



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 01:10 AM UTC

PDB ID : 7PE9 / pdb_00007pe9
EMDB ID : EMD-13349
Title : cryo-EM structure of DEPTOR bound to human mTOR complex 2, DEPT-bound subset local refinement
Authors : Waelchli, M.; Maier, T.
Deposited on : 2021-08-09
Resolution : 3.70 Å(reported)
Based on initial model : 6ZWM

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:

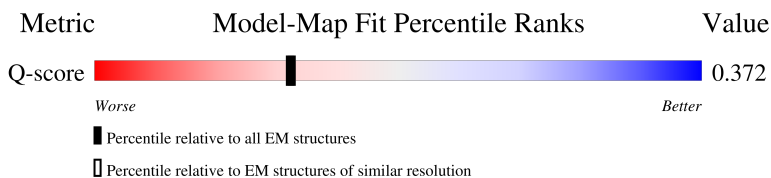
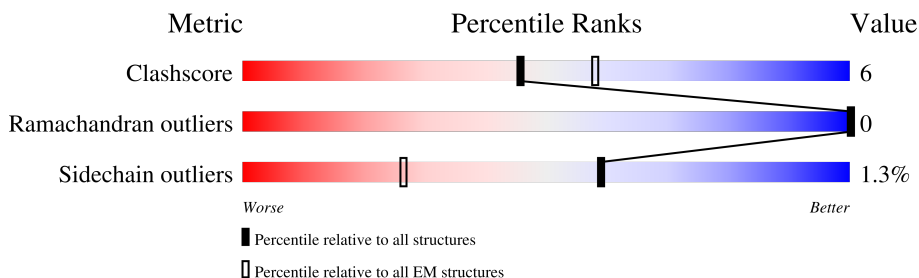
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

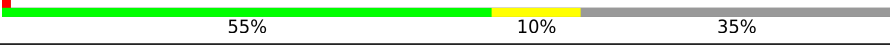
The reported resolution of this entry is 3.70 Å.

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	11569 (3.20 - 4.20)

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	2571	
2	C	326	
3	E	1708	
4	G	522	

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Mol	Chain	Length	Quality of chain
5	I	409	5% 51% 23% • 22%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 31076 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 Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2194	Total	C	N	O	S	0	0
			16419	10414	2922	2984	99		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246M	GLY	-	insertion	UNP P42345
A	246N	SER	-	insertion	UNP P42345
A	246O	THR	-	insertion	UNP P42345
A	246P	SER	-	insertion	UNP P42345
A	246Q	GLY	-	insertion	UNP P42345
A	246R	SER	-	insertion	UNP P42345
A	246S	GLY	-	insertion	UNP P42345
A	246T	ASP	-	insertion	UNP P42345
A	246U	TYR	-	insertion	UNP P42345
A	246V	LYS	-	insertion	UNP P42345
A	246W	ASP	-	insertion	UNP P42345
A	246X	ASP	-	insertion	UNP P42345
A	246Y	ASP	-	insertion	UNP P42345
A	246Z	ASP	-	insertion	UNP P42345
A	247A	LYS	-	insertion	UNP P42345
A	247B	GLY	-	insertion	UNP P42345
A	247C	SER	-	insertion	UNP P42345
A	247D	THR	-	insertion	UNP P42345
A	247E	SER	-	insertion	UNP P42345
A	247F	GLY	-	insertion	UNP P42345
A	247G	SER	-	insertion	UNP P42345
A	247H	GLY	-	insertion	UNP P42345

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	319	Total	C	N	O	S	0	0
			2465	1533	437	477	18		

- Molecule 3 is a protein called Rapamycin-insensitive companion of mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	1115	Total	C	N	O	S	0	0
			8917	5680	1582	1608	47		

- Molecule 4 is a protein called Target of rapamycin complex 2 subunit MAPKAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	98	Total	C	N	O	S	0	0
			655	399	125	127	4		

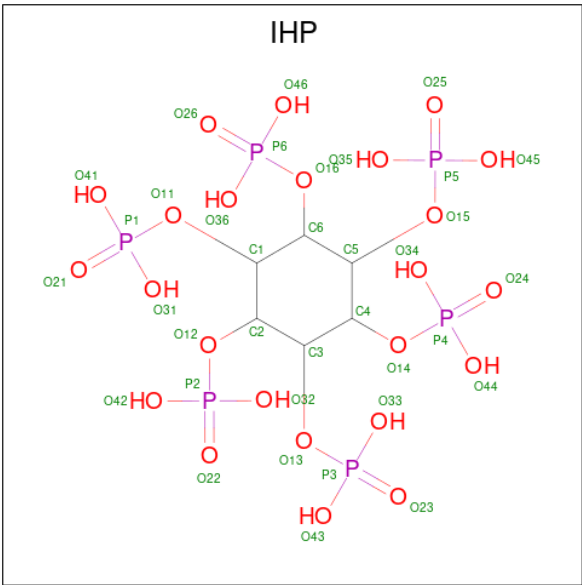
- Molecule 5 is a protein called DEP domain-containing mTOR-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	317	Total	C	N	O	S	0	0
			2580	1627	470	465	18		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	204	SER	ASN	variant	UNP Q8TB45
I	389	ASN	SER	variant	UNP Q8TB45

- Molecule 6 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).

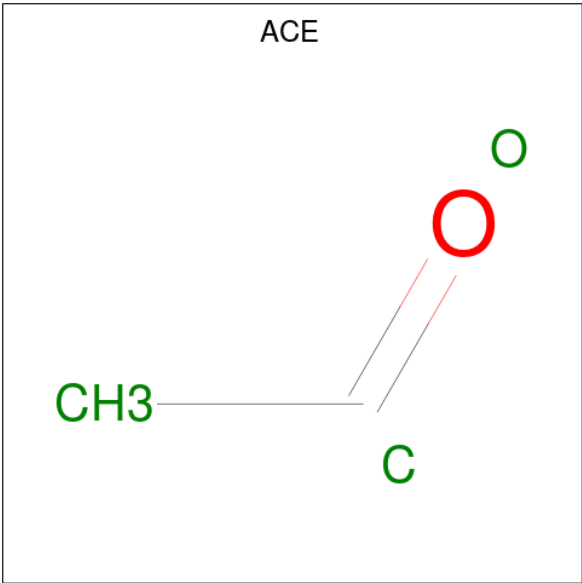


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	E	1	Total	Zn	0
			1	1	

- Molecule 8 is ACETYL GROUP (CCD ID: ACE) (formula: C₂H₄O).

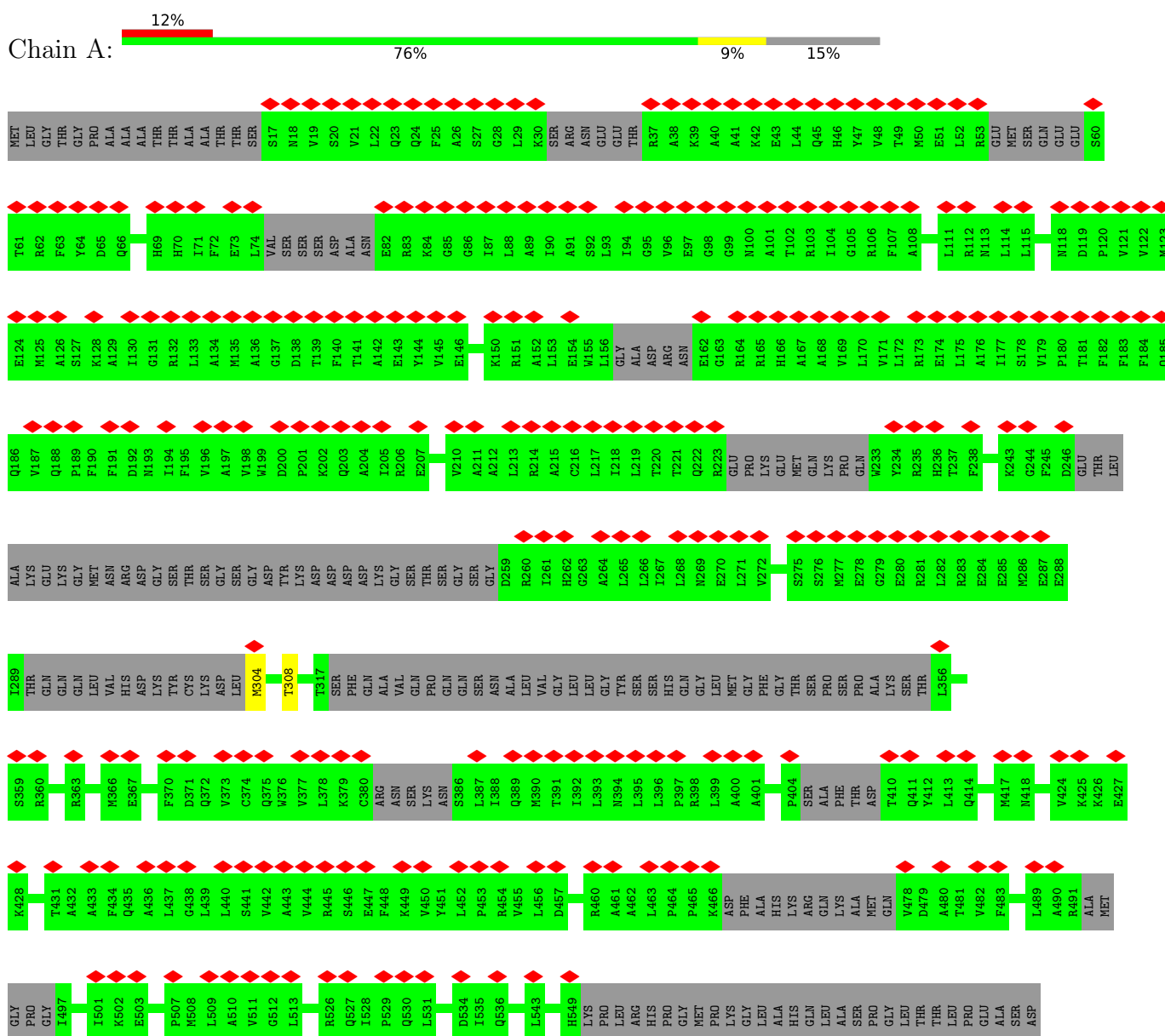


Mol	Chain	Residues	Atoms			AltConf
8	G	1	Total	C	O	0
			3	2	1	

3 Residue-property plots

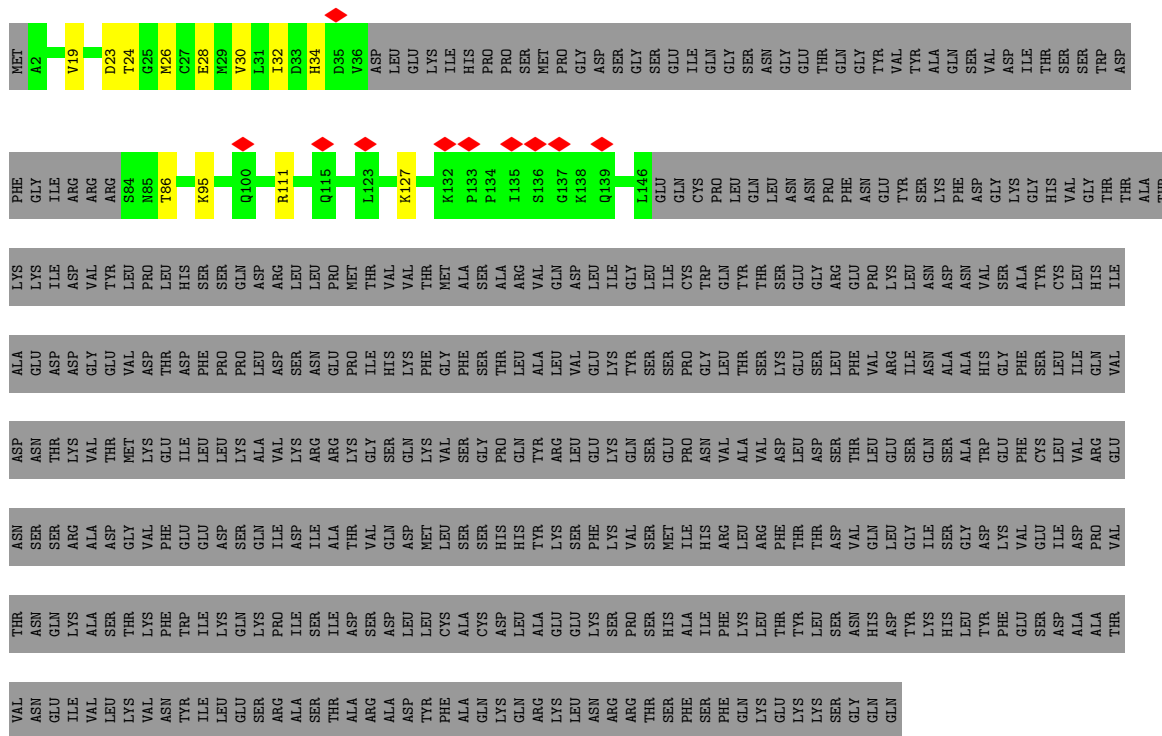
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

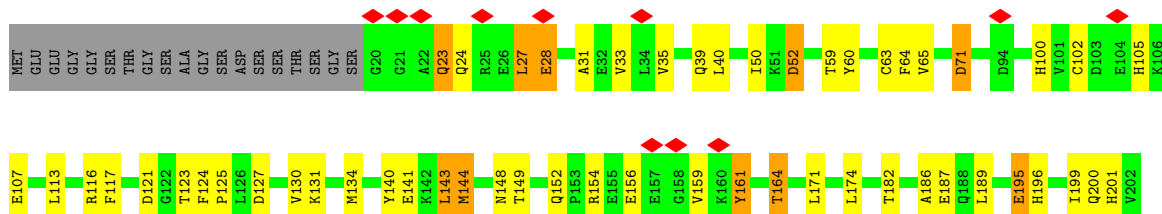




- Molecule 4: Target of rapamycin complex 2 subunit MAPKAP1



- Molecule 5: DEP domain-containing mTOR-interacting protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	132837	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.380	Depositor
Minimum map value	-0.484	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.205	Depositor
Map size ($\text{\AA}$)	507.84, 507.84, 507.84	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.058, 1.058, 1.058	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.13	0/16719	0.28	0/22710
2	C	0.13	0/2523	0.32	0/3438
3	E	0.13	0/9078	0.29	0/12281
4	G	0.12	0/660	0.30	0/900
5	I	0.11	0/2631	0.39	0/3539
All	All	0.13	0/31611	0.29	0/42868

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	16419	0	15461	147	0
2	C	2465	0	2351	58	0
3	E	8917	0	9064	115	0
4	G	655	0	519	11	0
5	I	2580	0	2592	65	0
6	A	36	0	6	0	0
7	E	1	0	0	0	0
8	G	3	0	3	0	0
All	All	31076	0	29996	381	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 6.

All (381) 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:773:GLU:HG2	1:A:774:PRO:HD3	1.62	0.82
1:A:631:THR:HA	1:A:682:ARG:HH22	1.45	0.82
1:A:737:ILE:HG23	1:A:753:SER:HB2	1.65	0.79
5:I:27:LEU:HD13	5:I:196:HIS:HA	1.66	0.77
2:C:39:GLN:HE22	2:C:41:GLN:HB2	1.51	0.76
5:I:105:HIS:HD2	5:I:107:GLU:H	1.33	0.75
1:A:1677:LEU:HD22	1:A:1690:PRO:HG2	1.73	0.70
1:A:727:MET:HG3	1:A:728:PRO:HD3	1.73	0.70
3:E:771:LEU:HD11	3:E:797:LEU:HD13	1.75	0.69
5:I:156:GLU:HB2	5:I:214:LEU:HD12	1.76	0.68
3:E:1492:ILE:HD12	3:E:1611:LEU:HD13	1.76	0.67
2:C:261:LYS:HA	2:C:270:ARG:HH12	1.60	0.66
2:C:78:ILE:HG13	2:C:79:ILE:HD12	1.78	0.66
1:A:2192:LEU:HD22	1:A:2235:GLY:HA3	1.77	0.66
1:A:2384:THR:HA	1:A:2387:MET:HE3	1.78	0.65
3:E:543:ASN:HD22	3:E:580:PHE:HE1	1.42	0.64
3:E:660:PHE:HA	3:E:663:ILE:HG22	1.78	0.64
3:E:830:LYS:HD3	3:E:835:TYR:HE1	1.63	0.63
1:A:1364:MET:HG3	1:A:1372:LEU:HD23	1.81	0.63
2:C:98:ARG:HH21	2:C:99:TRP:HE1	1.45	0.63
1:A:583:THR:HG22	1:A:618:ILE:HG13	1.80	0.63
2:C:122:GLN:NE2	4:G:111:ARG:O	2.27	0.62
3:E:139:ASN:ND2	3:E:142:GLU:OE1	2.32	0.62
3:E:380:ARG:NH2	3:E:780:ASP:OD2	2.32	0.62
2:C:178:ILE:HG12	2:C:185:MET:HG2	1.82	0.61
1:A:1686:ASP:OD1	1:A:1687:HIS:N	2.33	0.61
1:A:1950:ARG:HB2	1:A:1953:VAL:HG12	1.82	0.61
1:A:1722:GLN:O	1:A:1726:GLN:NE2	2.34	0.61
1:A:933:GLU:HG3	1:A:938:MET:HE2	1.82	0.61
3:E:833:ARG:NH2	3:E:834:GLU:OE2	2.32	0.61
1:A:304:MET:HE2	5:I:397:ARG:H	1.66	0.61
5:I:154:ARG:NH1	5:I:164:THR:O	2.35	0.60
5:I:218:ARG:HH12	5:I:219:MET:HB2	1.66	0.60
3:E:637:SER:HA	3:E:647:GLN:HB2	1.81	0.60
2:C:28:GLN:NE2	2:C:31:SER:OG	2.34	0.60
1:A:1736:ASP:HA	1:A:1740:LYS:HB3	1.82	0.60
3:E:436:THR:HG23	3:E:437:ILE:HG13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:539:GLN:HG3	3:E:540:HIS:CD2	2.37	0.60
3:E:557:TRP:CD2	3:E:558:PRO:HD2	2.38	0.59
1:A:1947:ASP:OD2	1:A:1987:ARG:NH1	2.35	0.59
5:I:40:LEU:HD13	5:I:227:LEU:HD11	1.85	0.59
3:E:136:GLN:OE1	3:E:143:ARG:NH1	2.36	0.58
1:A:1686:ASP:HB2	5:I:131:LYS:HD2	1.86	0.58
2:C:27:TRP:HH2	2:C:310:GLY:H	1.51	0.58
1:A:664:ILE:HG13	1:A:665:THR:HG23	1.85	0.58
2:C:146:GLY:HA3	2:C:173:ILE:HD11	1.86	0.57
3:E:45:VAL:HG22	3:E:90:LEU:HD12	1.86	0.57
2:C:173:ILE:HA	2:C:189:ASN:HA	1.86	0.57
3:E:755:LEU:HD21	3:E:773:ILE:HD11	1.85	0.57
4:G:32:ILE:HG22	4:G:34:HIS:H	1.69	0.57
3:E:835:TYR:HB2	3:E:838:LYS:HE3	1.86	0.57
5:I:333:ILE:HD11	5:I:360:PRO:HB2	1.86	0.57
1:A:1715:GLN:NE2	5:I:121:ASP:OD1	2.37	0.57
3:E:638:SER:O	3:E:694:GLN:NE2	2.38	0.56
2:C:11:ASP:O	2:C:54:ARG:NH1	2.38	0.56
1:A:1109:ASP:OD1	3:E:474:ASN:ND2	2.39	0.56
1:A:1031:MET:HE1	1:A:1059:ILE:HD13	1.87	0.56
1:A:809:SER:HB2	1:A:812:GLU:HB3	1.88	0.56
2:C:69:ASP:OD1	2:C:70:LEU:N	2.39	0.56
3:E:959:CYS:H	3:E:965:ARG:HH21	1.53	0.56
1:A:872:LEU:O	1:A:881:ARG:NH2	2.39	0.55
1:A:1226:GLU:O	3:E:485:ARG:NH1	2.37	0.55
3:E:533:ARG:HH12	3:E:569:GLN:HG2	1.72	0.55
1:A:709:GLU:OE2	1:A:759:HIS:NE2	2.40	0.55
3:E:539:GLN:HG3	3:E:540:HIS:HD2	1.70	0.55
5:I:71:ASP:OD1	5:I:71:ASP:N	2.40	0.55
1:A:1315:ARG:NH1	1:A:1352:GLU:OE2	2.40	0.55
1:A:1554:GLN:HG3	1:A:1556:LEU:HD13	1.88	0.55
5:I:218:ARG:HG2	5:I:218:ARG:HH11	1.71	0.55
2:C:137:HIS:HB2	2:C:142:GLU:HB2	1.88	0.55
3:E:557:TRP:HB3	3:E:560:VAL:HG22	1.90	0.54
3:E:809:LEU:HD23	3:E:886:LEU:HD13	1.89	0.54
3:E:916:LYS:HB2	3:E:919:GLU:HG2	1.89	0.54
5:I:331:PHE:N	5:I:401:MET:O	2.35	0.54
1:A:1432:VAL:HG22	1:A:2390:THR:HG21	1.88	0.54
1:A:1386:ARG:HH11	1:A:1389:LYS:HE2	1.73	0.54
3:E:710:ASP:HB2	3:E:714:ARG:NH2	2.23	0.54
2:C:131:ILE:HA	2:C:147:ASP:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:559:ASN:ND2	3:E:559:ASN:O	2.41	0.54
3:E:237:HIS:ND1	3:E:239:LYS:HG2	2.22	0.53
4:G:23:ASP:OD1	4:G:24:THR:N	2.41	0.53
1:A:1272:ALA:H	1:A:1274:ARG:NH1	2.05	0.53
1:A:1541:HIS:HD2	1:A:1571:LEU:HB2	1.72	0.53
1:A:2194:GLN:HG3	1:A:2421:PHE:HZ	1.74	0.53
3:E:237:HIS:HE1	3:E:239:LYS:HE3	1.73	0.53
3:E:537:VAL:HA	3:E:546:TRP:CD1	2.44	0.53
2:C:98:ARG:HA	2:C:115:ARG:HH12	1.72	0.53
3:E:968:CYS:HA	3:E:971:VAL:HG22	1.90	0.53
3:E:183:MET:HE3	4:G:26:MET:HB3	1.90	0.53
3:E:835:TYR:HB2	3:E:838:LYS:HB3	1.90	0.53
1:A:1527:ASP:O	5:I:345:ARG:NH1	2.38	0.53
5:I:201:HIS:HB3	5:I:205:LYS:HA	1.91	0.53
1:A:818:ASP:OD1	1:A:819:GLU:N	2.41	0.52
1:A:1386:ARG:HD3	1:A:1389:LYS:HE3	1.91	0.52
3:E:237:HIS:CG	3:E:238:PRO:HD2	2.44	0.52
2:C:141:ALA:HB2	4:G:127:LYS:HA	1.92	0.52
3:E:566:LYS:NZ	3:E:618:ASP:OD2	2.41	0.52
2:C:137:HIS:CG	2:C:138:PRO:HD2	2.45	0.52
5:I:164:THR:HB	5:I:214:LEU:HD22	1.90	0.52
5:I:24:GLN:O	5:I:28:GLU:HB3	2.08	0.52
5:I:152:GLN:O	5:I:164:THR:OG1	2.26	0.52
2:C:25:ARG:HB2	2:C:27:TRP:HE1	1.74	0.52
3:E:37:ASN:O	3:E:41:ILE:HG12	2.10	0.52
5:I:375:VAL:HG21	5:I:392:ILE:HG22	1.90	0.52
1:A:1097:LEU:HD22	1:A:1138:THR:HG21	1.92	0.52
1:A:854:VAL:HG23	1:A:855:VAL:HG23	1.92	0.51
1:A:719:SER:HB2	1:A:726:VAL:HG11	1.92	0.51
3:E:1607:MET:SD	3:E:1607:MET:N	2.84	0.51
3:E:409:VAL:HG13	3:E:452:LEU:HD13	1.91	0.51
3:E:959:CYS:O	3:E:965:ARG:NH2	2.43	0.51
2:C:202:GLY:HA3	2:C:207:VAL:HG22	1.92	0.51
3:E:689:CYS:HA	3:E:698:LEU:HD21	1.92	0.51
1:A:727:MET:CG	1:A:728:PRO:HD3	2.41	0.51
4:G:19:VAL:HG13	4:G:28:GLU:HG3	1.93	0.51
5:I:326:TYR:OH	5:I:328:ARG:NH2	2.44	0.51
5:I:373:VAL:O	5:I:380:VAL:N	2.40	0.51
1:A:1493:LEU:HD23	1:A:1519:ALA:HB2	1.93	0.50
3:E:186:ALA:HB1	4:G:30:VAL:HG11	1.93	0.50
3:E:942:LEU:H	3:E:942:LEU:HD23	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1211:VAL:HA	3:E:553:THR:HG21	1.93	0.50
5:I:310:LEU:HD21	5:I:369:CYS:HA	1.93	0.50
1:A:1358:LEU:HD23	1:A:1383:LEU:HD12	1.93	0.50
3:E:94:ASN:HD22	3:E:99:VAL:HG11	1.76	0.50
2:C:8:VAL:HG12	2:C:10:SER:H	1.77	0.50
2:C:63:GLN:NE2	2:C:85:ASN:O	2.40	0.50
3:E:36:ASP:HA	3:E:39:ARG:HH11	1.77	0.50
2:C:39:GLN:NE2	2:C:41:GLN:HB2	2.23	0.50
1:A:1085:ASP:HB3	1:A:1090:ARG:HH12	1.77	0.50
1:A:1072:PRO:HA	1:A:1075:ILE:HD12	1.94	0.50
2:C:292:ASN:ND2	2:C:312:GLN:O	2.45	0.50
2:C:200:THR:OG1	2:C:208:THR:HA	2.12	0.49
5:I:218:ARG:HH11	5:I:218:ARG:CG	2.25	0.49
1:A:1552:LEU:HD11	1:A:1603:ILE:HG12	1.94	0.49
3:E:1510:THR:HB	3:E:1610:ILE:HD11	1.93	0.49
1:A:2546:CYS:HB3	1:A:2549:TRP:HB2	1.93	0.49
3:E:831:TRP:NE1	3:E:835:TYR:OH	2.45	0.49
5:I:100:HIS:CE1	5:I:113:LEU:HB3	2.47	0.49
1:A:1501:TRP:HZ3	1:A:1512:MET:HG2	1.77	0.49
3:E:972:LEU:HA	3:E:975:ILE:HD12	1.94	0.49
1:A:2212:ASP:HB3	1:A:2215:SER:HB2	1.93	0.49
3:E:245:ARG:H	3:E:249:GLU:HG3	1.78	0.49
1:A:715:VAL:O	1:A:719:SER:N	2.45	0.49
3:E:586:LYS:HB3	3:E:590:ASN:OD1	2.13	0.49
1:A:751:GLU:HG2	1:A:797:ASN:HD22	1.77	0.49
2:C:137:HIS:HD1	2:C:139:ASN:CG	2.20	0.49
1:A:1159:ILE:HG21	1:A:1177:LEU:HD12	1.94	0.48
3:E:830:LYS:HD3	3:E:835:TYR:CE1	2.44	0.48
3:E:557:TRP:CG	3:E:558:PRO:HD2	2.48	0.48
3:E:880:ILE:HG23	3:E:885:GLN:HE21	1.78	0.48
3:E:538:LEU:O	3:E:541:LYS:NZ	2.46	0.48
1:A:1400:LYS:HD2	1:A:1400:LYS:HA	1.70	0.48
1:A:2025:GLU:OE1	1:A:2168:ARG:NH1	2.46	0.48
5:I:201:HIS:NE2	5:I:203:SER:OG	2.47	0.48
3:E:1649:ASP:OD1	3:E:1649:ASP:N	2.45	0.48
1:A:1285:ARG:O	1:A:1289:LEU:HD23	2.14	0.48
2:C:148:GLN:HA	2:C:172:SER:HB2	1.95	0.48
3:E:624:GLU:HG3	3:E:628:LYS:HE2	1.95	0.48
3:E:523:ASP:OD1	3:E:557:TRP:NE1	2.45	0.48
4:G:95:LYS:HA	4:G:95:LYS:HD3	1.64	0.48
1:A:2148:GLN:OE1	1:A:2149:PRO:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:ASP:OD2	2:C:108:THR:OG1	2.25	0.47
2:C:196:VAL:HG21	2:C:252:PHE:HE2	1.78	0.47
3:E:1609:ARG:HH12	3:E:1645:GLN:HG2	1.79	0.47
1:A:655:VAL:HA	1:A:658:LYS:HE2	1.96	0.47
1:A:2259:ILE:HG23	1:A:2263:ILE:HD12	1.96	0.47
1:A:1186:LYS:HG3	1:A:1225:GLU:HB2	1.96	0.47
3:E:238:PRO:HB3	3:E:960:GLU:HB3	1.95	0.47
1:A:2078:LEU:HD21	1:A:2107:VAL:HG11	1.96	0.47
2:C:144:ILE:HD11	2:C:178:ILE:HD11	1.96	0.47
1:A:895:ASP:OD1	1:A:895:ASP:N	2.44	0.47
1:A:2121:LEU:HD12	1:A:2160:LEU:HD11	1.95	0.47
3:E:360:ASP:O	3:E:363:ARG:NE	2.47	0.47
3:E:685:LEU:HD23	3:E:688:LEU:HD21	1.96	0.47
3:E:856:LYS:HG2	3:E:857:PRO:HD2	1.97	0.47
1:A:960:ARG:HG2	1:A:996:THR:HG21	1.97	0.47
1:A:2333:ILE:HD11	1:A:2404:MET:HE1	1.97	0.47
1:A:1091:ILE:HG22	1:A:1095:LYS:HE2	1.96	0.47
1:A:1541:HIS:CD2	1:A:1571:LEU:HD13	2.50	0.47
1:A:2006:VAL:O	1:A:2010:MET:HG2	2.15	0.47
1:A:2392:LEU:HD23	1:A:2392:LEU:H	1.79	0.47
5:I:144:MET:HE3	5:I:221:PHE:HD2	1.80	0.47
3:E:588:TYR:HA	3:E:591:LEU:HD23	1.97	0.46
3:E:827:GLN:O	3:E:831:TRP:N	2.44	0.46
5:I:334:VAL:HA	5:I:398:THR:HG22	1.97	0.46
1:A:2131:LEU:O	1:A:2134:ARG:NH1	2.47	0.46
3:E:563:ARG:O	3:E:563:ARG:NE	2.48	0.46
1:A:817:VAL:HG21	1:A:851:THR:HG21	1.96	0.46
1:A:1931:GLN:HG2	1:A:1933:ASP:H	1.79	0.46
3:E:237:HIS:CE1	3:E:239:LYS:HG2	2.50	0.46
3:E:434:ALA:HB1	3:E:438:LEU:HD12	1.97	0.46
5:I:326:TYR:CD2	5:I:404:MET:HG3	2.51	0.46
1:A:1140:ASP:OD1	1:A:1141:ARG:N	2.49	0.46
1:A:2069:SER:HB2	3:E:258:THR:HG22	1.97	0.46
3:E:217:ASP:OD1	3:E:217:ASP:N	2.45	0.46
3:E:562:LEU:O	3:E:566:LYS:NZ	2.46	0.46
3:E:676:LEU:HB3	3:E:681:VAL:HG12	1.97	0.46
3:E:737:ARG:HE	3:E:773:ILE:HG22	1.80	0.46
3:E:1000:LEU:HD23	3:E:1000:LEU:H	1.81	0.46
5:I:174:LEU:HD13	5:I:186:ALA:HB1	1.98	0.46
3:E:698:LEU:O	3:E:701:THR:HG22	2.15	0.46
3:E:1675:GLU:OE2	4:G:86:THR:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1044:MET:O	1:A:1049:GLN:NE2	2.48	0.46
1:A:2145:ASP:OD1	1:A:2148:GLN:HB3	2.16	0.46
2:C:51:THR:OG1	2:C:56:MET:O	2.30	0.46
1:A:1122:PHE:HB3	1:A:1135:ALA:HB3	1.96	0.46
2:C:69:ASP:HB2	2:C:78:ILE:HD13	1.97	0.46
1:A:1649:ASP:OD1	1:A:1649:ASP:N	2.48	0.46
1:A:2192:LEU:HD21	1:A:2237:ILE:HG13	1.97	0.46
3:E:224:ASN:HD22	3:E:286:MET:HE3	1.80	0.46
3:E:1613:ARG:NH2	3:E:1649:ASP:OD2	2.44	0.46
5:I:100:HIS:CE1	5:I:102:CYS:HB2	2.51	0.46
5:I:361:ALA:HB1	5:I:366:MET:HG2	1.96	0.45
1:A:619:ARG:HH21	1:A:671:ILE:HG13	1.81	0.45
1:A:630:LEU:HD22	1:A:652:VAL:HG23	1.97	0.45
3:E:831:TRP:O	3:E:836:ASN:HB2	2.17	0.45
1:A:1888:PHE:O	1:A:1892:ILE:HG13	2.16	0.45
3:E:1480:PHE:CD2	3:E:1614:LYS:HB3	2.52	0.45
1:A:2131:LEU:HD23	1:A:2131:LEU:H	1.81	0.45
3:E:41:ILE:HD12	3:E:1693:LEU:HD11	1.98	0.45
5:I:330:THR:HA	5:I:402:GLU:HA	1.99	0.45
1:A:1543:GLY:O	1:A:1547:ARG:NE	2.49	0.45
5:I:140:TYR:HE2	5:I:144:MET:HE2	1.82	0.45
1:A:703:GLN:HG3	1:A:704:VAL:HG13	1.99	0.45
1:A:1503:LEU:HD23	1:A:1503:LEU:H	1.81	0.45
2:C:182:ALA:HB1	2:C:199:LEU:HD11	1.97	0.45
5:I:50:ILE:HG12	5:I:64:PHE:CD2	2.52	0.45
1:A:630:LEU:HD23	1:A:630:LEU:HA	1.86	0.45
3:E:595:PHE:HE2	3:E:597:LYS:HB2	1.82	0.45
1:A:785:ASP:N	1:A:785:ASP:OD1	2.47	0.45
3:E:1527:GLU:N	3:E:1527:GLU:OE1	2.49	0.45
1:A:1800:ALA:O	1:A:1804:TYR:HD1	2.00	0.44
1:A:2162:VAL:HG22	1:A:2170:ARG:HG3	1.99	0.44
3:E:211:ILE:HB	3:E:231:ILE:HD11	1.98	0.44
1:A:2243:CYS:HB3	1:A:2345:MET:HE2	1.99	0.44
5:I:52:ASP:OD1	5:I:52:ASP:N	2.49	0.44
5:I:123:THR:HG23	5:I:124:PHE:H	1.81	0.44
5:I:143:LEU:HD22	5:I:148:ASN:CG	2.42	0.44
3:E:536:GLN:HB2	3:E:546:TRP:HA	2.00	0.44
5:I:389:ASN:O	5:I:392:ILE:HG12	2.17	0.44
2:C:119:LEU:HG	2:C:121:CYS:HB2	1.99	0.44
5:I:200:GLN:NE2	5:I:216:GLN:HB3	2.33	0.44
1:A:1012:LEU:HD23	1:A:1012:LEU:HA	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1455:GLU:OE1	1:A:1458:ASP:HB2	2.16	0.44
3:E:196:LEU:HD21	3:E:230:THR:HG23	1.99	0.44
1:A:856:GLU:N	1:A:857:PRO:HD2	2.33	0.44
1:A:941:LEU:HD12	1:A:942:PRO:HD2	2.00	0.44
1:A:1805:LYS:HE2	1:A:1805:LYS:HB3	1.87	0.44
2:C:192:GLY:HA3	2:C:219:HIS:O	2.18	0.44
2:C:196:VAL:HG21	2:C:252:PHE:CE2	2.52	0.44
2:C:267:GLU:HB2	2:C:270:ARG:HH21	1.83	0.44
2:C:272:TRP:N	2:C:290:SER:OG	2.51	0.44
3:E:293:ARG:HD3	3:E:851:LEU:HD12	2.00	0.44
5:I:349:PRO:HB2	5:I:371:PHE:HD2	1.82	0.44
1:A:1004:CYS:O	1:A:1009:ARG:NH2	2.51	0.44
3:E:121:LEU:HD13	3:E:162:PRO:HG3	2.00	0.44
5:I:23:GLN:NE2	5:I:195:GLU:O	2.47	0.44
5:I:60:TYR:HB3	5:I:63:CYS:SG	2.58	0.44
5:I:371:PHE:HB2	5:I:404:MET:HB3	2.00	0.44
2:C:201:GLY:H	2:C:209:GLN:NE2	2.16	0.44
2:C:293:LEU:HD11	2:C:295:ARG:CZ	2.48	0.44
3:E:631:VAL:HG22	3:E:681:VAL:HG23	2.00	0.44
1:A:1440:PHE:CD1	1:A:1441:GLY:N	2.86	0.43
1:A:2076:ARG:NH2	1:A:2080:GLU:OE1	2.51	0.43
2:C:100:MET:HB2	2:C:114:LEU:HD21	1.99	0.43
5:I:116:ARG:HG2	5:I:117:PHE:N	2.33	0.43
5:I:348:LYS:HB2	5:I:349:PRO:HD3	2.00	0.43
5:I:371:PHE:O	5:I:404:MET:N	2.39	0.43
1:A:2503:ARG:HA	1:A:2503:ARG:HD2	1.87	0.43
3:E:179:GLU:N	3:E:179:GLU:OE1	2.51	0.43
1:A:810:GLY:O	1:A:811:LEU:HG	2.18	0.43
1:A:2529:ILE:O	1:A:2533:THR:HG22	2.19	0.43
1:A:1116:PRO:HA	1:A:1119:VAL:HG12	2.00	0.43
2:C:27:TRP:HH2	2:C:310:GLY:N	2.15	0.43
2:C:41:GLN:HG3	2:C:42:ASP:N	2.33	0.43
5:I:201:HIS:HB3	5:I:205:LYS:CA	2.48	0.43
5:I:340:TRP:O	5:I:360:PRO:HD2	2.19	0.43
5:I:345:ARG:HB2	5:I:353:GLN:HB2	2.00	0.43
1:A:726:VAL:HG12	1:A:730:LEU:HG	2.00	0.43
1:A:1971:ALA:HB2	1:A:2144:TYR:CE2	2.53	0.43
1:A:2260:LEU:HB2	1:A:2263:ILE:HG13	2.00	0.43
2:C:25:ARG:HD3	2:C:37:THR:HG22	2.01	0.43
2:C:27:TRP:CZ3	2:C:308:TYR:HB3	2.54	0.43
3:E:1673:ILE:C	3:E:1675:GLU:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:23:GLN:O	5:I:27:LEU:HD12	2.19	0.43
5:I:33:VAL:HG23	5:I:230:LEU:HD13	2.01	0.43
5:I:352:ILE:HD12	5:I:370:GLN:HB2	2.01	0.43
1:A:1186:LYS:HE2	1:A:1186:LYS:HB3	1.83	0.43
5:I:159:VAL:HB	5:I:161:TYR:CZ	2.54	0.43
1:A:1085:ASP:HB3	1:A:1090:ARG:NH1	2.34	0.43
1:A:2381:ARG:HA	1:A:2384:THR:HG22	2.01	0.43
2:C:67:MET:HE2	2:C:67:MET:HB2	1.86	0.43
2:C:273:MET:HE3	2:C:287:THR:HB	2.01	0.43
2:C:295:ARG:HB2	2:C:297:TRP:HE1	1.83	0.43
5:I:324:ALA:HB3	5:I:326:TYR:HD1	1.84	0.43
5:I:336:ASP:HB2	5:I:360:PRO:HG2	2.01	0.43
1:A:1930:ILE:HD11	1:A:1935:TRP:CZ2	2.54	0.43
3:E:764:LYS:HB3	3:E:764:LYS:HE3	1.82	0.43
5:I:305:ASN:HB2	5:I:306:PRO:HD3	2.00	0.43
1:A:2245:THR:HG23	1:A:2248:ALA:H	1.84	0.42
2:C:245:LYS:HG2	2:C:257:GLU:HG2	2.00	0.42
3:E:182:ARG:HH12	4:G:26:MET:HE3	1.84	0.42
3:E:1682:PHE:HB3	3:E:1685:MET:HE3	2.01	0.42
3:E:439:PRO:HG2	3:E:442:HIS:ND1	2.34	0.42
3:E:794:LEU:HD21	3:E:804:LEU:HD23	2.00	0.42
1:A:757:LEU:HD21	1:A:775:ILE:HD13	2.02	0.42
1:A:1759:LEU:HG	1:A:1772:VAL:HG11	2.01	0.42
3:E:566:LYS:HB2	3:E:566:LYS:HE2	1.81	0.42
3:E:738:VAL:HG13	3:E:739:LEU:HD12	2.00	0.42
5:I:376:ASN:HA	5:I:400:VAL:HB	2.01	0.42
1:A:615:HIS:O	1:A:619:ARG:HG3	2.18	0.42
1:A:308:THR:O	1:A:1558:SER:OG	2.31	0.42
1:A:1767:SER:O	1:A:1770:PRO:HD2	2.18	0.42
1:A:2165:SER:OG	1:A:2166:LYS:N	2.51	0.42
1:A:2244:ASP:OD1	1:A:2244:ASP:N	2.53	0.42
3:E:182:ARG:NH1	4:G:26:MET:HE3	2.33	0.42
3:E:806:LEU:HD23	3:E:806:LEU:HA	1.75	0.42
2:C:201:GLY:H	2:C:209:GLN:HE22	1.66	0.42
5:I:31:ALA:O	5:I:35:VAL:HG23	2.20	0.42
5:I:124:PHE:N	5:I:125:PRO:HD3	2.35	0.42
5:I:201:HIS:HD2	5:I:204:SER:H	1.66	0.42
1:A:776:LEU:O	1:A:780:ILE:HG12	2.20	0.42
1:A:2136:LEU:O	1:A:2152:ARG:NH1	2.53	0.42
2:C:200:THR:HG22	2:C:202:GLY:H	1.85	0.42
3:E:134:ASP:OD1	3:E:134:ASP:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:430:LEU:HD23	3:E:430:LEU:HA	1.90	0.42
3:E:729:ARG:HH12	3:E:762:LYS:HZ3	1.68	0.42
3:E:1629:THR:O	3:E:1633:GLU:HG3	2.20	0.42
1:A:1306:LEU:HD23	1:A:1306:LEU:HA	1.85	0.42
5:I:218:ARG:HG2	5:I:218:ARG:NH1	2.34	0.42
1:A:1291:LEU:HB3	1:A:1321:ALA:HB1	2.01	0.41
1:A:1377:ASP:OD2	1:A:1406:LYS:NZ	2.49	0.41
5:I:105:HIS:CD2	5:I:107:GLU:H	2.23	0.41
5:I:324:ALA:HB3	5:I:326:TYR:CD1	2.55	0.41
1:A:955:LEU:HD22	1:A:971:VAL:HG23	2.01	0.41
3:E:352:SER:O	3:E:352:SER:OG	2.35	0.41
1:A:1686:ASP:OD1	1:A:1687:HIS:ND1	2.53	0.41
1:A:1873:LEU:HB3	1:A:1876:THR:HG23	2.03	0.41
1:A:668:ASP:OD1	1:A:668:ASP:N	2.52	0.41
3:E:245:ARG:HB2	3:E:249:GLU:HG2	2.02	0.41
1:A:1416:LEU:O	1:A:1420:ASN:ND2	2.53	0.41
1:A:2142:GLY:HA3	1:A:2228:ILE:HD11	2.03	0.41
2:C:32:GLY:N	2:C:306:ARG:HH21	2.19	0.41
2:C:150:GLY:HA2	2:C:173:ILE:HG23	2.02	0.41
1:A:776:LEU:HD11	1:A:813:MET:HE2	2.02	0.41
1:A:1063:LEU:HD12	1:A:1067:PHE:HD1	1.86	0.41
3:E:392:LEU:HD23	3:E:392:LEU:HA	1.91	0.41
3:E:546:TRP:HZ2	3:E:576:ARG:HH22	1.68	0.41
5:I:326:TYR:HD2	5:I:404:MET:HG3	1.85	0.41
1:A:1467:MET:HE1	1:A:1477:MET:HB3	2.02	0.41
2:C:84:VAL:HG12	2:C:110:ARG:NH1	2.36	0.41
2:C:110:ARG:HE	2:C:110:ARG:HB3	1.77	0.41
3:E:920:ILE:HG23	3:E:964:ILE:HD11	2.02	0.41
1:A:893:ALA:HA	1:A:1590:MET:HE2	2.03	0.41
1:A:1569:ASP:OD1	1:A:1570:LEU:N	2.53	0.41
1:A:1645:SER:HB3	1:A:1648:GLU:OE1	2.21	0.41
1:A:2022:LEU:H	1:A:2025:GLU:HG3	1.86	0.41
3:E:74:GLU:HG2	3:E:80:HIS:HA	2.03	0.41
3:E:269:ALA:HB3	3:E:272:GLN:HE22	1.86	0.41
3:E:633:TRP:CZ2	3:E:656:SER:HB3	2.56	0.41
3:E:719:LYS:HE3	3:E:719:LYS:HB3	1.84	0.41
3:E:555:LEU:HD13	3:E:608:PHE:HA	2.02	0.41
5:I:201:HIS:ND1	5:I:214:LEU:O	2.54	0.41
1:A:854:VAL:HG23	1:A:855:VAL:N	2.36	0.40
1:A:947:TYR:HB2	1:A:948:PRO:HD3	2.03	0.40
1:A:1063:LEU:HD23	1:A:1063:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2123:LEU:HD23	1:A:2158:PRO:C	2.46	0.40
2:C:219:HIS:CG	2:C:239:SER:HB3	2.56	0.40
2:C:258:LEU:HD23	2:C:297:TRP:CD2	2.56	0.40
2:C:274:TRP:CD1	2:C:290:SER:HB3	2.56	0.40
1:A:584:LEU:O	1:A:588:THR:HG23	2.21	0.40
1:A:1164:ASP:OD1	1:A:1165:GLN:N	2.54	0.40
1:A:723:PRO:O	1:A:727:MET:HG2	2.22	0.40
1:A:2262:ASN:HB2	1:A:2265:HIS:HB3	2.02	0.40
1:A:2304:TRP:HE3	1:A:2305:LEU:HD12	1.86	0.40
3:E:289:ILE:O	3:E:293:ARG:HG3	2.22	0.40
1:A:1537:PRO:O	1:A:1543:GLY:HA3	2.21	0.40
1:A:1878:LEU:HD12	1:A:1878:LEU:HA	1.87	0.40
1:A:1900:LEU:HD23	1:A:2204:LEU:HD13	2.03	0.40
1:A:2151:ILE:HD12	1:A:2178:ASN:ND2	2.37	0.40
2:C:216:ILE:HG13	2:C:216:ILE:O	2.22	0.40
3:E:540:HIS:ND1	3:E:545:GLU:HG2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2152/2571 (84%)	2095 (97%)	57 (3%)	0	100	100
2	C	317/326 (97%)	296 (93%)	21 (7%)	0	100	100
3	E	1101/1708 (64%)	1052 (96%)	49 (4%)	0	100	100
4	G	94/522 (18%)	91 (97%)	3 (3%)	0	100	100
5	I	313/409 (76%)	297 (95%)	16 (5%)	0	100	100
All	All	3977/5536 (72%)	3831 (96%)	146 (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	1571/2236 (70%)	1570 (100%)	1 (0%)	88	88
2	C	269/276 (98%)	269 (100%)	0	100	100
3	E	985/1539 (64%)	982 (100%)	3 (0%)	86	83
4	G	50/471 (11%)	50 (100%)	0	100	100
5	I	281/364 (77%)	243 (86%)	38 (14%)	4	20
All	All	3156/4886 (65%)	3114 (99%)	42 (1%)	59	71

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	739	THR
3	E	451	THR
3	E	696	HIS
3	E	710	ASP
5	I	23	GLN
5	I	27	LEU
5	I	28	GLU
5	I	39	GLN
5	I	52	ASP
5	I	59	THR
5	I	65	VAL
5	I	71	ASP
5	I	127	ASP
5	I	130	VAL
5	I	134	MET
5	I	141	GLU
5	I	143	LEU
5	I	144	MET
5	I	149	THR
5	I	161	TYR
5	I	164	THR
5	I	171	LEU
5	I	182	THR

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Mol	Chain	Res	Type
5	I	187	GLU
5	I	189	LEU
5	I	195	GLU
5	I	199	ILE
5	I	203	SER
5	I	205	LYS
5	I	208	PHE
5	I	218	ARG
5	I	221	PHE
5	I	223	ARG
5	I	224	ARG
5	I	225	ARG
5	I	309	VAL
5	I	314	VAL
5	I	315	THR
5	I	318	GLU
5	I	319	LEU
5	I	331	PHE
5	I	383	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	703	GLN
1	A	846	GLN
1	A	1015	GLN
1	A	1106	ASN
1	A	1233	GLN
1	A	1492	GLN
1	A	1561	GLN
1	A	1594	HIS
1	A	1695	GLN
1	A	1738	GLN
1	A	1920	ASN
1	A	1992	ASN
1	A	2063	GLN
1	A	2082	GLN
1	A	2178	ASN
2	C	39	GLN
2	C	153	HIS
3	E	80	HIS
3	E	112	GLN

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Mol	Chain	Res	Type
3	E	237	HIS
3	E	435	ASN
3	E	531	ASN
3	E	536	GLN
3	E	540	HIS
3	E	632	GLN
3	E	683	GLN
3	E	758	GLN
3	E	885	GLN
3	E	941	ASN
3	E	1434	ASN
3	E	1446	GLN
4	G	18	HIS
5	I	56	HIS
5	I	105	HIS

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	ACE	G	601	4	1,2,2	0.72	0	0,1,1	-	-
6	IHP	A	2601	-	36,36,36	0.70	1 (2%)	60,60,60	0.56	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	IHP	A	2601	-	-	1/30/54/54	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2601	IHP	P3-O13	2.94	1.64	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2601	IHP	P2-O12-C2	2.94	131.29	123.43

There are no chirality outliers.

All (1) torsion outliers are listed below:

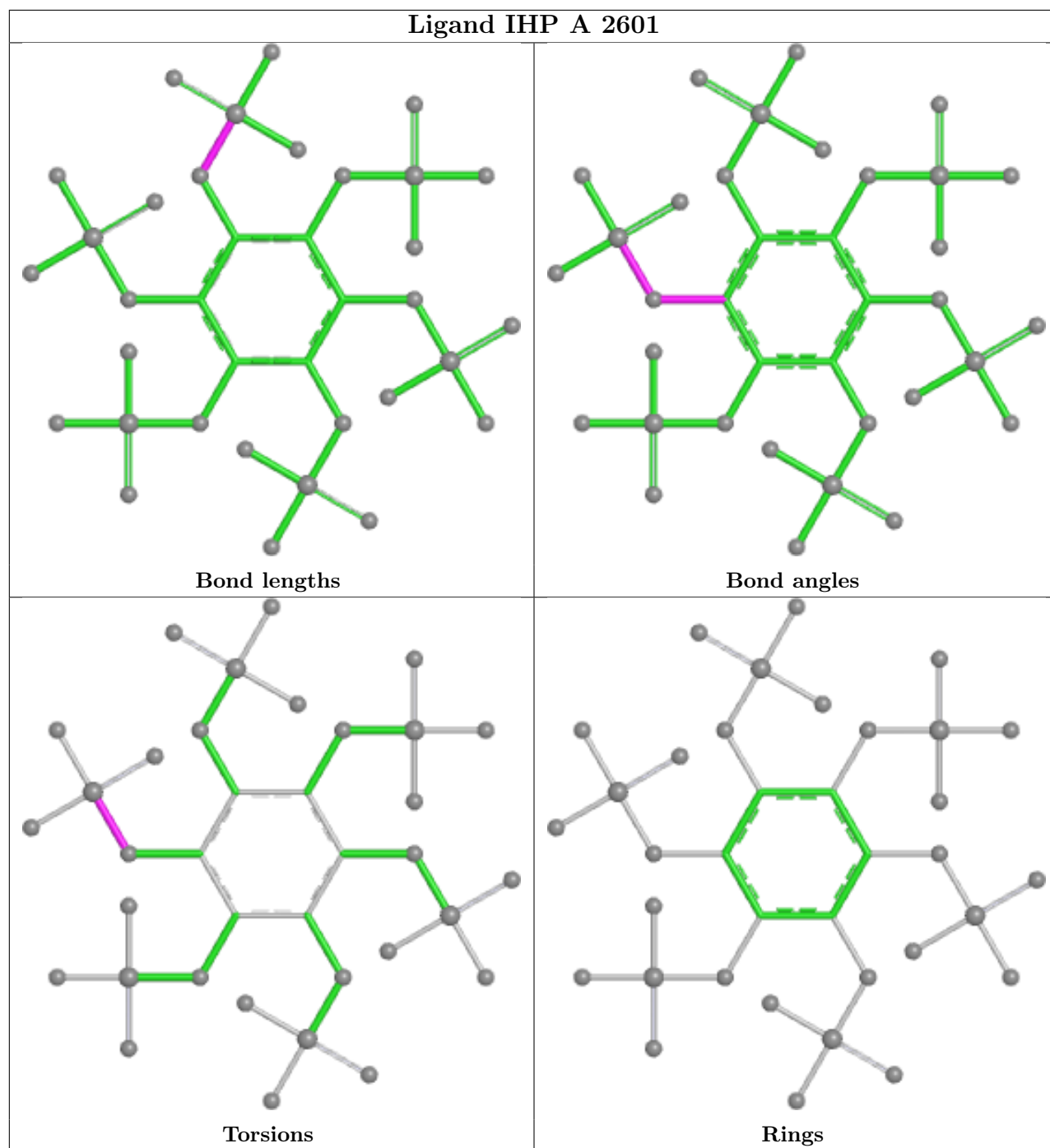
Mol	Chain	Res	Type	Atoms
6	A	2601	IHP	C2-O12-P2-O22

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

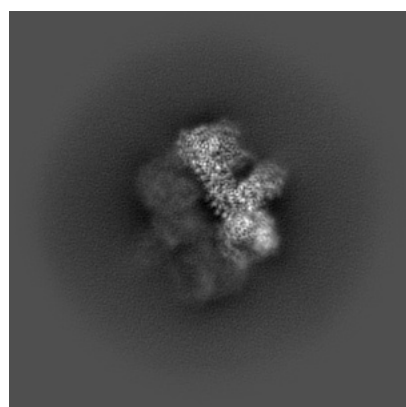
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13349. These allow visual inspection of the internal detail of the map and identification of artifacts.

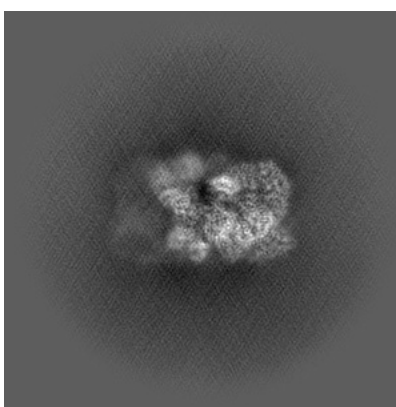
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

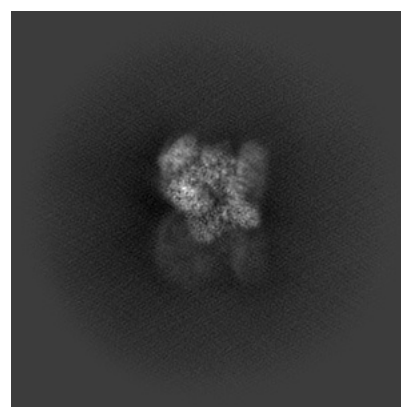
6.1.1 Primary map



X



Y

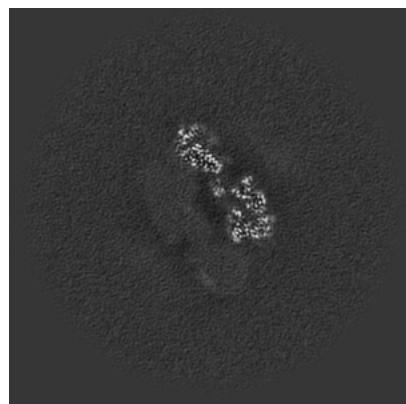


Z

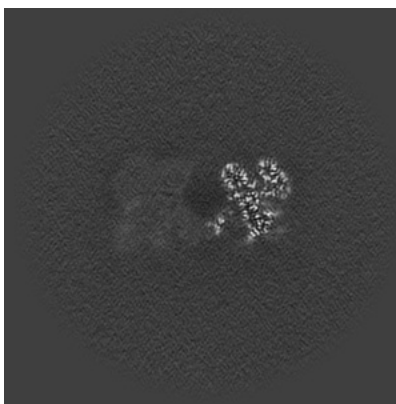
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

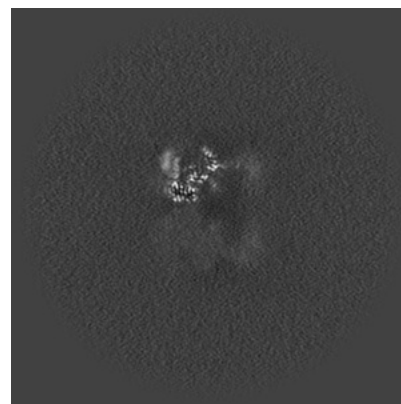
6.2.1 Primary map



X Index: 240



Y Index: 240

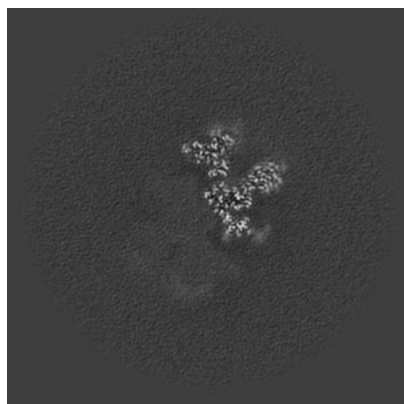


Z Index: 240

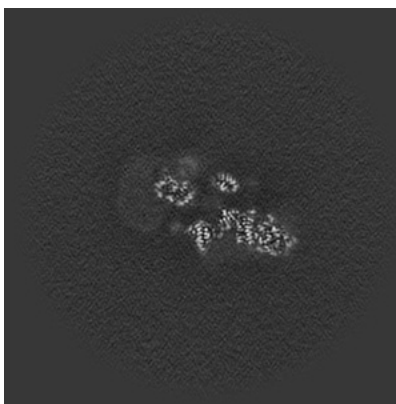
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

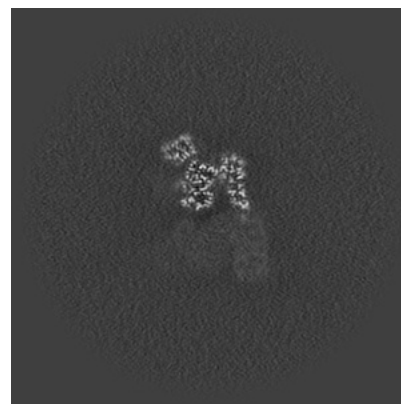
6.3.1 Primary map



X Index: 216



Y Index: 259

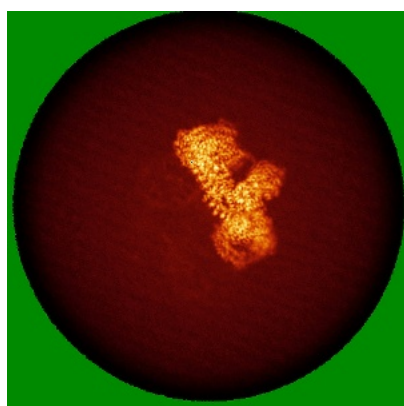


Z Index: 262

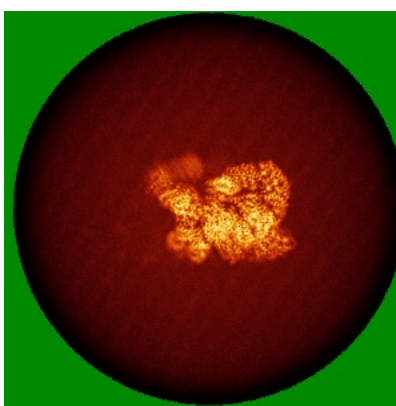
The images above show the largest variance slices of the map in three orthogonal directions.

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

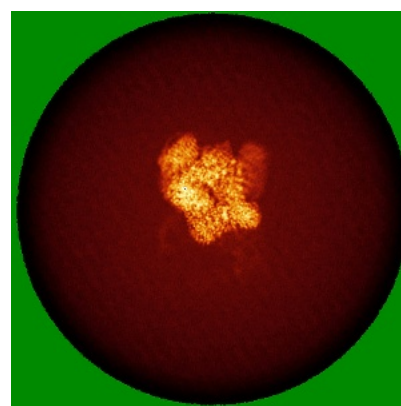
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

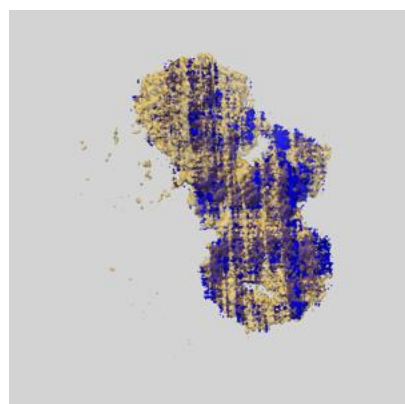
6.6 Mask visualisation [i](#)

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

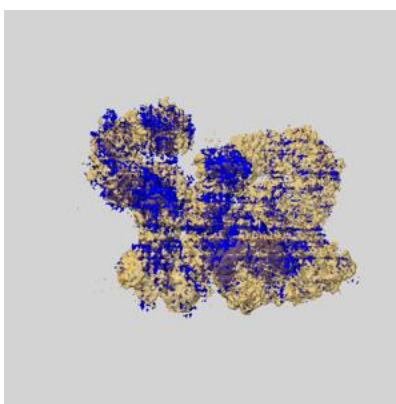
A mask typically either:

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

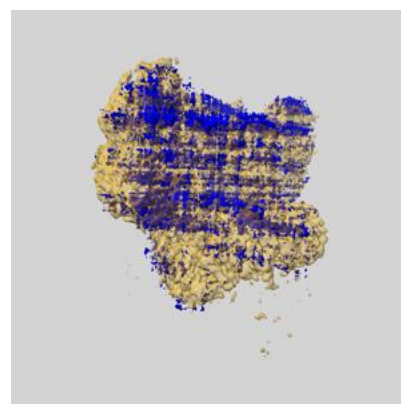
6.6.1 emd_13349_msk_1.map [i](#)



X



Y

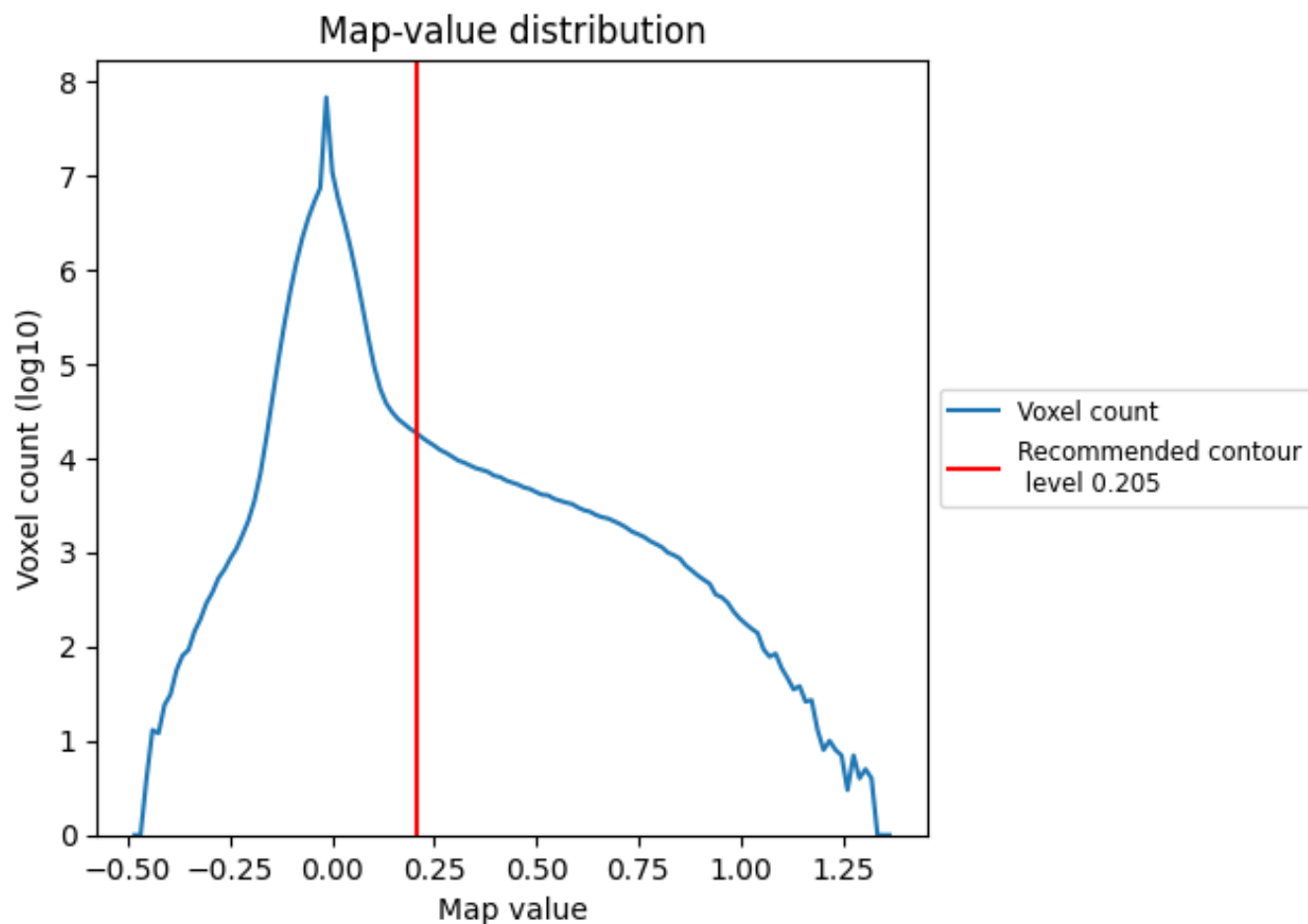


Z

7 Map analysis [i](#)

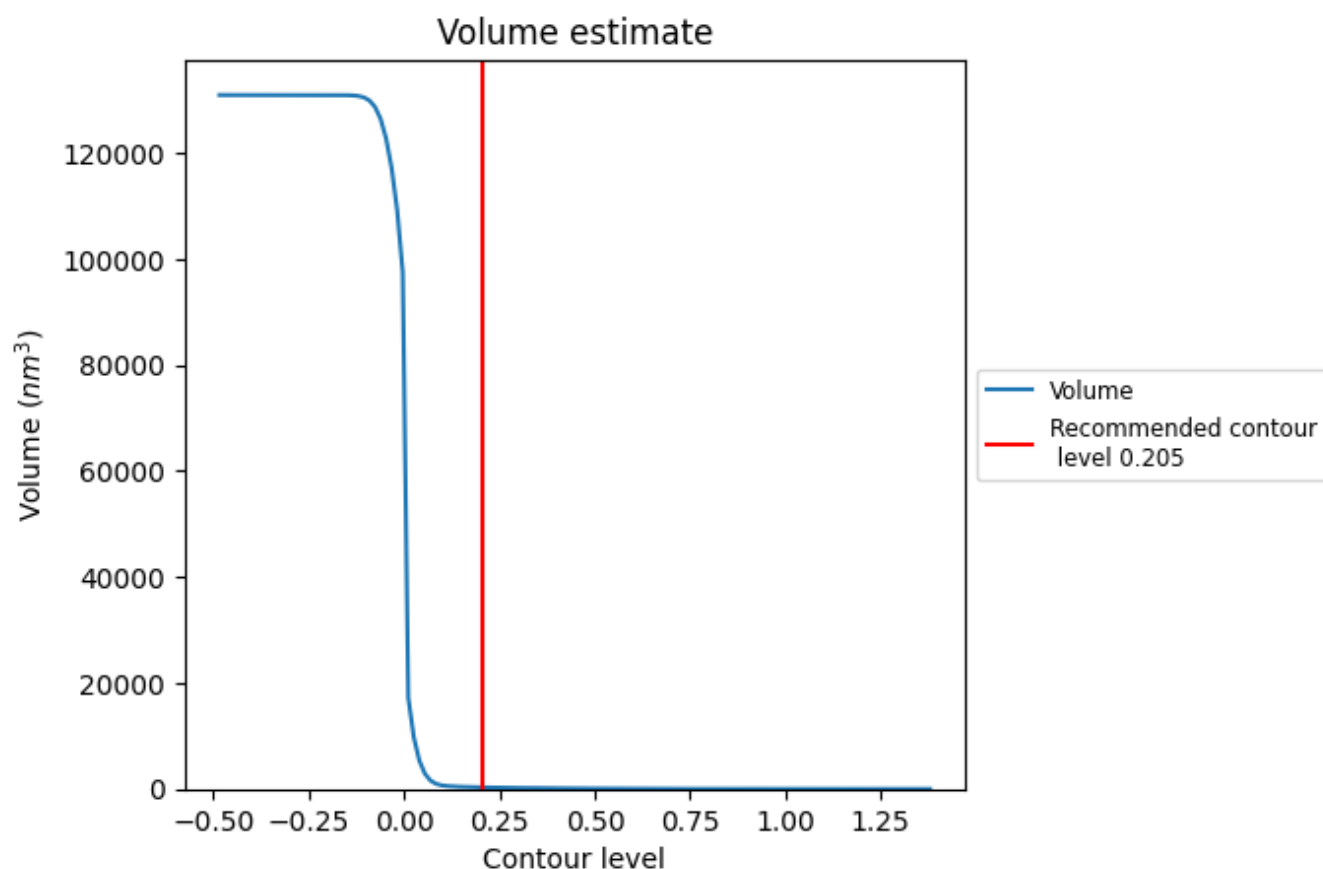
This section contains the results of statistical analysis of the map.

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.

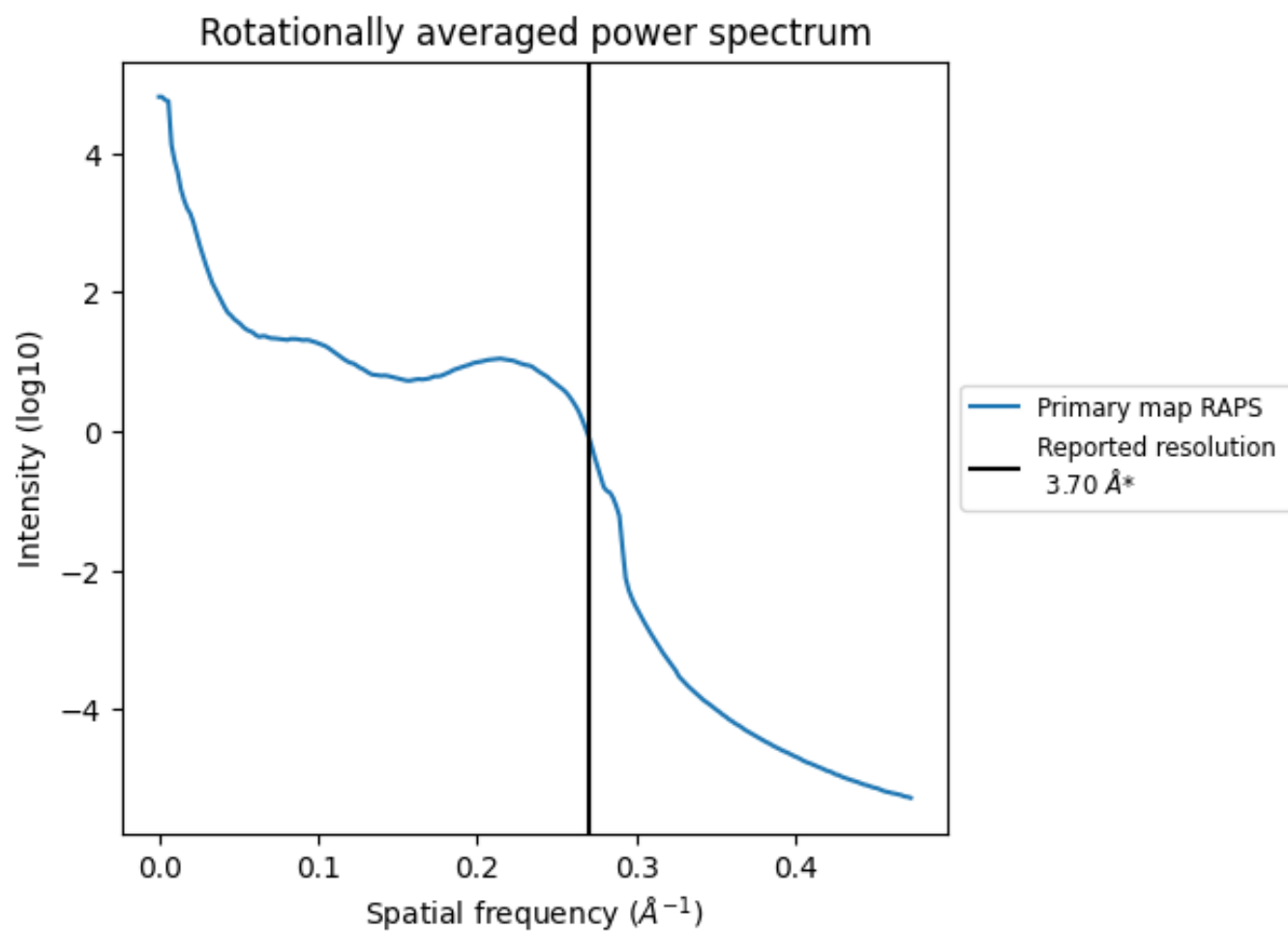
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 297 nm^3 ; this corresponds to an approximate mass of 268 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 0.270 Å⁻¹

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

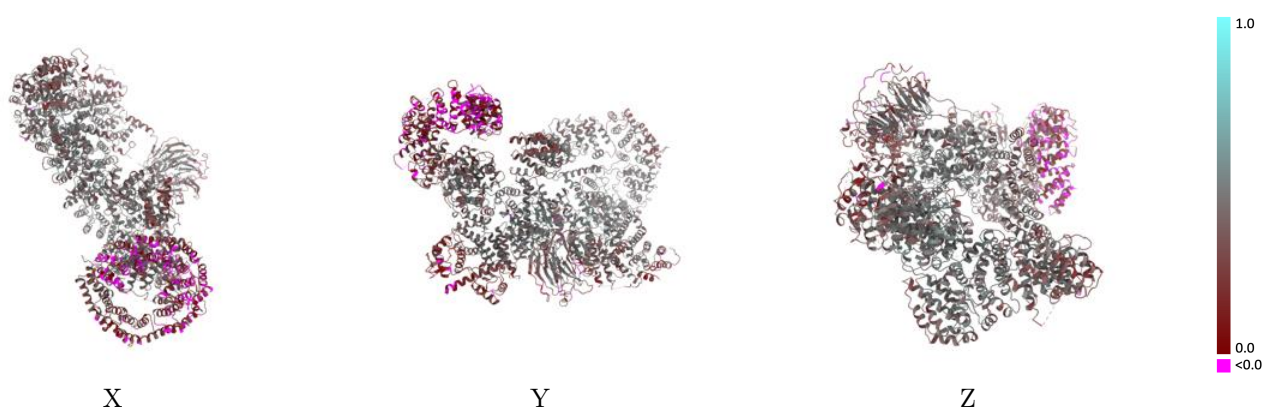
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-13349 and PDB model 7PE9. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

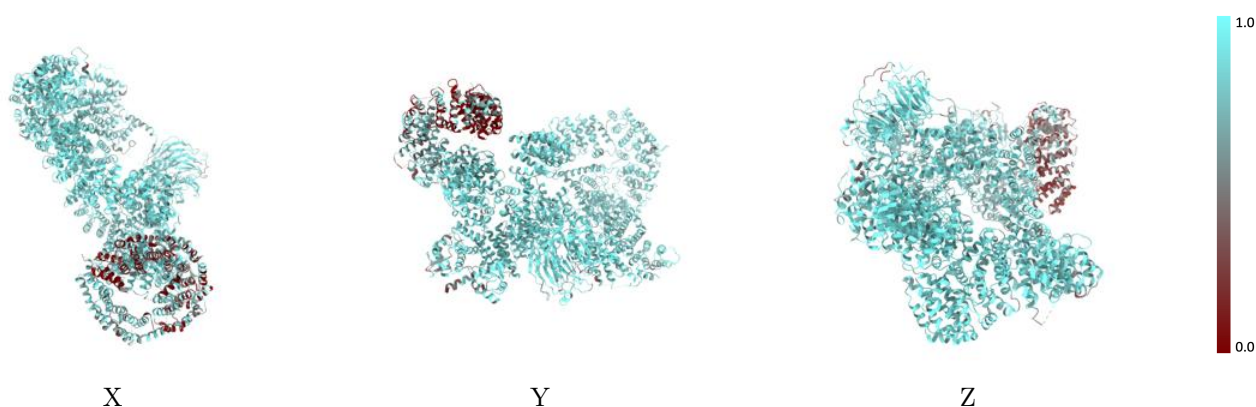
This section was not generated.

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



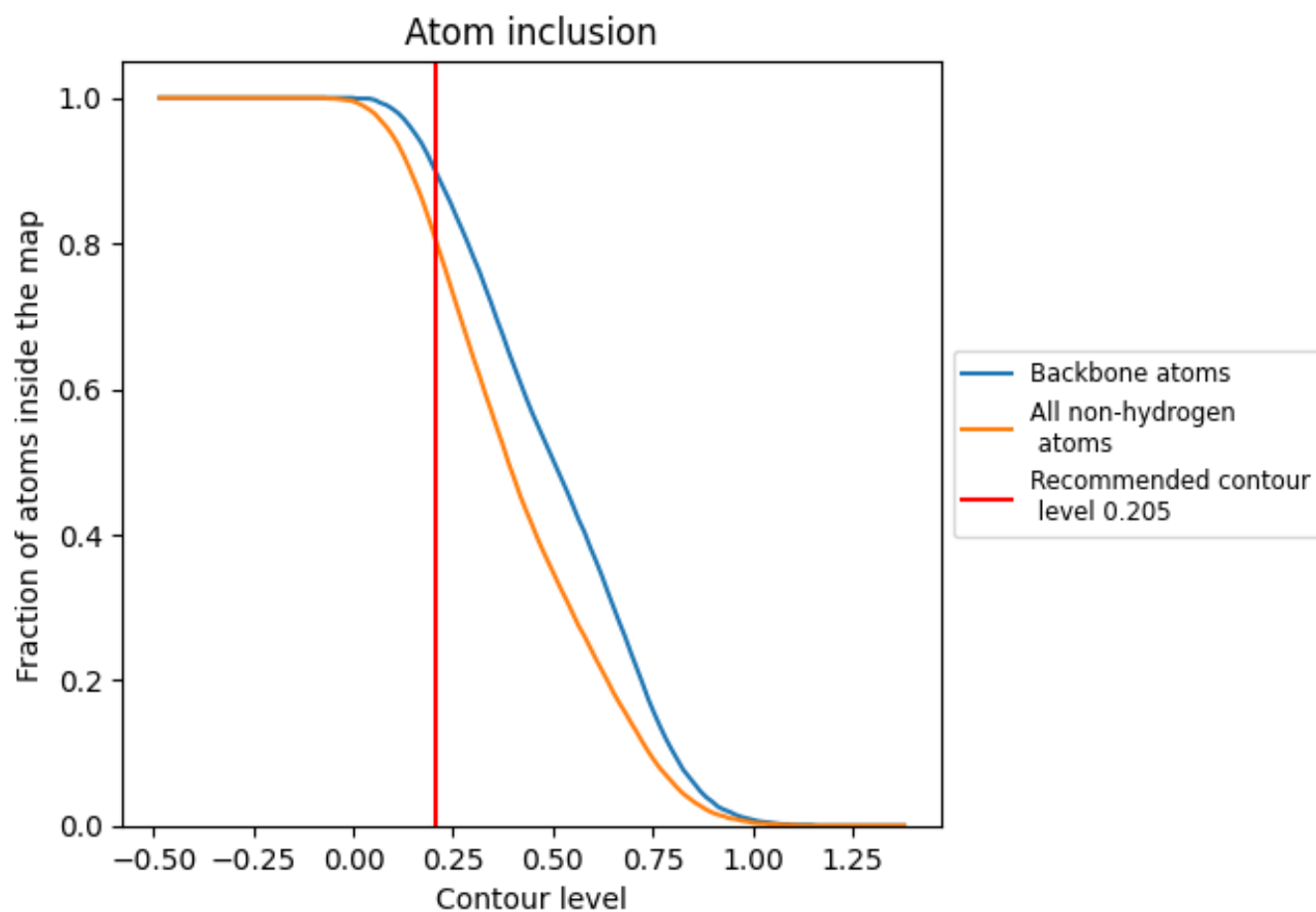
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.205).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 81% 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 (0.205) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8080	0.3720
A	0.7880	0.3720
C	0.8660	0.3740
E	0.8440	0.4140
G	0.8040	0.3460
I	0.7610	0.2310

