



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:47 AM UTC

PDB ID : 8X2H / pdb_00008x2h
EMDB ID : EMD-38010
Title : Cryo-EM structure of the TcsL at pH 5.0 in its closed conformation
Authors : Zhan, X.; Tao, L.
Deposited on : 2023-11-09
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

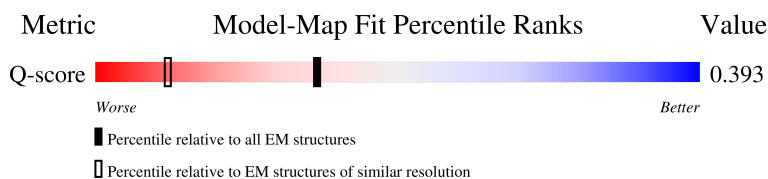
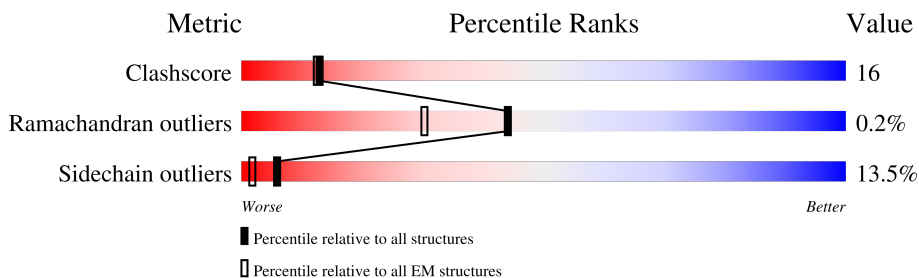
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2372	9% 57% 38% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19088 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 Cytotoxin-L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2363	Total	C	N	O	S	0	0
			19087	12219	3035	3786	47		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2365	HIS	-	expression tag	UNP T0D3N5
A	2366	HIS	-	expression tag	UNP T0D3N5
A	2367	HIS	-	expression tag	UNP T0D3N5
A	2368	HIS	-	expression tag	UNP T0D3N5
A	2369	HIS	-	expression tag	UNP T0D3N5
A	2370	HIS	-	expression tag	UNP T0D3N5
A	2371	HIS	-	expression tag	UNP T0D3N5
A	2372	HIS	-	expression tag	UNP T0D3N5

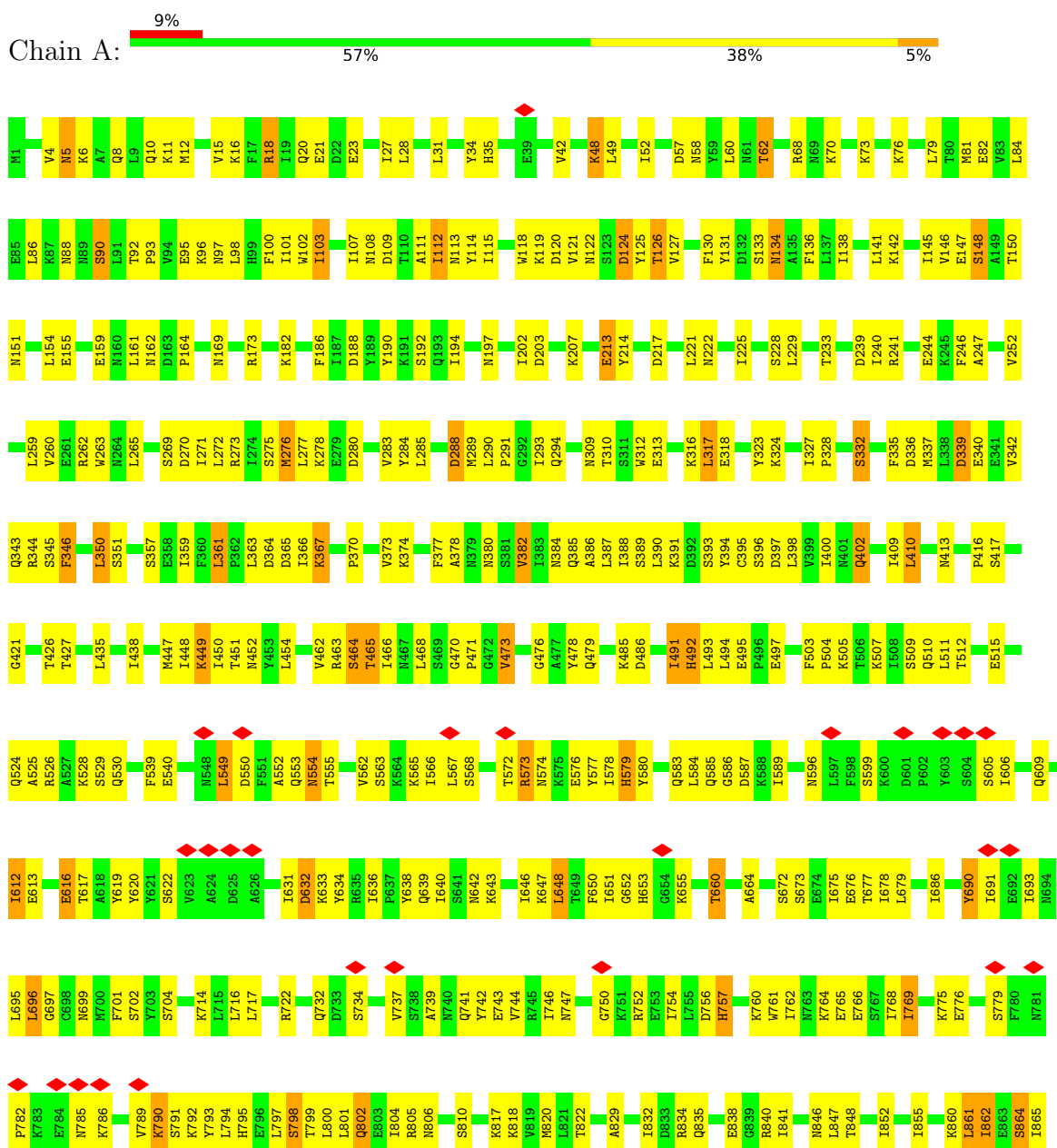
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

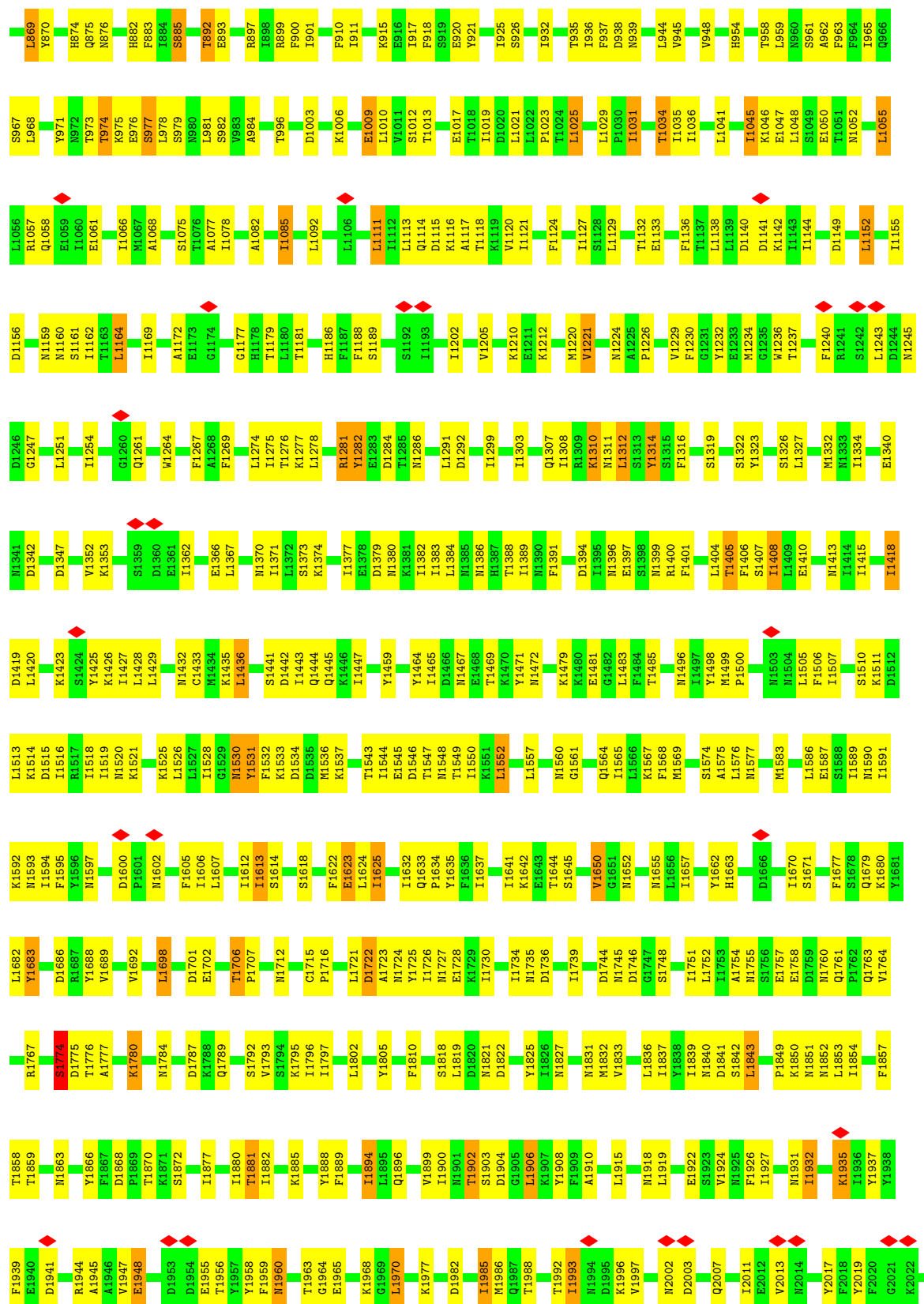
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	

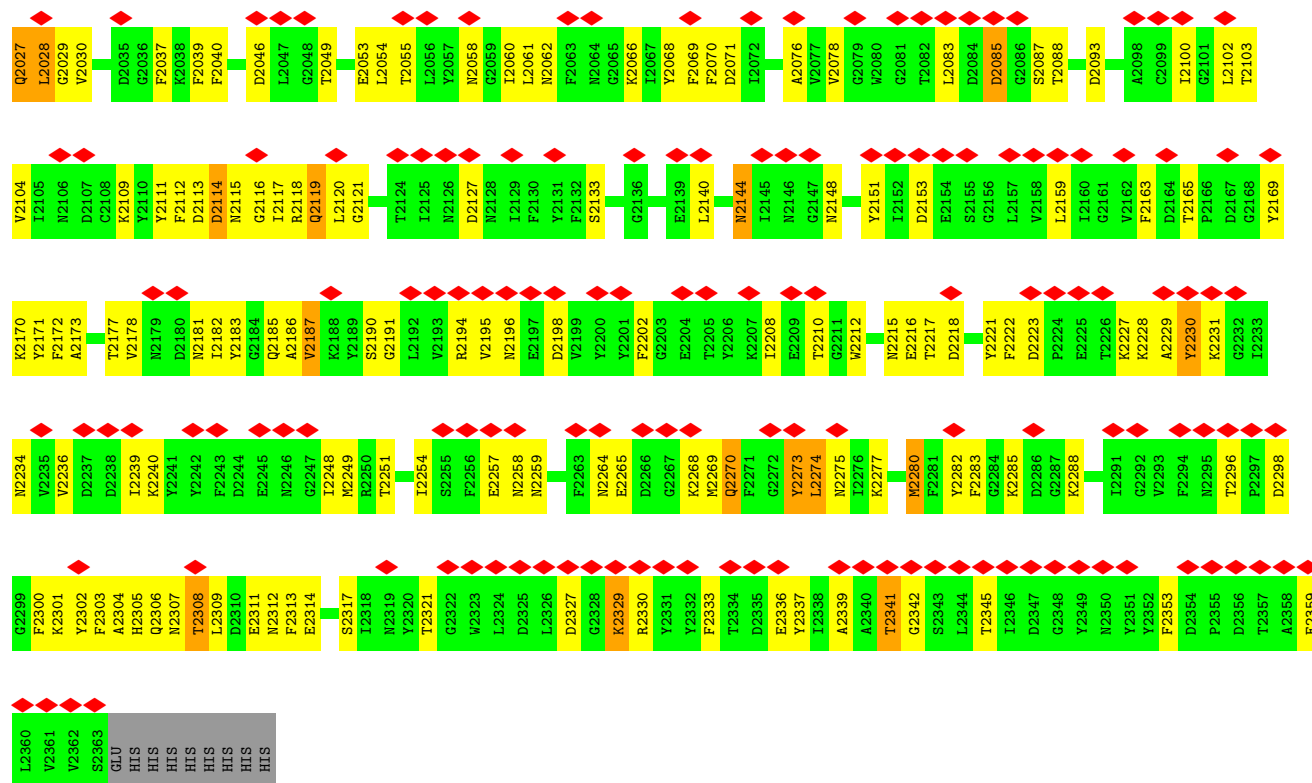
3 Residue-property plots

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: Cytotoxin-L







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	410049	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.347	Depositor
Minimum map value	-2.594	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.22	Depositor
Map size ($\text{\AA}$)	434.80002, 434.80002, 434.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.22	2/19471 (0.0%)	0.51	3/26343 (0.0%)

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	A	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1683	TYR	C-N	-5.34	1.25	1.33
1	A	1683	TYR	C-O	-5.20	1.17	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1683	TYR	CB-CA-C	-15.03	85.50	109.70
1	A	1650	VAL	CB-CA-C	-6.54	103.75	110.88
1	A	1683	TYR	CA-C-O	6.29	128.07	121.15

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1068	ALA	Peptide
1	A	1774	SER	Peptide

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Mol	Chain	Res	Type	Group
1	A	841	ILE	Peptide

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	19087	0	18641	621	0
2	A	1	0	0	0	0
All	All	19088	0	18641	621	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 16.

All (621) 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:578:ILE:O	1:A:647:LYS:HB3	1.66	0.96
1:A:2028:LEU:HA	1:A:2040:PHE:O	1.73	0.89
1:A:2307:ASN:ND2	1:A:2312:ASN:O	2.05	0.88
1:A:1052:ASN:HD21	1:A:1057:ARG:HB3	1.40	0.86
1:A:1547:THR:O	1:A:1597:ASN:ND2	2.10	0.84
1:A:410:LEU:HD13	1:A:468:LEU:HD11	1.60	0.83
1:A:2058:ASN:ND2	1:A:2071:ASP:O	2.12	0.81
1:A:1760:ASN:HA	1:A:1849:PRO:HD3	1.62	0.81
1:A:12:MET:SD	1:A:975:LYS:NZ	2.55	0.80
1:A:5:ASN:OD1	1:A:5:ASN:N	2.15	0.79
1:A:84:LEU:O	1:A:88:ASN:ND2	2.16	0.77
1:A:1116:LYS:HZ3	1:A:1118:THR:HG22	1.49	0.77
1:A:1590:ASN:OD1	1:A:1593:ASN:ND2	2.19	0.76
1:A:2307:ASN:O	1:A:2309:LEU:N	2.12	0.76
1:A:124:ASP:OD1	1:A:124:ASP:N	2.17	0.76
1:A:1432:ASN:HB3	1:A:1435:LYS:HB2	1.67	0.76
1:A:2259:ASN:HB3	1:A:2288:LYS:HG2	1.67	0.76
1:A:339:ASP:OD1	1:A:339:ASP:N	2.16	0.75
1:A:1234:MET:HE1	1:A:1264:TRP:HA	1.68	0.75
1:A:1574:SER:HB2	1:A:1836:LEU:HG	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2240:LYS:NZ	1:A:2269:MET:SD	2.59	0.74
1:A:109:ASP:O	1:A:113:ASN:ND2	2.21	0.74
1:A:1377:ILE:HD11	1:A:1420:LEU:HD23	1.70	0.74
1:A:119:LYS:HB3	1:A:127:VAL:HG21	1.68	0.73
1:A:1960:ASN:OD1	1:A:1960:ASN:N	2.22	0.73
1:A:1377:ILE:HD11	1:A:1420:LEU:HA	1.71	0.73
1:A:2264:ASN:HB3	1:A:2270:GLN:HE22	1.54	0.72
1:A:125:TYR:OH	1:A:363:LEU:O	2.04	0.72
1:A:2222:PHE:HA	1:A:2229:ALA:HA	1.71	0.72
1:A:366:ILE:HG12	1:A:507:LYS:HE2	1.71	0.72
1:A:1832:MET:HE3	1:A:1851:ASN:HD22	1.55	0.71
1:A:95:GLU:OE1	1:A:95:GLU:N	2.18	0.71
1:A:646:ILE:HG23	1:A:691:ILE:HA	1.71	0.71
1:A:58:ASN:O	1:A:62:THR:OG1	2.09	0.71
1:A:373:VAL:HG23	1:A:395:CYS:HB3	1.73	0.71
1:A:1863:ASN:HD22	1:A:1894:ILE:HD13	1.56	0.71
1:A:801:LEU:HD21	1:A:805:ARG:HH11	1.56	0.71
1:A:1758:GLU:HB2	1:A:1761:GLN:HG3	1.72	0.70
1:A:754:ILE:HD11	1:A:764:LYS:HB3	1.72	0.70
1:A:1115:ASP:O	1:A:1277:LYS:NZ	2.23	0.70
1:A:1121:ILE:HD13	1:A:1245:ASN:HD21	1.56	0.70
1:A:1680:LYS:O	1:A:1683:TYR:HD2	1.74	0.70
1:A:528:LYS:NZ	1:A:699:ASN:OD1	2.24	0.69
1:A:578:ILE:HB	1:A:646:ILE:HA	1.74	0.69
1:A:148:SER:OG	1:A:182:LYS:NZ	2.24	0.69
1:A:549:LEU:HD21	1:A:589:ILE:HD12	1.73	0.69
1:A:435:LEU:HD21	1:A:447:MET:HB3	1.75	0.68
1:A:2329:LYS:HG3	1:A:2359:GLU:HG3	1.74	0.68
1:A:283:VAL:HG11	1:A:363:LEU:HD21	1.73	0.68
1:A:976:GLU:OE1	1:A:982:SER:N	2.24	0.68
1:A:2300:PHE:HB2	1:A:2339:ALA:HB3	1.76	0.68
1:A:752:ARG:HD3	1:A:752:ARG:H	1.58	0.68
1:A:2296:THR:OG1	1:A:2298:ASP:OD2	2.11	0.68
1:A:1469:THR:HG22	1:A:1471:TYR:HE2	1.57	0.68
1:A:8:GLN:NE2	1:A:870:TYR:OH	2.27	0.67
1:A:1744:ASP:OD1	1:A:1745:ASN:N	2.24	0.67
1:A:690:TYR:HB2	1:A:734:SER:HB3	1.76	0.67
1:A:1124:PHE:HA	1:A:1127:ILE:HD12	1.77	0.67
1:A:1230:PHE:HB3	1:A:1278:LEU:HD11	1.75	0.67
1:A:1156:ASP:OD1	1:A:1159:ASN:N	2.27	0.66
1:A:90:SER:O	1:A:90:SER:OG	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1326:SER:HA	1:A:1347:ASP:HB3	1.76	0.66
1:A:2103:THR:O	1:A:2109:LYS:HA	1.94	0.66
1:A:207:LYS:NZ	1:A:222:ASN:OD1	2.29	0.66
1:A:273:ARG:NH1	1:A:284:TYR:OH	2.29	0.66
1:A:1340:GLU:HA	1:A:1399:ASN:HD21	1.60	0.65
1:A:802:GLN:O	1:A:806:ASN:ND2	2.24	0.65
1:A:2148:ASN:OD1	1:A:2185:GLN:NE2	2.29	0.65
1:A:795:HIS:CE1	1:A:1802:LEU:HD12	2.31	0.65
1:A:364:ASP:OD1	1:A:365:ASP:N	2.29	0.65
1:A:2144:ASN:OD1	1:A:2144:ASN:N	2.29	0.65
1:A:1531:TYR:OH	1:A:1589:ILE:O	2.10	0.65
1:A:73:LYS:HE3	1:A:1726:ILE:HG12	1.77	0.65
1:A:11:LYS:NZ	1:A:977:SER:O	2.28	0.65
1:A:655:LYS:O	1:A:699:ASN:ND2	2.27	0.65
1:A:1956:THR:HB	1:A:1986:MET:HB3	1.78	0.65
1:A:2113:ASP:HB3	1:A:2119:GLN:HE21	1.62	0.65
1:A:1307:GLN:HA	1:A:1310:LYS:HB2	1.78	0.64
1:A:1935:LYS:NZ	1:A:1965:GLU:OE2	2.29	0.64
1:A:2257:GLU:O	1:A:2259:ASN:ND2	2.31	0.64
1:A:479:GLN:HE21	1:A:493:LEU:HG	1.62	0.64
1:A:1505:LEU:HD13	1:A:1507:ILE:HD11	1.79	0.64
1:A:1407:SER:OG	1:A:1413:ASN:OD1	2.13	0.64
1:A:374:LYS:HD3	1:A:503:PHE:HA	1.79	0.63
1:A:1899:VAL:HG23	1:A:1932:ILE:HD11	1.79	0.63
1:A:1992:THR:HG22	1:A:1997:VAL:HG22	1.81	0.63
1:A:463:ARG:O	1:A:465:THR:N	2.31	0.63
1:A:1652:ASN:O	1:A:1655:ASN:ND2	2.30	0.63
1:A:1116:LYS:NZ	1:A:1118:THR:HG22	2.13	0.62
1:A:650:PHE:HB2	1:A:695:LEU:HD23	1.80	0.62
1:A:937:PHE:HB3	1:A:945:VAL:HG23	1.80	0.62
1:A:651:ILE:HG23	1:A:696:LEU:HB3	1.82	0.62
1:A:2215:ASN:HD21	1:A:2218:ASP:HB2	1.65	0.62
1:A:340:GLU:OE1	1:A:344:ARG:NH1	2.33	0.62
1:A:1407:SER:HA	1:A:1413:ASN:HA	1.82	0.62
1:A:363:LEU:HA	1:A:507:LYS:HE3	1.80	0.62
1:A:16:LYS:H	1:A:16:LYS:HD2	1.65	0.62
1:A:289:MET:HE3	1:A:385:GLN:HB3	1.82	0.61
1:A:1367:LEU:HD11	1:A:1408:ILE:HA	1.80	0.61
1:A:97:ASN:ND2	1:A:280:ASP:OD1	2.33	0.61
1:A:932:ILE:HD11	1:A:962:ALA:HA	1.81	0.61
1:A:794:LEU:O	1:A:798:SER:OG	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2112:PHE:HA	1:A:2118:ARG:HA	1.82	0.61
1:A:93:PRO:HA	1:A:367:LYS:HA	1.82	0.61
1:A:883:PHE:HB2	1:A:984:ALA:HB2	1.81	0.61
1:A:1970:LEU:HD12	1:A:1993:ILE:HD12	1.81	0.61
1:A:2182:ILE:N	1:A:2185:GLN:OE1	2.30	0.61
1:A:2215:ASN:O	1:A:2217:THR:N	2.27	0.61
1:A:1793:VAL:O	1:A:1797:ILE:HG13	2.01	0.61
1:A:2282:TYR:HB2	1:A:2303:PHE:CZ	2.36	0.61
1:A:2114:ASP:OD2	1:A:2115:ASN:ND2	2.35	0.60
1:A:1948:GLU:HB3	1:A:1958:TYR:CZ	2.36	0.60
1:A:1029:LEU:HB2	1:A:1031:ILE:HG12	1.83	0.60
1:A:1927:ILE:HD12	1:A:1941:ASP:HA	1.83	0.60
1:A:870:TYR:HB2	1:A:979:SER:HB3	1.83	0.60
1:A:2239:ILE:HG12	1:A:2268:LYS:HE3	1.84	0.60
1:A:1352:VAL:HG21	1:A:1406:PHE:HB2	1.82	0.60
1:A:925:ILE:HD13	1:A:968:LEU:HD21	1.83	0.60
1:A:1827:ASN:OD1	1:A:1831:ASN:N	2.34	0.59
1:A:2228:LYS:HZ2	1:A:2231:LYS:HE3	1.66	0.59
1:A:1530:ASN:HD22	1:A:1537:LYS:HG3	1.67	0.59
1:A:113:ASN:HB3	1:A:328:PRO:HD2	1.84	0.59
1:A:526:ARG:HH11	1:A:526:ARG:HG3	1.67	0.59
1:A:1400:ARG:NH2	1:A:1419:ASP:OD2	2.35	0.59
1:A:479:GLN:HE22	1:A:492:HIS:H	1.51	0.58
1:A:1276:THR:HG22	1:A:1277:LYS:H	1.67	0.58
1:A:2210:THR:HA	1:A:2222:PHE:HB2	1.84	0.58
1:A:1686:ASP:OD2	1:A:1712:ASN:ND2	2.36	0.58
1:A:239:ASP:OD1	1:A:241:ARG:N	2.26	0.58
1:A:2078:VAL:HG11	1:A:2093:ASP:HA	1.85	0.58
1:A:336:ASP:HA	1:A:343:GLN:HE22	1.68	0.58
1:A:2171:TYR:HB3	1:A:2187:VAL:HG12	1.86	0.58
1:A:169:ASN:O	1:A:173:ARG:HG3	2.03	0.58
1:A:899:ARG:HH21	1:A:901:ILE:HD11	1.69	0.58
1:A:2113:ASP:OD1	1:A:2117:ILE:N	2.36	0.58
1:A:70:LYS:HG3	1:A:1698:LEU:HD11	1.84	0.58
1:A:1221:VAL:HG22	1:A:1299:ILE:HD13	1.86	0.58
1:A:1236:TRP:HB2	1:A:2254:ILE:HA	1.85	0.58
1:A:148:SER:HG	1:A:182:LYS:NZ	2.02	0.57
1:A:1902:THR:OG1	1:A:1903:SER:N	2.37	0.57
1:A:136:PHE:H	1:A:203:ASP:CG	2.11	0.57
1:A:363:LEU:HG	1:A:366:ILE:HD11	1.86	0.57
1:A:2171:TYR:O	1:A:2187:VAL:N	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2307:ASN:O	1:A:2312:ASN:ND2	2.38	0.57
1:A:1046:LYS:HG2	1:A:1066:ILE:HD13	1.85	0.57
1:A:1520:ASN:HD22	1:A:1525:LYS:HG3	1.70	0.57
1:A:1774:SER:O	1:A:1776:THR:HG22	2.05	0.57
1:A:1868:ASP:OD1	1:A:1870:THR:HG22	2.04	0.57
1:A:1948:GLU:O	1:A:1958:TYR:HA	2.04	0.57
1:A:10:GLN:HE21	1:A:20:GLN:HE22	1.53	0.57
1:A:2039:PHE:O	1:A:2055:THR:OG1	2.21	0.57
1:A:402:GLN:HB3	1:A:473:VAL:HG22	1.87	0.57
1:A:1680:LYS:O	1:A:1683:TYR:CD2	2.57	0.56
1:A:101:ILE:HD12	1:A:284:TYR:HE1	1.70	0.56
1:A:1397:GLU:OE1	1:A:1400:ARG:NH1	2.38	0.56
1:A:1577:ASN:O	1:A:1632:ILE:N	2.31	0.56
1:A:2195:VAL:HG22	1:A:2196:ASN:H	1.69	0.56
1:A:801:LEU:HG	1:A:805:ARG:HE	1.70	0.56
1:A:865:ILE:HG12	1:A:921:TYR:CZ	2.40	0.56
1:A:1822:ASP:OD2	1:A:1850:LYS:NZ	2.29	0.56
1:A:2120:LEU:HD21	1:A:2133:SER:O	2.05	0.56
1:A:134:ASN:O	1:A:202:ILE:HB	2.06	0.56
1:A:756:ASP:OD1	1:A:757:HIS:N	2.39	0.56
1:A:1405:THR:O	1:A:1405:THR:OG1	2.22	0.56
1:A:2327:ASP:C	1:A:2329:LYS:H	2.14	0.56
1:A:573:ARG:HH21	1:A:1805:TYR:HB3	1.70	0.56
1:A:672:SER:HA	1:A:675:ILE:HD12	1.88	0.56
1:A:764:LYS:O	1:A:768:ILE:HG13	2.05	0.56
1:A:1926:PHE:HB3	1:A:1939:PHE:CD1	2.41	0.56
1:A:103:ILE:HD12	1:A:265:LEU:HD22	1.88	0.56
1:A:23:GLU:N	1:A:23:GLU:OE1	2.39	0.56
1:A:648:LEU:HG	1:A:678:ILE:HD13	1.88	0.56
1:A:1937:TYR:OH	1:A:1963:THR:O	2.19	0.55
1:A:1625:ILE:HD12	1:A:1633:GLN:HG3	1.89	0.55
1:A:2305:HIS:CG	1:A:2306:GLN:H	2.24	0.55
1:A:1144:ILE:HB	1:A:1220:MET:HG3	1.88	0.55
1:A:1754:ALA:HB3	1:A:1764:VAL:HB	1.89	0.55
1:A:2181:ASN:ND2	1:A:2182:ILE:O	2.40	0.55
1:A:126:THR:O	1:A:126:THR:OG1	2.25	0.55
1:A:95:GLU:OE2	1:A:391:LYS:HB2	2.06	0.55
1:A:1202:ILE:O	1:A:1205:VAL:HG22	2.07	0.55
1:A:52:ILE:HG22	1:A:79:LEU:HD11	1.87	0.54
1:A:60:LEU:HD13	1:A:73:LYS:HE2	1.89	0.54
1:A:800:LEU:O	1:A:804:ILE:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1078:ILE:HG21	1:A:1415:ILE:HD11	1.89	0.54
1:A:2019:TYR:O	1:A:2027:GLN:NE2	2.31	0.54
1:A:1722:ASP:OD1	1:A:1722:ASP:N	2.40	0.54
1:A:549:LEU:HD22	1:A:587:ASP:HB2	1.90	0.54
1:A:1111:LEU:HD13	1:A:1282:TYR:CE2	2.42	0.54
1:A:1111:LEU:HD13	1:A:1282:TYR:HE2	1.73	0.54
1:A:790:LYS:HG3	1:A:791:SER:H	1.73	0.54
1:A:1048:LEU:C	1:A:1050:GLU:H	2.16	0.54
1:A:1400:ARG:HA	1:A:1420:LEU:HD12	1.90	0.54
1:A:148:SER:OG	1:A:148:SER:O	2.17	0.53
1:A:246:PHE:CD2	1:A:252:VAL:HG12	2.43	0.53
1:A:846:ASN:HD21	1:A:1767:ARG:HH22	1.56	0.53
1:A:289:MET:HE1	1:A:510:GLN:HG3	1.90	0.53
1:A:2190:SER:HA	1:A:2202:PHE:HB2	1.90	0.53
1:A:1152:LEU:HD22	1:A:1164:LEU:HA	1.89	0.53
1:A:1881:THR:O	1:A:1881:THR:OG1	2.24	0.53
1:A:31:LEU:O	1:A:35:HIS:HD2	1.92	0.53
1:A:1327:LEU:HD11	1:A:1389:ILE:HD11	1.91	0.53
1:A:1594:ILE:HG13	1:A:1595:PHE:H	1.73	0.53
1:A:932:ILE:HG21	1:A:1021:LEU:HD22	1.91	0.53
1:A:1224:ASN:N	1:A:1224:ASN:OD1	2.41	0.53
1:A:485:LYS:HG2	1:A:486:ASP:H	1.74	0.53
1:A:1955:GLU:HB3	1:A:1985:ILE:HG23	1.90	0.53
1:A:2177:THR:OG1	1:A:2181:ASN:OD1	2.22	0.53
1:A:100:PHE:O	1:A:101:ILE:HG13	2.09	0.53
1:A:1429:LEU:HD11	1:A:1447:ILE:HD11	1.91	0.53
1:A:1677:PHE:CZ	1:A:1692:VAL:HG11	2.43	0.53
1:A:332:SER:O	1:A:332:SER:OG	2.25	0.52
1:A:566:ILE:HG12	1:A:599:SER:HA	1.91	0.52
1:A:596:ASN:ND2	1:A:743:GLU:OE2	2.42	0.52
1:A:1113:LEU:HD23	1:A:1114:GLN:HG2	1.91	0.52
1:A:1160:ASN:O	1:A:1212:LYS:N	2.41	0.52
1:A:373:VAL:O	1:A:478:TYR:OH	2.16	0.52
1:A:975:LYS:O	1:A:979:SER:OG	2.17	0.52
1:A:1432:ASN:O	1:A:1436:LEU:N	2.36	0.52
1:A:1469:THR:HG22	1:A:1471:TYR:CE2	2.43	0.52
1:A:1988:THR:HG21	1:A:2002:ASN:HA	1.91	0.52
1:A:108:ASN:O	1:A:112:ILE:HD12	2.10	0.52
1:A:696:LEU:HD11	1:A:742:TYR:O	2.09	0.52
1:A:869:LEU:HD11	1:A:979:SER:HB2	1.91	0.52
1:A:393:SER:OG	1:A:394:TYR:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:GLY:HA3	1:A:427:THR:HB	1.92	0.52
1:A:744:VAL:HG22	1:A:754:ILE:HG22	1.92	0.52
1:A:1377:ILE:HG23	1:A:1423:LYS:HA	1.91	0.52
1:A:2302:TYR:HB2	1:A:2333:PHE:CZ	2.45	0.52
1:A:1730:ILE:HG12	1:A:1780:LYS:HB3	1.90	0.52
1:A:1832:MET:HE3	1:A:1851:ASN:ND2	2.25	0.52
1:A:573:ARG:HG3	1:A:574:ASN:N	2.24	0.51
1:A:1284:ASP:HA	1:A:1311:ASN:HB3	1.92	0.51
1:A:1531:TYR:HD2	1:A:1532:PHE:N	2.08	0.51
1:A:1264:TRP:HB2	1:A:1275:ILE:HB	1.92	0.51
1:A:1625:ILE:HD11	1:A:1635:TYR:HD2	1.76	0.51
1:A:239:ASP:OD1	1:A:240:ILE:N	2.42	0.51
1:A:655:LYS:HB2	1:A:660:THR:HB	1.92	0.51
1:A:479:GLN:NE2	1:A:493:LEU:HG	2.26	0.51
1:A:1384:LEU:HD22	1:A:1404:LEU:HD13	1.92	0.51
1:A:2083:LEU:HG	1:A:2085:ASP:H	1.76	0.51
1:A:2306:GLN:NE2	1:A:2307:ASN:OD1	2.44	0.51
1:A:1136:PHE:HE2	1:A:1162:ILE:HG21	1.75	0.51
1:A:1728:GLU:OE1	1:A:1728:GLU:N	2.36	0.51
1:A:695:LEU:H	1:A:739:ALA:HA	1.75	0.51
1:A:161:LEU:HD23	1:A:162:ASN:H	1.75	0.51
1:A:504:PRO:HB2	1:A:507:LYS:HB2	1.93	0.51
1:A:1841:ASP:O	1:A:1842:SER:OG	2.23	0.51
1:A:246:PHE:HE1	1:A:272:LEU:HD12	1.76	0.51
1:A:606:ILE:HG12	1:A:620:TYR:HB2	1.93	0.51
1:A:1836:LEU:HD22	1:A:1843:LEU:HD11	1.92	0.51
1:A:270:ASP:HA	1:A:273:ARG:HE	1.75	0.50
1:A:1970:LEU:HD22	1:A:1977:LYS:HD3	1.93	0.50
1:A:1058:GLN:HA	1:A:1061:GLU:HG2	1.93	0.50
1:A:959:LEU:HD13	1:A:1023:PRO:HD2	1.91	0.50
1:A:1152:LEU:HD11	1:A:1162:ILE:HD12	1.93	0.50
1:A:148:SER:O	1:A:182:LYS:NZ	2.44	0.50
1:A:421:GLY:HA2	1:A:426:THR:HG22	1.94	0.50
1:A:1379:ASP:OD1	1:A:1380:ASN:N	2.45	0.50
1:A:885:SER:OG	1:A:885:SER:O	2.30	0.50
1:A:2163:PHE:HB2	1:A:2172:PHE:HE2	1.77	0.50
1:A:42:VAL:HG11	1:A:90:SER:OG	2.11	0.50
1:A:587:ASP:OD1	1:A:587:ASP:N	2.44	0.50
1:A:852:ILE:HD13	1:A:1721:LEU:HD21	1.92	0.50
1:A:1569:MET:HG2	1:A:1576:LEU:HD13	1.92	0.50
1:A:765:GLU:HG2	1:A:766:GLU:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1880:ILE:HG22	1:A:1882:ILE:HG13	1.93	0.50
1:A:103:ILE:HD11	1:A:269:SER:HB2	1.93	0.49
1:A:493:LEU:HD22	1:A:497:GLU:HG2	1.93	0.49
1:A:973:THR:HG22	1:A:975:LYS:H	1.77	0.49
1:A:1116:LYS:O	1:A:1120:VAL:HG23	2.11	0.49
1:A:1237:THR:HB	1:A:1240:PHE:HE1	1.76	0.49
1:A:1382:ILE:HD13	1:A:1418:ILE:HD12	1.94	0.49
1:A:1613:ILE:HG13	1:A:1614:SER:N	2.23	0.49
1:A:2218:ASP:HB3	1:A:2248:ILE:HG23	1.94	0.49
1:A:1777:ALA:HB1	1:A:1780:LYS:HD3	1.94	0.49
1:A:1481:GLU:OE1	1:A:1496:ASN:ND2	2.46	0.49
1:A:57:ASP:OD1	1:A:76:LYS:NZ	2.29	0.49
1:A:277:LEU:HD13	1:A:389:SER:HB3	1.94	0.49
1:A:829:ALA:O	1:A:832:ILE:HG13	2.13	0.49
1:A:96:LYS:HD2	1:A:124:ASP:HB2	1.95	0.49
1:A:892:THR:OG1	1:A:893:GLU:N	2.45	0.49
1:A:1046:LYS:HD3	1:A:1519:ILE:HG21	1.93	0.49
1:A:1036:ILE:HG21	1:A:1521:LYS:HG2	1.93	0.49
1:A:1164:LEU:HD12	1:A:1164:LEU:H	1.78	0.49
1:A:402:GLN:HE21	1:A:402:GLN:HA	1.77	0.49
1:A:552:ALA:N	1:A:586:GLY:O	2.46	0.49
1:A:1292:ASP:O	1:A:1323:TYR:OH	2.20	0.49
1:A:1418:ILE:HG23	1:A:1425:TYR:HB3	1.95	0.49
1:A:1723:ALA:HB3	1:A:1725:TYR:CZ	2.48	0.49
1:A:244:GLU:CD	1:A:244:GLU:H	2.21	0.49
1:A:1035:ILE:HD12	1:A:1612:ILE:HD11	1.94	0.49
1:A:1138:LEU:HG	1:A:1141:ASP:HA	1.95	0.49
1:A:1314:TYR:HE2	1:A:1332:MET:HG2	1.77	0.49
1:A:283:VAL:HG22	1:A:388:ILE:HG23	1.94	0.49
1:A:936:ILE:HD13	1:A:944:LEU:HD22	1.94	0.49
1:A:1284:ASP:OD1	1:A:1311:ASN:ND2	2.45	0.49
1:A:2030:VAL:HG12	1:A:2037:PHE:HB3	1.95	0.49
1:A:2273:TYR:CE2	1:A:2280:MET:HG3	2.48	0.49
1:A:309:ASN:OD1	1:A:310:THR:N	2.46	0.48
1:A:386:ALA:O	1:A:387:LEU:HD23	2.13	0.48
1:A:631:ILE:HG22	1:A:632:ASP:N	2.28	0.48
1:A:765:GLU:HG2	1:A:766:GLU:N	2.27	0.48
1:A:915:LYS:HB3	1:A:917:ILE:HG22	1.94	0.48
1:A:550:ASP:O	1:A:553:GLN:HG2	2.12	0.48
1:A:1377:ILE:HD12	1:A:1382:ILE:HG12	1.95	0.48
1:A:2212:TRP:CE2	1:A:2221:TYR:HD2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ASN:O	1:A:8:GLN:N	2.45	0.48
1:A:860:LYS:HB3	1:A:860:LYS:HE2	1.50	0.48
1:A:1082:ALA:HB1	1:A:1085:ILE:HG12	1.94	0.48
1:A:2173:ALA:HB1	1:A:2177:THR:HG21	1.94	0.48
1:A:691:ILE:HG12	1:A:693:ILE:HG13	1.96	0.48
1:A:1592:LYS:HE2	1:A:1605:PHE:CD2	2.49	0.48
1:A:1612:ILE:HG12	1:A:1625:ILE:HG22	1.96	0.48
1:A:1857:PHE:CE1	1:A:1866:TYR:HB2	2.49	0.48
1:A:119:LYS:HG3	1:A:120:ASP:OD1	2.14	0.48
1:A:217:ASP:OD2	1:A:217:ASP:N	2.36	0.48
1:A:1132:THR:OG1	1:A:1133:GLU:OE2	2.32	0.48
1:A:1245:ASN:OD1	1:A:1247:GLY:N	2.45	0.48
1:A:1533:LYS:HD3	1:A:1590:ASN:HD22	1.79	0.48
1:A:818:LYS:O	1:A:822:THR:OG1	2.24	0.48
1:A:1118:THR:O	1:A:1121:ILE:HG13	2.14	0.48
1:A:2230:TYR:HB3	1:A:2234:ASN:ND2	2.29	0.48
1:A:397:ASP:OD1	1:A:398:LEU:N	2.47	0.48
1:A:449:LYS:O	1:A:464:SER:HA	2.14	0.48
1:A:584:LEU:HB2	1:A:651:ILE:O	2.14	0.48
1:A:1380:ASN:HB2	1:A:1391:PHE:O	2.13	0.48
1:A:2100:ILE:HA	1:A:2112:PHE:HB2	1.95	0.48
1:A:151:ASN:O	1:A:155:GLU:N	2.46	0.48
1:A:578:ILE:O	1:A:647:LYS:CB	2.53	0.48
1:A:675:ILE:O	1:A:679:LEU:HG	2.14	0.48
1:A:954:HIS:O	1:A:958:THR:HG23	2.14	0.47
1:A:1177:GLY:HA3	1:A:1188:PHE:CD2	2.49	0.47
1:A:1514:LYS:HB3	1:A:1515:ASP:OD1	2.14	0.47
1:A:1787:ASP:OD1	1:A:1787:ASP:N	2.40	0.47
1:A:15:VAL:HG12	1:A:18:ARG:HB2	1.97	0.47
1:A:1169:ILE:HB	1:A:1202:ILE:HD11	1.96	0.47
1:A:1340:GLU:HA	1:A:1399:ASN:ND2	2.28	0.47
1:A:1682:LEU:HD12	1:A:1689:VAL:HG21	1.96	0.47
1:A:1498:TYR:CE1	1:A:1500:PRO:HD2	2.49	0.47
1:A:1908:TYR:CE1	1:A:1910:ALA:HB2	2.48	0.47
1:A:963:PHE:O	1:A:967:SER:OG	2.28	0.47
1:A:1269:PHE:CZ	1:A:2277:LYS:HG2	2.49	0.47
1:A:1291:LEU:HD21	1:A:1316:PHE:HD1	1.79	0.47
1:A:1948:GLU:H	1:A:1948:GLU:HG3	1.26	0.47
1:A:2342:GLY:HA2	1:A:2353:PHE:O	2.14	0.47
1:A:861:LEU:O	1:A:865:ILE:HG13	2.14	0.47
1:A:1229:VAL:HG13	1:A:1281:ARG:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2049:THR:HG21	1:A:2055:THR:HG22	1.96	0.47
1:A:2112:PHE:CE1	1:A:2118:ARG:HB2	2.50	0.47
1:A:34:TYR:HB2	1:A:48:LYS:HG2	1.97	0.47
1:A:834:ARG:O	1:A:838:GLU:HG2	2.14	0.47
1:A:1382:ILE:HG13	1:A:1391:PHE:HE2	1.79	0.47
1:A:2037:PHE:HB2	1:A:2076:ALA:HB3	1.96	0.47
1:A:791:SER:HB3	1:A:840:ARG:O	2.14	0.47
1:A:1319:SER:O	1:A:1319:SER:OG	2.32	0.47
1:A:1698:LEU:HB3	1:A:1724:ASN:O	2.15	0.47
1:A:1919:LEU:H	1:A:1922:GLU:CD	2.23	0.47
1:A:2308:THR:HB	1:A:2312:ASN:HD21	1.79	0.47
1:A:747:ASN:OD1	1:A:750:GLY:N	2.48	0.47
1:A:2275:ASN:HB3	1:A:2280:MET:HE1	1.97	0.47
1:A:313:GLU:HB2	1:A:511:LEU:HD12	1.96	0.46
1:A:1025:LEU:HB2	1:A:1623:GLU:OE2	2.15	0.46
1:A:1600:ASP:HB2	1:A:1602:ASN:OD1	2.15	0.46
1:A:1679:GLN:HA	1:A:1682:LEU:HD23	1.96	0.46
1:A:917:ILE:HD11	1:A:921:TYR:OH	2.15	0.46
1:A:1532:PHE:HB3	1:A:1534:ASP:H	1.80	0.46
1:A:288:ASP:N	1:A:288:ASP:OD2	2.48	0.46
1:A:932:ILE:HD13	1:A:1021:LEU:HD22	1.97	0.46
1:A:1352:VAL:HG21	1:A:1406:PHE:CB	2.46	0.46
1:A:1840:ASN:C	1:A:1840:ASN:HD22	2.22	0.46
1:A:294:GLN:HE21	1:A:361:LEU:HB2	1.80	0.46
1:A:870:TYR:CD2	1:A:978:LEU:HB3	2.51	0.46
1:A:1186:HIS:CD2	1:A:1267:PHE:HB3	2.50	0.46
1:A:1251:LEU:O	1:A:1254:ILE:HG22	2.15	0.46
1:A:1746:ASP:HB2	1:A:1751:ILE:HD11	1.96	0.46
1:A:1937:TYR:CE1	1:A:1964:GLY:HA3	2.49	0.46
1:A:269:SER:O	1:A:269:SER:OG	2.31	0.46
1:A:1575:ALA:HB3	1:A:1577:ASN:OD1	2.16	0.46
1:A:1583:MET:HE3	1:A:1586:LEU:HB2	1.98	0.46
1:A:1959:PHE:HA	1:A:1965:GLU:O	2.16	0.46
1:A:23:GLU:O	1:A:27:ILE:HG13	2.15	0.46
1:A:114:TYR:HE1	1:A:327:ILE:HG21	1.81	0.46
1:A:631:ILE:HG22	1:A:632:ASP:H	1.81	0.46
1:A:1077:ALA:O	1:A:1082:ALA:N	2.49	0.46
1:A:213:GLU:HB3	1:A:214:TYR:HD2	1.81	0.46
1:A:577:TYR:O	1:A:643:LYS:HG3	2.16	0.46
1:A:676:GLU:OE2	1:A:722:ARG:NE	2.49	0.46
1:A:820:MET:HE3	1:A:820:MET:HB3	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:ILE:HG12	1:A:921:TYR:CE2	2.51	0.46
1:A:1560:ASN:O	1:A:1564:GLN:HG2	2.15	0.46
1:A:1926:PHE:O	1:A:1927:ILE:HD13	2.15	0.46
1:A:2181:ASN:HD22	1:A:2185:GLN:HG2	1.81	0.46
1:A:2274:LEU:HD21	1:A:2283:PHE:HD2	1.81	0.46
1:A:512:THR:O	1:A:515:GLU:HB3	2.16	0.46
1:A:1226:PRO:HD3	1:A:1308:ILE:HG23	1.97	0.46
1:A:312:TRP:NE1	1:A:316:LYS:HE3	2.32	0.45
1:A:554:ASN:HB3	1:A:612:ILE:HG12	1.97	0.45
1:A:1433:CYS:HA	1:A:1436:LEU:HB2	1.98	0.45
1:A:2007:GLN:HB3	1:A:2011:ILE:HD13	1.96	0.45
1:A:335:PHE:HE1	1:A:346:PHE:HD1	1.65	0.45
1:A:478:TYR:N	1:A:478:TYR:CD1	2.84	0.45
1:A:1237:THR:HB	1:A:1240:PHE:CE1	2.51	0.45
1:A:2223:ASP:N	1:A:2228:LYS:O	2.46	0.45
1:A:1496:ASN:HB3	1:A:1506:PHE:CD2	2.51	0.45
1:A:1085:ILE:H	1:A:1085:ILE:HG13	1.39	0.45
1:A:1548:ASN:ND2	1:A:1600:ASP:OD1	2.37	0.45
1:A:221:LEU:O	1:A:225:ILE:HG13	2.17	0.45
1:A:882:HIS:HD2	1:A:900:PHE:HB3	1.81	0.45
1:A:115:ILE:O	1:A:118:TRP:N	2.50	0.45
1:A:769:ILE:HG12	1:A:804:ILE:HD11	1.97	0.45
1:A:865:ILE:HA	1:A:921:TYR:CE1	2.51	0.45
1:A:1441:SER:OG	1:A:1500:PRO:O	2.35	0.45
1:A:1525:LYS:O	1:A:1543:THR:HG23	2.17	0.45
1:A:775:LYS:O	1:A:792:LYS:HE2	2.17	0.45
1:A:976:GLU:OE1	1:A:981:LEU:N	2.50	0.45
1:A:1968:LYS:HD3	1:A:1982:ASP:HA	1.98	0.45
1:A:466:ILE:HA	1:A:470:GLY:HA3	1.99	0.45
1:A:1189:SER:HB3	1:A:2311:GLU:OE2	2.16	0.45
1:A:283:VAL:HG21	1:A:366:ILE:HD12	1.98	0.45
1:A:309:ASN:HD21	1:A:786:LYS:HE2	1.81	0.45
1:A:378:ALA:O	1:A:380:ASN:N	2.50	0.45
1:A:1442:ASP:OD1	1:A:1442:ASP:N	2.48	0.45
1:A:1877:ILE:HA	1:A:1889:PHE:HB2	1.99	0.45
1:A:2069:PHE:C	1:A:2070:PHE:HD2	2.25	0.45
1:A:382:VAL:HG23	1:A:471:PRO:HB3	1.99	0.44
1:A:402:GLN:HE21	1:A:402:GLN:CA	2.30	0.44
1:A:526:ARG:HG3	1:A:526:ARG:NH1	2.32	0.44
1:A:1370:ASN:HB3	1:A:1373:SER:OG	2.17	0.44
1:A:1863:ASN:ND2	1:A:1894:ILE:HD13	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2170:LYS:HZ2	1:A:2186:ALA:HB1	1.82	0.44
1:A:2341:THR:O	1:A:2353:PHE:HB2	2.17	0.44
1:A:130:PHE:CE2	1:A:276:MET:HG2	2.51	0.44
1:A:549:LEU:HD23	1:A:549:LEU:HA	1.81	0.44
1:A:583:GLN:NE2	1:A:585:GLN:O	2.50	0.44
1:A:1058:GLN:HA	1:A:1061:GLU:CG	2.46	0.44
1:A:1394:ASP:HB3	1:A:1396:ASN:HD22	1.82	0.44
1:A:48:LYS:HE2	1:A:48:LYS:HA	2.00	0.44
1:A:555:THR:O	1:A:609:GLN:NE2	2.43	0.44
1:A:1442:ASP:HA	1:A:1445:GLN:HG3	2.00	0.44
1:A:1583:MET:O	1:A:1587:GLU:HG3	2.16	0.44
1:A:377:PHE:CE1	1:A:382:VAL:HG12	2.52	0.44
1:A:396:SER:O	1:A:400:ILE:HD12	2.17	0.44
1:A:2302:TYR:O	1:A:2317:SER:HA	2.17	0.44
1:A:549:LEU:HD11	1:A:653:HIS:CE1	2.53	0.44
1:A:673:SER:O	1:A:677:THR:HG23	2.18	0.44
1:A:795:HIS:HE1	1:A:1802:LEU:HD12	1.80	0.44
1:A:862:ILE:HG21	1:A:971:TYR:HD2	1.83	0.44
1:A:973:THR:HG22	1:A:974:THR:N	2.32	0.44
1:A:1140:ASP:O	1:A:1142:LYS:HG3	2.17	0.44
1:A:2111:TYR:O	1:A:2119:GLN:N	2.49	0.44
1:A:2285:LYS:HB2	1:A:2285:LYS:HE2	1.72	0.44
1:A:1888:TYR:O	1:A:1896:GLN:HB2	2.18	0.44
1:A:2172:PHE:HA	1:A:2186:ALA:HA	2.00	0.44
1:A:102:TRP:CE3	1:A:107:ILE:HG13	2.53	0.44
1:A:161:LEU:HD23	1:A:162:ASN:N	2.32	0.44
1:A:835:GLN:NE2	1:A:840:ARG:HD2	2.32	0.44
1:A:2029:GLY:O	1:A:2039:PHE:HA	2.18	0.44
1:A:2314:GLU:CD	1:A:2314:GLU:H	2.26	0.44
1:A:539:PHE:HB2	1:A:540:GLU:HG2	1.99	0.44
1:A:869:LEU:HA	1:A:918:PHE:HZ	1.83	0.44
1:A:1075:SER:HA	1:A:1078:ILE:HD12	2.00	0.44
1:A:1444:GLN:HG3	1:A:1499:MET:HB3	1.99	0.44
1:A:1885:LYS:HD3	1:A:1922:GLU:CD	2.43	0.44
1:A:1918:ASN:HB2	1:A:1922:GLU:HB2	2.00	0.44
1:A:2190:SER:OG	1:A:2191:GLY:N	2.50	0.44
1:A:118:TRP:CE3	1:A:291:PRO:HG3	2.53	0.43
1:A:366:ILE:HD13	1:A:388:ILE:HD13	1.98	0.43
1:A:246:PHE:HD2	1:A:252:VAL:HG12	1.82	0.43
1:A:580:TYR:OH	1:A:633:LYS:O	2.35	0.43
1:A:765:GLU:HA	1:A:768:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1545:GLU:OE2	1:A:1546:ASP:HB2	2.18	0.43
1:A:2066:LYS:HB3	1:A:2068:TYR:CE2	2.53	0.43
1:A:1370:ASN:HD22	1:A:1370:ASN:HA	1.65	0.43
1:A:2053:GLU:HG2	1:A:2054:LEU:N	2.33	0.43
1:A:259:LEU:HD12	1:A:259:LEU:HA	1.81	0.43
1:A:2163:PHE:O	1:A:2169:TYR:HA	2.18	0.43
1:A:2190:SER:OG	1:A:2202:PHE:O	2.34	0.43
1:A:42:VAL:HG21	1:A:370:PRO:HG2	2.00	0.43
1:A:622:SER:HA	1:A:639:GLN:HE22	1.84	0.43
1:A:716:LEU:HB2	1:A:737:VAL:HG21	2.00	0.43
1:A:1181:THR:HB	1:A:1186:HIS:CE1	2.52	0.43
1:A:1210:LYS:HE3	1:A:1210:LYS:HB2	1.83	0.43
1:A:2100:ILE:HG22	1:A:2116:GLY:HA2	2.01	0.43
1:A:2181:ASN:HB2	1:A:2185:GLN:CD	2.43	0.43
1:A:2341:THR:HG22	1:A:2342:GLY:H	1.83	0.43
1:A:466:ILE:HG23	1:A:471:PRO:HD2	1.99	0.43
1:A:579:HIS:HB3	1:A:605:SER:HA	2.00	0.43
1:A:702:SER:CB	1:A:776:GLU:H	2.31	0.43
1:A:869:LEU:CD1	1:A:979:SER:HB2	2.48	0.43
1:A:1918:ASN:HD22	1:A:1924:VAL:HG12	1.83	0.43
1:A:2102:LEU:HD21	1:A:2109:LYS:HB2	2.00	0.43
1:A:2215:ASN:ND2	1:A:2218:ASP:HB2	2.30	0.43
1:A:573:ARG:NH2	1:A:1805:TYR:HB3	2.32	0.43
1:A:1374:LYS:NZ	1:A:1386:ASN:OD1	2.48	0.43
1:A:102:TRP:HZ3	1:A:111:ALA:HB2	1.83	0.43
1:A:1513:LEU:HD12	1:A:1530:ASN:O	2.18	0.43
1:A:766:GLU:HG3	1:A:820:MET:SD	2.59	0.43
1:A:897:ARG:HE	1:A:910:PHE:HE1	1.66	0.43
1:A:1352:VAL:HG12	1:A:1371:ILE:HG12	2.01	0.43
1:A:339:ASP:O	1:A:342:VAL:HG12	2.19	0.43
1:A:1352:VAL:HG23	1:A:1353:LYS:HG3	2.00	0.43
1:A:317:LEU:HA	1:A:317:LEU:HD23	1.87	0.42
1:A:553:GLN:HE21	1:A:587:ASP:HA	1.83	0.42
1:A:2307:ASN:HA	1:A:2312:ASN:O	2.19	0.42
1:A:6:LYS:HD2	1:A:28:LEU:HB3	2.02	0.42
1:A:49:LEU:HD11	1:A:82:GLU:HG3	2.01	0.42
1:A:438:ILE:HG13	1:A:447:MET:HE1	2.00	0.42
1:A:525:ALA:HB2	1:A:701:PHE:CG	2.55	0.42
1:A:1464:TYR:C	1:A:1465:ILE:HD12	2.45	0.42
1:A:1594:ILE:HG13	1:A:1595:PHE:N	2.34	0.42
1:A:1625:ILE:H	1:A:1625:ILE:HG13	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2120:LEU:HD13	1:A:2121:GLY:N	2.33	0.42
1:A:213:GLU:HB3	1:A:214:TYR:CD2	2.54	0.42
1:A:447:MET:HA	1:A:450:ILE:HG12	2.01	0.42
1:A:732:GLN:HB2	1:A:782:PRO:HG3	2.01	0.42
1:A:876:ASN:ND2	1:A:911:ILE:HG23	2.35	0.42
1:A:1622:PHE:HD1	1:A:1637:ILE:HG23	1.84	0.42
1:A:1758:GLU:H	1:A:1758:GLU:CD	2.27	0.42
1:A:324:LYS:HA	1:A:324:LYS:HD3	1.83	0.42
1:A:643:LYS:O	1:A:686:ILE:HD11	2.20	0.42
1:A:817:LYS:HB3	1:A:817:LYS:HE3	1.78	0.42
1:A:2301:LYS:HG3	1:A:2317:SER:OG	2.20	0.42
1:A:131:TYR:HE2	1:A:133:SER:HB3	1.85	0.42
1:A:1009:GLU:O	1:A:1013:THR:HG22	2.20	0.42
1:A:1055:LEU:HD22	1:A:1401:PHE:CZ	2.54	0.42
1:A:2151:TYR:HB3	1:A:2159:LEU:HB2	2.00	0.42
1:A:2330:ARG:HD3	1:A:2330:ARG:N	2.35	0.42
1:A:154:LEU:HD23	1:A:154:LEU:HA	1.90	0.42
1:A:188:ASP:O	1:A:192:SER:OG	2.31	0.42
1:A:476:GLY:HA2	1:A:491:ILE:HD11	2.01	0.42
1:A:764:LYS:HE2	1:A:764:LYS:HA	2.00	0.42
1:A:1142:LYS:HE3	1:A:1142:LYS:HB2	1.67	0.42
1:A:1948:GLU:HB3	1:A:1958:TYR:CE2	2.55	0.42
1:A:634:TYR:CD2	1:A:678:ILE:HG13	2.54	0.42
1:A:653:HIS:O	1:A:664:ALA:N	2.51	0.42
1:A:864:SER:OG	1:A:921:TYR:OH	2.37	0.42
1:A:1427:ILE:C	1:A:1428:LEU:HD12	2.45	0.42
1:A:2275:ASN:OD1	1:A:2275:ASN:N	2.53	0.42
1:A:2301:LYS:NZ	1:A:2337:TYR:HB3	2.34	0.42
1:A:2304:ALA:HB1	1:A:2308:THR:HG21	2.01	0.42
1:A:1232:TYR:HB3	1:A:1278:LEU:HD13	2.02	0.42
1:A:1915:LEU:HD22	1:A:1924:VAL:HB	2.02	0.42
1:A:1371:ILE:HD12	1:A:1371:ILE:HA	1.91	0.42
1:A:1515:ASP:OD1	1:A:1515:ASP:N	2.53	0.42
1:A:1516:ILE:HA	1:A:1528:ILE:O	2.20	0.42
1:A:1544:ILE:HG12	1:A:1550:ILE:HG12	2.01	0.42
1:A:1567:LYS:NZ	1:A:1567:LYS:HB3	2.34	0.42
1:A:34:TYR:HD1	1:A:48:LYS:HG2	1.85	0.42
1:A:247:ALA:HA	1:A:275:SER:HB3	2.02	0.42
1:A:716:LEU:HD21	1:A:779:SER:C	2.45	0.42
1:A:1679:GLN:HE22	1:A:1716:PRO:HD2	1.85	0.42
1:A:2182:ILE:HG22	1:A:2183:TYR:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2208:ILE:HG23	1:A:2227:LYS:HE3	2.02	0.42
1:A:122:ASN:HB3	1:A:125:TYR:CD1	2.55	0.41
1:A:1536:MET:HE1	1:A:1564:GLN:HG3	2.02	0.41
1:A:1552:LEU:HD22	1:A:1552:LEU:HA	1.85	0.41
1:A:452:ASN:HB3	1:A:462:VAL:HG13	2.03	0.41
1:A:505:LYS:HB3	1:A:505:LYS:HE3	1.74	0.41
1:A:616:GLU:HG3	1:A:633:LYS:HB2	2.02	0.41
1:A:652:GLY:O	1:A:697:GLY:HA3	2.19	0.41
1:A:2198:ASP:HA	1:A:2228:LYS:NZ	2.35	0.41
1:A:1557:LEU:HB3	1:A:1561:GLY:HA3	2.03	0.41
1:A:1568:PHE:CE1	1:A:1576:LEU:HD12	2.55	0.41
1:A:76:LYS:HB3	1:A:76:LYS:HE3	1.68	0.41
1:A:413:ASN:O	1:A:416:PRO:HD2	2.21	0.41
1:A:1543:THR:HG22	1:A:1544:ILE:H	1.85	0.41
1:A:10:GLN:HE21	1:A:20:GLN:NE2	2.19	0.41
1:A:1034:THR:O	1:A:1035:ILE:HG13	2.20	0.41
1:A:1520:ASN:ND2	1:A:1525:LYS:HG3	2.34	0.41
1:A:1565:ILE:HG12	1:A:1569:MET:HE3	2.02	0.41
1:A:96:LYS:HA	1:A:125:TYR:CE2	2.56	0.41
1:A:246:PHE:HE1	1:A:272:LEU:CD1	2.33	0.41
1:A:1531:TYR:CD2	1:A:1531:TYR:C	2.99	0.41
1:A:1904:ASP:O	1:A:1944:ARG:NH1	2.54	0.41
1:A:1996:LYS:HA	1:A:1996:LYS:HE3	2.01	0.41
1:A:346:PHE:HD2	1:A:346:PHE:HA	1.79	0.41
1:A:714:LYS:HB2	1:A:714:LYS:HE2	1.75	0.41
1:A:793:TYR:HD1	1:A:793:TYR:HA	1.69	0.41
1:A:899:ARG:HE	1:A:901:ILE:HD11	1.85	0.41
1:A:917:ILE:O	1:A:920:GLU:HB2	2.20	0.41
1:A:1172:ALA:N	1:A:1261:GLN:O	2.49	0.41
1:A:1299:ILE:HD12	1:A:1299:ILE:H	1.86	0.41
1:A:1308:ILE:O	1:A:1312:LEU:HB2	2.21	0.41
1:A:1682:LEU:CD1	1:A:1689:VAL:HG21	2.51	0.41
1:A:1757:GLU:HB2	1:A:1758:GLU:OE1	2.19	0.41
1:A:524:GLN:C	1:A:526:ARG:H	2.29	0.41
1:A:567:LEU:HD12	1:A:568:SER:N	2.35	0.41
1:A:835:GLN:HE22	1:A:840:ARG:NH1	2.18	0.41
1:A:1276:THR:HG22	1:A:1277:LYS:HD2	2.02	0.41
1:A:1469:THR:CG2	1:A:1471:TYR:HE2	2.31	0.41
1:A:1479:LYS:NZ	1:A:1481:GLU:OE2	2.52	0.41
1:A:1899:VAL:CG2	1:A:1932:ILE:HD11	2.49	0.41
1:A:2153:ASP:HB3	1:A:2159:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:MET:HE2	1:A:337:MET:HB3	1.97	0.41
1:A:2060:ILE:O	1:A:2061:LEU:HD22	2.21	0.41
1:A:2280:MET:HB3	1:A:2317:SER:HB2	2.02	0.41
1:A:323:TYR:HD2	1:A:350:LEU:HG	1.86	0.40
1:A:1899:VAL:HG23	1:A:1932:ILE:CD1	2.48	0.40
1:A:2062:ASN:HA	1:A:2066:LYS:O	2.21	0.40
1:A:363:LEU:HD12	1:A:507:LYS:HD3	2.03	0.40
1:A:563:SER:O	1:A:566:ILE:HB	2.22	0.40
1:A:1003:ASP:HB3	1:A:1006:LYS:HD2	2.04	0.40
1:A:1116:LYS:HG2	1:A:1117:ALA:H	1.86	0.40
1:A:1152:LEU:HD22	1:A:1152:LEU:HA	1.95	0.40
1:A:1706:THR:HA	1:A:1707:PRO:HD3	1.88	0.40
1:A:1825:TYR:CZ	1:A:1839:ILE:HG12	2.56	0.40
1:A:1906:LEU:HB3	1:A:1945:ALA:HB3	2.03	0.40
1:A:271:ILE:H	1:A:271:ILE:HG13	1.67	0.40
1:A:760:LYS:HE3	1:A:760:LYS:HB3	1.81	0.40
1:A:1041:LEU:O	1:A:1045:ILE:HG12	2.21	0.40
1:A:142:LYS:HG3	1:A:263:TRP:HE3	1.85	0.40
1:A:1114:GLN:HB2	1:A:1120:VAL:HG22	2.03	0.40
1:A:1841:ASP:C	1:A:1842:SER:HG	2.24	0.40
1:A:164:PRO:HB3	1:A:756:ASP:CG	2.46	0.40
1:A:760:LYS:HG2	1:A:761:TRP:N	2.37	0.40
1:A:1426:LYS:HB3	1:A:1426:LYS:HE3	1.72	0.40
1:A:1443:ILE:O	1:A:1447:ILE:HG13	2.22	0.40
1:A:1634:PRO:HG3	1:A:1688:TYR:CD1	2.56	0.40
1:A:1755:ASN:ND2	1:A:1763:GLN:HE21	2.20	0.40
1:A:2120:LEU:HD22	1:A:2120:LEU:HA	1.91	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	2361/2372 (100%)	2151 (91%)	206 (9%)	4 (0%)	43 72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	464	SER
1	A	1775	ASP
1	A	2308	THR
1	A	2216	GLU

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	2137/2146 (100%)	1849 (86%)	288 (14%)	4 12

All (288) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	5	ASN
1	A	18	ARG
1	A	21	GLU
1	A	48	LYS
1	A	62	THR
1	A	68	ARG
1	A	81	MET
1	A	86	LEU
1	A	90	SER
1	A	92	THR
1	A	98	LEU
1	A	103	ILE
1	A	112	ILE
1	A	121	VAL
1	A	124	ASP
1	A	126	THR

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Mol	Chain	Res	Type
1	A	134	ASN
1	A	138	ILE
1	A	141	LEU
1	A	145	ILE
1	A	146	VAL
1	A	147	GLU
1	A	148	SER
1	A	150	THR
1	A	159	GLU
1	A	186	PHE
1	A	190	TYR
1	A	194	ILE
1	A	197	ASN
1	A	213	GLU
1	A	228	SER
1	A	229	LEU
1	A	233	THR
1	A	260	VAL
1	A	262	ARG
1	A	276	MET
1	A	278	LYS
1	A	285	LEU
1	A	288	ASP
1	A	290	LEU
1	A	293	ILE
1	A	317	LEU
1	A	318	GLU
1	A	332	SER
1	A	339	ASP
1	A	345	SER
1	A	346	PHE
1	A	350	LEU
1	A	351	SER
1	A	357	SER
1	A	359	ILE
1	A	361	LEU
1	A	367	LYS
1	A	382	VAL
1	A	384	ASN
1	A	390	LEU
1	A	402	GLN
1	A	409	ILE

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Mol	Chain	Res	Type
1	A	410	LEU
1	A	417	SER
1	A	448	ILE
1	A	449	LYS
1	A	451	THR
1	A	454	LEU
1	A	465	THR
1	A	473	VAL
1	A	491	ILE
1	A	492	HIS
1	A	494	LEU
1	A	495	GLU
1	A	509	SER
1	A	529	SER
1	A	530	GLN
1	A	549	LEU
1	A	554	ASN
1	A	562	VAL
1	A	565	LYS
1	A	572	THR
1	A	573	ARG
1	A	576	GLU
1	A	579	HIS
1	A	612	ILE
1	A	613	GLU
1	A	616	GLU
1	A	617	THR
1	A	619	TYR
1	A	632	ASP
1	A	636	ILE
1	A	638	TYR
1	A	640	ILE
1	A	642	ASN
1	A	648	LEU
1	A	660	THR
1	A	690	TYR
1	A	696	LEU
1	A	704	SER
1	A	717	LEU
1	A	741	GLN
1	A	746	ILE
1	A	757	HIS

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Mol	Chain	Res	Type
1	A	762	ILE
1	A	769	ILE
1	A	785	ASN
1	A	789	VAL
1	A	790	LYS
1	A	797	LEU
1	A	798	SER
1	A	799	THR
1	A	802	GLN
1	A	810	SER
1	A	847	LEU
1	A	848	THR
1	A	855	ILE
1	A	861	LEU
1	A	862	ILE
1	A	864	SER
1	A	869	LEU
1	A	874	HIS
1	A	875	GLN
1	A	885	SER
1	A	892	THR
1	A	926	SER
1	A	935	THR
1	A	938	ASP
1	A	939	ASN
1	A	948	VAL
1	A	961	SER
1	A	965	ILE
1	A	974	THR
1	A	977	SER
1	A	996	THR
1	A	1009	GLU
1	A	1010	LEU
1	A	1012	SER
1	A	1017	GLU
1	A	1019	ILE
1	A	1025	LEU
1	A	1031	ILE
1	A	1034	THR
1	A	1045	ILE
1	A	1047	GLU
1	A	1055	LEU

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Mol	Chain	Res	Type
1	A	1085	ILE
1	A	1092	LEU
1	A	1111	LEU
1	A	1129	LEU
1	A	1149	ASP
1	A	1152	LEU
1	A	1155	ILE
1	A	1161	SER
1	A	1164	LEU
1	A	1179	THR
1	A	1221	VAL
1	A	1243	LEU
1	A	1274	LEU
1	A	1281	ARG
1	A	1282	TYR
1	A	1286	ASN
1	A	1303	ILE
1	A	1310	LYS
1	A	1312	LEU
1	A	1314	TYR
1	A	1322	SER
1	A	1334	ILE
1	A	1342	ASP
1	A	1362	ILE
1	A	1366	GLU
1	A	1383	ILE
1	A	1388	THR
1	A	1405	THR
1	A	1408	ILE
1	A	1410	GLU
1	A	1418	ILE
1	A	1436	LEU
1	A	1459	TYR
1	A	1467	ASN
1	A	1472	ASN
1	A	1483	LEU
1	A	1485	THR
1	A	1510	SER
1	A	1511	LYS
1	A	1518	ILE
1	A	1526	LEU
1	A	1530	ASN

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Mol	Chain	Res	Type
1	A	1531	TYR
1	A	1549	THR
1	A	1552	LEU
1	A	1591	ILE
1	A	1606	ILE
1	A	1607	LEU
1	A	1613	ILE
1	A	1618	SER
1	A	1623	GLU
1	A	1624	LEU
1	A	1625	ILE
1	A	1641	ILE
1	A	1642	LYS
1	A	1644	THR
1	A	1645	SER
1	A	1650	VAL
1	A	1657	ILE
1	A	1662	TYR
1	A	1663	HIS
1	A	1670	ILE
1	A	1671	SER
1	A	1698	LEU
1	A	1701	ASP
1	A	1702	GLU
1	A	1706	THR
1	A	1715	CYS
1	A	1722	ASP
1	A	1727	ASN
1	A	1734	ILE
1	A	1735	ASN
1	A	1736	ASP
1	A	1739	ILE
1	A	1748	SER
1	A	1752	LEU
1	A	1774	SER
1	A	1780	LYS
1	A	1784	ASN
1	A	1789	GLN
1	A	1792	SER
1	A	1795	LYS
1	A	1796	ILE
1	A	1810	PHE

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Mol	Chain	Res	Type
1	A	1818	SER
1	A	1819	LEU
1	A	1821	ASN
1	A	1833	VAL
1	A	1837	ILE
1	A	1843	LEU
1	A	1852	ASN
1	A	1853	LEU
1	A	1854	ILE
1	A	1858	THR
1	A	1859	THR
1	A	1872	SER
1	A	1881	THR
1	A	1894	ILE
1	A	1900	ILE
1	A	1902	THR
1	A	1906	LEU
1	A	1931	ASN
1	A	1932	ILE
1	A	1935	LYS
1	A	1947	VAL
1	A	1948	GLU
1	A	1960	ASN
1	A	1970	LEU
1	A	1985	ILE
1	A	1993	ILE
1	A	2003	ASP
1	A	2013	VAL
1	A	2017	TYR
1	A	2027	GLN
1	A	2028	LEU
1	A	2046	ASP
1	A	2085	ASP
1	A	2087	SER
1	A	2088	THR
1	A	2104	VAL
1	A	2114	ASP
1	A	2119	GLN
1	A	2127	ASP
1	A	2140	LEU
1	A	2144	ASN
1	A	2165	THR

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Mol	Chain	Res	Type
1	A	2178	VAL
1	A	2187	VAL
1	A	2194	ARG
1	A	2230	TYR
1	A	2236	VAL
1	A	2249	MET
1	A	2251	THR
1	A	2258	ASN
1	A	2265	GLU
1	A	2270	GLN
1	A	2273	TYR
1	A	2274	LEU
1	A	2280	MET
1	A	2313	PHE
1	A	2321	THR
1	A	2329	LYS
1	A	2336	GLU
1	A	2341	THR
1	A	2345	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	10	GLN
1	A	20	GLN
1	A	35	HIS
1	A	36	ASN
1	A	53	ASN
1	A	113	ASN
1	A	193	GLN
1	A	212	ASN
1	A	236	ASN
1	A	238	ASN
1	A	294	GLN
1	A	343	GLN
1	A	379	ASN
1	A	380	ASN
1	A	402	GLN
1	A	405	ASN
1	A	415	ASN
1	A	479	GLN

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Mol	Chain	Res	Type
1	A	510	GLN
1	A	579	HIS
1	A	596	ASN
1	A	611	ASN
1	A	639	GLN
1	A	653	HIS
1	A	659	ASN
1	A	785	ASN
1	A	802	GLN
1	A	835	GLN
1	A	853	ASN
1	A	907	ASN
1	A	972	ASN
1	A	999	ASN
1	A	1052	ASN
1	A	1186	HIS
1	A	1257	HIS
1	A	1294	ASN
1	A	1307	GLN
1	A	1370	ASN
1	A	1399	ASN
1	A	1456	HIS
1	A	1472	ASN
1	A	1490	ASN
1	A	1504	ASN
1	A	1520	ASN
1	A	1530	ASN
1	A	1553	ASN
1	A	1570	ASN
1	A	1610	ASN
1	A	1617	ASN
1	A	1676	ASN
1	A	1735	ASN
1	A	1763	GLN
1	A	1840	ASN
1	A	1851	ASN
1	A	1901	ASN
1	A	1925	ASN
1	A	1976	ASN
1	A	2023	ASN
1	A	2119	GLN
1	A	2126	ASN

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Mol	Chain	Res	Type
1	A	2196	ASN
1	A	2234	ASN
1	A	2270	GLN
1	A	2295	ASN
1	A	2312	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 1 ligands modelled in this entry, 1 is 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 [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-38010. These allow visual inspection of the internal detail of the map and identification of artifacts.

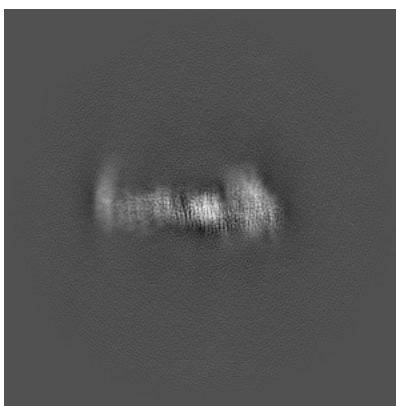
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

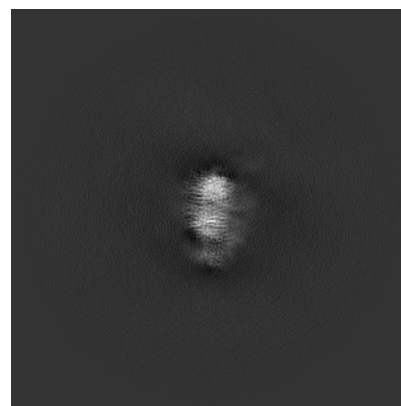
6.1.1 Primary map



X



Y

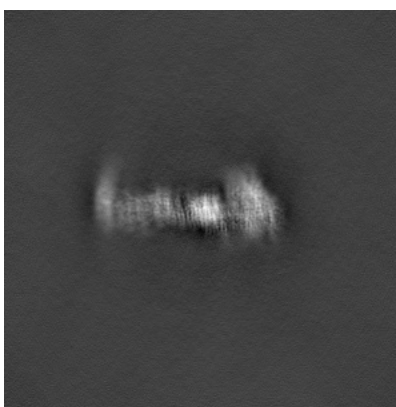


Z

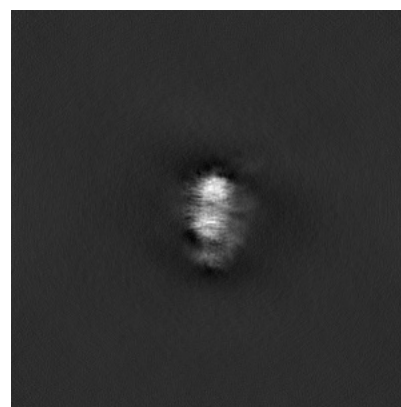
6.1.2 Raw map



X



Y

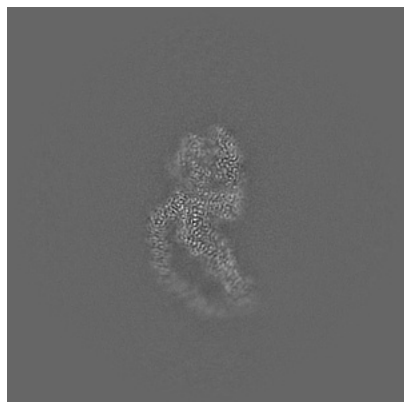


Z

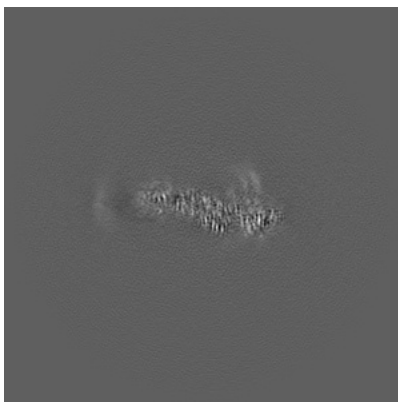
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

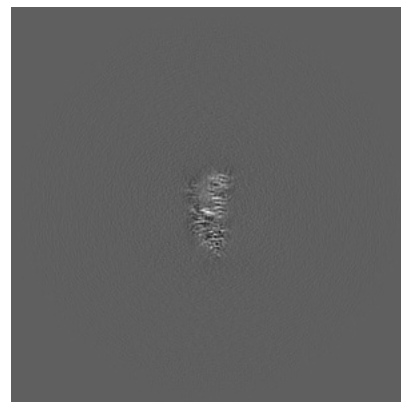
6.2.1 Primary map



X Index: 200

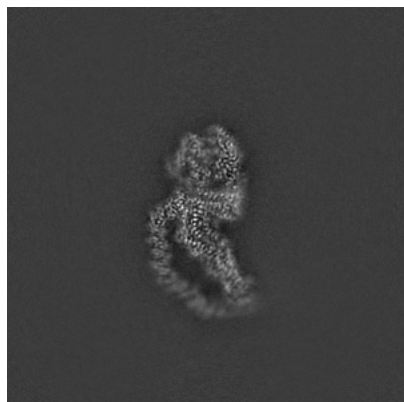


Y Index: 200

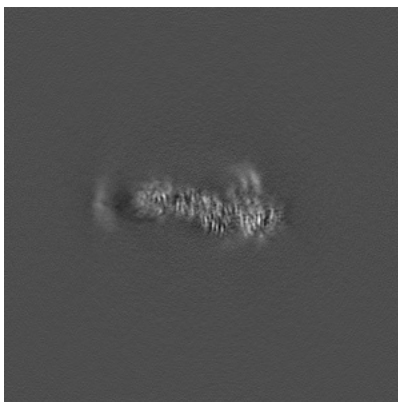


Z Index: 200

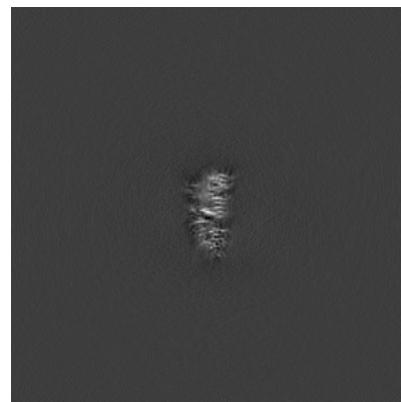
6.2.2 Raw map



X Index: 200



Y Index: 200

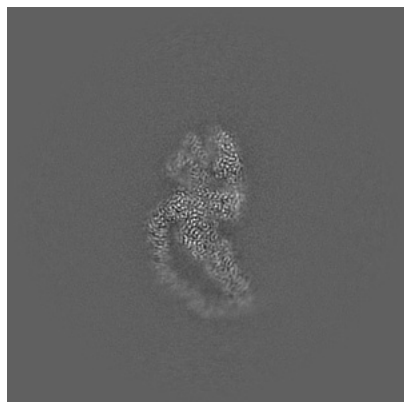


Z Index: 200

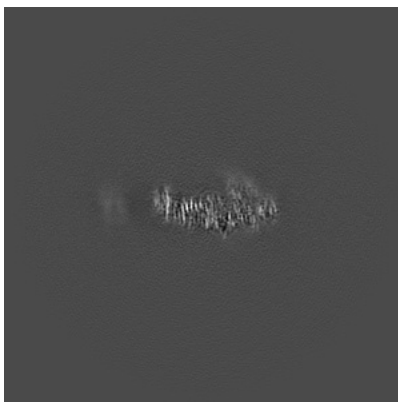
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 202

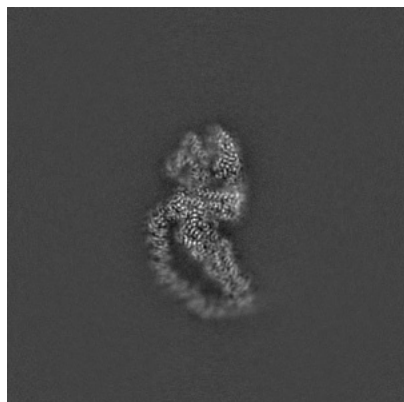


Y Index: 187

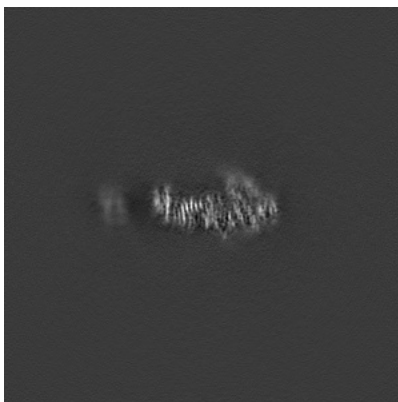


Z Index: 201

6.3.2 Raw map



X Index: 202



Y Index: 187

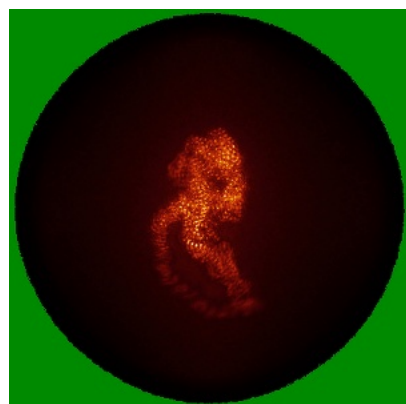


Z Index: 201

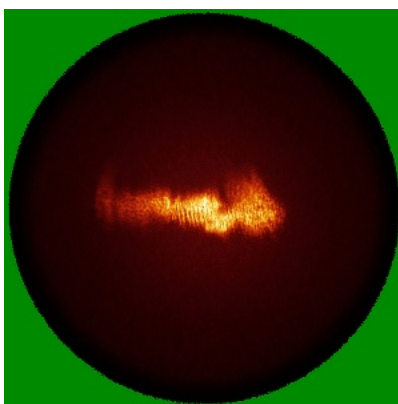
The images above show the largest variance slices of the map in three orthogonal directions.

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

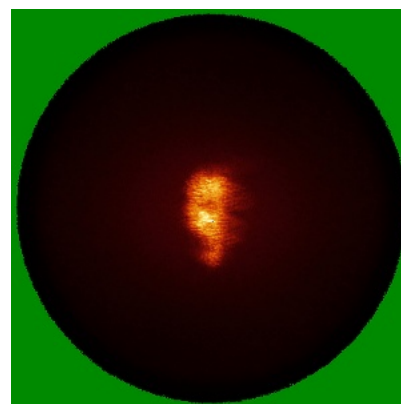
6.4.1 Primary map



X

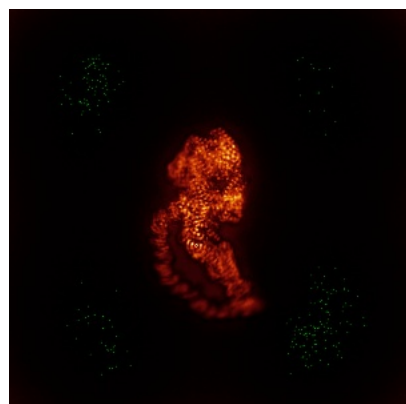


Y

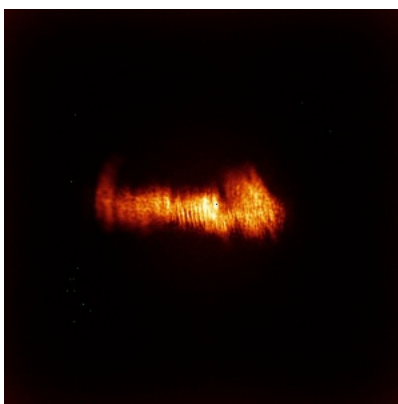


Z

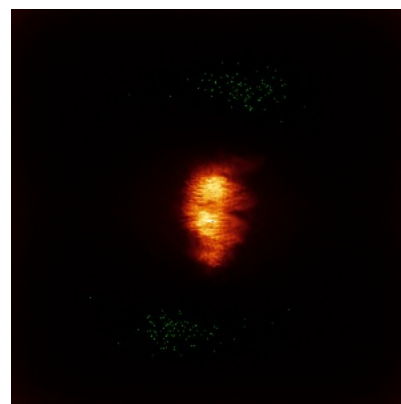
6.4.2 Raw map



X



Y



Z

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

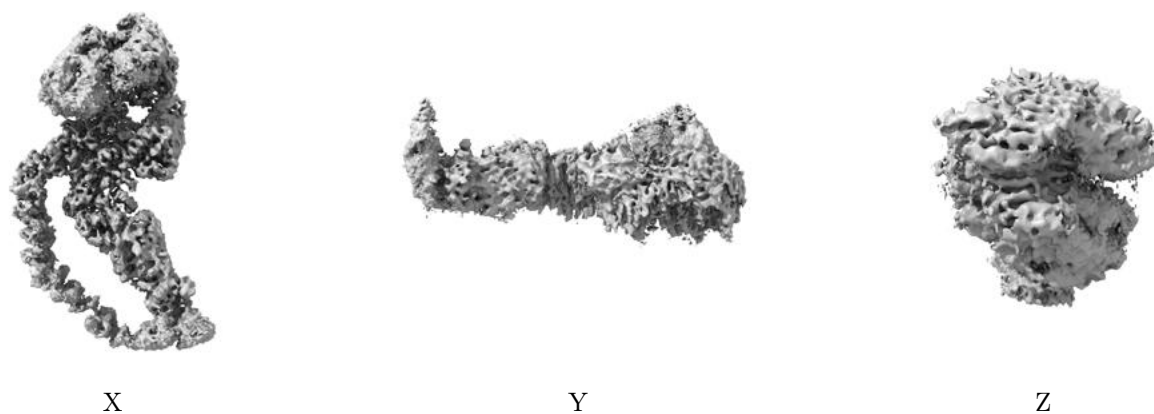
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.22. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

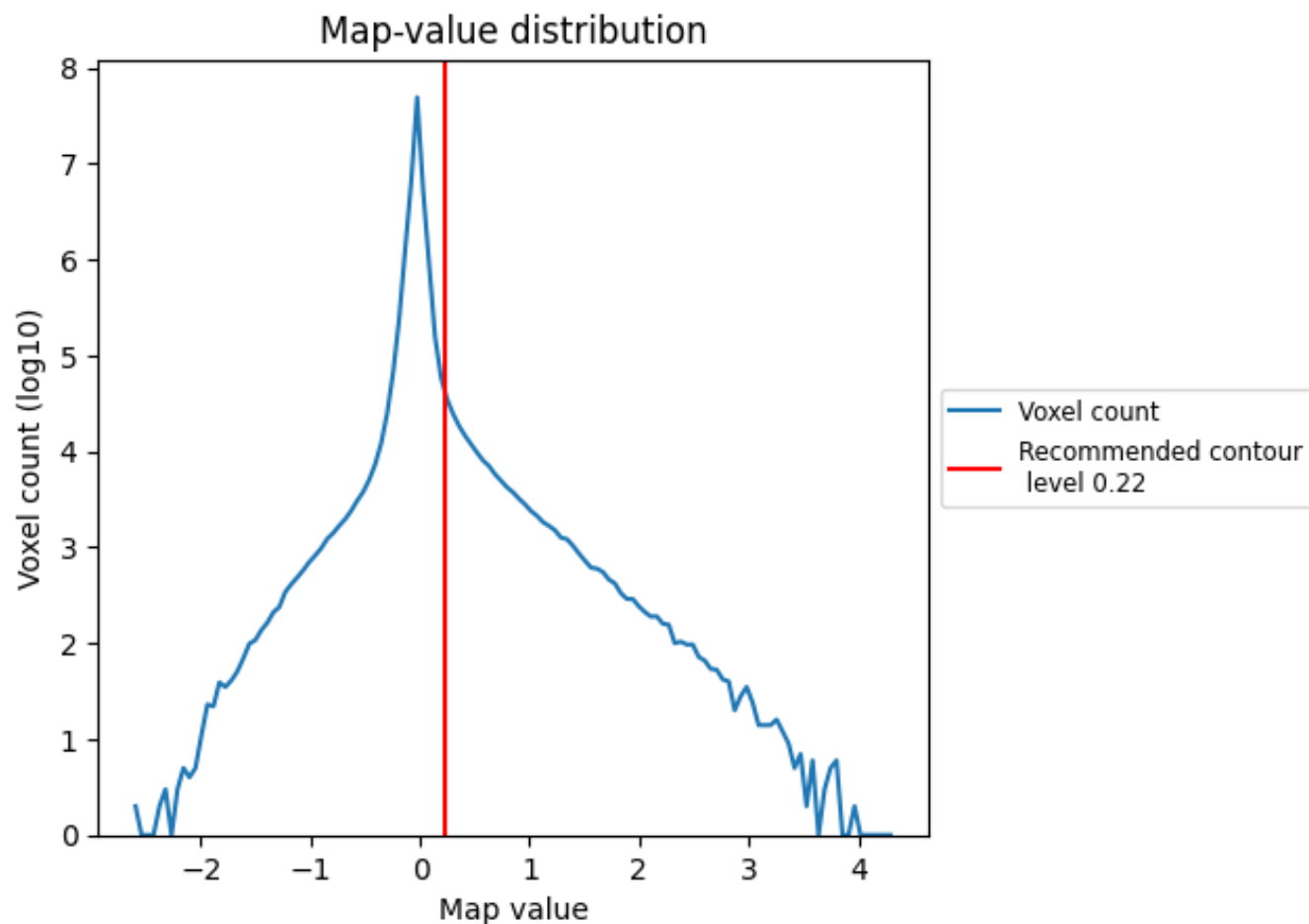
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

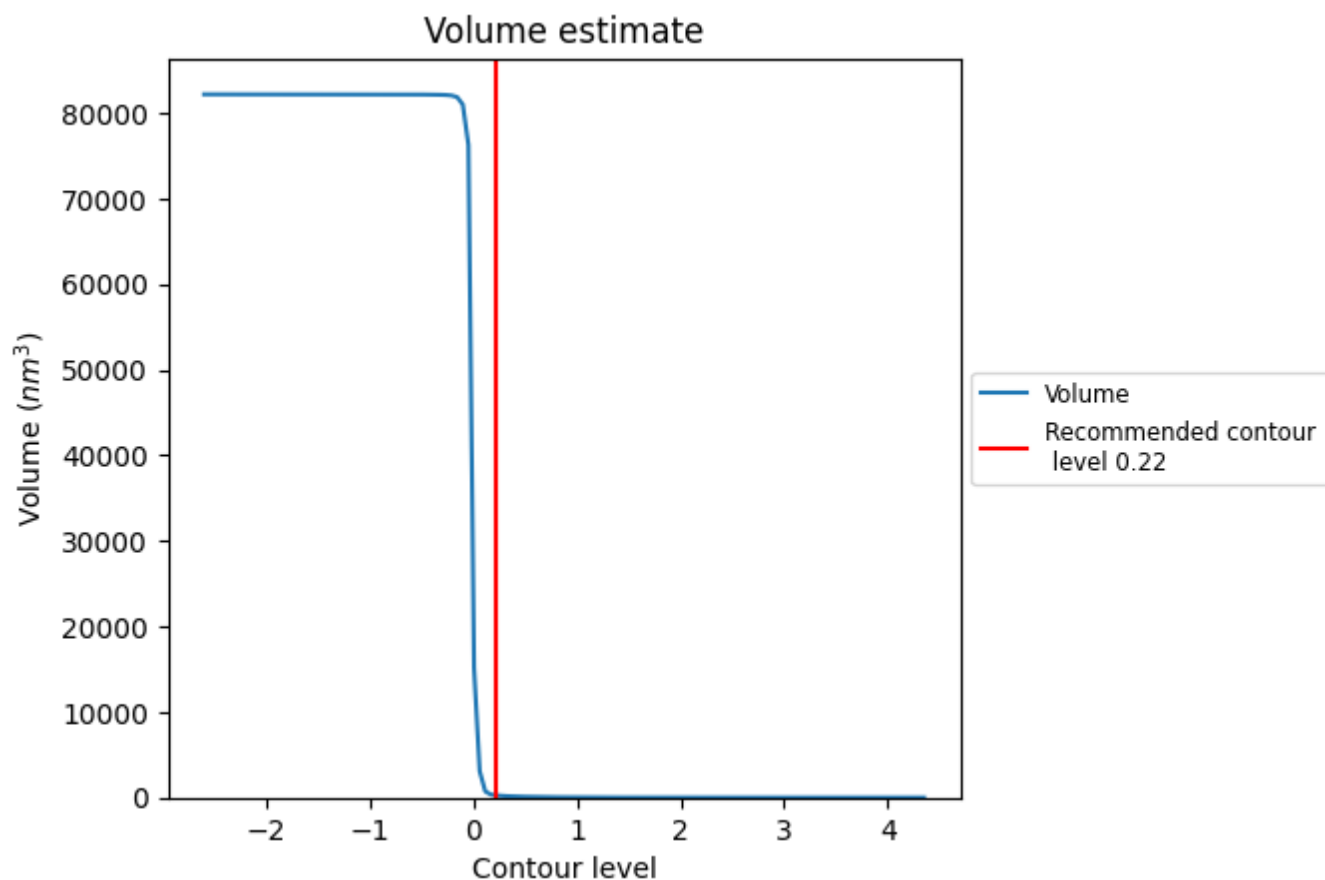
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

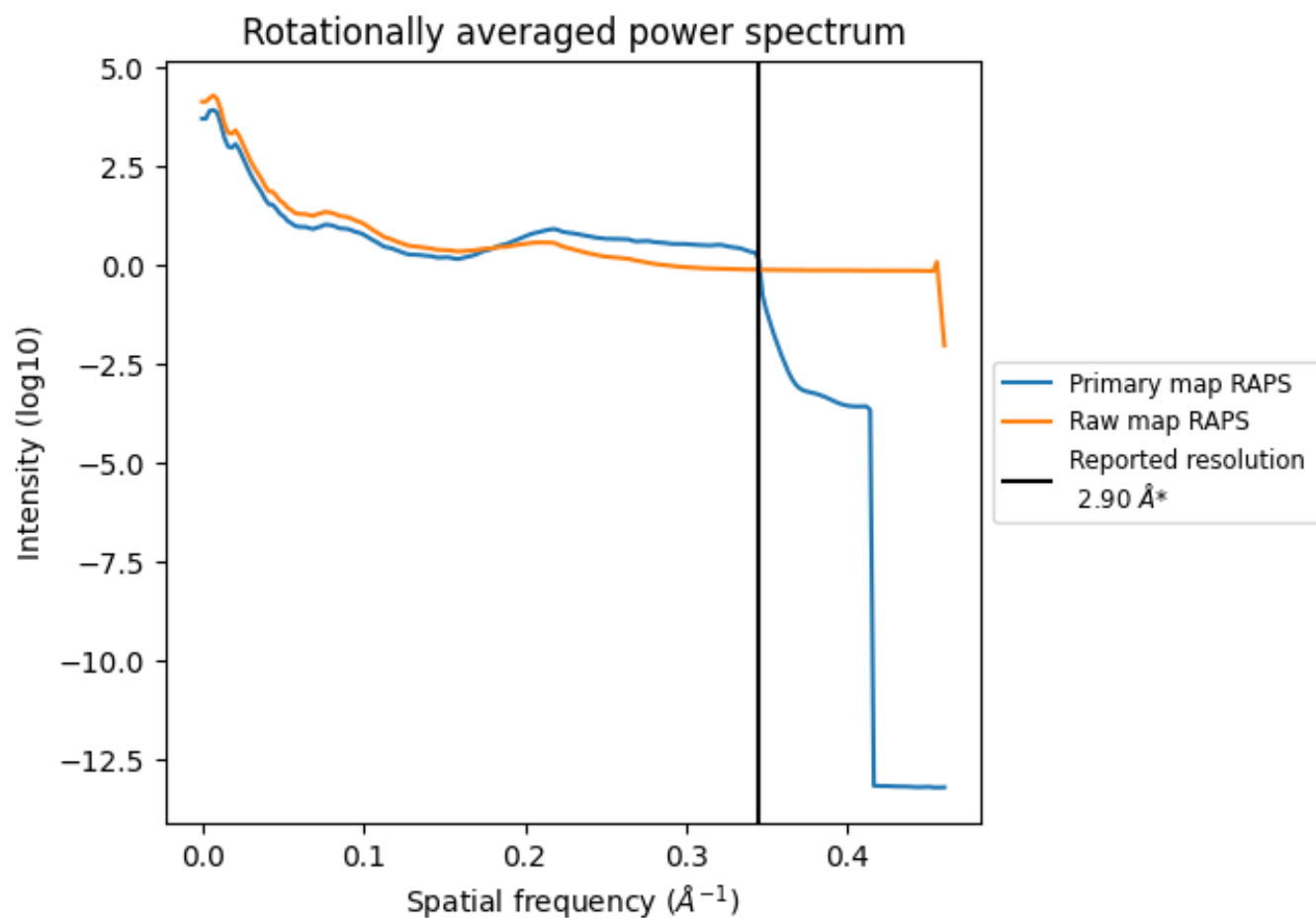
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 260 nm³; this corresponds to an approximate mass of 235 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

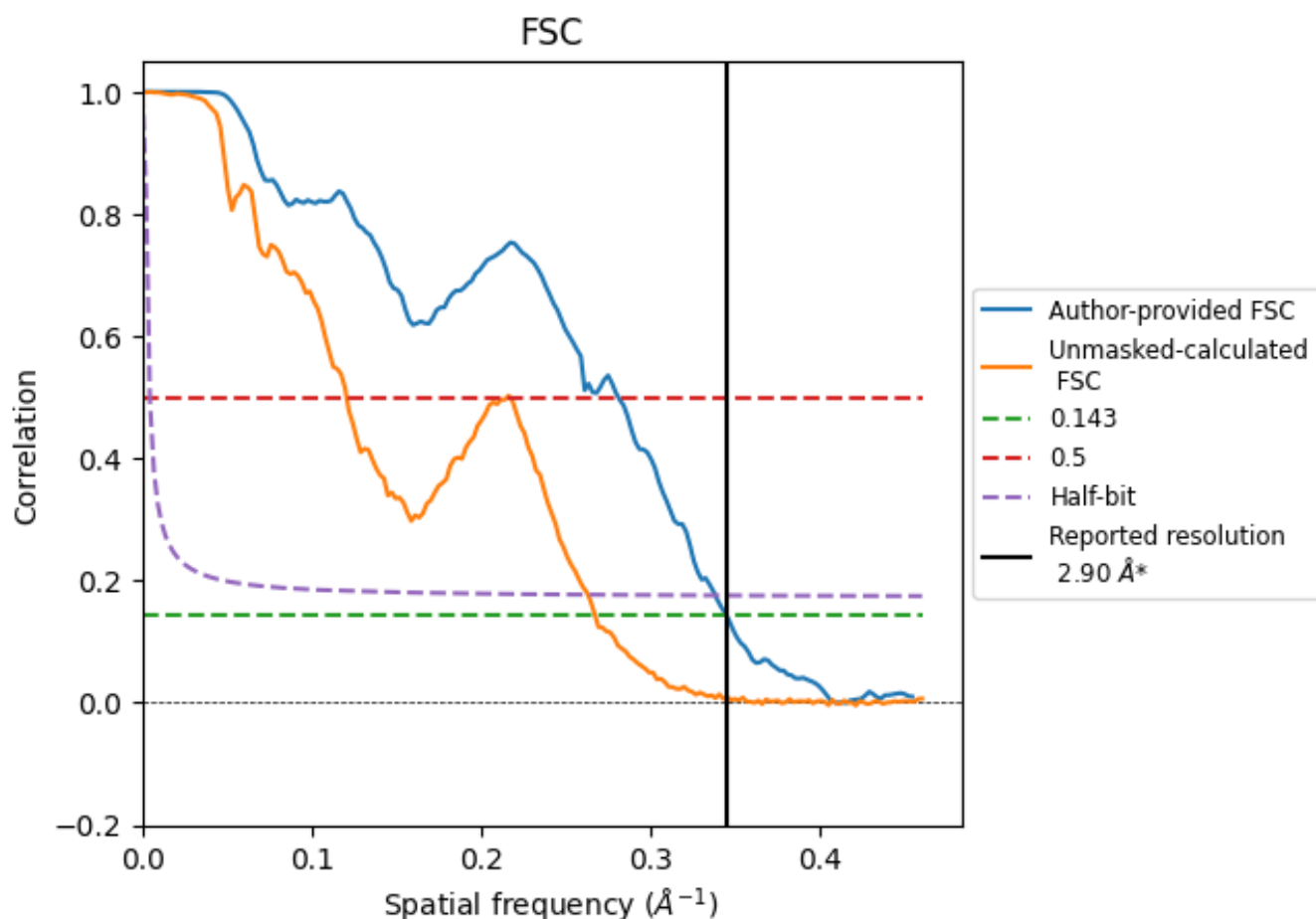


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.56	2.96
Unmasked-calculated*	3.74	8.30	3.81

*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 3.74 differs from the reported value 2.9 by more than 10 %

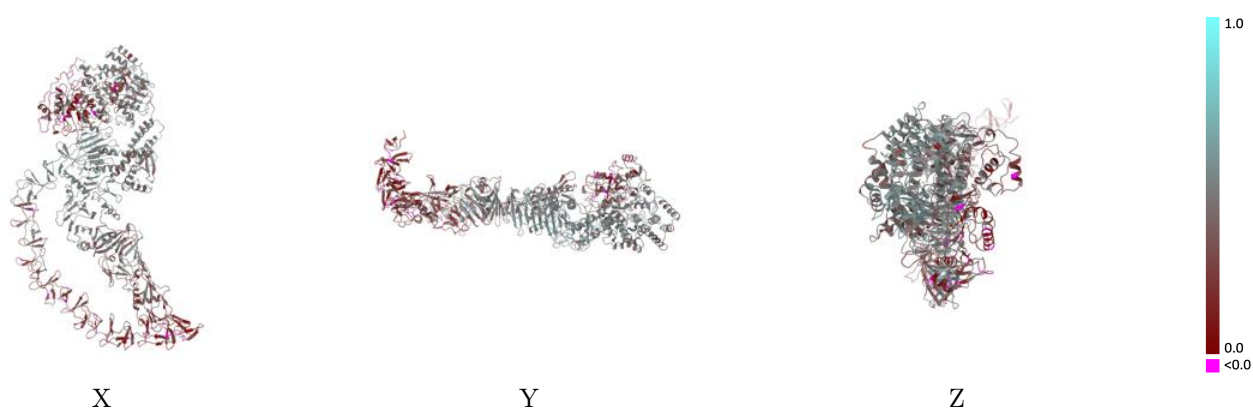
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-38010 and PDB model 8X2H. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

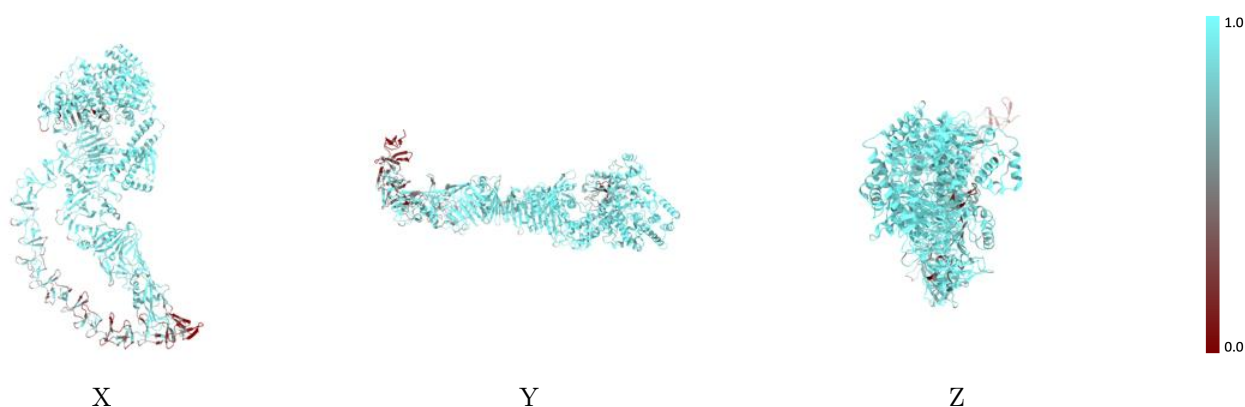
This section was not generated.

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



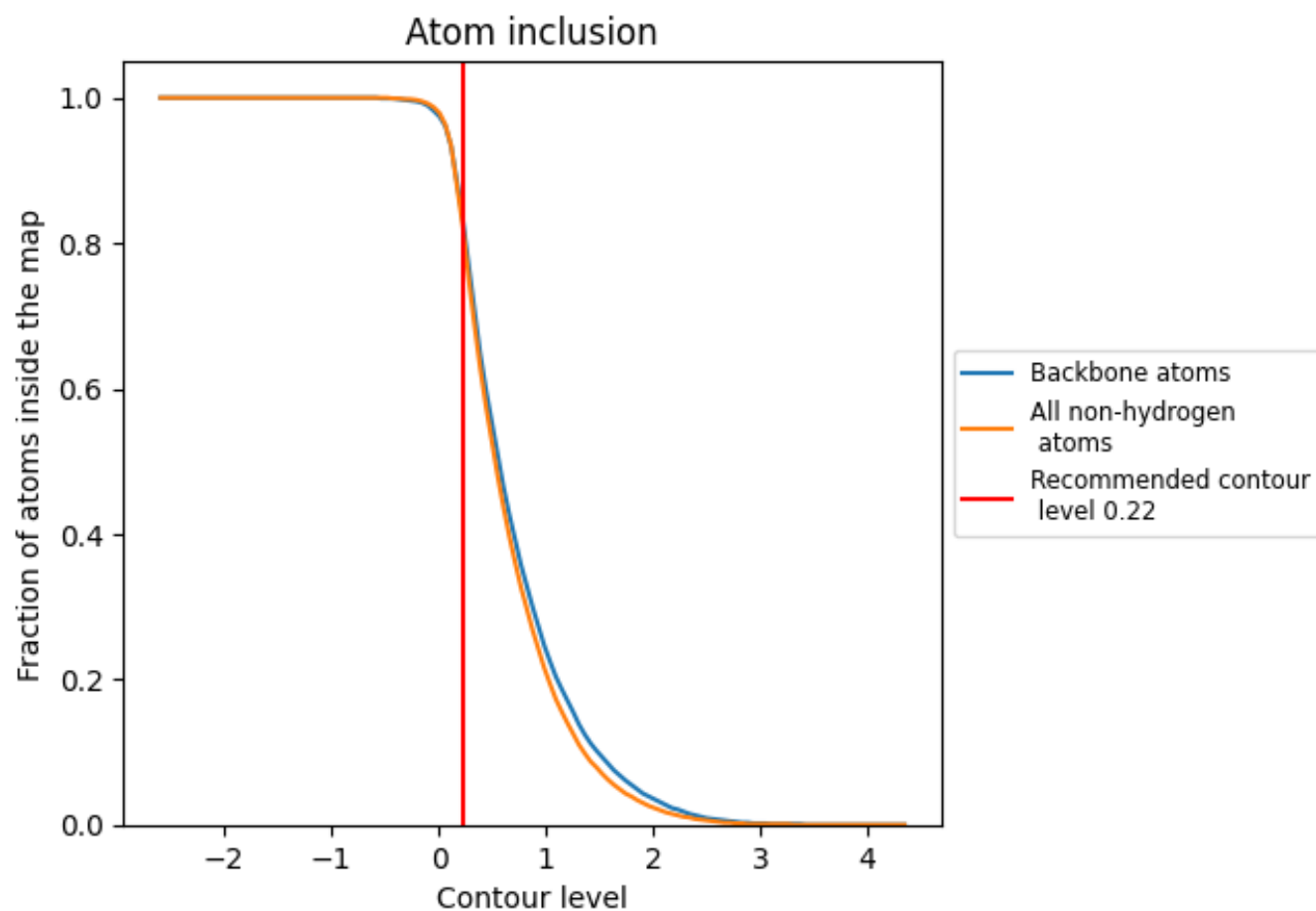
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.22).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 83% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8310	0.3930
A	0.8310	0.3930

