B:1314:ILE:HG23	1.77	0.66
1:B:2227:THR:HB	1:B:2321:ILE:HA	1.77	0.66
1:B:2233:GLN:HB2	1:B:2274:LEU:HD22	1.76	0.66
1:B:2249:VAL:HA	1:B:2288:ARG:HH21	1.60	0.66
1:A:332:SER:HG	1:A:396:TRP:CG	2.15	0.65
1:A:369:VAL:HG23	1:A:415:MET:HE2	1.78	0.65
1:B:1909:PHE:HB3	1:B:1942:LEU:HD23	1.77	0.65
1:A:382:ILE:HG13	1:A:383:HIS:HD1	1.60	0.65
1:B:1489:THR:HG22	1:B:1514:LYS:HB2	1.78	0.65
1:A:129:MET:HE1	1:A:155:GLY:HA2	1.79	0.65
1:A:1310:ILE:O	1:A:1314:ILE:HG13	1.96	0.65
1:B:591:ILE:HG21	1:B:614:PRO:HB2	1.77	0.65
1:B:2392:SER:O	1:B:2396:VAL:HG23	1.97	0.65
1:B:332:SER:HG	1:B:396:TRP:CG	2.15	0.65
1:A:2392:SER:O	1:A:2396:VAL:HG23	1.97	0.64
1:A:123:THR:HB	1:A:168:LEU:HG	1.79	0.64
1:B:382:ILE:HG13	1:B:383:HIS:HD1	1.61	0.64
1:B:1736:MET:HE3	1:B:1740:LEU:HD11	1.80	0.63
1:A:1920:VAL:HG13	1:A:1930:VAL:HG13	1.80	0.63
1:B:610:ILE:HD11	1:B:671:ASN:HB2	1.78	0.63
1:A:1872:SER:H	1:A:1921:ALA:HB2	1.64	0.63
1:A:2224:LEU:HB3	1:A:2228:ILE:HD11	1.81	0.63
1:A:747:LYS:HA	1:A:750:MET:HE1	1.80	0.63
1:A:1667:SER:H	1:A:1677:TYR:HE2	1.47	0.63
1:A:2084:GLY:H	1:A:2106:THR:HG21	1.64	0.63
1:B:1254:ILE:HG21	1:B:1624:GLU:HB3	1.81	0.62
1:B:1872:SER:H	1:B:1921:ALA:HB2	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1920:VAL:HG13	1:B:1930:VAL:HG13	1.82	0.62
1:A:1736:MET:HE3	1:A:1740:LEU:HD11	1.80	0.61
1:A:2378:ILE:HG22	1:A:2382:ILE:HG22	1.81	0.61
1:B:1659:TYR:HA	1:B:1714:ASN:HB3	1.82	0.61
1:A:510:ARG:HH12	1:A:878:GLY:HA2	1.65	0.61
1:B:1667:SER:H	1:B:1677:TYR:HE2	1.48	0.61
1:B:1492:SER:HB3	1:B:1497:ILE:HG12	1.80	0.61
1:B:1565:LYS:HG3	1:B:1640:ASP:HA	1.83	0.61
1:B:1883:ASN:HD21	1:B:1911:LEU:HB2	1.66	0.61
1:A:1127:ASN:H	1:A:1130:ILE:HD12	1.64	0.61
1:B:369:VAL:HG23	1:B:415:MET:HE2	1.83	0.61
1:B:680:LEU:HD23	1:B:713:ILE:HD11	1.82	0.61
1:B:462:LEU:HD21	1:B:868:LYS:HD2	1.83	0.61
1:B:884:ALA:HA	1:B:889:LEU:HD12	1.83	0.61
1:B:2084:GLY:H	1:B:2106:THR:HG21	1.66	0.61
1:B:1711:ILE:HD11	1:B:1750:LEU:HD13	1.83	0.61
1:B:2483:MET:HB3	1:B:2487:MET:HE3	1.81	0.61
1:A:1711:ILE:HD11	1:A:1750:LEU:HD13	1.83	0.61
1:A:1883:ASN:HD21	1:A:1911:LEU:HB2	1.66	0.61
1:A:789:VAL:HA	1:A:792:ILE:HD12	1.82	0.60
1:A:950:LEU:HD11	1:A:1016:GLN:NE2	2.15	0.60
1:A:680:LEU:HD23	1:A:713:ILE:HD11	1.82	0.60
1:B:231:ARG:HG2	1:B:234:ASP:HB2	1.83	0.60
1:A:884:ALA:HA	1:A:889:LEU:HD12	1.83	0.60
1:B:1460:ASN:HB3	1:B:1462:GLN:HG2	1.82	0.60
1:A:1997:ALA:HB2	1:A:2032:ALA:HB1	1.83	0.60
1:A:1074:THR:HG21	1:A:2276:ASN:HB2	1.82	0.60
1:B:1127:ASN:H	1:B:1130:ILE:HD12	1.65	0.60
1:A:1877:VAL:HG12	1:A:2190:PHE:HD2	1.66	0.60
1:B:1877:VAL:HG12	1:B:2190:PHE:HD2	1.66	0.60
1:B:1032:PHE:HB3	1:B:1042:TRP:HB3	1.84	0.60
1:B:1789:PHE:HD1	1:B:1816:ARG:HB3	1.67	0.60
1:B:1992:ILE:HG23	1:B:2030:ILE:HG23	1.84	0.60
1:A:1023:THR:HG22	1:A:1024:LYS:H	1.67	0.60
1:B:1516:ARG:HD2	1:B:2494:TYR:HD2	1.66	0.60
1:A:680:LEU:HB3	1:A:720:LEU:HD22	1.84	0.60
1:A:462:LEU:HD21	1:A:868:LYS:HD2	1.84	0.59
1:B:1074:THR:HG21	1:B:2276:ASN:HB2	1.82	0.59
1:B:1830:ILE:HD13	1:B:2487:MET:HE2	1.84	0.59
1:A:1992:ILE:HG23	1:A:2030:ILE:HG23	1.84	0.59
1:A:576:ILE:HD11	1:A:618:LEU:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1657:SER:H	1:A:1688:PHE:HB3	1.68	0.59
1:A:1800:ASN:HB3	1:A:1803:LEU:HB2	1.85	0.59
1:B:1782:GLU:HA	1:B:2482:GLN:HE22	1.66	0.59
1:A:231:ARG:HG2	1:A:234:ASP:HB2	1.84	0.59
1:B:57:TYR:CG	1:B:65:GLU:HB3	2.37	0.59
1:B:653:VAL:HG12	1:B:654:ILE:HG23	1.83	0.59
1:B:789:VAL:HA	1:B:792:ILE:HD12	1.84	0.59
1:A:152:GLY:HA2	1:A:161:ARG:HH12	1.68	0.58
1:A:748:GLN:HB2	1:A:797:ARG:HD3	1.85	0.58
1:A:954:PHE:HD2	1:A:1014:HIS:HE1	1.50	0.58
1:A:1032:PHE:HB3	1:A:1042:TRP:HB3	1.85	0.58
1:A:1659:TYR:HA	1:A:1714:ASN:HB3	1.84	0.58
1:B:2415:ASN:HB2	1:B:2467:MET:HB2	1.84	0.58
1:B:240:TYR:HB3	1:B:318:THR:HB	1.84	0.58
1:A:933:ARG:HB3	1:A:942:HIS:CE1	2.37	0.58
1:A:1460:ASN:HB3	1:A:1462:GLN:HG2	1.84	0.58
1:B:1997:ALA:HB2	1:B:2032:ALA:HB1	1.84	0.58
1:A:100:LEU:HB3	1:A:162:LEU:HD21	1.84	0.58
1:A:1830:ILE:HD13	1:A:2487:MET:HE2	1.85	0.58
1:B:2017:LYS:HA	1:B:2022:SER:HA	1.84	0.58
1:B:2420:ASP:HA	1:B:2442:LEU:HD13	1.85	0.58
1:A:97:GLN:O	1:A:101:MET:HE3	2.03	0.58
1:A:902:SER:HA	1:A:905:LYS:HG3	1.86	0.58
1:A:798:MET:HA	1:A:798:MET:HE2	1.86	0.58
1:B:798:MET:HE2	1:B:798:MET:HA	1.85	0.58
1:B:864:LEU:HD23	1:B:864:LEU:H	1.69	0.58
1:A:1492:SER:HB3	1:A:1497:ILE:HG12	1.85	0.58
1:B:344:PRO:HG3	1:B:399:ARG:HE	1.68	0.57
1:B:561:MET:HE3	1:B:561:MET:HA	1.86	0.57
1:B:1679:GLN:HG2	1:B:1683:ASP:HA	1.86	0.57
1:B:674:MET:N	1:B:674:MET:HE2	2.18	0.57
1:B:1457:ILE:HG22	1:B:1492:SER:HA	1.85	0.57
1:B:1323:LEU:HD22	1:B:1327:LYS:HE2	1.87	0.57
1:A:653:VAL:HG12	1:A:654:ILE:HG23	1.85	0.57
1:A:1266:ASN:HB3	1:A:1317:LEU:HB3	1.87	0.57
1:A:2420:ASP:HA	1:A:2442:LEU:HD13	1.87	0.57
1:A:1686:GLU:HB2	1:A:1801:LEU:HD23	1.86	0.57
1:B:1535:ASP:HA	1:B:1563:LEU:HB2	1.86	0.57
1:A:1789:PHE:HD1	1:A:1816:ARG:HB3	1.70	0.57
1:A:1840:SER:H	1:A:1843:TYR:HE2	1.51	0.57
1:A:101:MET:HG3	1:A:162:LEU:HD23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1781:LEU:HD11	1:B:1816:ARG:HD2	1.87	0.57
1:A:548:ILE:HG12	1:A:636:ILE:HB	1.86	0.56
1:A:864:LEU:H	1:A:864:LEU:HD23	1.70	0.56
1:B:902:SER:HA	1:B:905:LYS:HG3	1.86	0.56
1:A:240:TYR:HB3	1:A:318:THR:HB	1.86	0.56
1:A:2116:PHE:HB2	1:B:2112:ASP:O	2.06	0.56
1:A:2143:ASP:O	1:A:2147:GLU:HG2	2.06	0.56
1:A:2483:MET:HB3	1:A:2487:MET:HE3	1.88	0.56
1:B:548:ILE:HG12	1:B:636:ILE:HB	1.86	0.56
1:A:911:LEU:HD13	1:A:912:PRO:HD2	1.88	0.56
1:A:1792:ASP:HB3	1:A:1819:ILE:HG12	1.87	0.56
1:B:1644:MET:H	1:B:1806:ARG:HD3	1.71	0.56
1:A:1057:PRO:O	1:A:1060:ASN:HB2	2.06	0.56
1:A:94:ASP:OD1	1:A:96:GLN:HG3	2.06	0.56
1:A:307:PRO:HB2	1:A:338:ASN:HD21	1.69	0.56
1:B:1253:LYS:HE3	1:B:1630:SER:HA	1.88	0.56
1:A:1570:LEU:HB3	1:A:1634:VAL:HG23	1.87	0.55
1:B:484:GLN:HG3	1:B:522:LEU:HD11	1.88	0.55
1:B:1853:ASN:HA	1:B:1943:SER:HB2	1.87	0.55
1:A:344:PRO:HG3	1:A:399:ARG:HE	1.72	0.55
1:A:1679:GLN:HG2	1:A:1683:ASP:HA	1.87	0.55
1:B:438:TYR:HA	1:B:441:LEU:HB2	1.87	0.55
1:B:1266:ASN:HB3	1:B:1317:LEU:HB3	1.88	0.55
1:B:1800:ASN:HB3	1:B:1803:LEU:HB2	1.88	0.55
1:A:1565:LYS:H	1:A:1638:LYS:HB3	1.72	0.55
1:A:279:ASN:ND2	1:B:169:ARG:HH12	2.03	0.55
1:A:438:TYR:HA	1:A:441:LEU:HB2	1.87	0.55
1:A:2017:LYS:HA	1:A:2022:SER:HA	1.87	0.55
1:A:864:LEU:O	1:A:868:LYS:HG2	2.05	0.55
1:A:1253:LYS:HE3	1:A:1630:SER:HA	1.88	0.55
1:B:1852:LEU:HG	1:B:2197:ILE:HD13	1.88	0.55
1:B:864:LEU:O	1:B:868:LYS:HG2	2.05	0.55
1:B:1735:THR:HG22	1:B:1773:LEU:HG	1.89	0.55
1:A:182:SER:O	1:A:186:VAL:HG23	2.07	0.55
1:B:1998:THR:HG21	1:B:2039:LYS:HB3	1.89	0.55
1:A:1565:LYS:HG3	1:A:1640:ASP:HA	1.89	0.55
1:A:778:GLY:HA2	1:A:805:ALA:HB2	1.90	0.54
1:A:1459:GLN:HG2	1:A:1460:ASN:H	1.72	0.54
1:B:606:ILE:HA	1:B:611:LEU:HD23	1.89	0.54
1:B:933:ARG:HB3	1:B:942:HIS:CE1	2.41	0.54
1:B:1310:ILE:O	1:B:1314:ILE:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:TYR:CG	1:A:65:GLU:HB3	2.42	0.54
1:A:1457:ILE:HG22	1:A:1492:SER:HA	1.88	0.54
1:B:1254:ILE:HD12	1:B:1621:ASP:HB2	1.90	0.54
1:B:1028:LYS:HE3	1:B:2111:ASN:HB3	1.90	0.54
1:B:954:PHE:HD2	1:B:1014:HIS:HE1	1.54	0.54
1:B:1431:VAL:HG11	1:B:1470:GLN:HG2	1.89	0.54
1:A:1516:ARG:HD2	1:A:2494:TYR:HD2	1.73	0.54
1:B:2404:ARG:HE	1:B:2411:SER:HB3	1.72	0.54
1:B:510:ARG:HH12	1:B:878:GLY:HA2	1.73	0.54
1:A:2179:GLU:HB3	1:A:2181:VAL:HG22	1.89	0.54
1:A:554:GLN:HB2	1:A:642:PHE:HB2	1.90	0.54
1:B:101:MET:HG3	1:B:162:LEU:HD23	1.89	0.54
1:B:2009:LEU:HD13	1:B:2030:ILE:HD13	1.88	0.54
1:A:186:VAL:HA	1:A:203:VAL:HG11	1.89	0.54
1:A:207:ASN:HB2	1:A:359:SER:HB3	1.89	0.54
1:B:242:ARG:HG2	1:B:358:GLU:HB2	1.90	0.54
1:B:554:GLN:HB2	1:B:642:PHE:HB2	1.90	0.54
1:B:1657:SER:H	1:B:1688:PHE:HB3	1.72	0.54
1:B:1570:LEU:HB3	1:B:1634:VAL:HG23	1.90	0.53
1:A:2227:THR:C	1:A:2228:ILE:HD13	2.33	0.53
1:B:680:LEU:HB3	1:B:720:LEU:HD22	1.90	0.53
1:A:1111:PHE:CE1	1:A:1137:GLY:HA3	2.44	0.53
1:B:558:TRP:HD1	1:B:560:ASP:H	1.54	0.53
1:B:1431:VAL:HG21	1:B:1470:GLN:HG2	1.90	0.53
1:A:1789:PHE:HE1	1:A:1816:ARG:HD3	1.73	0.53
1:A:2204:GLU:HG3	1:A:2206:GLU:H	1.73	0.53
1:A:130:MET:HG2	1:A:178:ALA:HB2	1.91	0.53
1:A:579:CYS:HA	1:A:582:LEU:HD12	1.91	0.53
1:B:182:SER:O	1:B:186:VAL:HG23	2.08	0.53
1:B:207:ASN:HB2	1:B:359:SER:HB3	1.91	0.53
1:B:1674:PRO:HB3	1:B:1694:ILE:HG21	1.90	0.53
1:B:1934:VAL:HG12	1:B:1955:LEU:HA	1.91	0.53
1:B:2480:ALA:HB1	1:B:2483:MET:HE2	1.91	0.53
1:A:994:ILE:HG22	1:A:1158:PHE:HB3	1.91	0.53
1:B:1695:ILE:HG21	1:B:1703:LEU:HG	1.91	0.53
1:A:493:PHE:O	1:A:497:VAL:HG23	2.09	0.52
1:A:1704:THR:HG22	1:A:1744:ILE:HD13	1.91	0.52
1:B:940:LEU:HD11	1:B:951:MET:HG3	1.90	0.52
1:A:1524:LEU:H	1:A:1524:LEU:HD12	1.73	0.52
1:A:1486:ILE:HB	1:A:1511:LEU:HD22	1.92	0.52
1:B:493:PHE:O	1:B:497:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:CYS:HA	1:B:582:LEU:HD12	1.91	0.52
1:A:1448:LEU:HD22	1:A:2489:HIS:CE1	2.45	0.52
1:A:1559:TYR:HA	1:A:1562:LEU:HD12	1.92	0.52
1:B:22:ARG:HB2	1:B:99:LEU:HD21	1.92	0.52
1:A:284:ILE:HG21	1:B:157:PHE:CE2	2.44	0.52
1:A:320:THR:HG22	1:A:322:VAL:H	1.75	0.52
1:B:130:MET:HG2	1:B:178:ALA:HB2	1.92	0.52
1:B:1579:SER:HA	1:B:1582:LEU:HD12	1.92	0.52
1:A:561:MET:HB3	1:A:619:ILE:HD11	1.91	0.52
1:A:1078:LYS:HE2	1:A:1097:GLN:HB3	1.92	0.52
1:A:1781:LEU:HD11	1:A:1816:ARG:HD2	1.92	0.52
1:B:1792:ASP:HB3	1:B:1819:ILE:HG12	1.92	0.52
1:A:860:LYS:HB2	1:A:861:LYS:HE2	1.90	0.52
1:A:940:LEU:HD11	1:A:951:MET:HG3	1.91	0.52
1:A:1323:LEU:HD22	1:A:1327:LYS:HE2	1.91	0.52
1:B:175:LEU:HD11	1:B:188:LEU:HD12	1.91	0.52
1:B:1111:PHE:CE1	1:B:1137:GLY:HA3	2.44	0.52
1:B:2199:LYS:O	1:B:2203:GLN:HB2	2.10	0.52
1:A:169:ARG:HH12	1:B:279:ASN:ND2	2.08	0.51
1:B:860:LYS:HB2	1:B:861:LYS:HE2	1.92	0.51
1:A:157:PHE:HE2	1:B:284:ILE:HG21	1.74	0.51
1:A:1535:ASP:HA	1:A:1563:LEU:HB2	1.91	0.51
1:B:484:GLN:HE22	1:B:488:LYS:HD2	1.75	0.51
1:A:157:PHE:CE2	1:B:284:ILE:HG21	2.46	0.51
1:A:1754:PHE:HB3	1:A:1788:THR:HG23	1.92	0.51
1:A:1802:THR:HA	1:A:1805:LEU:HD12	1.91	0.51
1:B:55:SER:HA	1:B:58:GLU:OE2	2.09	0.51
1:A:1674:PRO:HB3	1:A:1694:ILE:HG21	1.92	0.51
1:A:2084:GLY:N	1:A:2106:THR:HG21	2.26	0.51
1:B:186:VAL:HA	1:B:203:VAL:HG11	1.93	0.51
1:B:1115:MET:HG3	1:B:1171:ILE:HG23	1.93	0.51
1:B:759:LEU:HD12	1:B:762:LEU:HD11	1.92	0.51
1:B:2228:ILE:HD12	1:B:2323:SER:HB2	1.91	0.51
1:A:1184:SER:HA	1:A:1208:THR:HA	1.92	0.51
1:B:1448:LEU:HD23	1:B:1829:LYS:HE3	1.91	0.51
1:B:1564:PRO:HB3	1:B:1641:ILE:HB	1.93	0.51
1:B:1704:THR:HG22	1:B:1744:ILE:HD13	1.91	0.51
1:A:175:LEU:HD11	1:A:188:LEU:HD12	1.92	0.51
1:A:2198:LEU:HD23	1:A:2202:LEU:HD12	1.93	0.51
1:B:1852:LEU:HB3	1:B:1860:PHE:CD1	2.46	0.51
1:A:1423:ASN:HB3	1:A:1463:LEU:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:LEU:HD12	1:A:762:LEU:HD11	1.94	0.50
1:A:1270:ILE:HD11	1:A:1317:LEU:HB2	1.93	0.50
1:B:1184:SER:HA	1:B:1208:THR:HA	1.92	0.50
1:A:1248:LYS:HB2	1:A:1620:ASP:H	1.75	0.50
1:A:1736:MET:HE1	1:A:2340:THR:HA	1.92	0.50
1:B:1448:LEU:HD22	1:B:2489:HIS:CE1	2.46	0.50
1:A:951:MET:HE3	1:A:951:MET:HA	1.94	0.50
1:B:2163:LYS:HG2	1:B:2165:PHE:HE1	1.77	0.50
1:A:1221:PRO:HG3	1:A:2451:CYS:HB2	1.93	0.50
1:A:1579:SER:HA	1:A:1582:LEU:HD12	1.93	0.50
1:B:1057:PRO:O	1:B:1060:ASN:HB2	2.11	0.50
1:A:1268:TYR:CZ	1:A:1341:ILE:HG13	2.47	0.50
1:A:1842:ASN:HD21	1:A:2220:THR:H	1.60	0.50
1:B:951:MET:HA	1:B:951:MET:HE3	1.92	0.50
1:B:1311:LEU:HD23	1:B:1314:ILE:HD12	1.93	0.50
1:A:484:GLN:HG3	1:A:522:LEU:HD11	1.92	0.50
1:B:1882:ILE:HG22	1:B:2177:ILE:HD12	1.93	0.50
1:A:773:PHE:CE1	1:A:780:GLN:HB3	2.47	0.50
1:A:1257:GLU:HG3	1:A:1627:GLN:HB2	1.93	0.50
1:B:152:GLY:HA2	1:B:161:ARG:HH12	1.77	0.50
1:B:778:GLY:HA2	1:B:805:ALA:HB2	1.94	0.50
1:A:2369:LEU:HB2	1:A:2404:ARG:HH22	1.76	0.49
1:A:289:MET:HE1	1:A:329:GLU:HB3	1.94	0.49
1:A:1448:LEU:HD23	1:A:1829:LYS:HE3	1.93	0.49
1:A:993:ASP:HB3	1:A:1055:HIS:CE1	2.48	0.49
1:B:2084:GLY:N	1:B:2106:THR:HG21	2.27	0.49
1:B:2227:THR:C	1:B:2228:ILE:HD13	2.37	0.49
1:B:312:TYR:HB3	1:B:415:MET:HB3	1.93	0.49
1:B:1078:LYS:HE2	1:B:1097:GLN:HB3	1.93	0.49
1:B:320:THR:HG22	1:B:322:VAL:H	1.77	0.49
1:B:1852:LEU:HB3	1:B:1860:PHE:HD1	1.77	0.49
1:B:2415:ASN:O	1:B:2467:MET:HG2	2.12	0.49
1:A:103:THR:HG23	1:A:248:VAL:HG22	1.95	0.49
1:A:242:ARG:HG2	1:A:358:GLU:HB2	1.94	0.49
1:B:1454:LEU:HD11	1:B:1518:PHE:CD2	2.46	0.49
1:A:1056:ASN:HB3	1:B:2061:GLU:HB2	1.93	0.49
1:A:2009:LEU:HD13	1:A:2030:ILE:HD13	1.94	0.49
1:B:1639:ARG:HH21	1:B:1644:MET:HB3	1.78	0.49
1:A:1268:TYR:CE1	1:A:1341:ILE:HG13	2.48	0.49
1:A:1976:TYR:HB3	1:A:2144:ILE:HD13	1.95	0.49
1:A:1115:MET:HG3	1:A:1171:ILE:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:911:LEU:HD13	1:B:912:PRO:HD2	1.95	0.49
1:B:994:ILE:HG22	1:B:1158:PHE:HB3	1.93	0.49
1:B:1536:LEU:HD13	1:B:1567:GLN:HB2	1.95	0.49
1:A:664:TYR:CZ	1:A:668:LEU:HD11	2.48	0.48
1:A:1264:LEU:HD12	1:A:1322:ASP:HA	1.95	0.48
1:A:1819:ILE:HB	1:A:1826:PHE:HB2	1.95	0.48
1:A:2114:LEU:HD11	1:A:2119:PHE:HE1	1.77	0.48
1:B:462:LEU:HB2	1:B:883:PHE:HE1	1.77	0.48
1:B:1023:THR:HG22	1:B:1024:LYS:H	1.77	0.48
1:A:1564:PRO:HA	1:A:1638:LYS:HD3	1.93	0.48
1:A:2134:THR:HG22	1:A:2141:VAL:HG11	1.95	0.48
1:B:1067:LEU:HD12	1:B:1192:MET:HE1	1.95	0.48
1:A:1014:HIS:HD2	1:A:1034:LYS:HE2	1.78	0.48
1:B:214:ILE:HA	1:B:217:THR:HG22	1.96	0.48
1:B:1268:TYR:CZ	1:B:1341:ILE:HG13	2.49	0.48
1:B:1423:ASN:HB3	1:B:1463:LEU:HA	1.95	0.48
1:A:1852:LEU:HB3	1:A:1860:PHE:CD1	2.47	0.48
1:B:100:LEU:HD21	1:B:206:VAL:HB	1.94	0.48
1:B:985:ILE:HD11	1:B:1029:VAL:HG11	1.94	0.48
1:B:1686:GLU:HB2	1:B:1801:LEU:HD23	1.95	0.48
1:B:1976:TYR:HB3	1:B:2144:ILE:HD13	1.94	0.48
1:B:1993:LEU:HD21	1:B:1995:HIS:HE1	1.78	0.48
1:B:2220:THR:HA	1:B:2251:ASN:HD21	1.77	0.48
1:A:2482:GLN:HG2	1:A:2483:MET:SD	2.54	0.48
1:B:2114:LEU:HD12	1:B:2114:LEU:H	1.78	0.48
1:B:2224:LEU:HB3	1:B:2228:ILE:HD11	1.95	0.48
1:B:21:PHE:HD2	1:B:367:ILE:HD13	1.78	0.48
1:B:802:PHE:O	1:B:806:ILE:HG12	2.14	0.48
1:B:1305:GLU:O	1:B:1308:GLN:HG3	2.14	0.48
1:B:1343:LEU:HA	1:B:1346:LYS:HD3	1.96	0.48
1:A:120:GLY:HA2	1:A:169:ARG:HE	1.79	0.48
1:B:1428:LYS:HA	1:B:1431:VAL:HG22	1.96	0.48
1:A:156:SER:HB3	1:B:177:THR:HA	1.96	0.48
1:A:576:ILE:HD12	1:A:576:ILE:HA	1.77	0.48
1:A:1226:TYR:HB2	1:A:2467:MET:SD	2.54	0.48
1:A:1536:LEU:HD13	1:A:1567:GLN:HB2	1.95	0.47
1:B:1108:CYS:HB3	1:B:1176:LYS:HE3	1.96	0.47
1:B:1829:LYS:HA	1:B:1829:LYS:HD3	1.71	0.47
1:A:62:ILE:HG13	1:A:216:MET:HG2	1.96	0.47
1:A:462:LEU:HB2	1:A:883:PHE:HE1	1.79	0.47
1:A:1067:LEU:HD12	1:A:1192:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:CYS:HB3	1:A:1176:LYS:HE3	1.96	0.47
1:A:1428:LYS:HA	1:A:1431:VAL:HG22	1.96	0.47
1:A:1700:SER:O	1:A:1704:THR:HG23	2.14	0.47
1:B:103:THR:HG23	1:B:248:VAL:HG22	1.97	0.47
1:B:1577:VAL:HB	1:B:1580:PHE:HB3	1.97	0.47
1:A:583:LEU:HD23	1:A:660:VAL:HG13	1.97	0.47
1:A:1998:THR:HG21	1:A:2039:LYS:HB3	1.96	0.47
1:B:154:ALA:HB3	1:B:157:PHE:CD1	2.50	0.47
1:B:1565:LYS:N	1:B:1638:LYS:HB3	2.29	0.47
1:B:2179:GLU:HB3	1:B:2181:VAL:HG22	1.96	0.47
1:A:284:ILE:HG21	1:B:157:PHE:HE2	1.79	0.47
1:A:985:ILE:HD11	1:A:1029:VAL:HG11	1.96	0.47
1:A:1343:LEU:HA	1:A:1346:LYS:HD3	1.96	0.47
1:B:1268:TYR:CE1	1:B:1341:ILE:HG13	2.49	0.47
1:B:1270:ILE:HD11	1:B:1317:LEU:HB2	1.96	0.47
1:B:1641:ILE:HD11	1:B:1813:ILE:HD13	1.97	0.47
1:B:1700:SER:O	1:B:1704:THR:HG23	2.14	0.47
1:A:2055:TYR:HE2	1:A:2065:GLU:HG2	1.80	0.47
1:A:558:TRP:HD1	1:A:560:ASP:H	1.63	0.47
1:A:747:LYS:HE2	1:A:747:LYS:HB2	1.79	0.47
1:A:1034:LYS:HD3	1:A:1042:TRP:CH2	2.50	0.47
1:A:1524:LEU:HB3	1:A:1561:LEU:HD21	1.96	0.47
1:B:1348:ILE:HA	1:B:1351:ILE:HG22	1.95	0.47
1:B:2194:GLU:HG3	1:B:2198:LEU:HD12	1.97	0.47
1:A:484:GLN:HE22	1:A:488:LYS:HD2	1.80	0.47
1:A:1489:THR:HB	1:A:1516:ARG:NH2	2.30	0.47
1:B:805:ALA:O	1:B:809:ILE:HG23	2.15	0.47
1:A:154:ALA:HB3	1:A:157:PHE:CD1	2.49	0.46
1:A:466:SER:HB2	1:A:507:LEU:H	1.80	0.46
1:A:971:LYS:HA	1:A:971:LYS:HD3	1.75	0.46
1:A:757:LYS:HA	1:A:757:LYS:HD3	1.72	0.46
1:A:1538:ILE:HG22	1:A:1571:MET:HE1	1.97	0.46
1:A:1218:ILE:HD11	1:A:2243:TRP:HE1	1.81	0.46
1:A:1695:ILE:HG21	1:A:1703:LEU:HG	1.98	0.46
1:A:2108:LEU:HD11	1:B:2121:TYR:CZ	2.49	0.46
1:A:2195:GLN:O	1:A:2199:LYS:HG3	2.15	0.46
1:B:664:TYR:CZ	1:B:668:LEU:HD11	2.50	0.46
1:B:678:ARG:HG2	1:B:717:GLU:HG3	1.97	0.46
1:A:15:ALA:HB1	1:A:264:ILE:HG23	1.98	0.46
1:A:1852:LEU:HB3	1:A:1860:PHE:HD1	1.80	0.46
1:A:2220:THR:HA	1:A:2251:ASN:HD21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:TRP:CE3	1:B:95:PRO:HB2	2.50	0.46
1:B:561:MET:HB3	1:B:619:ILE:HD11	1.97	0.46
1:B:1896:GLN:HE22	1:B:1904:ILE:HB	1.80	0.46
1:A:806:ILE:HB	1:A:840:CYS:SG	2.55	0.46
1:A:941:GLY:HA3	1:A:953:LEU:HB2	1.96	0.46
1:A:1678:ILE:HB	1:A:1684:ILE:HG22	1.97	0.46
1:B:549:TYR:CG	1:B:634:PRO:HB3	2.50	0.46
1:B:2208:PRO:HB3	1:B:2213:LYS:HG2	1.96	0.46
1:B:2441:LEU:HD12	1:B:2442:LEU:N	2.31	0.46
1:A:177:THR:HA	1:B:156:SER:HB3	1.98	0.46
1:A:558:TRP:CD1	1:A:560:ASP:H	2.33	0.46
1:A:678:ARG:HG2	1:A:717:GLU:HG3	1.98	0.46
1:B:120:GLY:H	1:B:167:ASP:HB3	1.81	0.46
1:B:609:PRO:HD2	1:B:674:MET:HE1	1.96	0.46
1:B:993:ASP:HB3	1:B:1055:HIS:ND1	2.31	0.46
1:B:1789:PHE:HE2	1:B:1808:VAL:HG23	1.80	0.46
1:A:114:LYS:O	1:A:117:THR:HG22	2.16	0.46
1:A:332:SER:HG	1:A:396:TRP:CD1	2.34	0.46
1:A:1431:VAL:HG21	1:A:1470:GLN:HG2	1.98	0.46
1:A:2236:ILE:O	1:A:2240:ILE:HG12	2.16	0.46
1:B:369:VAL:HG21	1:B:417:ILE:HD11	1.97	0.46
1:B:1257:GLU:HG3	1:B:1627:GLN:HB2	1.96	0.46
1:B:1643:SER:HA	1:B:1806:ARG:NE	2.30	0.46
1:B:2110:GLU:C	1:B:2112:ASP:H	2.24	0.46
1:B:2245:ILE:HG23	1:B:2289:PHE:HE2	1.80	0.46
1:A:22:ARG:HB2	1:A:99:LEU:HD21	1.96	0.46
1:A:137:CYS:O	1:A:140:ARG:HG2	2.16	0.46
1:A:593:GLN:HA	1:A:596:ARG:HB2	1.98	0.46
1:A:1068:LYS:HE2	1:A:1110:PHE:CE2	2.51	0.46
1:A:2108:LEU:HD12	1:A:2108:LEU:HA	1.78	0.46
1:A:2208:PRO:HB3	1:A:2213:LYS:HB3	1.97	0.46
1:B:1900:THR:HG21	1:B:2131:GLU:HG3	1.97	0.46
1:B:1968:VAL:HG13	1:B:1972:TYR:CD2	2.51	0.46
1:A:312:TYR:HB3	1:A:415:MET:HB3	1.98	0.46
1:B:378:LEU:HG	1:B:407:PHE:HE1	1.80	0.46
1:A:1565:LYS:N	1:A:1638:LYS:HB3	2.31	0.46
1:A:1896:GLN:HE22	1:A:1904:ILE:HB	1.81	0.46
1:A:2335:LEU:HG	1:A:2386:LYS:HD2	1.98	0.46
1:B:212:PRO:O	1:B:216:MET:HG3	2.16	0.46
1:B:480:LEU:HD21	1:B:496:PHE:CZ	2.51	0.46
1:B:1486:ILE:HB	1:B:1511:LEU:HD22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1876:LYS:O	1:B:1915:GLY:HA3	2.16	0.46
1:A:549:TYR:CG	1:A:634:PRO:HB3	2.51	0.45
1:A:805:ALA:O	1:A:809:ILE:HG23	2.17	0.45
1:A:1305:GLU:O	1:A:1308:GLN:HG3	2.16	0.45
1:A:2066:ILE:HG21	1:A:2075:VAL:HG13	1.98	0.45
1:B:558:TRP:CE3	1:B:859:LYS:HB3	2.51	0.45
1:B:806:ILE:HA	1:B:809:ILE:HG12	1.99	0.45
1:B:1495:LYS:HD3	1:B:1495:LYS:HA	1.76	0.45
1:B:1854:THR:HG23	1:B:1940:HIS:HE1	1.80	0.45
1:B:2229:LEU:HB3	1:B:2324:VAL:HG23	1.98	0.45
1:A:767:VAL:H	1:A:784:LYS:NZ	2.14	0.45
1:A:1431:VAL:HA	1:A:1434:PHE:HB2	1.98	0.45
1:A:2441:LEU:HD12	1:A:2442:LEU:N	2.31	0.45
1:B:1014:HIS:O	1:B:1033:ILE:HA	2.16	0.45
1:B:1156:MET:HB2	1:B:1202:ILE:HG12	1.98	0.45
1:B:2166:PRO:HD2	1:B:2169:GLN:HB2	1.98	0.45
1:A:174:THR:HB	1:B:176:ASP:OD2	2.17	0.45
1:A:1348:ILE:HA	1:A:1351:ILE:HG22	1.98	0.45
1:A:2229:LEU:HB3	1:A:2324:VAL:HG23	1.99	0.45
1:B:583:LEU:HD23	1:B:660:VAL:HG13	1.97	0.45
1:B:1218:ILE:HD11	1:B:2243:TRP:HE1	1.81	0.45
1:A:605:GLU:HA	1:A:608:HIS:CG	2.51	0.45
1:A:2271:LYS:HE3	1:A:2271:LYS:HB3	1.84	0.45
1:B:114:LYS:O	1:B:117:THR:HG22	2.16	0.45
1:B:1777:PHE:O	1:B:1781:LEU:HD23	2.17	0.45
1:A:100:LEU:HD21	1:A:206:VAL:HB	1.98	0.45
1:B:1273:LEU:HD13	1:B:1310:ILE:HG23	1.98	0.45
1:A:768:PRO:HB2	1:A:770:VAL:O	2.17	0.45
1:A:1174:PHE:HZ	1:A:1176:LYS:HD2	1.81	0.45
1:B:1174:PHE:HZ	1:B:1176:LYS:HD2	1.81	0.45
1:A:609:PRO:HA	1:A:612:ALA:HB3	1.99	0.45
1:B:137:CYS:O	1:B:140:ARG:HG2	2.17	0.45
1:B:1349:LYS:O	1:B:1352:VAL:HG12	2.17	0.45
1:A:378:LEU:HG	1:A:407:PHE:HE1	1.82	0.45
1:A:1156:MET:HB2	1:A:1202:ILE:HG12	1.98	0.45
1:A:1909:PHE:HB3	1:A:1942:LEU:HD23	1.98	0.45
1:B:332:SER:HG	1:B:396:TRP:CD1	2.34	0.45
1:B:768:PRO:HB2	1:B:770:VAL:O	2.17	0.45
1:B:1073:PHE:HE2	1:B:2280:GLN:HA	1.82	0.45
1:B:1239:LEU:HD11	1:B:1637:GLU:HG3	1.99	0.45
1:B:1248:LYS:HE2	1:B:1248:LYS:HB3	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2204:GLU:HG3	1:B:2206:GLU:H	1.81	0.45
1:A:806:ILE:O	1:A:809:ILE:HG12	2.17	0.45
1:A:946:ALA:HA	1:B:1042:TRP:CZ2	2.52	0.45
1:A:1700:SER:HA	1:A:1703:LEU:HD12	1.98	0.45
1:B:15:ALA:HB1	1:B:264:ILE:HG23	1.98	0.45
1:B:1034:LYS:HD3	1:B:1042:TRP:CH2	2.52	0.45
1:A:2166:PRO:HD2	1:A:2169:GLN:HB2	1.99	0.45
1:B:717:GLU:HA	1:B:720:LEU:HD12	1.99	0.45
1:B:1740:LEU:HA	1:B:1743:GLN:HE21	1.82	0.45
1:A:140:ARG:HH12	1:B:142:ILE:HD11	1.81	0.44
1:B:971:LYS:HD3	1:B:971:LYS:HA	1.74	0.44
1:B:2335:LEU:HA	1:B:2386:LYS:HB2	2.00	0.44
1:A:1218:ILE:HG23	1:A:2450:GLY:HA2	1.98	0.44
1:A:1349:LYS:O	1:A:1352:VAL:HG12	2.17	0.44
1:A:1829:LYS:HA	1:A:1829:LYS:HD3	1.68	0.44
1:A:1876:LYS:O	1:A:1915:GLY:HA3	2.18	0.44
1:A:1424:GLN:HE21	1:A:1428:LYS:NZ	2.16	0.44
1:A:1577:VAL:HB	1:A:1580:PHE:HB3	1.99	0.44
1:A:2242:LYS:HB2	1:A:2242:LYS:HE2	1.66	0.44
1:B:135:GLN:HB2	1:B:153:SER:OG	2.18	0.44
1:B:775:THR:HB	1:B:800:VAL:HG13	1.98	0.44
1:B:2357:ASN:O	1:B:2361:LEU:HG	2.17	0.44
1:A:1789:PHE:CE1	1:A:1816:ARG:HD3	2.51	0.44
1:A:2119:PHE:CE2	1:B:2125:TYR:HD2	2.36	0.44
1:B:773:PHE:CE1	1:B:780:GLN:HB3	2.52	0.44
1:A:1616:ASN:HB3	1:A:1629:PRO:HB3	2.00	0.44
1:A:1868:LEU:HD23	1:A:1869:PRO:HD2	1.99	0.44
1:B:492:LEU:HB2	1:B:495:ASP:OD1	2.18	0.44
1:B:1028:LYS:HE2	1:B:1030:GLU:CD	2.42	0.44
1:B:1226:TYR:HD2	1:B:2467:MET:HE1	1.83	0.44
1:A:176:ASP:OD2	1:B:174:THR:HB	2.16	0.44
1:A:1073:PHE:HE2	1:A:2280:GLN:HA	1.83	0.44
1:A:1234:ASP:HB3	1:A:1641:ILE:HG21	2.00	0.44
1:A:2245:ILE:HG23	1:A:2289:PHE:HE2	1.82	0.44
1:B:1678:ILE:HB	1:B:1684:ILE:HG22	1.99	0.44
1:A:255:SER:O	1:A:258:ILE:HG13	2.18	0.44
1:A:269:LYS:HB2	1:A:430:ILE:HG22	2.00	0.44
1:A:480:LEU:HD21	1:A:496:PHE:CZ	2.53	0.44
1:A:1350:ARG:HA	1:A:1350:ARG:HD3	1.88	0.44
1:A:2360:ASN:O	1:A:2364:GLU:HG2	2.18	0.44
1:B:671:ASN:C	1:B:674:MET:HE3	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:767:VAL:H	1:B:784:LYS:NZ	2.16	0.44
1:B:1613:GLU:O	1:B:1634:VAL:HA	2.18	0.44
1:A:1732:LYS:HB2	1:A:1732:LYS:HE3	1.83	0.44
1:B:233:PHE:CZ	1:B:328:ILE:HD11	2.53	0.44
1:B:1108:CYS:HB3	1:B:1176:LYS:HG3	2.00	0.44
1:B:1448:LEU:HD21	1:B:1450:LYS:HE3	2.00	0.44
1:A:301:LYS:HE3	1:A:301:LYS:HB3	1.67	0.43
1:A:373:LEU:HD23	1:A:373:LEU:HA	1.84	0.43
1:A:554:GLN:HA	1:A:616:ILE:HD12	1.99	0.43
1:A:1613:GLU:O	1:A:1634:VAL:HA	2.18	0.43
1:A:2206:GLU:HB3	1:A:2211:LEU:HD11	2.00	0.43
1:A:2357:ASN:O	1:A:2361:LEU:HG	2.18	0.43
1:B:1248:LYS:HB2	1:B:1620:ASP:H	1.83	0.43
1:B:1516:ARG:HG2	1:B:2494:TYR:HB3	2.00	0.43
1:B:1550:ASP:HB3	1:B:1553:GLU:HG3	2.00	0.43
1:B:1802:THR:HA	1:B:1805:LEU:HD12	2.00	0.43
1:B:1840:SER:HB2	1:B:2457:GLN:NE2	2.32	0.43
1:B:1868:LEU:HD23	1:B:1869:PRO:HD2	1.99	0.43
1:A:806:ILE:HA	1:A:809:ILE:HG12	1.99	0.43
1:A:1900:THR:HG21	1:A:2131:GLU:HG3	2.01	0.43
1:B:510:ARG:NH1	1:B:878:GLY:HA2	2.33	0.43
1:B:935:PRO:HA	1:B:954:PHE:HE1	1.82	0.43
1:A:492:LEU:HB2	1:A:495:ASP:OD1	2.17	0.43
1:A:636:ILE:HD13	1:A:771:PRO:HB2	2.00	0.43
1:A:392:LYS:HB3	1:A:395:ASP:HB2	2.00	0.43
1:B:2336:PRO:HA	1:B:2339:ILE:HD11	2.00	0.43
1:A:2416:TRP:CZ3	1:A:2468:LEU:HD23	2.53	0.43
1:B:30:PRO:HB3	1:B:371:LEU:HD21	2.01	0.43
1:B:37:LEU:HD23	1:B:37:LEU:HA	1.82	0.43
1:A:700:ILE:HD11	1:A:713:ILE:HB	2.00	0.43
1:A:707:ASP:HA	1:A:803:THR:OG1	2.19	0.43
1:A:1108:CYS:HB3	1:A:1176:LYS:HG3	2.01	0.43
1:A:1840:SER:HB2	1:A:2457:GLN:NE2	2.34	0.43
1:A:2226:ASN:HB2	1:A:2322:LYS:HG3	2.00	0.43
1:B:255:SER:O	1:B:258:ILE:HG13	2.18	0.43
1:B:1446:LYS:HG2	1:B:1483:ASN:HA	2.01	0.43
1:B:1865:LYS:HE2	1:B:1865:LYS:HB3	1.91	0.43
1:B:2129:ASP:OD2	1:B:2132:ARG:HG3	2.18	0.43
1:A:573:LYS:O	1:A:576:ILE:HG22	2.19	0.43
1:A:775:THR:HB	1:A:800:VAL:HG13	2.00	0.43
1:A:1597:GLU:HG2	1:A:1601:LYS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1713:LYS:HE2	1:A:1753:ARG:HH21	1.84	0.43
1:B:1220:TYR:HB2	1:B:2212:ASN:HB3	2.00	0.43
1:B:1489:THR:HB	1:B:1516:ARG:NH2	2.34	0.43
1:B:2326:HIS:O	1:B:2375:PHE:HB2	2.19	0.43
1:A:933:ARG:HH21	1:A:942:HIS:HB3	1.83	0.43
1:A:1273:LEU:HD13	1:A:1310:ILE:HG23	2.00	0.43
1:A:1524:LEU:HD11	1:A:1557:LYS:HG2	1.99	0.43
1:A:1550:ASP:HB3	1:A:1553:GLU:HG3	2.00	0.43
1:A:1682:PHE:CD1	1:A:1801:LEU:HD22	2.54	0.43
1:A:2378:ILE:HD11	1:A:2469:SER:OG	2.19	0.43
1:B:58:GLU:HB3	1:B:1121:PHE:CE1	2.54	0.43
1:B:747:LYS:HE2	1:B:747:LYS:HB2	1.79	0.43
1:B:1202:ILE:HG21	1:B:1205:VAL:HG23	2.00	0.43
1:B:1451:ILE:HG12	1:B:1536:LEU:HB3	2.00	0.43
1:B:1795:LYS:HD3	1:B:1795:LYS:HA	1.79	0.43
1:B:2192:ASN:O	1:B:2195:GLN:HG3	2.17	0.43
1:A:30:PRO:HB3	1:A:371:LEU:HD21	2.01	0.43
1:A:1258:LYS:HA	1:A:1258:LYS:HD2	1.82	0.43
1:A:2046:LYS:HA	1:A:2046:LYS:HD2	1.93	0.43
1:B:126:PHE:O	1:B:203:VAL:HA	2.18	0.43
1:B:989:PHE:CD1	1:B:1052:LEU:HD11	2.53	0.43
1:B:1068:LYS:HE2	1:B:1110:PHE:CE2	2.53	0.43
1:B:1356:LYS:HE3	1:B:1356:LYS:HB3	1.84	0.43
1:B:1538:ILE:HG12	1:B:1569:ILE:HD12	2.00	0.43
1:B:1842:ASN:HD21	1:B:2220:THR:H	1.67	0.43
1:A:154:ALA:HB3	1:A:157:PHE:HD1	1.84	0.43
1:A:1067:LEU:HD23	1:A:1067:LEU:HA	1.73	0.43
1:A:1538:ILE:HG12	1:A:1569:ILE:HD12	2.01	0.43
1:B:269:LYS:HB2	1:B:430:ILE:HG22	2.01	0.43
1:B:466:SER:HB2	1:B:507:LEU:H	1.84	0.43
1:B:2226:ASN:HB2	1:B:2322:LYS:HG3	2.01	0.43
1:B:2264:ILE:HB	1:B:2293:TYR:HB2	2.01	0.43
1:B:2325:LEU:HD22	1:B:2373:ILE:HB	2.01	0.43
1:A:1034:LYS:HD3	1:A:1042:TRP:CZ2	2.54	0.42
1:B:130:MET:HE2	1:B:130:MET:O	2.19	0.42
1:B:2007:ASN:HB3	1:B:2157:LEU:HD11	2.01	0.42
1:B:2335:LEU:HG	1:B:2386:LYS:HD2	2.01	0.42
1:A:640:HIS:CG	1:A:641:SER:H	2.37	0.42
1:A:2094:LEU:HD11	1:A:2100:ILE:HG12	2.01	0.42
1:A:2335:LEU:HA	1:A:2386:LYS:HB2	2.00	0.42
1:B:968:HIS:HB2	1:B:1096:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1340:GLU:O	1:B:1344:ILE:HG13	2.19	0.42
1:B:1524:LEU:HG	1:B:1561:LEU:HD11	2.00	0.42
1:B:1713:LYS:HE2	1:B:1753:ARG:HH21	1.84	0.42
1:A:1082:TYR:CZ	1:A:1097:GLN:HA	2.55	0.42
1:A:2264:ILE:HB	1:A:2293:TYR:HB2	2.02	0.42
1:B:97:GLN:O	1:B:101:MET:HE3	2.19	0.42
1:B:706:ASN:HB3	1:B:836:TYR:CG	2.53	0.42
1:B:1014:HIS:HD2	1:B:1036:ASN:HA	1.84	0.42
1:B:1564:PRO:HA	1:B:1638:LYS:HD3	2.01	0.42
1:B:1723:LEU:HD21	1:B:1757:LEU:HG	2.02	0.42
1:B:1728:ILE:HG23	1:B:1729:GLU:HG3	2.00	0.42
1:B:2012:LYS:HD2	1:B:2012:LYS:HA	1.93	0.42
1:B:2236:ILE:O	1:B:2240:ILE:HG12	2.19	0.42
1:B:2251:ASN:ND2	1:B:2257:GLN:HE21	2.16	0.42
1:A:126:PHE:O	1:A:203:VAL:HA	2.18	0.42
1:A:969:LYS:O	1:A:1091:PRO:HG2	2.19	0.42
1:A:1435:ASP:HA	1:A:1438:ILE:HG12	2.00	0.42
1:A:1723:LEU:HD21	1:A:1757:LEU:HG	2.01	0.42
1:B:871:ILE:HD13	1:B:871:ILE:HA	1.94	0.42
1:B:1616:ASN:HB3	1:B:1629:PRO:HB3	2.02	0.42
1:A:2125:TYR:HD2	1:B:2119:PHE:HE2	1.66	0.42
1:A:2326:HIS:O	1:A:2375:PHE:HB2	2.19	0.42
1:B:467:ALA:HB3	1:B:473:LEU:HB2	2.01	0.42
1:B:857:LEU:HD11	1:B:863:GLU:HB3	2.02	0.42
1:B:950:LEU:HD11	1:B:1016:GLN:NE2	2.34	0.42
1:B:1138:LEU:HD11	1:B:1187:GLY:HA3	2.02	0.42
1:B:2094:LEU:HD23	1:B:2094:LEU:HA	1.89	0.42
1:B:2360:ASN:O	1:B:2364:GLU:HG2	2.18	0.42
1:A:1042:TRP:CZ2	1:B:946:ALA:HA	2.55	0.42
1:A:1840:SER:HB2	1:A:2457:GLN:HE21	1.85	0.42
1:A:1882:ILE:HG22	1:A:2177:ILE:HD12	2.02	0.42
1:B:154:ALA:HB3	1:B:157:PHE:HD1	1.84	0.42
1:B:640:HIS:CG	1:B:641:SER:H	2.37	0.42
1:B:1082:TYR:CZ	1:B:1097:GLN:HA	2.55	0.42
1:B:1353:SER:HA	1:B:1356:LYS:HE3	2.01	0.42
1:A:233:PHE:CZ	1:A:328:ILE:HD11	2.55	0.42
1:A:263:ARG:HD3	1:A:906:GLU:HA	2.02	0.42
1:A:2336:PRO:HA	1:A:2339:ILE:HD11	2.01	0.42
1:B:558:TRP:CD1	1:B:560:ASP:H	2.35	0.42
1:B:583:LEU:HD23	1:B:583:LEU:HA	1.83	0.42
1:B:2368:LYS:HE3	1:B:2368:LYS:HB3	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2441:LEU:HD12	1:B:2442:LEU:H	1.85	0.42
1:A:21:PHE:HD2	1:A:367:ILE:HD13	1.84	0.42
1:A:627:TYR:CE2	1:A:825:LEU:HD21	2.55	0.42
1:B:512:VAL:HG21	1:B:872:SER:HA	2.00	0.42
1:B:1115:MET:HE3	1:B:1115:MET:HB3	1.95	0.42
1:B:1475:LEU:HD23	1:B:1510:LEU:HB2	2.01	0.42
1:B:1538:ILE:HG22	1:B:1571:MET:HE1	2.02	0.42
1:A:140:ARG:NH1	1:B:142:ILE:HD11	2.34	0.42
1:A:311:TYR:HB3	1:A:413:ILE:HG23	2.01	0.42
1:A:989:PHE:CD1	1:A:1052:LEU:HD11	2.54	0.42
1:B:1459:GLN:HG2	1:B:1460:ASN:H	1.83	0.42
1:B:1819:ILE:HB	1:B:1826:PHE:HB2	2.01	0.42
1:A:837:ILE:HD13	1:A:837:ILE:HA	1.83	0.42
1:A:2249:VAL:HG21	1:A:2285:TYR:CZ	2.54	0.42
1:A:2261:ASP:OD1	1:A:2290:ARG:HB2	2.19	0.42
1:B:373:LEU:HD23	1:B:373:LEU:HA	1.86	0.42
1:B:757:LYS:HA	1:B:757:LYS:HD3	1.74	0.42
1:B:806:ILE:O	1:B:809:ILE:HG12	2.20	0.42
1:B:1212:ARG:HB2	1:B:1905:TYR:CE2	2.55	0.42
1:B:1425:LEU:HD13	1:B:1617:ILE:HD13	2.01	0.42
1:B:2301:LEU:HD12	1:B:2302:ASN:N	2.35	0.42
1:A:802:PHE:O	1:A:806:ILE:HG12	2.18	0.41
1:A:968:HIS:HB2	1:A:1096:PHE:CE2	2.54	0.41
1:B:62:ILE:HG13	1:B:216:MET:HG2	2.02	0.41
1:B:1541:LEU:HD22	1:B:1544:VAL:HG21	2.02	0.41
1:B:1682:PHE:CD1	1:B:1801:LEU:HD22	2.55	0.41
1:B:2010:LYS:HE3	1:B:2010:LYS:HB2	1.78	0.41
1:A:212:PRO:O	1:A:216:MET:HG3	2.20	0.41
1:A:369:VAL:HG21	1:A:417:ILE:HD11	2.01	0.41
1:B:933:ARG:HH21	1:B:942:HIS:HB3	1.84	0.41
1:A:1023:THR:HA	1:B:2112:ASP:OD2	2.20	0.41
1:A:1959:ASN:HD21	1:A:2153:SER:HA	1.85	0.41
1:B:578:HIS:NE2	1:B:582:LEU:HD11	2.35	0.41
1:B:1350:ARG:HA	1:B:1350:ARG:HD3	1.86	0.41
1:B:1913:CYS:HB2	1:B:1941:SER:OG	2.20	0.41
1:A:682:ILE:HD11	1:A:711:ILE:HG12	2.01	0.41
1:A:717:GLU:HA	1:A:720:LEU:HD12	2.02	0.41
1:A:1202:ILE:HG21	1:A:1205:VAL:HG23	2.02	0.41
1:A:1233:LYS:H	1:A:1826:PHE:HA	1.86	0.41
1:A:2199:LYS:O	1:A:2203:GLN:HB2	2.21	0.41
1:A:2325:LEU:HD22	1:A:2373:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ARG:HD3	1:B:906:GLU:HA	2.02	0.41
1:B:935:PRO:HA	1:B:954:PHE:CE1	2.54	0.41
1:B:1073:PHE:HB2	1:B:1104:ILE:O	2.21	0.41
1:B:1686:GLU:OE1	1:B:1801:LEU:HB3	2.20	0.41
1:A:578:HIS:NE2	1:A:582:LEU:HD11	2.35	0.41
1:A:1212:ARG:HB2	1:A:1905:TYR:CE2	2.55	0.41
1:A:1851:TYR:CD2	1:A:1945:LEU:HB2	2.56	0.41
1:A:1958:GLU:CD	1:A:1958:GLU:H	2.29	0.41
1:A:2192:ASN:O	1:A:2195:GLN:HG3	2.21	0.41
1:B:752:LYS:O	1:B:755:ILE:HG13	2.19	0.41
1:B:969:LYS:O	1:B:1091:PRO:HG2	2.21	0.41
1:B:2487:MET:HG2	1:B:2490:HIS:CE1	2.56	0.41
1:A:191:GLN:O	1:A:195:THR:HG23	2.21	0.41
1:A:554:GLN:CD	1:A:613:GLN:HG2	2.45	0.41
1:A:752:LYS:O	1:A:755:ILE:HG13	2.20	0.41
1:A:1014:HIS:O	1:A:1033:ILE:HA	2.21	0.41
1:A:1340:GLU:O	1:A:1344:ILE:HG13	2.20	0.41
1:B:311:TYR:HB3	1:B:413:ILE:HG23	2.02	0.41
1:B:1312:LYS:HB3	1:B:1312:LYS:HE2	1.82	0.41
1:B:1470:GLN:O	1:B:1473:GLN:HG2	2.21	0.41
1:B:1597:GLU:HG2	1:B:1601:LYS:HD2	2.02	0.41
1:A:706:ASN:HB3	1:A:836:TYR:CG	2.56	0.41
1:A:1353:SER:HA	1:A:1356:LYS:HE3	2.03	0.41
1:A:2301:LEU:HD12	1:A:2302:ASN:N	2.35	0.41
1:B:621:VAL:HA	1:B:624:VAL:HG22	2.03	0.41
1:B:2195:GLN:O	1:B:2200:PRO:HD3	2.20	0.41
1:B:2452:LEU:HA	1:B:2455:VAL:HG12	2.03	0.41
1:A:467:ALA:HB3	1:A:473:LEU:HB2	2.03	0.41
1:A:1475:LEU:HA	1:A:1475:LEU:HD12	1.84	0.41
1:A:1499:SER:HA	1:A:1502:GLU:HG2	2.03	0.41
1:A:2487:MET:HG2	1:A:2490:HIS:CE1	2.55	0.41
1:B:58:GLU:HB3	1:B:1121:PHE:CZ	2.55	0.41
1:B:1271:ARG:CZ	1:B:1322:ASP:HB3	2.50	0.41
1:A:512:VAL:HG21	1:A:872:SER:HA	2.01	0.41
1:A:1438:ILE:HD12	1:A:1478:LEU:HD21	2.02	0.41
1:A:2114:LEU:HD13	1:B:2116:PHE:HE1	1.85	0.41
1:A:2351:LYS:HE2	1:A:2390:TYR:CE1	2.56	0.41
1:A:2368:LYS:HE3	1:A:2368:LYS:HB3	1.74	0.41
1:A:2441:LEU:HD12	1:A:2442:LEU:H	1.84	0.41
1:B:233:PHE:CE1	1:B:317:GLY:HA3	2.55	0.41
1:B:437:ASN:HD21	1:B:440:GLU:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:752:LYS:HD2	1:B:793:TYR:CZ	2.56	0.41
1:B:939:LEU:O	1:B:953:LEU:HD22	2.21	0.41
1:B:993:ASP:HB3	1:B:1055:HIS:CE1	2.55	0.41
1:B:1497:ILE:HD13	1:B:1497:ILE:HA	1.93	0.41
1:B:1754:PHE:HB3	1:B:1788:THR:HG23	2.03	0.41
1:B:2008:LEU:HD23	1:B:2008:LEU:HA	1.89	0.41
1:B:2152:ILE:HD13	1:B:2152:ILE:HA	1.94	0.41
1:B:2163:LYS:HG2	1:B:2165:PHE:CE1	2.55	0.41
1:A:120:GLY:H	1:A:167:ASP:HB3	1.86	0.41
1:A:1153:LEU:HD13	1:A:1202:ILE:HD13	2.02	0.41
1:A:1312:LYS:HE2	1:A:1312:LYS:HB3	1.81	0.41
1:A:1475:LEU:HD23	1:A:1510:LEU:HB2	2.03	0.41
1:A:1541:LEU:HD22	1:A:1544:VAL:HG21	2.03	0.41
1:A:1865:LYS:HE2	1:A:1865:LYS:HB3	1.85	0.41
1:A:1875:ILE:HD11	1:A:1953:ILE:HD13	2.03	0.41
1:A:2174:ILE:O	1:A:2177:ILE:HG22	2.21	0.41
1:A:2373:ILE:HA	1:A:2412:THR:O	2.21	0.41
1:B:1234:ASP:HB3	1:B:1641:ILE:HG21	2.03	0.41
1:B:1866:GLU:OE2	1:B:1866:GLU:N	2.54	0.41
1:B:2477:LEU:HD13	1:B:2484:LYS:HG2	2.03	0.41
1:A:366:LEU:HD12	1:A:366:LEU:HA	1.96	0.40
1:A:679:LEU:HD22	1:A:714:THR:OG1	2.21	0.40
1:A:1495:LYS:HD3	1:A:1495:LYS:HA	1.77	0.40
1:A:1536:LEU:HD11	1:A:1569:ILE:HD11	2.01	0.40
1:B:609:PRO:HA	1:B:612:ALA:HB3	2.02	0.40
1:B:671:ASN:O	1:B:674:MET:HE3	2.21	0.40
1:B:2351:LYS:HE2	1:B:2390:TYR:CE1	2.55	0.40
1:A:671:ASN:O	1:A:674:MET:HG2	2.22	0.40
1:A:840:CYS:SG	1:A:840:CYS:O	2.79	0.40
1:A:2251:ASN:ND2	1:A:2257:GLN:HE21	2.18	0.40
1:A:2432:ALA:O	1:A:2435:LEU:HD12	2.21	0.40
1:B:191:GLN:O	1:B:195:THR:HG23	2.20	0.40
1:B:301:LYS:HE3	1:B:301:LYS:HB3	1.67	0.40
1:B:919:GLU:HB3	1:B:921:TYR:CE1	2.57	0.40
1:B:1135:PHE:N	1:B:1135:PHE:CD1	2.89	0.40
1:B:1253:LYS:HD2	1:B:1627:GLN:HG3	2.02	0.40
1:A:57:TYR:CD2	1:A:65:GLU:HB3	2.57	0.40
1:A:510:ARG:HH12	1:A:878:GLY:CA	2.30	0.40
1:A:1041:LYS:HE2	1:A:1041:LYS:HB3	1.87	0.40
1:A:1356:LYS:HE3	1:A:1356:LYS:HB3	1.85	0.40
1:A:1497:ILE:HD13	1:A:1497:ILE:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2431:VAL:O	1:A:2435:LEU:HG	2.21	0.40
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.92	0.40
1:B:392:LYS:HB3	1:B:395:ASP:HB2	2.02	0.40
1:B:1226:TYR:HD1	1:B:1832:LYS:HA	1.86	0.40
1:B:1438:ILE:HD11	1:B:1484:ILE:HG21	2.04	0.40
1:B:1936:GLY:HA3	1:B:1953:ILE:HG22	2.02	0.40
1:B:2145:LEU:HD23	1:B:2145:LEU:HA	1.93	0.40
1:B:2249:VAL:HG21	1:B:2285:TYR:CZ	2.56	0.40
1:A:823:ILE:HG23	1:A:852:ILE:HB	2.03	0.40
1:A:859:LYS:HB3	1:A:859:LYS:HE2	1.88	0.40
1:A:919:GLU:HB3	1:A:921:TYR:CE1	2.56	0.40
1:A:1266:ASN:HB3	1:A:1317:LEU:HD22	2.03	0.40
1:A:1597:GLU:HG3	1:A:1632:LEU:HD22	2.04	0.40
1:A:1639:ARG:HH21	1:A:1644:MET:HA	1.86	0.40
1:A:1646:LEU:HA	1:A:1809:ASP:OD1	2.21	0.40
1:B:627:TYR:CE2	1:B:825:LEU:HD21	2.55	0.40
1:B:837:ILE:HD13	1:B:837:ILE:HA	1.82	0.40
1:B:1514:LYS:HB3	1:B:1516:ARG:HD3	2.03	0.40
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.86	0.40
1:A:1452:ILE:HD11	1:A:1534:TYR:CG	2.56	0.40
1:A:1896:GLN:HA	1:A:1899:PHE:CD2	2.56	0.40
1:B:75:TRP:HE1	1:B:244:GLU:CD	2.30	0.40
1:B:1789:PHE:CE1	1:B:1816:ARG:HD3	2.57	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	2357/2603 (90%)	2257 (96%)	100 (4%)	0	100	100
1	B	2357/2603 (90%)	2250 (96%)	107 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4714/5206 (90%)	4507 (96%)	207 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	2145/2360 (91%)	2050 (96%)	95 (4%)	25	49
1	B	2145/2360 (91%)	2061 (96%)	84 (4%)	28	51
All	All	4290/4720 (91%)	4111 (96%)	179 (4%)	28	50

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	SER
1	A	93	ILE
1	A	101	MET
1	A	108	PHE
1	A	168	LEU
1	A	174	THR
1	A	216	MET
1	A	232	SER
1	A	255	SER
1	A	302	LYS
1	A	327	GLU
1	A	401	VAL
1	A	402	THR
1	A	422	LEU
1	A	442	LEU
1	A	480	LEU
1	A	587	PHE
1	A	598	LEU
1	A	606	ILE
1	A	619	ILE

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Mol	Chain	Res	Type
1	A	630	PHE
1	A	672	LEU
1	A	699	GLU
1	A	713	ILE
1	A	741	CYS
1	A	744	HIS
1	A	773	PHE
1	A	795	ASN
1	A	802	PHE
1	A	836	TYR
1	A	847	ILE
1	A	853	ILE
1	A	871	ILE
1	A	872	SER
1	A	874	LEU
1	A	918	PHE
1	A	937	ASN
1	A	949	THR
1	A	950	LEU
1	A	954	PHE
1	A	955	ILE
1	A	995	THR
1	A	1014	HIS
1	A	1015	LEU
1	A	1016	GLN
1	A	1017	THR
1	A	1052	LEU
1	A	1086	LEU
1	A	1096	PHE
1	A	1149	VAL
1	A	1153	LEU
1	A	1154	GLN
1	A	1166	THR
1	A	1234	ASP
1	A	1341	ILE
1	A	1346	LYS
1	A	1351	ILE
1	A	1418	PHE
1	A	1437	LEU
1	A	1466	LEU
1	A	1497	ILE
1	A	1509	ASN

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Mol	Chain	Res	Type
1	A	1516	ARG
1	A	1542	LEU
1	A	1594	ILE
1	A	1596	SER
1	A	1603	LEU
1	A	1634	VAL
1	A	1696	GLU
1	A	1721	VAL
1	A	1752	THR
1	A	1777	PHE
1	A	1833	GLU
1	A	1883	ASN
1	A	1884	TYR
1	A	1930	VAL
1	A	1970	VAL
1	A	1992	ILE
1	A	2001	VAL
1	A	2009	LEU
1	A	2016	LEU
1	A	2025	SER
1	A	2079	LEU
1	A	2083	SER
1	A	2092	ARG
1	A	2097	VAL
1	A	2103	LEU
1	A	2116	PHE
1	A	2127	THR
1	A	2129	ASP
1	A	2178	ASN
1	A	2187	VAL
1	A	2199	LYS
1	A	2311	VAL
1	A	2476	LEU
1	B	55	SER
1	B	58	GLU
1	B	70	LEU
1	B	101	MET
1	B	103	THR
1	B	108	PHE
1	B	174	THR
1	B	255	SER
1	B	302	LYS

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Mol	Chain	Res	Type
1	B	327	GLU
1	B	402	THR
1	B	442	LEU
1	B	576	ILE
1	B	587	PHE
1	B	600	SER
1	B	606	ILE
1	B	619	ILE
1	B	644	GLU
1	B	699	GLU
1	B	769	CYS
1	B	773	PHE
1	B	795	ASN
1	B	800	VAL
1	B	836	TYR
1	B	847	ILE
1	B	853	ILE
1	B	871	ILE
1	B	872	SER
1	B	874	LEU
1	B	918	PHE
1	B	937	ASN
1	B	949	THR
1	B	950	LEU
1	B	954	PHE
1	B	955	ILE
1	B	995	THR
1	B	1017	THR
1	B	1043	THR
1	B	1052	LEU
1	B	1074	THR
1	B	1086	LEU
1	B	1096	PHE
1	B	1149	VAL
1	B	1153	LEU
1	B	1154	GLN
1	B	1166	THR
1	B	1341	ILE
1	B	1346	LYS
1	B	1352	VAL
1	B	1418	PHE
1	B	1464	SER

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Mol	Chain	Res	Type
1	B	1497	ILE
1	B	1516	ARG
1	B	1542	LEU
1	B	1594	ILE
1	B	1634	VAL
1	B	1777	PHE
1	B	1833	GLU
1	B	1847	THR
1	B	1865	LYS
1	B	1883	ASN
1	B	1884	TYR
1	B	1930	VAL
1	B	1951	ASP
1	B	1963	ASN
1	B	1970	VAL
1	B	1992	ILE
1	B	1996	SER
1	B	2009	LEU
1	B	2016	LEU
1	B	2031	TYR
1	B	2055	TYR
1	B	2063	CYS
1	B	2079	LEU
1	B	2092	ARG
1	B	2097	VAL
1	B	2103	LEU
1	B	2114	LEU
1	B	2127	THR
1	B	2203	GLN
1	B	2296	VAL
1	B	2311	VAL
1	B	2406	SER
1	B	2468	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	32	GLN
1	A	64	ASN
1	A	226	HIS
1	A	338	ASN

Continued on next page...

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Mol	Chain	Res	Type
1	A	353	ASN
1	A	381	ASN
1	A	484	GLN
1	A	526	ASN
1	A	554	GLN
1	A	585	ASN
1	A	844	ASN
1	A	887	GLN
1	A	962	HIS
1	A	1056	ASN
1	A	1255	ASN
1	A	1342	ASN
1	A	1424	GLN
1	A	1460	ASN
1	A	1472	ASN
1	A	1473	GLN
1	A	1496	ASN
1	A	1527	ASN
1	A	1586	ASN
1	A	1787	ASN
1	A	1822	ASN
1	A	1896	GLN
1	A	2251	ASN
1	A	2457	GLN
1	B	28	ASN
1	B	32	GLN
1	B	35	ASN
1	B	64	ASN
1	B	160	ASN
1	B	226	HIS
1	B	484	GLN
1	B	526	ASN
1	B	554	GLN
1	B	585	ASN
1	B	613	GLN
1	B	706	ASN
1	B	844	ASN
1	B	962	HIS
1	B	988	GLN
1	B	1415	ASN
1	B	1460	ASN
1	B	1472	ASN

Continued on next page...

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Mol	Chain	Res	Type
1	B	1496	ASN
1	B	1527	ASN
1	B	1531	ASN
1	B	1586	ASN
1	B	1691	ASN
1	B	1787	ASN
1	B	1896	GLN
1	B	2021	ASN
1	B	2239	HIS
1	B	2251	ASN
1	B	2457	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.

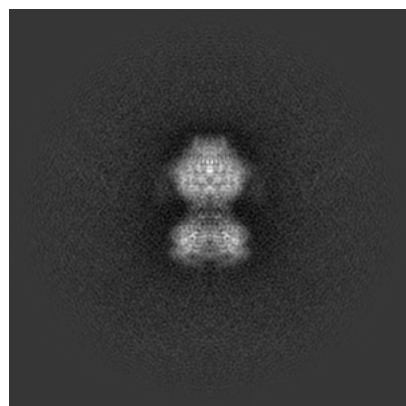
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49491. These allow visual inspection of the internal detail of the map and identification of artifacts.

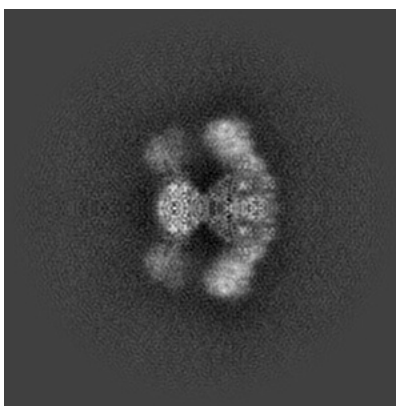
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

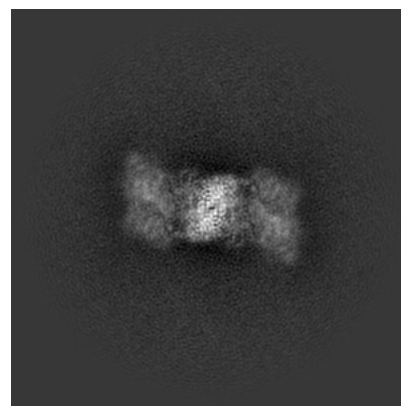
6.1.1 Primary map



X

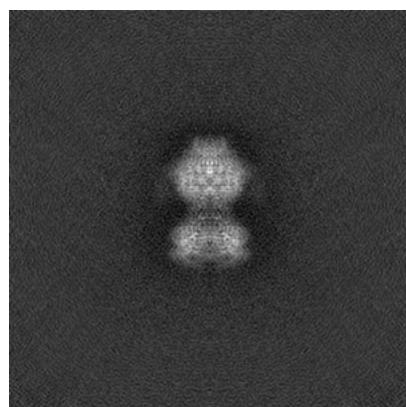


Y

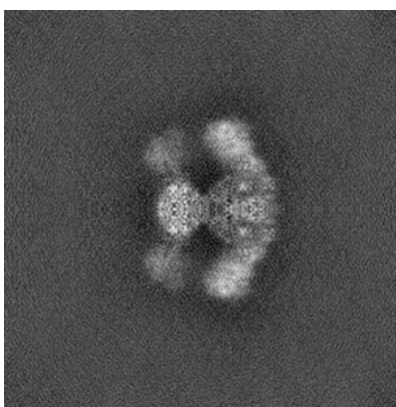


Z

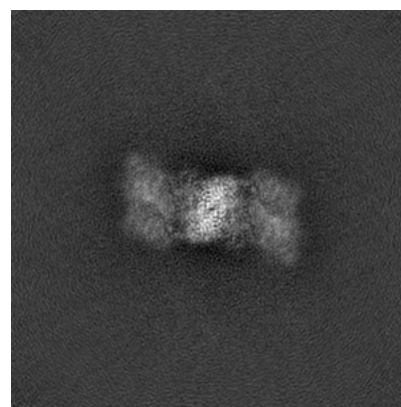
6.1.2 Raw map



X



Y

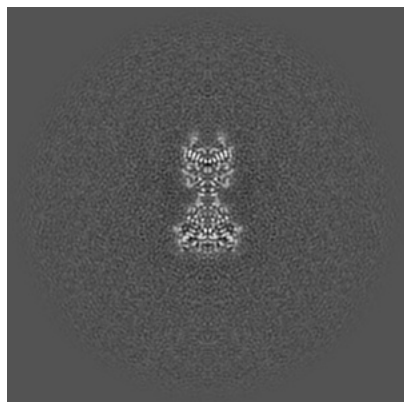


Z

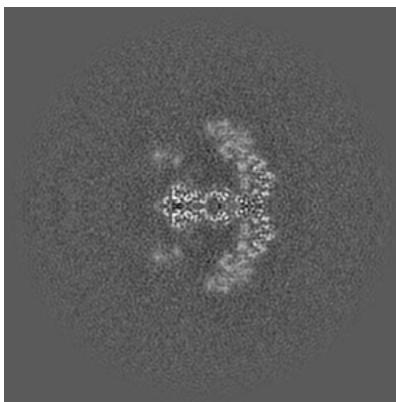
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

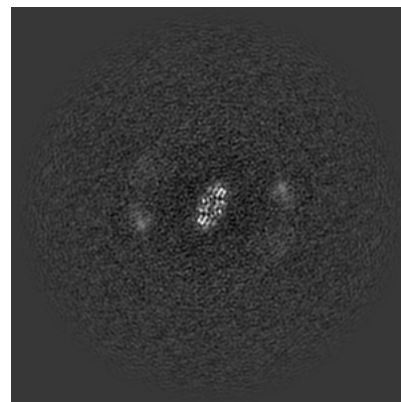
6.2.1 Primary map



X Index: 128

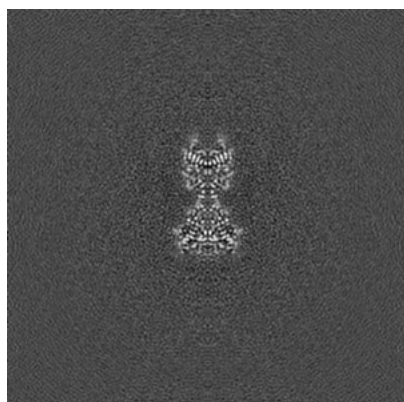


Y Index: 128

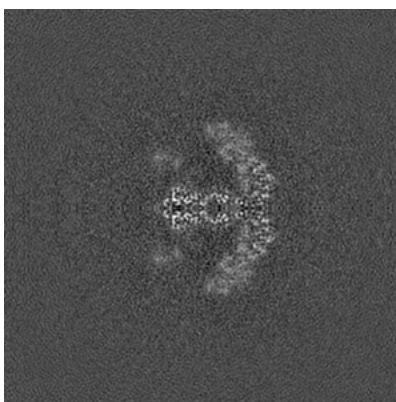


Z Index: 128

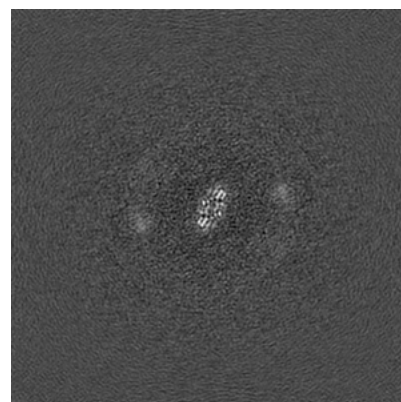
6.2.2 Raw map



X Index: 128



Y Index: 128

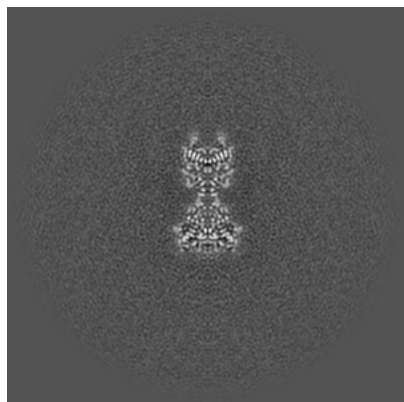


Z Index: 128

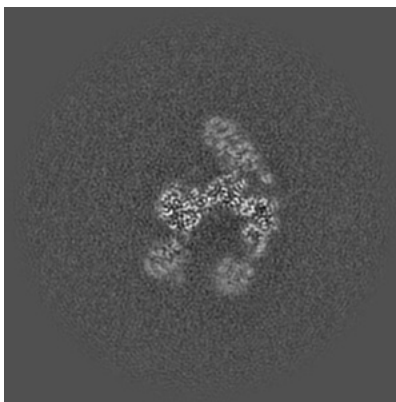
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

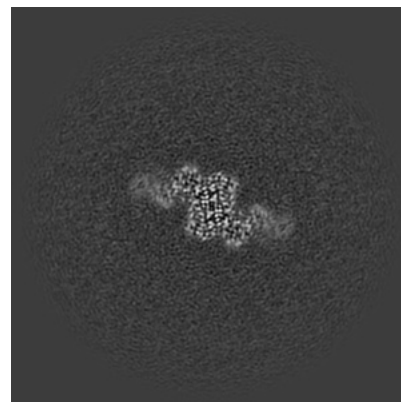
6.3.1 Primary map



X Index: 128

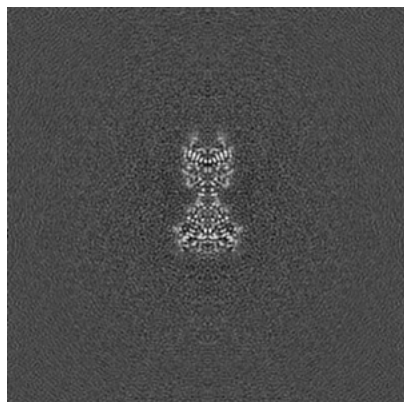


Y Index: 135

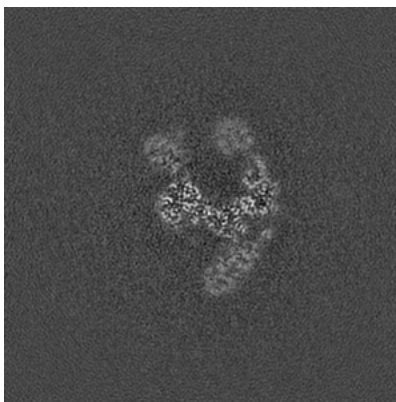


Z Index: 110

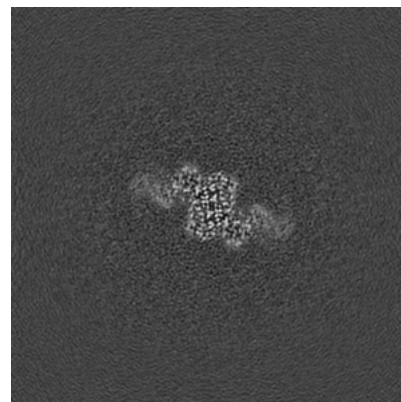
6.3.2 Raw map



X Index: 128



Y Index: 121

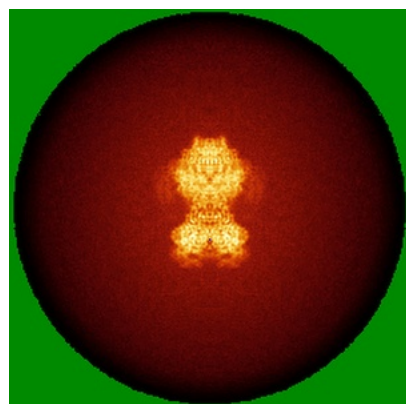


Z Index: 110

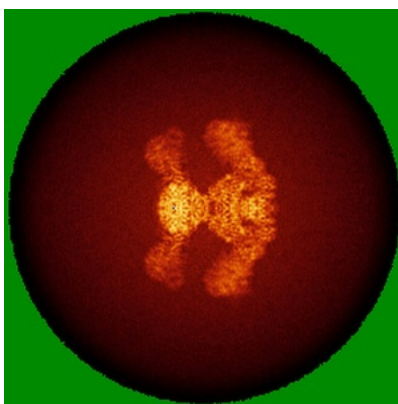
The images above show the largest variance slices of the map in three orthogonal directions.

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

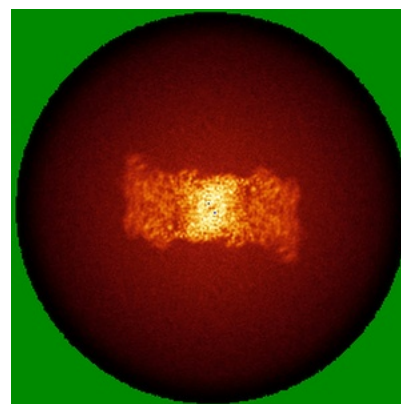
6.4.1 Primary map



X

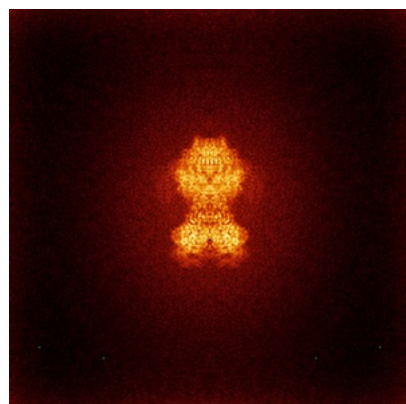


Y

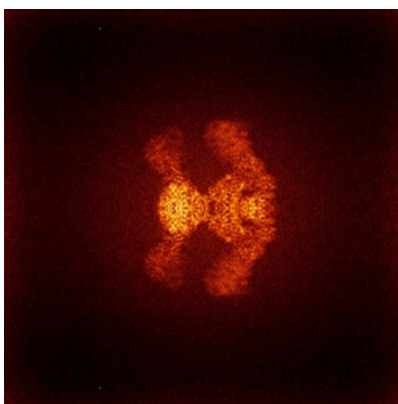


Z

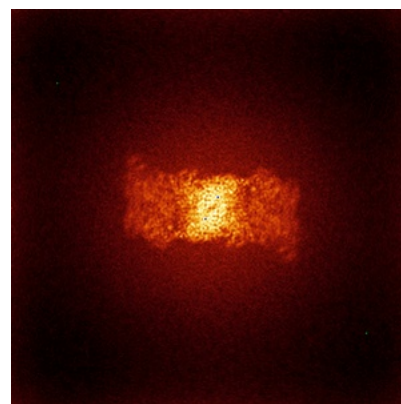
6.4.2 Raw map



X



Y



Z

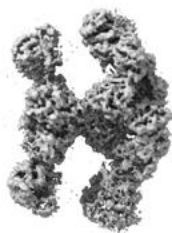
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.239. 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.

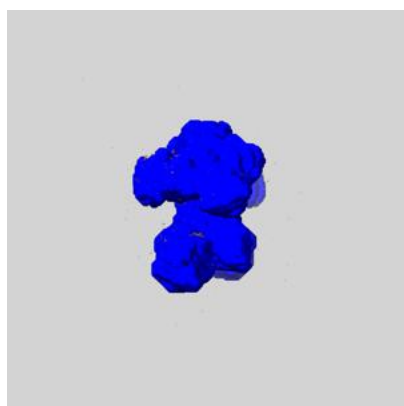
6.6 Mask visualisation [i](#)

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

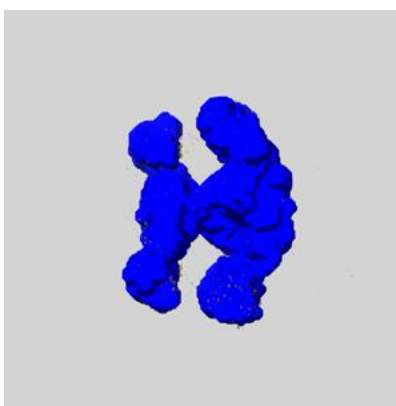
A mask typically either:

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

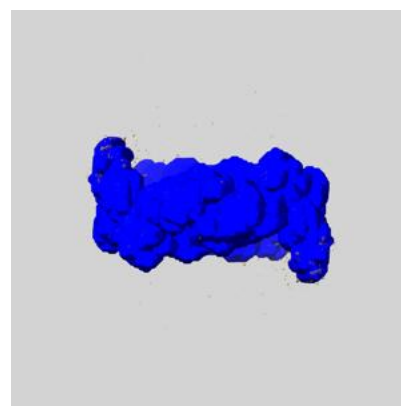
6.6.1 emd_49491_msk_1.map [i](#)



X



Y

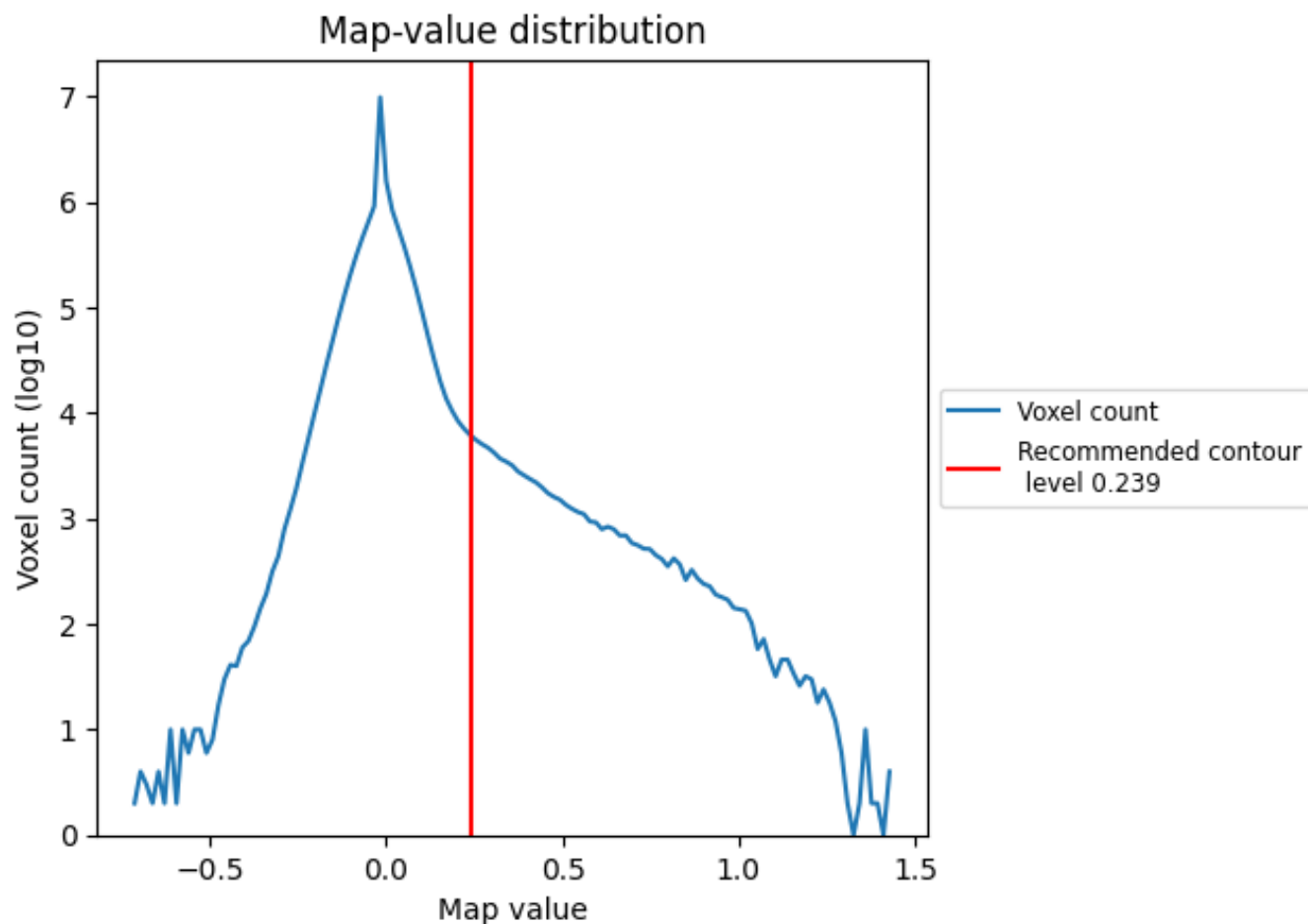


Z

7 Map analysis [i](#)

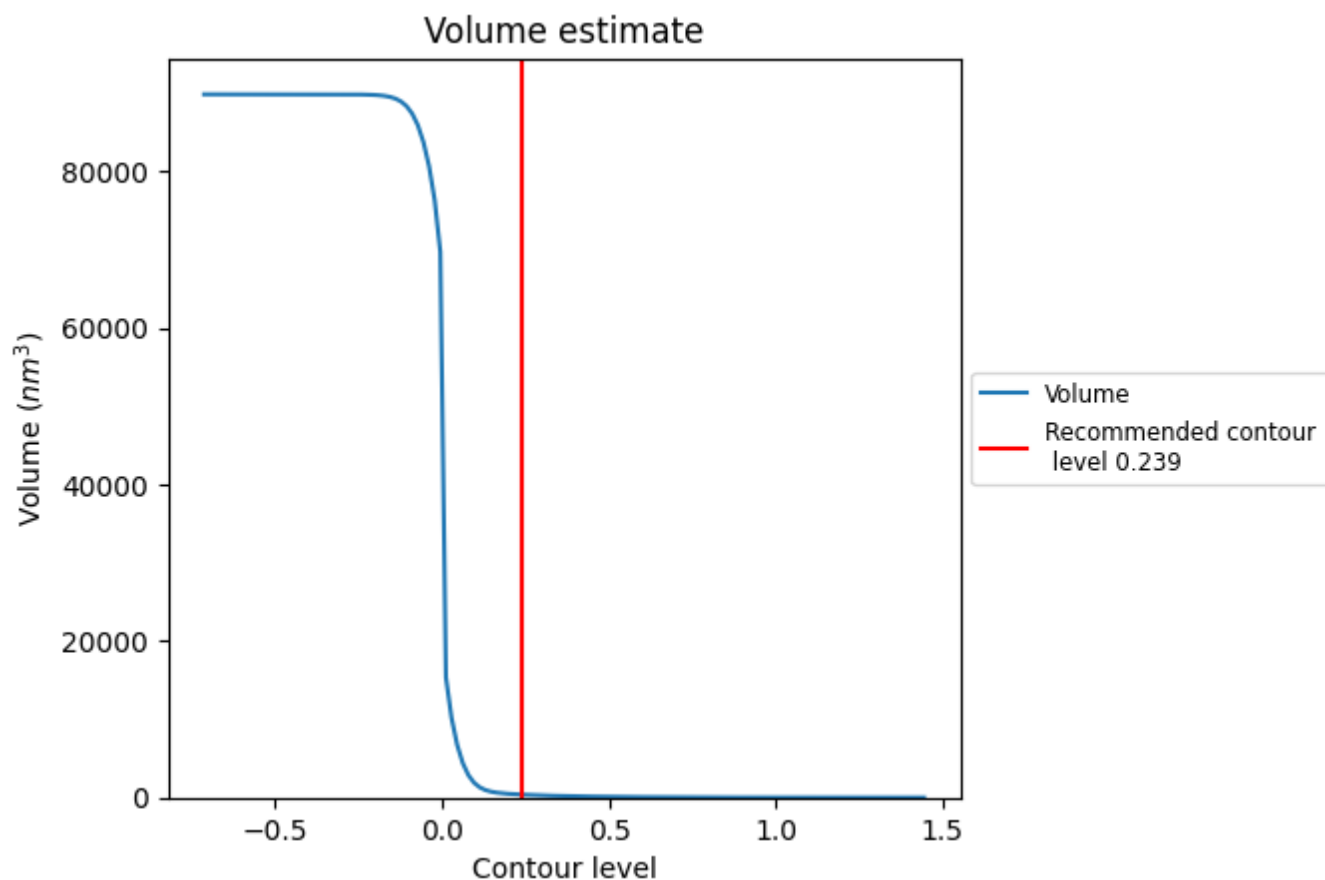
This section contains the results of statistical analysis of the map.

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.

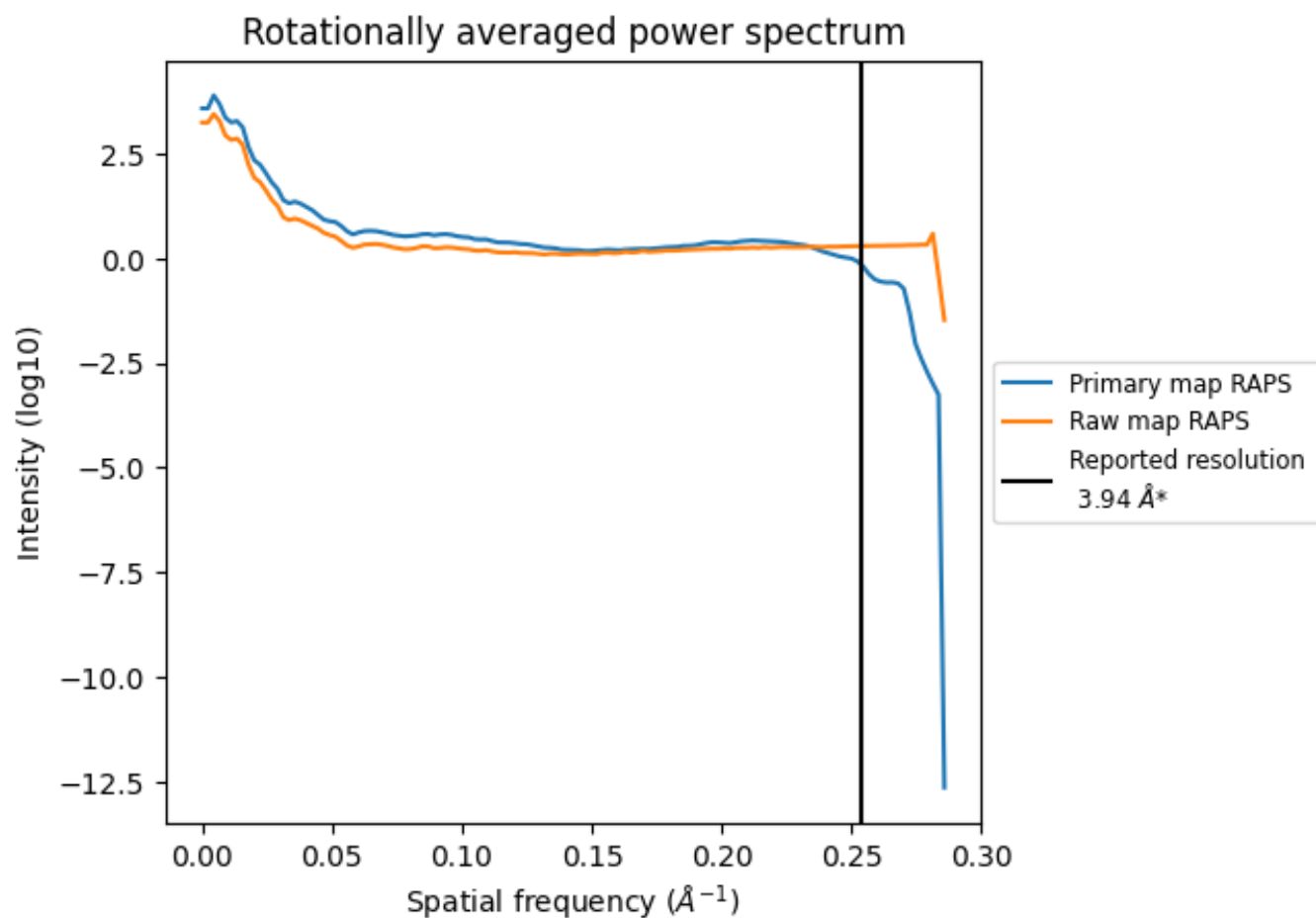
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 376 nm³; this corresponds to an approximate mass of 340 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 ⓘ

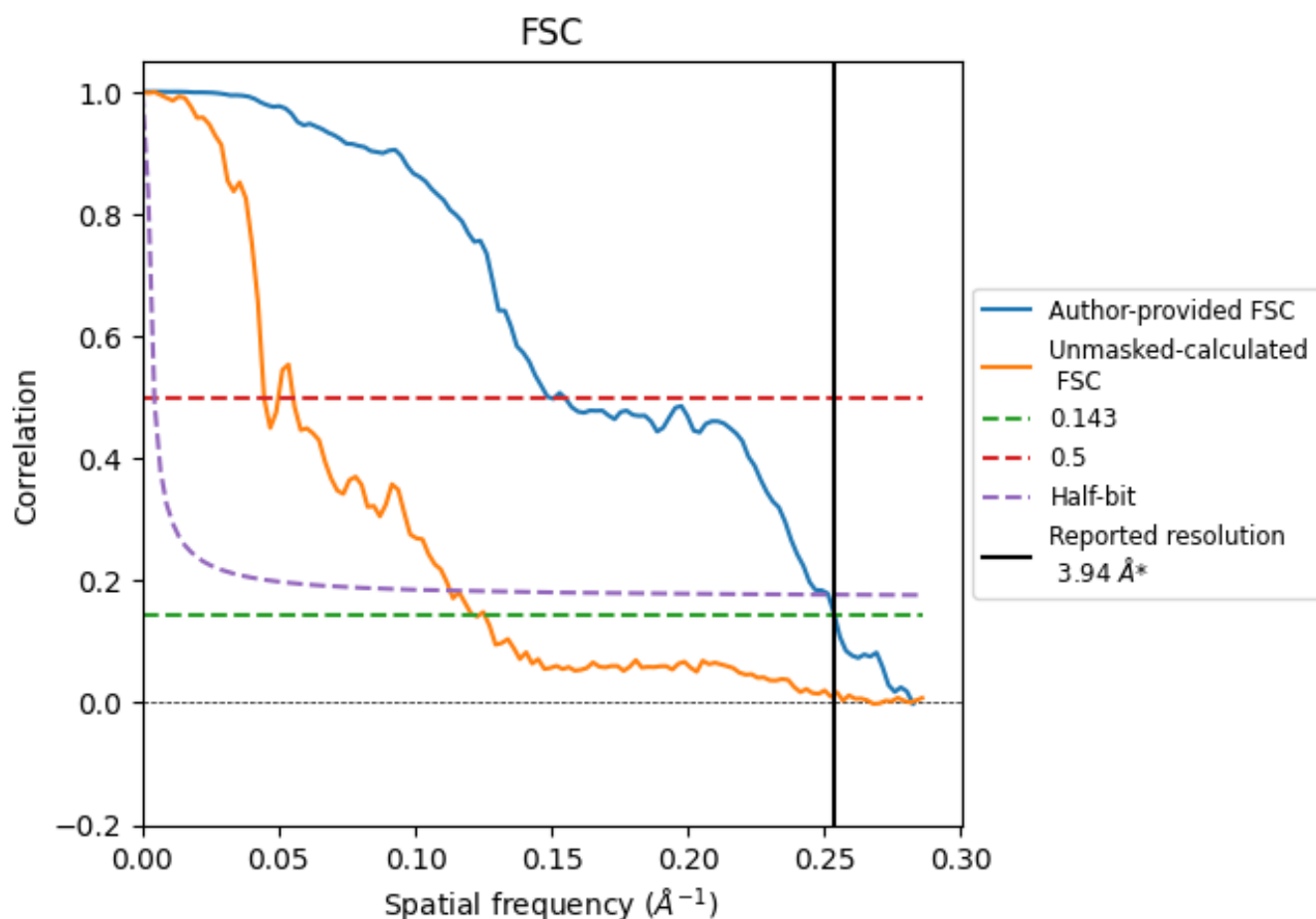


*Reported resolution corresponds to spatial frequency of 0.254 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.254 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

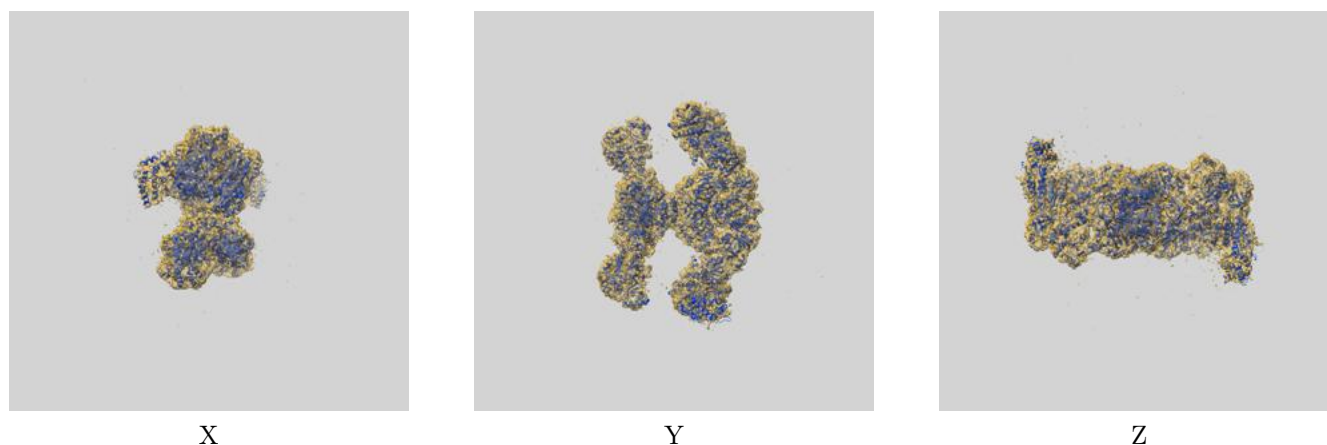
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.94	-	-
Author-provided FSC curve	3.94	6.71	3.98
Unmasked-calculated*	8.22	22.42	8.87

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.22 differs from the reported value 3.94 by more than 10 %

9 Map-model fit [i](#)

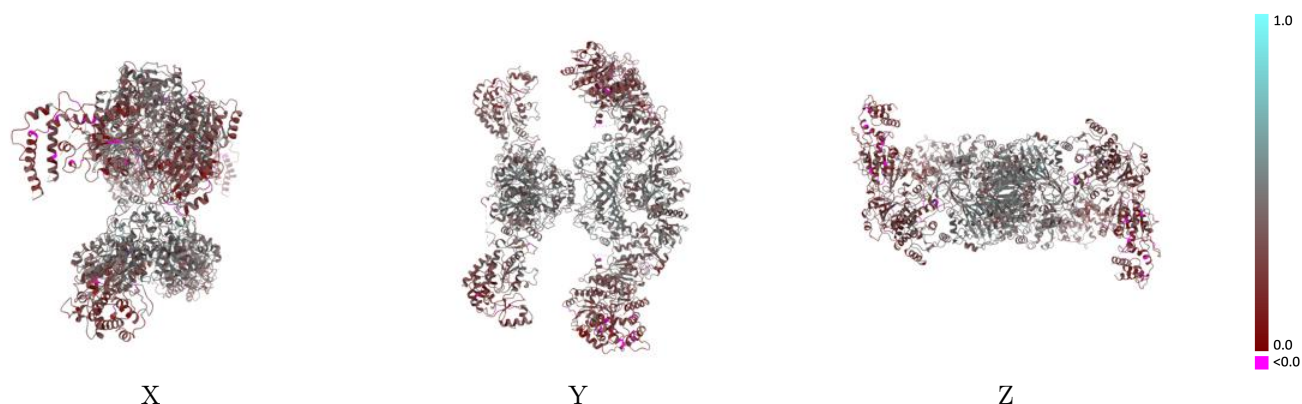
This section contains information regarding the fit between EMDB map EMD-49491 and PDB model 9NJU. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



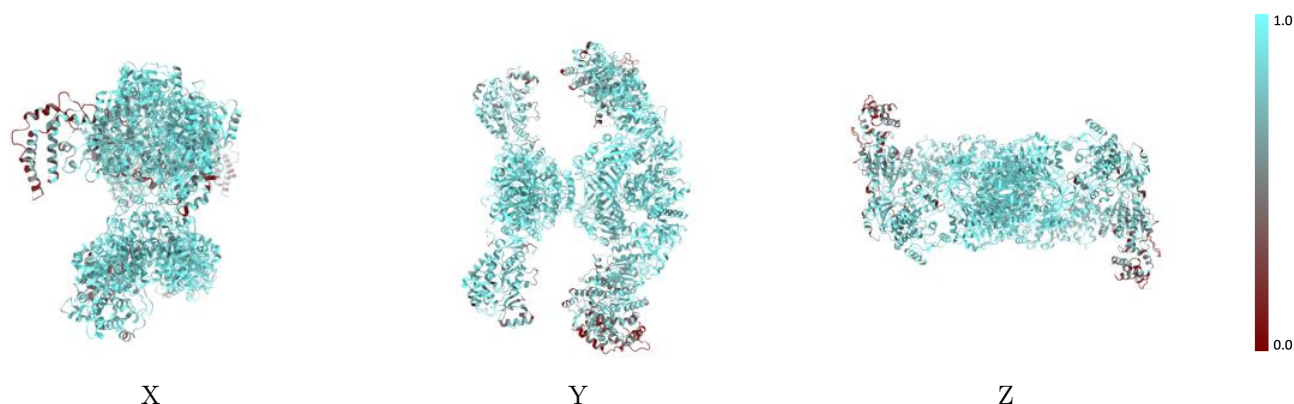
The images above show the 3D surface view of the map at the recommended contour level 0.239 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



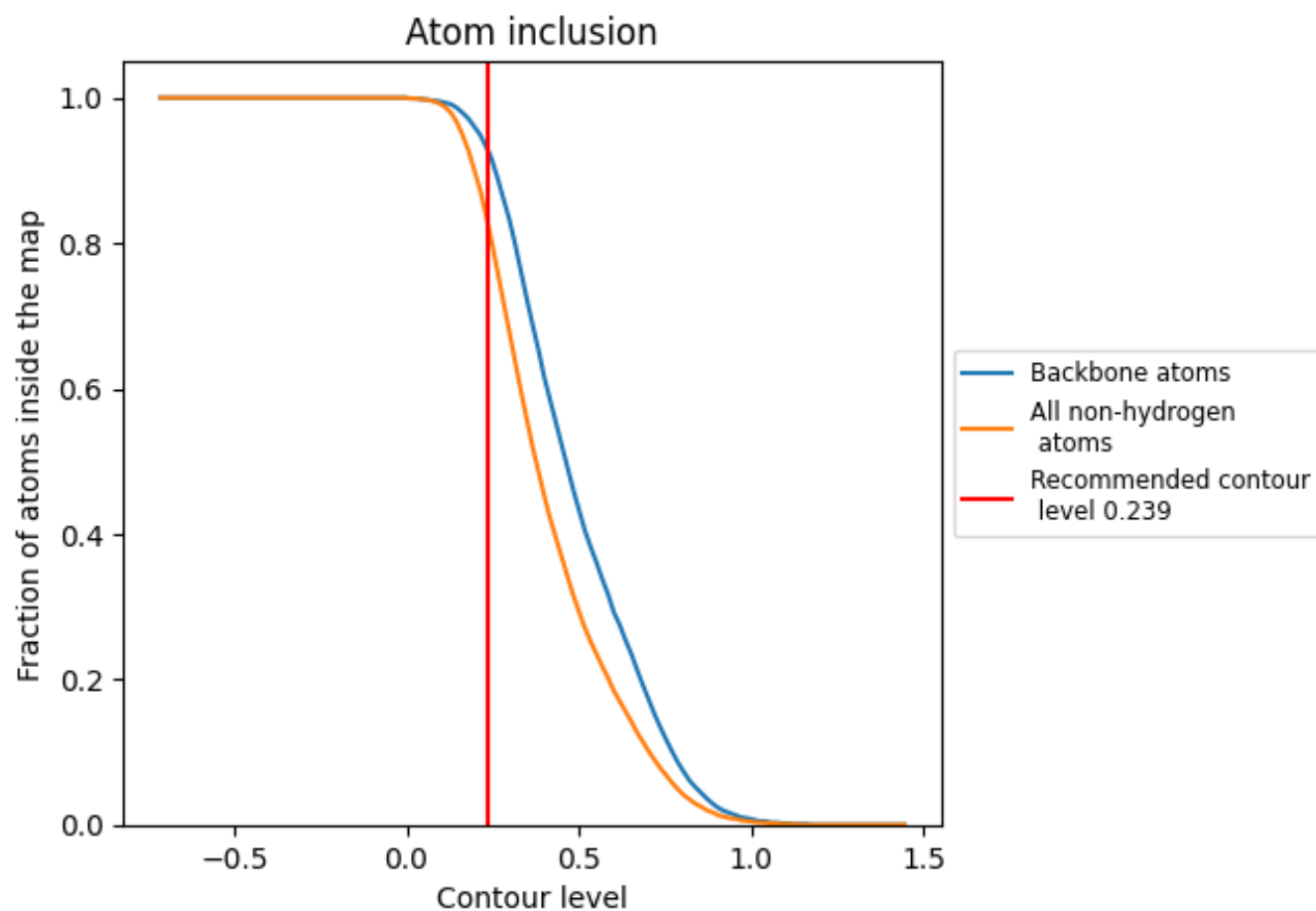
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.239).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 82% 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 (0.239) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8210	0.3720
A	0.8210	0.3720
B	0.8210	0.3710

