



## Full wwPDB EM Validation Report ⓘ

May 26, 2025 – 01:59 PM EDT

PDB ID : 7RZH / pdb\_00007rzh  
EMDB ID : EMD-24760  
Title : Insulin Degrading Enzyme O/O  
Authors : Mancl, J.M.; Liang, W.G.; Tang, W.J.  
Deposited on : 2021-08-27  
Resolution : 3.80 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

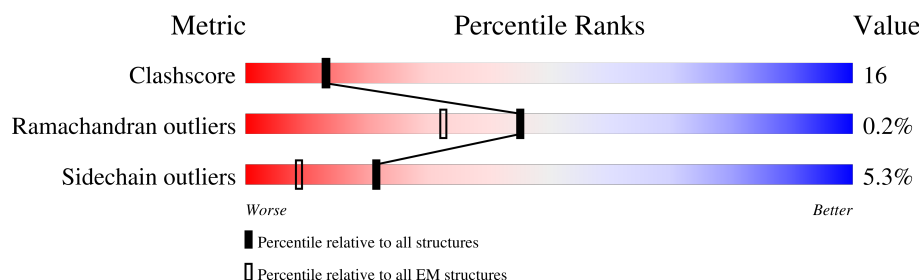
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	1011	<div> <div>10%</div> <div>65%</div> <div>25%</div> <div>8%</div> </div>
1	B	1011	<div> <div>5%</div> <div>68%</div> <div>23%</div> <div>8%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15300 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.

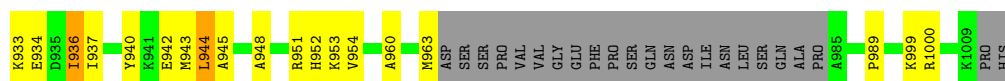
- Molecule 1 is a protein called Cysteine-free Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	932	Total	C	N	O	S	0	0
			7637	4924	1275	1416	22		
1	B	935	Total	C	N	O	S	0	0
			7663	4942	1284	1416	21		

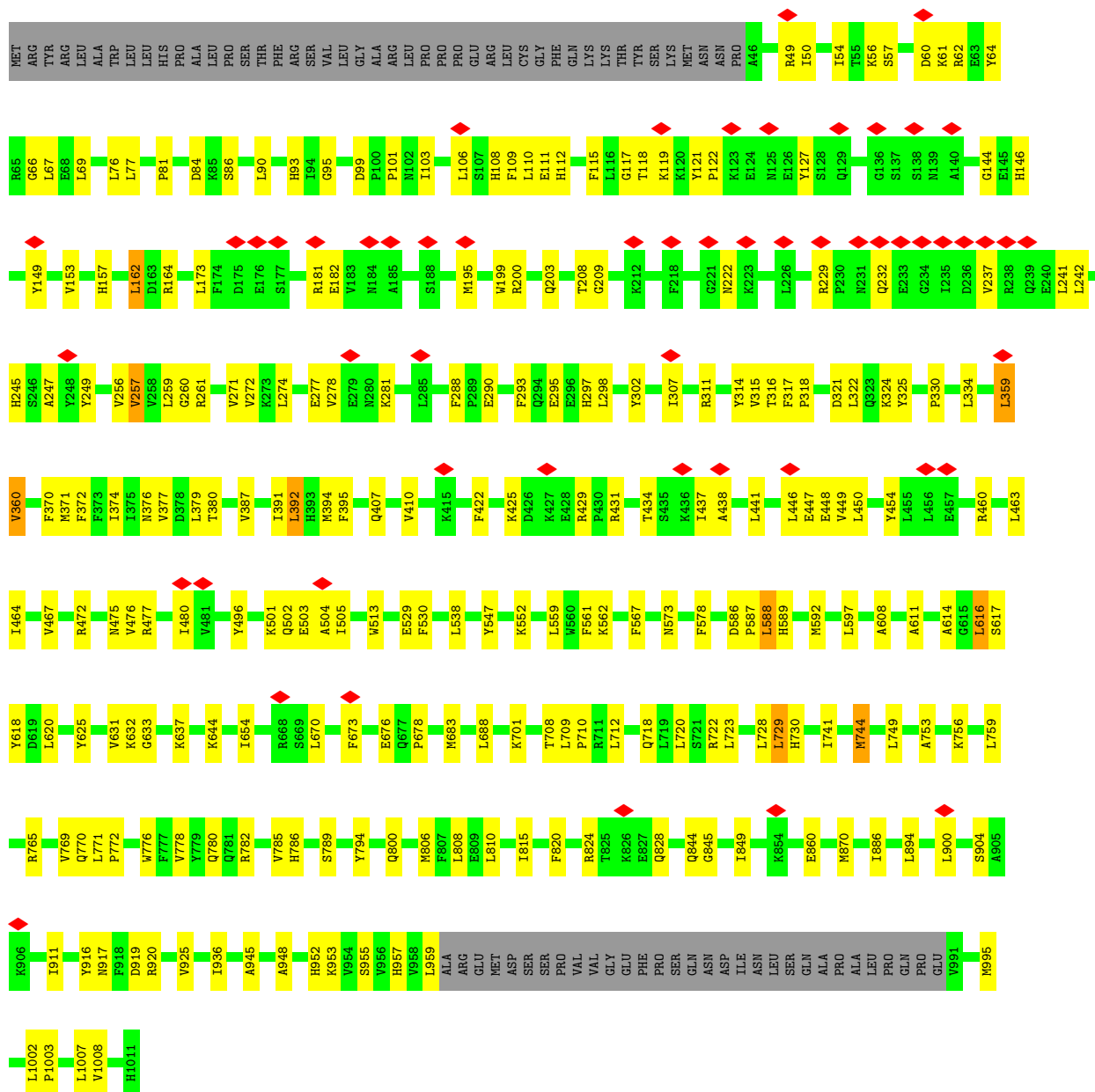
There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	LEU	CYS	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	SER	CYS	engineered mutation	UNP P14735
A	974	SER	CYS	engineered mutation	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	SER	CYS	engineered mutation	UNP P14735
B	974	SER	CYS	engineered mutation	UNP P14735





● Molecule 1: Cysteine-free Insulin-degrading enzyme



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77973	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.076	Depositor
Minimum map value	-0.047	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	277.5552, 277.5552, 277.5552	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0842, 1.0842, 1.0842	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.96	0/7827	1.18	4/10585 (0.0%)
1	B	0.97	0/7854	1.18	1/10620 (0.0%)
All	All	0.96	0/15681	1.18	5/21205 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	PHE	N-CA-C	-5.78	106.21	113.72
1	A	91	ASP	CA-C-O	-5.53	115.36	121.33
1	A	221	GLY	CA-C-O	-5.34	117.96	122.29
1	A	281	LYS	N-CA-C	-5.13	106.80	113.16
1	A	587	PRO	N-CA-C	-5.07	106.49	113.53

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	7637	0	7574	248	0
1	B	7663	0	7610	257	0
All	All	15300	0	15184	487	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 (487) 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:115:PHE:CE1	1:A:127:TYR:CD2	1.85	1.64
1:A:115:PHE:CE1	1:A:127:TYR:HD2	1.06	1.63
1:B:317:PHE:CZ	1:B:476:VAL:HG22	1.29	1.60
1:A:1000:ARG:CD	1:B:1007:LEU:HD23	1.39	1.48
1:B:317:PHE:CZ	1:B:476:VAL:CG2	1.99	1.46
1:B:530:PHE:CZ	1:B:611:ALA:HA	1.57	1.37
1:A:115:PHE:CD1	1:A:127:TYR:HD2	1.46	1.34
1:B:608:ALA:HB1	1:B:618:TYR:CE2	1.64	1.32
1:B:567:PHE:CB	1:B:900:LEU:HD21	1.57	1.32
1:A:115:PHE:HE1	1:A:127:TYR:CD2	1.33	1.29
1:B:771:LEU:CD2	1:B:952:HIS:HA	1.59	1.29
1:B:317:PHE:CE1	1:B:476:VAL:CG2	2.15	1.27
1:B:317:PHE:CE1	1:B:476:VAL:HG23	1.67	1.27
1:B:771:LEU:CD2	1:B:952:HIS:CA	2.09	1.27
1:B:769:VAL:CG1	1:B:1002:LEU:HB2	1.73	1.19
1:B:771:LEU:HD21	1:B:952:HIS:CA	1.68	1.19
1:A:1000:ARG:HD3	1:B:1007:LEU:CD2	1.72	1.19
1:B:771:LEU:CD2	1:B:952:HIS:HB3	1.71	1.18
1:B:771:LEU:CD1	1:B:772:PRO:HD2	1.74	1.17
1:B:530:PHE:HZ	1:B:611:ALA:CA	1.56	1.17
1:A:1000:ARG:NE	1:B:1007:LEU:HD23	1.58	1.17
1:B:608:ALA:CB	1:B:618:TYR:CE2	2.27	1.16
1:B:771:LEU:CD2	1:B:952:HIS:CB	2.22	1.16
1:B:567:PHE:HB3	1:B:900:LEU:HD21	1.26	1.16
1:B:530:PHE:HE1	1:B:614:ALA:CB	1.58	1.16
1:B:771:LEU:HD23	1:B:952:HIS:CB	1.74	1.16
1:B:769:VAL:HG11	1:B:1002:LEU:HD12	1.17	1.15
1:B:334:LEU:HD11	1:B:467:VAL:CG2	1.78	1.14
1:B:334:LEU:CD1	1:B:467:VAL:CG2	2.26	1.13
1:B:530:PHE:HE1	1:B:614:ALA:HB3	1.10	1.13
1:B:771:LEU:HD21	1:B:952:HIS:HA	1.13	1.12
1:B:530:PHE:CE1	1:B:614:ALA:CB	2.33	1.11
1:B:769:VAL:CG1	1:B:1002:LEU:CB	2.27	1.11
1:B:769:VAL:HG13	1:B:1002:LEU:HB2	1.12	1.11
1:B:103:ILE:HD11	1:B:106:LEU:HD13	1.18	1.11
1:B:769:VAL:HG13	1:B:1002:LEU:CB	1.82	1.10
1:A:1000:ARG:HG3	1:B:1007:LEU:HB3	1.17	1.09
1:B:334:LEU:HD11	1:B:467:VAL:HG23	1.31	1.09
1:A:579:PHE:HD2	1:A:758:LEU:CD1	1.66	1.08
1:B:334:LEU:CD1	1:B:467:VAL:HG23	1.82	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1000:ARG:CG	1:B:1007:LEU:HB3	1.85	1.05
1:B:778:VAL:HG22	1:B:955:SER:HB3	1.41	1.02
1:A:200:ARG:HG3	1:A:498:THR:CG2	1.90	1.02
1:A:1000:ARG:CD	1:B:1007:LEU:CD2	2.34	1.02
1:B:608:ALA:HB3	1:B:618:TYR:CZ	1.95	1.02
1:B:66:GLY:HA3	1:B:446:LEU:CD2	1.90	1.01
1:B:771:LEU:HD12	1:B:772:PRO:HD2	1.04	1.01
1:B:530:PHE:CE1	1:B:614:ALA:HB3	1.94	1.01
1:B:769:VAL:CG1	1:B:1002:LEU:HD12	1.91	1.01
1:B:567:PHE:CB	1:B:900:LEU:CD2	2.40	1.00
1:A:200:ARG:HG3	1:A:498:THR:HG22	1.41	1.00
1:A:115:PHE:HZ	1:A:128:SER:N	1.59	1.00
1:B:771:LEU:HD22	1:B:952:HIS:HB3	1.39	0.99
1:B:66:GLY:HA3	1:B:446:LEU:HD22	1.44	0.99
1:B:769:VAL:CG1	1:B:1002:LEU:CD1	2.41	0.98
1:A:117:GLY:O	1:A:173:LEU:HD13	1.61	0.98
1:B:769:VAL:HG11	1:B:1002:LEU:CD1	1.92	0.98
1:A:200:ARG:HB2	1:A:498:THR:CG2	1.94	0.97
1:B:317:PHE:CE1	1:B:476:VAL:HG22	1.90	0.97
1:A:1000:ARG:HD3	1:B:1007:LEU:HD23	0.98	0.96
1:B:567:PHE:CG	1:B:900:LEU:CD2	2.50	0.95
1:A:579:PHE:CD2	1:A:758:LEU:CD1	2.50	0.94
1:B:771:LEU:HD12	1:B:772:PRO:CD	1.98	0.94
1:B:334:LEU:CD1	1:B:467:VAL:HG21	1.93	0.94
1:A:391:ILE:HB	1:A:513:TRP:CH2	2.03	0.93
1:A:200:ARG:CG	1:A:498:THR:HG22	1.98	0.93
1:B:334:LEU:HD12	1:B:467:VAL:HG21	1.49	0.92
1:A:115:PHE:CD1	1:A:127:TYR:CD2	2.34	0.91
1:A:573:ASN:OD1	1:A:900:LEU:HD23	1.71	0.90
1:B:103:ILE:HD11	1:B:106:LEU:CD1	2.01	0.89
1:B:103:ILE:CD1	1:B:106:LEU:HD13	2.03	0.89
1:B:567:PHE:HB2	1:B:900:LEU:HD21	1.53	0.89
1:A:301:LEU:CD1	1:A:505:ILE:HD11	2.03	0.88
1:B:771:LEU:HD23	1:B:952:HIS:HA	1.47	0.88
1:B:317:PHE:HE1	1:B:476:VAL:HG23	1.11	0.88
1:B:317:PHE:HZ	1:B:476:VAL:HG22	1.14	0.88
1:A:115:PHE:CZ	1:A:128:SER:N	2.43	0.87
1:B:567:PHE:CG	1:B:900:LEU:HD21	2.10	0.87
1:B:567:PHE:CG	1:B:900:LEU:HD23	2.10	0.86
1:B:529:GLU:OE1	1:B:644:LYS:NZ	2.08	0.86
1:B:778:VAL:HG22	1:B:955:SER:CB	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ARG:CG	1:A:498:THR:CG2	2.54	0.86
1:A:1000:ARG:NE	1:B:1007:LEU:CD2	2.37	0.85
1:B:771:LEU:HD21	1:B:952:HIS:C	2.01	0.85
1:B:501:LYS:HG3	1:B:503:GLU:HB2	1.57	0.85
1:A:200:ARG:CB	1:A:498:THR:CG2	2.55	0.84
1:A:201:LEU:O	1:A:204:LEU:HG	1.75	0.84
1:A:301:LEU:HD13	1:A:505:ILE:HD11	1.59	0.83
1:B:776:TRP:CH2	1:B:778:VAL:HG21	2.13	0.83
1:B:608:ALA:CB	1:B:618:TYR:CZ	2.58	0.83
1:A:388:GLU:O	1:A:513:TRP:HH2	1.62	0.82
1:A:264:LEU:CD1	1:A:265:ASP:OD1	2.28	0.82
1:B:317:PHE:HZ	1:B:476:VAL:CG2	1.64	0.81
1:B:359:LEU:HD13	1:B:359:LEU:C	2.04	0.81
1:A:392:LEU:HG	1:A:513:TRP:CZ3	2.15	0.81
1:A:115:PHE:CE1	1:A:127:TYR:CG	2.68	0.80
1:B:501:LYS:CG	1:B:503:GLU:HB2	2.10	0.80
1:B:808:LEU:HD22	1:B:844:GLN:HB3	1.64	0.80
1:B:334:LEU:HD12	1:B:467:VAL:CG2	2.09	0.80
1:A:579:PHE:HD2	1:A:758:LEU:HD11	1.47	0.79
1:B:771:LEU:HD23	1:B:952:HIS:CA	1.91	0.79
1:A:388:GLU:O	1:A:513:TRP:CH2	2.35	0.78
1:B:567:PHE:CD2	1:B:900:LEU:HD23	2.18	0.78
1:B:76:LEU:HD13	1:B:446:LEU:HD11	1.64	0.78
1:A:1000:ARG:HG3	1:B:1007:LEU:CB	2.09	0.77
1:B:530:PHE:HZ	1:B:611:ALA:HA	0.67	0.77
1:B:769:VAL:HG12	1:B:1002:LEU:CD1	2.13	0.77
1:B:315:VAL:HG13	1:B:476:VAL:HG13	1.66	0.77
1:A:200:ARG:HB2	1:A:498:THR:HG23	1.63	0.77
1:B:62:ARG:HH12	1:B:259:LEU:HD22	1.49	0.76
1:A:684:TYR:CE1	1:A:687:ARG:NH2	2.54	0.76
1:A:117:GLY:O	1:A:173:LEU:CD1	2.33	0.75
1:B:76:LEU:HD13	1:B:446:LEU:HD21	1.69	0.75
1:A:264:LEU:HD11	1:A:265:ASP:OD1	1.86	0.74
1:B:103:ILE:HG13	1:B:106:LEU:HB2	1.69	0.74
1:A:229:ARG:HG3	1:A:230:PRO:HD3	1.69	0.74
1:A:106:LEU:O	1:A:110:LEU:HD13	1.88	0.74
1:A:264:LEU:HD12	1:A:265:ASP:N	2.03	0.74
1:B:771:LEU:HD23	1:B:952:HIS:HB3	1.44	0.74
1:A:392:LEU:HG	1:A:513:TRP:CH2	2.22	0.74
1:B:437:ILE:O	1:B:441:LEU:HG	1.86	0.74
1:A:960:ALA:HB3	1:A:963:MET:HB3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:GLN:HE21	1:B:587:PRO:CD	2.01	0.73
1:A:1000:ARG:HE	1:B:1007:LEU:CD2	2.00	0.73
1:A:573:ASN:OD1	1:A:900:LEU:CD2	2.36	0.73
1:B:530:PHE:CE1	1:B:614:ALA:HB2	2.23	0.72
1:A:115:PHE:CZ	1:A:127:TYR:HB3	2.25	0.71
1:B:567:PHE:HB2	1:B:900:LEU:CD2	2.16	0.71
1:A:155:HIS:HB2	1:A:261:ARG:HD3	1.72	0.71
1:B:769:VAL:CG1	1:B:1002:LEU:HB3	2.17	0.71
1:A:532:PRO:HA	1:A:636:ASP:HB3	1.71	0.71
1:A:299:LYS:HD2	1:A:474:GLU:HA	1.72	0.71
1:A:200:ARG:HG3	1:A:498:THR:HG21	1.71	0.70
1:A:301:LEU:HD13	1:A:505:ILE:CD1	2.21	0.70
1:B:293:PHE:CZ	1:B:477:ARG:NH1	2.59	0.70
1:B:608:ALA:HB1	1:B:618:TYR:HE2	1.50	0.70
1:A:444:TYR:HB2	1:A:449:VAL:HB	1.72	0.70
1:B:608:ALA:HB1	1:B:618:TYR:CD2	2.27	0.69
1:A:392:LEU:N	1:A:513:TRP:HZ3	1.91	0.68
1:A:264:LEU:HD12	1:A:265:ASP:OD1	1.94	0.68
1:B:359:LEU:HD13	1:B:360:VAL:N	2.08	0.68
1:B:769:VAL:HG12	1:B:1002:LEU:HD13	1.76	0.68
1:B:771:LEU:HD23	1:B:952:HIS:CG	2.28	0.68
1:A:392:LEU:N	1:A:513:TRP:CZ3	2.63	0.67
1:A:254:MET:HE3	1:A:256:VAL:CG2	2.25	0.67
1:A:301:LEU:HD13	1:A:505:ILE:CG1	2.25	0.67
1:A:301:LEU:HA	1:A:478:VAL:HB	1.77	0.66
1:A:287:GLU:HB3	1:A:368:ARG:HD3	1.76	0.66
1:A:210:ASN:HB3	1:A:213:HIS:HB2	1.76	0.66
1:B:311:ARG:HB3	1:B:379:LEU:HB2	1.78	0.66
1:A:285:LEU:HD12	1:A:285:LEU:O	1.96	0.66
1:A:392:LEU:HD23	1:A:513:TRP:CE3	2.31	0.65
1:A:1000:ARG:HE	1:B:1007:LEU:HD23	1.52	0.65
1:A:573:ASN:ND2	1:A:632:LYS:HB3	2.11	0.65
1:A:1000:ARG:HD3	1:B:1007:LEU:CG	2.26	0.65
1:A:366:GLY:HA3	1:A:371:MET:HA	1.78	0.65
1:B:770:GLN:HB3	1:B:1003:PRO:HD2	1.78	0.65
1:A:301:LEU:HD12	1:A:505:ILE:HD11	1.78	0.64
1:A:489:THR:HA	1:A:501:LYS:HB2	1.77	0.64
1:B:769:VAL:HG12	1:B:1002:LEU:CB	2.27	0.64
1:A:579:PHE:CD2	1:A:758:LEU:HD13	2.32	0.64
1:B:530:PHE:HB2	1:B:637:LYS:HB3	1.80	0.64
1:B:76:LEU:CD1	1:B:446:LEU:HD21	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:HIS:HB3	1:A:253:LEU:HD13	1.80	0.63
1:A:110:LEU:HD11	1:A:241:LEU:CD2	2.29	0.63
1:B:76:LEU:HD13	1:B:446:LEU:CD1	2.28	0.63
1:B:162:LEU:HD23	1:B:274:LEU:HD12	1.81	0.63
1:B:76:LEU:HD13	1:B:446:LEU:CG	2.29	0.63
1:B:771:LEU:CD2	1:B:952:HIS:C	2.67	0.62
1:B:608:ALA:HB3	1:B:618:TYR:OH	1.98	0.62
1:B:209:GLY:HA2	1:B:293:PHE:HE1	1.64	0.62
1:B:359:LEU:C	1:B:359:LEU:CD1	2.72	0.62
1:A:115:PHE:HZ	1:A:128:SER:CA	2.12	0.62
1:A:561:PHE:HB2	1:A:729:LEU:HD12	1.82	0.62
1:B:771:LEU:CG	1:B:772:PRO:HD2	2.28	0.62
1:B:95:GLY:HA3	1:B:144:GLY:O	2.00	0.62
1:A:391:ILE:HB	1:A:513:TRP:HH2	1.62	0.61
1:A:415:LYS:HE3	1:A:457:GLU:HA	1.82	0.61
1:A:91:ASP:HB3	1:A:255:ALA:HB3	1.81	0.61
1:B:66:GLY:HA3	1:B:446:LEU:HD21	1.78	0.61
1:A:942:GLU:HG3	1:A:943:MET:HG2	1.80	0.61
1:A:179:LYS:HD2	1:A:237:VAL:HB	1.83	0.60
1:B:334:LEU:HD21	1:B:464:ILE:HG23	1.82	0.60
1:A:115:PHE:CE1	1:A:127:TYR:HB3	2.35	0.59
1:B:90:LEU:HG	1:B:256:VAL:HG12	1.83	0.59
1:A:810:LEU:HD22	1:A:931:LEU:HD23	1.84	0.59
1:A:548:PRO:HG3	1:A:562:LYS:HB2	1.84	0.59
1:A:64:TYR:HE1	1:A:447:GLU:OE1	1.85	0.59
1:B:769:VAL:CG1	1:B:1002:LEU:CG	2.81	0.59
1:B:76:LEU:HD13	1:B:446:LEU:CD2	2.31	0.59
1:B:395:PHE:HZ	1:B:476:VAL:HG21	1.67	0.59
1:B:302:TYR:HD1	1:B:502:GLN:HA	1.67	0.59
1:B:578:PHE:HB3	1:B:723:LEU:HD13	1.85	0.58
1:A:119:LYS:HB2	1:A:173:LEU:HD11	1.85	0.58
1:A:204:LEU:HD12	1:A:205:GLU:N	2.18	0.58
1:B:314:TYR:HB3	1:B:374:ILE:HD11	1.84	0.58
1:A:579:PHE:CD2	1:A:758:LEU:HD11	2.32	0.58
1:A:837:PRO:HB2	1:A:839:ARG:HH12	1.67	0.58
1:B:199:TRP:HD1	1:B:496:TYR:HE2	1.51	0.58
1:A:200:ARG:CB	1:A:498:THR:HG21	2.33	0.58
1:A:437:ILE:HD12	1:A:446:LEU:HD13	1.86	0.58
1:A:579:PHE:HD2	1:A:758:LEU:HD12	1.63	0.58
1:B:501:LYS:HG2	1:B:503:GLU:HB2	1.85	0.58
1:A:509:VAL:O	1:A:513:TRP:CD1	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:LEU:HD13	1:A:723:LEU:HD11	1.85	0.57
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.86	0.57
1:A:729:LEU:HD13	1:A:738:ALA:HB1	1.87	0.57
1:A:722:ARG:HG2	1:A:756:LYS:HB2	1.86	0.57
1:B:917:ASN:HB3	1:B:920:ARG:HB3	1.85	0.57
1:B:769:VAL:HG12	1:B:1002:LEU:HB3	1.84	0.57
1:B:293:PHE:CE2	1:B:477:ARG:NH1	2.73	0.57
1:B:608:ALA:HB3	1:B:618:TYR:CE2	2.15	0.57
1:A:392:LEU:CG	1:A:513:TRP:CZ3	2.87	0.57
1:B:76:LEU:CD1	1:B:446:LEU:HD11	2.32	0.57
1:A:319:ILE:HG13	1:A:371:MET:HB2	1.87	0.56
1:B:81:PRO:HA	1:B:261:ARG:HB2	1.88	0.56
1:B:586:ASP:HB2	1:B:589:HIS:HD1	1.68	0.56
1:A:79:SER:HA	1:A:260:GLY:O	2.05	0.56
1:B:391:ILE:HA	1:B:394:MET:HE2	1.88	0.56
1:B:69:LEU:HD21	1:B:272:VAL:HG22	1.88	0.56
1:B:673:PHE:HA	1:B:676:GLU:HB2	1.86	0.56
1:B:771:LEU:HD21	1:B:953:LYS:N	2.20	0.56
1:A:894:LEU:HG	1:A:925:VAL:HG11	1.88	0.56
1:B:325:TYR:CD1	1:B:460:ARG:HD3	2.41	0.56
1:A:554:THR:HG22	1:A:556:MET:H	1.71	0.55
1:A:295:GLU:HA	1:A:298:LEU:HG	1.88	0.55
1:B:208:THR:O	1:B:293:PHE:CE1	2.60	0.55
1:B:316:THR:HB	1:B:477:ARG:HB2	1.88	0.55
1:B:810:LEU:HD11	1:B:886:ILE:HG22	1.89	0.55
1:B:561:PHE:HD1	1:B:729:LEU:HD11	1.72	0.55
1:A:392:LEU:CD2	1:A:513:TRP:CE3	2.90	0.55
1:A:110:LEU:CD1	1:A:241:LEU:HD22	2.37	0.54
1:A:392:LEU:CA	1:A:513:TRP:HZ3	2.19	0.54
1:A:153:VAL:HG11	1:A:158:LEU:HA	1.88	0.54
1:A:579:PHE:CE2	1:A:758:LEU:HD13	2.42	0.54
1:A:788:ASN:HB2	1:A:851:GLN:HE21	1.72	0.54
1:A:227:GLU:HG2	1:A:237:VAL:HG21	1.90	0.54
1:B:112:HIS:HB3	1:B:182:GLU:CD	2.33	0.54
1:A:776:TRP:HB2	1:A:951:ARG:HH22	1.73	0.54
1:B:422:PHE:HB2	1:B:454:TYR:HB3	1.88	0.54
1:A:799:MET:HA	1:A:843:ILE:HD13	1.90	0.54
1:B:315:VAL:HG12	1:B:317:PHE:CE2	2.43	0.54
1:B:625:TYR:HE2	1:B:765:ARG:HA	1.73	0.54
1:A:683:MET:HE2	1:A:849:ILE:HD13	1.90	0.53
1:A:201:LEU:HA	1:A:204:LEU:CD2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ASP:HA	1:A:371:MET:HG2	1.90	0.53
1:A:108:HIS:O	1:A:111:GLU:HG3	2.08	0.53
1:A:317:PHE:HD1	1:A:475:ASN:HB3	1.73	0.53
1:A:350:LEU:HB3	1:A:356:VAL:HB	1.90	0.53
1:B:60:ASP:HB2	1:B:425:LYS:HD3	1.89	0.53
1:A:73:ILE:HG21	1:A:254:MET:HE2	1.91	0.53
1:A:675:ALA:HA	1:A:785:VAL:HG21	1.90	0.53
1:B:778:VAL:HG13	1:B:957:HIS:CD2	2.42	0.53
1:A:148:ASN:HD21	1:A:435:SER:HB2	1.72	0.53
1:B:330:PRO:HG3	1:B:463:LEU:HB3	1.89	0.53
1:A:101:PRO:HA	1:A:217:LYS:HE2	1.91	0.53
1:B:616:LEU:HD12	1:B:633:GLY:HA3	1.90	0.53
1:B:776:TRP:CZ2	1:B:778:VAL:HG21	2.43	0.53
1:A:115:PHE:CE1	1:A:127:TYR:CB	2.92	0.53
1:B:589:HIS:HA	1:B:592:MET:SD	2.49	0.53
1:B:683:MET:HE2	1:B:849:ILE:HD13	1.90	0.53
1:B:530:PHE:CZ	1:B:611:ALA:CA	2.48	0.53
1:B:122:PRO:HB2	1:B:181:ARG:HH12	1.74	0.52
1:A:87:SER:HA	1:A:152:ASP:HA	1.90	0.52
1:A:400:LYS:HG2	1:A:522:PHE:HB2	1.91	0.52
1:A:153:VAL:HG22	1:A:154:SER:H	1.75	0.52
1:A:646:ILE:HA	1:A:649:MET:HE2	1.90	0.52
1:B:118:THR:HG21	1:B:173:LEU:HB2	1.91	0.52
1:B:153:VAL:HB	1:B:157:HIS:HB2	1.91	0.52
1:A:119:LYS:CB	1:A:173:LEU:HD11	2.39	0.52
1:A:600:LEU:HD21	1:A:649:MET:HB3	1.91	0.52
1:B:86:SER:HB3	1:B:260:GLY:HA2	1.91	0.52
1:B:93:HIS:HA	1:B:146:HIS:HB3	1.90	0.52
1:A:809:GLU:HG3	1:A:889:LEU:HD21	1.92	0.52
1:A:945:ALA:HB3	1:A:948:ALA:HB2	1.92	0.52
1:B:117:GLY:HA3	1:B:121:TYR:HB2	1.91	0.52
1:B:209:GLY:HA2	1:B:293:PHE:CE1	2.44	0.52
1:B:708:THR:HB	1:B:710:PRO:HD2	1.92	0.51
1:A:806:MET:HE3	1:A:924:GLU:HB3	1.93	0.51
1:B:49:ARG:HA	1:B:67:LEU:HB2	1.92	0.51
1:A:811:PHE:HB2	1:A:936:ILE:HD11	1.93	0.51
1:B:109:PHE:HE2	1:B:241:LEU:HD11	1.75	0.51
1:A:509:VAL:O	1:A:513:TRP:HD1	1.94	0.51
1:A:183:VAL:HG11	1:A:227:GLU:HB2	1.93	0.51
1:A:641:LEU:O	1:A:645:ILE:HG12	2.11	0.50
1:B:720:LEU:HB3	1:B:753:ALA:HB1	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ILE:HG23	1:A:254:MET:HB3	1.93	0.50
1:A:814:ILE:HG21	1:A:874:ILE:HD11	1.93	0.50
1:B:776:TRP:CZ2	1:B:778:VAL:CG2	2.94	0.50
1:A:264:LEU:HD12	1:A:264:LEU:C	2.36	0.50
1:A:392:LEU:CA	1:A:513:TRP:CZ3	2.94	0.50
1:B:820:PHE:HD1	1:B:824:ARG:HD3	1.77	0.50
1:B:828:GLN:HG2	1:B:828:GLN:O	2.12	0.50
1:B:894:LEU:HG	1:B:925:VAL:HG11	1.94	0.50
1:A:762:GLN:HE21	1:B:587:PRO:CG	2.24	0.49
1:A:285:LEU:HD12	1:A:285:LEU:C	2.37	0.49
1:A:344:GLY:HA3	1:A:523:LYS:H	1.76	0.49
1:A:573:ASN:ND2	1:A:632:LYS:CB	2.74	0.49
1:B:794:TYR:CE1	1:B:845:GLY:HA3	2.47	0.49
1:A:684:TYR:HE1	1:A:687:ARG:NH2	2.11	0.48
1:B:245:HIS:HA	1:B:249:TYR:CD1	2.47	0.48
1:B:447:GLU:HG2	1:B:448:GLU:HG3	1.95	0.48
1:B:911:ILE:HG23	1:B:916:TYR:CE2	2.48	0.48
1:A:153:VAL:HG21	1:A:161:ALA:HB2	1.96	0.48
1:B:127:TYR:HD1	1:B:164:ARG:HE	1.61	0.48
1:B:259:LEU:HG	1:B:434:THR:HG22	1.94	0.48
1:B:195:MET:CE	1:B:307:ILE:HD13	2.44	0.48
1:B:298:LEU:HD23	1:B:477:ARG:HE	1.79	0.48
1:A:200:ARG:NE	1:A:498:THR:HG22	2.28	0.48
1:A:301:LEU:CD1	1:A:505:ILE:CD1	2.82	0.48
1:B:195:MET:HE1	1:B:307:ILE:HD13	1.95	0.48
1:B:670:LEU:HD13	1:B:701:LYS:HB2	1.96	0.48
1:A:201:LEU:HA	1:A:204:LEU:HD21	1.94	0.48
1:A:360:VAL:HG13	1:A:376:ASN:HB2	1.96	0.48
1:A:329:ASN:HB2	1:A:456:LEU:HD11	1.95	0.47
1:B:302:TYR:CD1	1:B:502:GLN:HA	2.49	0.47
1:B:288:PHE:HD2	1:B:370:PHE:HE1	1.61	0.47
1:A:121:TYR:HB2	1:A:126:GLU:HG2	1.95	0.47
1:A:897:PRO:HG2	1:A:903:GLU:HB3	1.96	0.47
1:A:151:PHE:HE2	1:A:161:ALA:HB1	1.78	0.47
1:B:108:HIS:O	1:B:111:GLU:HG3	2.15	0.47
1:B:392:LEU:HG	1:B:513:TRP:CD1	2.49	0.47
1:B:552:LYS:HB3	1:B:559:LEU:HD23	1.96	0.47
1:B:562:LYS:HD3	1:B:730:HIS:CE1	2.50	0.47
1:A:74:LYS:HB3	1:A:441:LEU:HG	1.96	0.47
1:A:340:HIS:CE1	1:A:525:PRO:HB3	2.50	0.47
1:A:313:LEU:HD23	1:A:480:ILE:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:TYR:HE1	1:A:838:ARG:HB3	1.80	0.46
1:A:839:ARG:NE	1:A:844:GLN:HG2	2.29	0.46
1:B:237:VAL:O	1:B:241:LEU:HG	2.15	0.46
1:A:251:SER:HB2	1:A:281:LYS:HB2	1.97	0.46
1:B:769:VAL:HG11	1:B:1002:LEU:HB2	1.82	0.46
1:A:115:PHE:CZ	1:A:127:TYR:C	2.94	0.46
1:A:579:PHE:CD2	1:A:758:LEU:HD12	2.43	0.46
1:A:794:TYR:CZ	1:A:845:GLY:HA3	2.51	0.46
1:B:54:ILE:HD13	1:B:447:GLU:HA	1.96	0.46
1:B:911:ILE:HG23	1:B:916:TYR:HE2	1.80	0.46
1:A:237:VAL:O	1:A:241:LEU:HG	2.15	0.46
1:A:75:VAL:HA	1:A:256:VAL:O	2.16	0.46
1:A:110:LEU:HD11	1:A:241:LEU:HD22	1.98	0.46
1:A:110:LEU:CD1	1:A:241:LEU:CD2	2.94	0.46
1:A:254:MET:HE3	1:A:256:VAL:HG23	1.96	0.46
1:A:509:VAL:HG12	1:A:513:TRP:HE1	1.81	0.46
1:A:573:ASN:HD22	1:A:632:LYS:CB	2.28	0.46
1:A:315:VAL:HG22	1:A:375:ILE:HG22	1.97	0.46
1:A:837:PRO:HB2	1:A:839:ARG:NH1	2.29	0.46
1:A:940:TYR:HA	1:A:944:LEU:HB2	1.98	0.46
1:B:810:LEU:HD23	1:B:936:ILE:HG13	1.97	0.46
1:A:200:ARG:CG	1:A:498:THR:HG21	2.34	0.45
1:A:505:ILE:HG22	1:A:509:VAL:HB	1.99	0.45
1:A:506:PRO:HB2	1:A:508:GLU:HG3	1.98	0.45
1:B:429:ARG:HH21	1:B:431:ARG:HB3	1.81	0.45
1:A:800:GLN:HG2	1:A:844:GLN:HG3	1.98	0.45
1:B:318:PRO:HA	1:B:372:PHE:CD1	2.51	0.45
1:B:617:SER:HB3	1:B:632:LYS:HB2	1.98	0.45
1:B:722:ARG:HG2	1:B:756:LYS:HG3	1.99	0.45
1:A:200:ARG:CD	1:A:498:THR:HG22	2.47	0.45
1:A:317:PHE:CZ	1:A:476:VAL:HG22	2.52	0.45
1:A:897:PRO:HB3	1:A:902:ALA:HB3	1.98	0.45
1:B:561:PHE:HA	1:B:729:LEU:HG	1.99	0.45
1:A:115:PHE:HZ	1:A:127:TYR:C	2.21	0.45
1:A:338:ILE:H	1:A:338:ILE:HG12	1.59	0.45
1:A:491:ARG:HH22	1:A:502:GLN:HB2	1.82	0.45
1:A:643:LYS:HA	1:A:646:ILE:HD12	1.98	0.45
1:A:933:LYS:O	1:A:936:ILE:HG22	2.16	0.45
1:B:547:TYR:CE2	1:B:919:ASP:HB3	2.51	0.45
1:A:110:LEU:HD11	1:A:241:LEU:HD23	1.97	0.45
1:A:1000:ARG:HE	1:B:1007:LEU:HD22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:625:TYR:CE2	1:B:765:ARG:HA	2.51	0.45
1:A:450:LEU:HD12	1:A:450:LEU:HA	1.84	0.45
1:B:64:TYR:OH	1:B:450:LEU:HD12	2.16	0.45
1:B:103:ILE:CG1	1:B:106:LEU:HB2	2.42	0.45
1:B:438:ALA:HA	1:B:441:LEU:HD12	1.99	0.45
1:A:446:LEU:HA	1:A:449:VAL:HG12	1.99	0.44
1:A:883:GLN:O	1:A:886:ILE:HG12	2.16	0.44
1:B:782:ARG:HA	1:B:959:LEU:HB2	1.99	0.44
1:A:391:ILE:C	1:A:513:TRP:HZ3	2.25	0.44
1:B:103:ILE:HD11	1:B:106:LEU:CG	2.47	0.44
1:B:293:PHE:CG	1:B:477:ARG:NH2	2.85	0.44
1:B:317:PHE:HE1	1:B:472:ARG:O	2.01	0.44
1:B:371:MET:O	1:B:372:PHE:HD1	2.01	0.44
1:A:64:TYR:CG	1:A:64:TYR:O	2.70	0.44
1:B:776:TRP:CH2	1:B:778:VAL:CG2	2.93	0.44
1:A:109:PHE:HE2	1:A:241:LEU:HD11	1.83	0.44
1:A:341:GLU:HG2	1:A:347:LEU:HD23	1.99	0.44
1:A:934:GLU:HA	1:A:937:ILE:HD12	1.98	0.44
1:B:288:PHE:CD2	1:B:370:PHE:HE1	2.36	0.44
1:B:295:GLU:HG2	1:B:298:LEU:HD12	2.00	0.44
1:A:301:LEU:HD13	1:A:505:ILE:HG13	1.98	0.44
1:A:538:LEU:H	1:A:732:ASN:HD21	1.65	0.44
1:B:446:LEU:O	1:B:449:VAL:HG22	2.18	0.44
1:B:741:ILE:O	1:B:744:MET:HG3	2.18	0.44
1:B:920:ARG:HE	1:B:920:ARG:HB2	1.64	0.43
1:B:77:LEU:HD21	1:B:271:VAL:HG11	1.99	0.43
1:B:588:LEU:HD13	1:B:588:LEU:HA	1.86	0.43
1:B:995:MET:HE3	1:B:995:MET:HB3	1.88	0.43
1:A:229:ARG:O	1:A:232:GLN:HG2	2.19	0.43
1:A:762:GLN:HE21	1:B:587:PRO:HD2	1.81	0.43
1:A:928:LEU:HD12	1:A:931:LEU:HD22	1.99	0.43
1:B:894:LEU:HD21	1:B:925:VAL:HG21	2.00	0.43
1:B:76:LEU:HA	1:B:446:LEU:HD11	2.00	0.43
1:B:460:ARG:HE	1:B:463:LEU:HG	1.84	0.43
1:A:128:SER:HA	1:A:131:LEU:HD12	2.00	0.43
1:A:827:GLU:O	1:A:828:GLN:HG2	2.19	0.43
1:A:257:VAL:HG21	1:A:437:ILE:HG22	2.00	0.43
1:A:300:GLN:HE22	1:A:504:ALA:HB2	1.83	0.43
1:A:847:ARG:HD2	1:A:849:ILE:HD11	2.00	0.43
1:B:103:ILE:HA	1:B:229:ARG:HH11	1.83	0.43
1:B:245:HIS:HA	1:B:249:TYR:HD1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:PRO:HD2	1:B:475:ASN:HB3	2.00	0.43
1:A:109:PHE:O	1:A:113:MET:HG2	2.18	0.43
1:B:257:VAL:HG21	1:B:437:ILE:HD11	2.01	0.43
1:B:573:ASN:HD21	1:B:904:SER:CB	2.30	0.43
1:A:321:ASP:CG	1:A:324:LYS:HB2	2.44	0.43
1:A:762:GLN:NE2	1:B:587:PRO:HG2	2.34	0.43
1:A:936:ILE:HD12	1:A:936:ILE:HA	1.82	0.43
1:B:749:LEU:HD12	1:B:749:LEU:HA	1.90	0.43
1:A:392:LEU:HA	1:A:513:TRP:HZ3	1.83	0.43
1:A:817:GLU:HB2	1:A:818:PRO:HD3	2.01	0.43
1:A:115:PHE:CZ	1:A:127:TYR:CB	2.99	0.42
1:B:561:PHE:HB2	1:B:729:LEU:HD21	2.00	0.42
1:B:208:THR:O	1:B:293:PHE:HE1	2.02	0.42
1:B:800:GLN:HA	1:B:844:GLN:NE2	2.34	0.42
1:A:126:GLU:O	1:A:129:GLN:HG3	2.18	0.42
1:A:252:ASN:HB3	1:A:253:LEU:HG	2.01	0.42
1:A:762:GLN:NE2	1:B:587:PRO:CD	2.78	0.42
1:A:889:LEU:HD23	1:A:928:LEU:HD11	2.02	0.42
1:B:56:LYS:O	1:B:57:SER:C	2.62	0.42
1:A:574:LEU:HD21	1:A:733:ILE:HD12	2.00	0.42
1:B:953:LYS:HE2	1:B:953:LYS:HB3	1.94	0.42
1:A:200:ARG:C	1:A:498:THR:HG21	2.45	0.42
1:A:573:ASN:ND2	1:A:632:LYS:HG2	2.35	0.42
1:A:661:ILE:HD12	1:A:661:ILE:HA	1.95	0.42
1:B:93:HIS:HA	1:B:146:HIS:CB	2.50	0.42
1:B:122:PRO:HB2	1:B:181:ARG:NH1	2.34	0.42
1:B:530:PHE:CZ	1:B:611:ALA:CB	3.02	0.42
1:B:815:ILE:HG22	1:B:870:MET:HE2	2.01	0.42
1:A:97:LEU:HD22	1:A:215:PHE:HA	2.01	0.42
1:A:236:ASP:HB3	1:A:239:GLN:HB2	2.02	0.42
1:A:240:GLU:HA	1:A:243:LYS:HG2	2.01	0.41
1:B:360:VAL:HG13	1:B:376:ASN:HB3	2.01	0.41
1:A:317:PHE:CD1	1:A:475:ASN:HB3	2.54	0.41
1:A:422:PHE:HE1	1:A:450:LEU:HG	1.84	0.41
1:A:787:ASN:O	1:A:960:ALA:HB1	2.20	0.41
1:B:771:LEU:HD23	1:B:952:HIS:CD2	2.55	0.41
1:B:785:VAL:HG23	1:B:786:HIS:CD2	2.55	0.41
1:A:364:LYS:HB2	1:A:374:ILE:HG12	2.02	0.41
1:A:460:ARG:HB2	1:A:463:LEU:HB2	2.03	0.41
1:A:689:LEU:HA	1:A:999:LYS:HE2	2.01	0.41
1:B:670:LEU:HB2	1:B:701:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PHE:CZ	1:A:128:SER:CA	2.99	0.41
1:A:821:ASN:HA	1:A:825:THR:HB	2.03	0.41
1:B:66:GLY:HA3	1:B:446:LEU:CD1	2.50	0.41
1:B:103:ILE:HD11	1:B:106:LEU:HD22	2.01	0.41
1:B:200:ARG:O	1:B:203:GLN:HG3	2.20	0.41
1:A:254:MET:HE3	1:A:256:VAL:HG21	2.00	0.41
1:A:294:GLN:O	1:A:295:GLU:HB2	2.19	0.41
1:B:84:ASP:HA	1:B:261:ARG:HH21	1.86	0.41
1:A:121:TYR:C	1:A:123:LYS:H	2.29	0.41
1:A:445:PRO:HD2	1:A:448:GLU:HB3	2.02	0.41
1:B:321:ASP:O	1:B:322:LEU:HG	2.20	0.41
1:B:530:PHE:O	1:B:530:PHE:CD1	2.73	0.41
1:A:395:PHE:HZ	1:A:476:VAL:HG21	1.85	0.41
1:A:572:ALA:HA	1:A:731:GLY:HA3	2.02	0.41
1:B:103:ILE:HG12	1:B:106:LEU:HD22	2.02	0.41
1:A:307:ILE:HD13	1:A:307:ILE:HA	1.91	0.41
1:A:631:VAL:HG12	1:A:638:GLN:HG3	2.03	0.41
1:B:103:ILE:CG1	1:B:106:LEU:HD22	2.51	0.41
1:B:229:ARG:HA	1:B:232:GLN:HE21	1.85	0.41
1:B:463:LEU:HD23	1:B:463:LEU:HA	1.86	0.41
1:B:678:PRO:HD3	1:B:786:HIS:CD2	2.56	0.41
1:B:776:TRP:HD1	1:B:953:LYS:HB3	1.86	0.41
1:A:472:ARG:O	1:A:476:VAL:HG23	2.20	0.41
1:A:771:LEU:HB2	1:A:952:HIS:HB3	2.03	0.41
1:B:50:ILE:HG12	1:B:67:LEU:HA	2.02	0.41
1:B:504:ALA:O	1:B:505:ILE:C	2.64	0.41
1:A:501:LYS:HD2	1:A:501:LYS:HA	1.86	0.40
1:B:247:ALA:HA	1:B:281:LYS:HG3	2.02	0.40
1:A:573:ASN:HD21	1:A:632:LYS:HB3	1.83	0.40
1:B:118:THR:HG23	1:B:119:LYS:H	1.86	0.40
1:A:415:LYS:HG3	1:A:455:LEU:O	2.22	0.40
1:A:433:TYR:O	1:A:436:LYS:HG2	2.22	0.40
1:A:505:ILE:HG23	1:A:506:PRO:HD2	2.03	0.40
1:A:506:PRO:HG2	1:A:509:VAL:CG2	2.51	0.40
1:A:837:PRO:HB2	1:A:839:ARG:HH22	1.86	0.40
1:B:945:ALA:HB3	1:B:948:ALA:HB2	2.04	0.40
1:A:506:PRO:HG2	1:A:509:VAL:HG23	2.02	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	928/1011 (92%)	904 (97%)	22 (2%)	2 (0%)	44	74
1	B	931/1011 (92%)	904 (97%)	26 (3%)	1 (0%)	48	79
All	All	1859/2022 (92%)	1808 (97%)	48 (3%)	3 (0%)	45	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	PRO
1	B	101	PRO
1	A	989	PRO

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	831/901 (92%)	785 (94%)	46 (6%)	18	43
1	B	834/901 (93%)	792 (95%)	42 (5%)	20	45
All	All	1665/1802 (92%)	1577 (95%)	88 (5%)	21	44

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	VAL
1	A	98	SER
1	A	114	LEU

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Mol	Chain	Res	Type
1	A	116	LEU
1	A	162	LEU
1	A	242	LEU
1	A	267	LEU
1	A	280	ASN
1	A	290	GLU
1	A	298	LEU
1	A	307	ILE
1	A	338	ILE
1	A	349	GLU
1	A	359	LEU
1	A	360	VAL
1	A	387	VAL
1	A	401	LEU
1	A	440	ILE
1	A	450	LEU
1	A	455	LEU
1	A	456	LEU
1	A	478	VAL
1	A	491	ARG
1	A	517	ASP
1	A	545	THR
1	A	598	GLU
1	A	604	LEU
1	A	620	LEU
1	A	623	THR
1	A	642	LEU
1	A	688	LEU
1	A	707	VAL
1	A	709	LEU
1	A	745	VAL
1	A	751	GLU
1	A	759	LEU
1	A	769	VAL
1	A	771	LEU
1	A	809	GLU
1	A	814	ILE
1	A	849	ILE
1	A	931	LEU
1	A	936	ILE
1	A	944	LEU
1	A	953	LYS

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Mol	Chain	Res	Type
1	A	954	VAL
1	B	61	LYS
1	B	99	ASP
1	B	110	LEU
1	B	149	TYR
1	B	162	LEU
1	B	222	ASN
1	B	242	LEU
1	B	257	VAL
1	B	277	GLU
1	B	278	VAL
1	B	290	GLU
1	B	297	HIS
1	B	324	LYS
1	B	359	LEU
1	B	360	VAL
1	B	377	VAL
1	B	380	THR
1	B	387	VAL
1	B	392	LEU
1	B	407	GLN
1	B	410	VAL
1	B	480	ILE
1	B	538	LEU
1	B	588	LEU
1	B	597	LEU
1	B	616	LEU
1	B	620	LEU
1	B	631	VAL
1	B	654	ILE
1	B	688	LEU
1	B	709	LEU
1	B	712	LEU
1	B	718	GLN
1	B	728	LEU
1	B	729	LEU
1	B	744	MET
1	B	759	LEU
1	B	780	GLN
1	B	789	SER
1	B	806	MET
1	B	860	GLU

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Mol	Chain	Res	Type
1	B	1008	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	A	112	HIS
1	A	148	ASN
1	A	245	HIS
1	A	280	ASN
1	A	297	HIS
1	A	300	GLN
1	A	323	GLN
1	A	340	HIS
1	A	386	HIS
1	A	407	GLN
1	A	502	GLN
1	A	534	ASN
1	A	573	ASN
1	A	671	ASN
1	A	677	GLN
1	A	724	HIS
1	A	762	GLN
1	A	786	HIS
1	A	788	ASN
1	A	841	ASN
1	A	851	GLN
1	A	957	HIS
1	B	125	ASN
1	B	190	HIS
1	B	232	GLN
1	B	282	ASN
1	B	323	GLN
1	B	418	ASN
1	B	475	ASN
1	B	515	ASN
1	B	519	ASN
1	B	534	ASN
1	B	573	ASN
1	B	672	ASN
1	B	718	GLN
1	B	730	HIS

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Mol	Chain	Res	Type
1	B	786	HIS
1	B	821	ASN
1	B	851	GLN
1	B	915	GLN
1	B	922	ASN
1	B	993	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



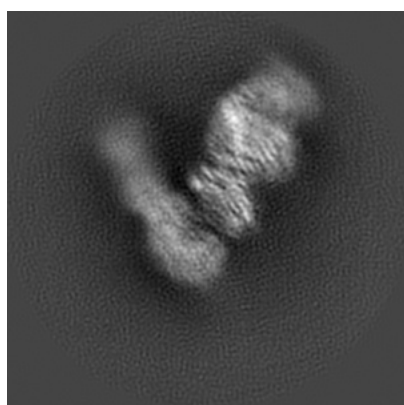
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24760. These allow visual inspection of the internal detail of the map and identification of artifacts.

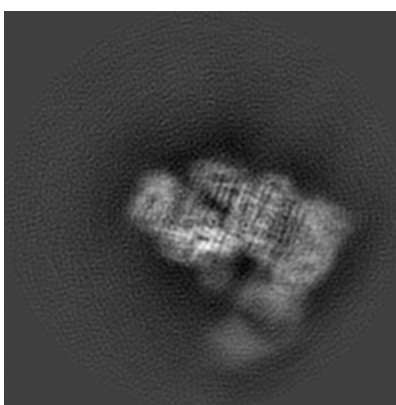
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

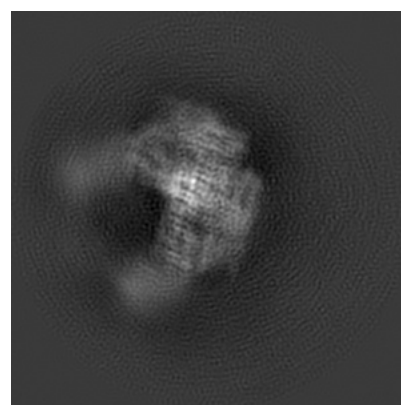
#### 6.1.1 Primary map



X



Y

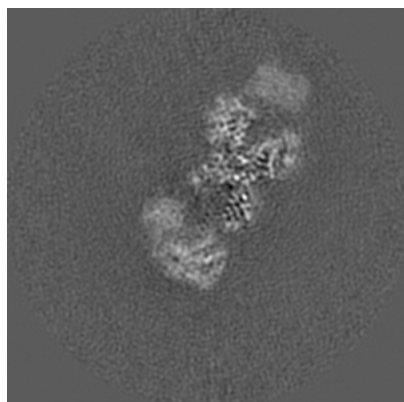


Z

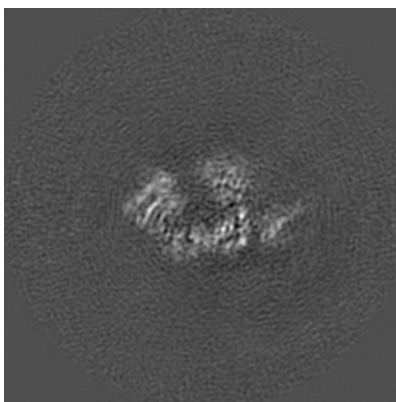
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

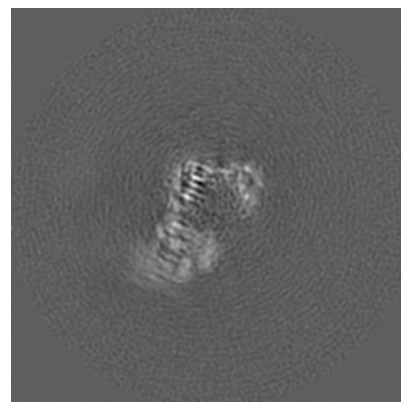
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

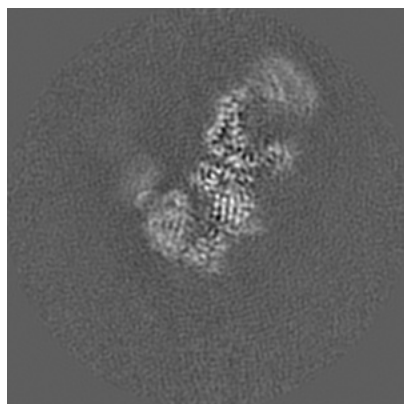


Z Index: 128

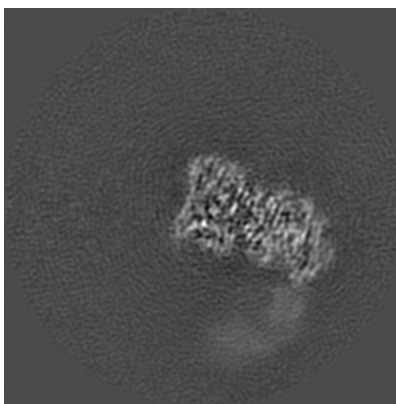
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

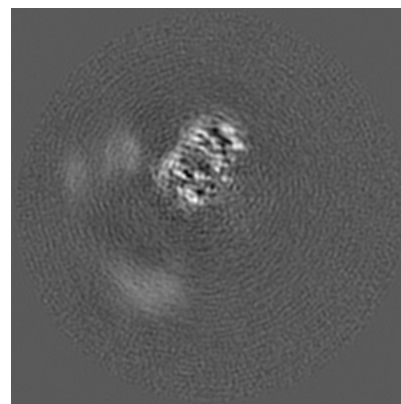
### 6.3.1 Primary map



X Index: 115



Y Index: 147

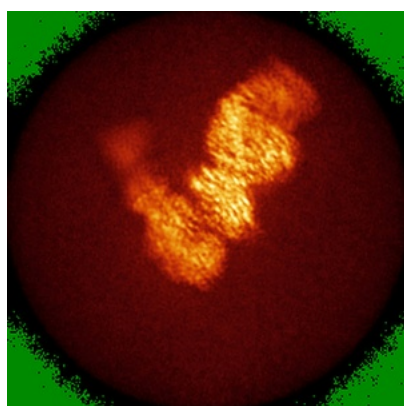


Z Index: 164

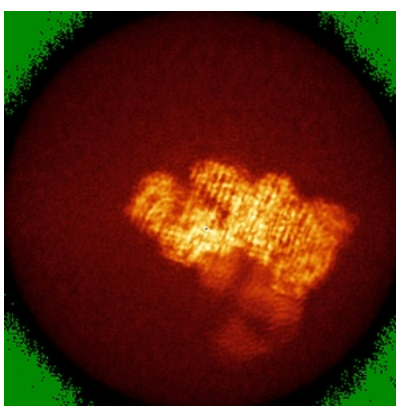
The images above show the largest variance slices of the map in three orthogonal directions.

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

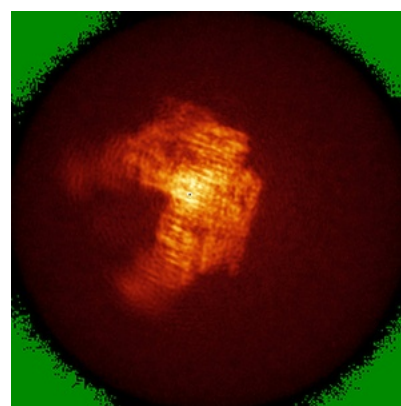
### 6.4.1 Primary map



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 [i](#)

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

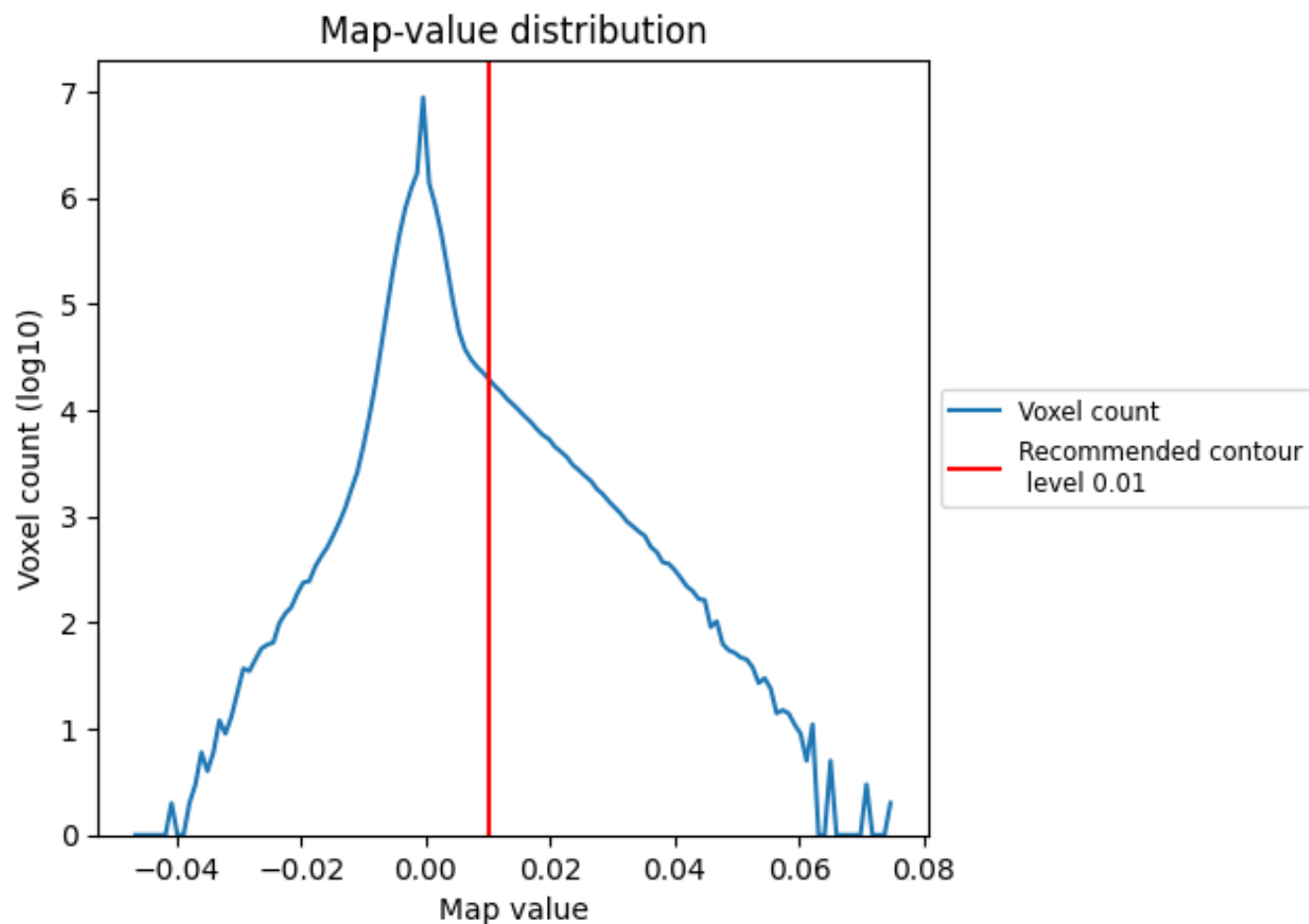
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

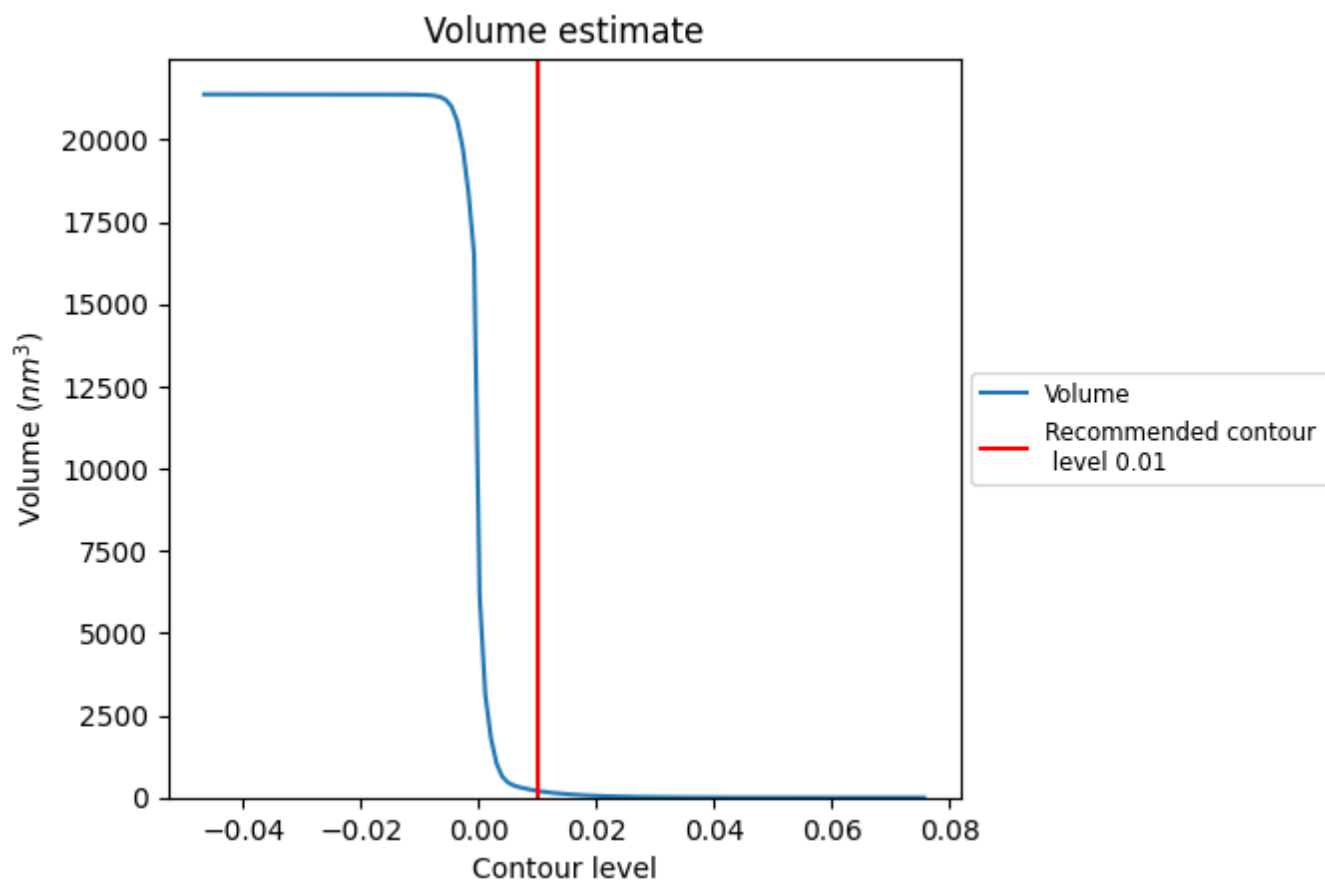
This section contains the results of statistical analysis of the map.

### 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.

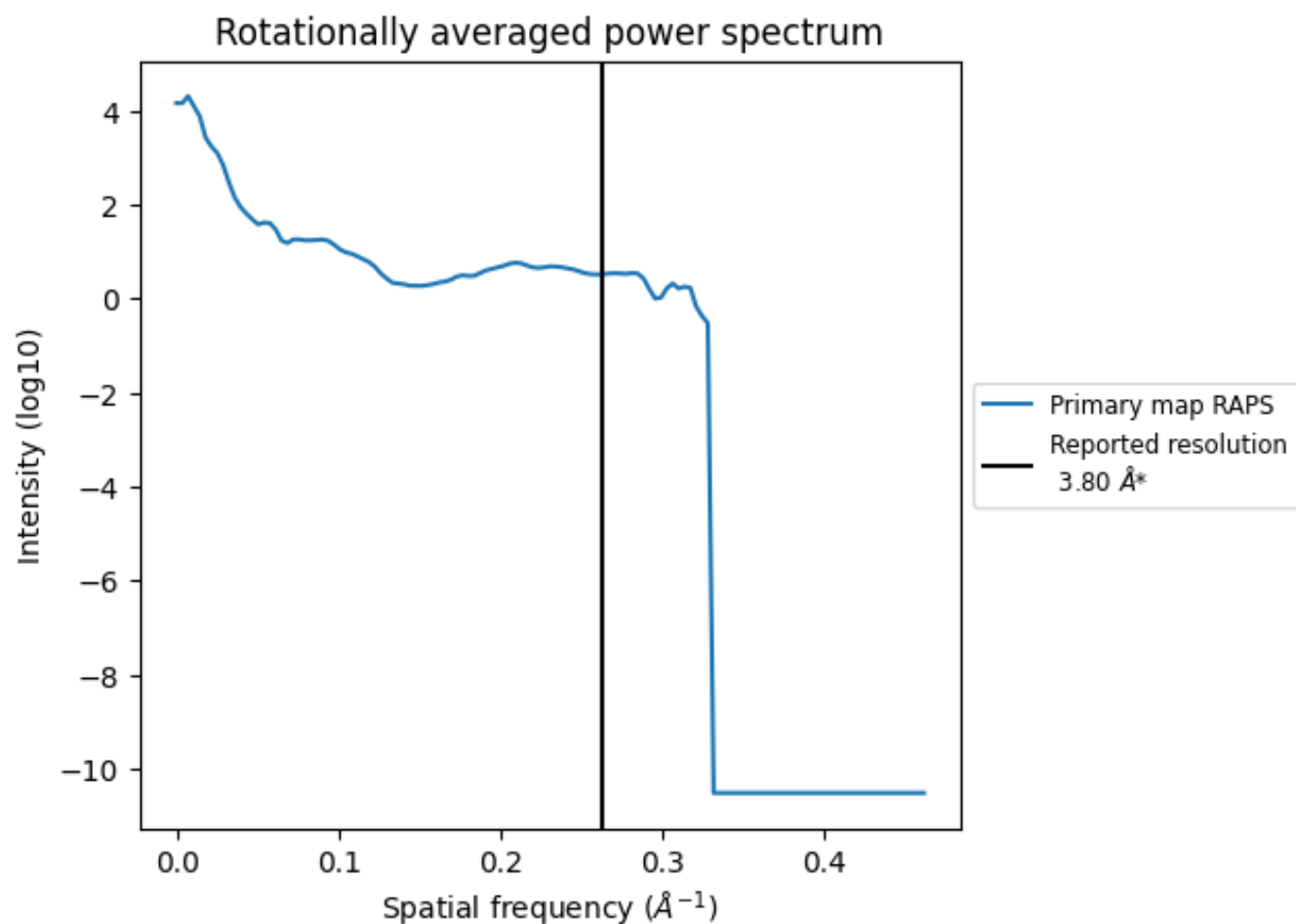
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 204 nm<sup>3</sup>; this corresponds to an approximate mass of 184 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 0.263 Å<sup>-1</sup>

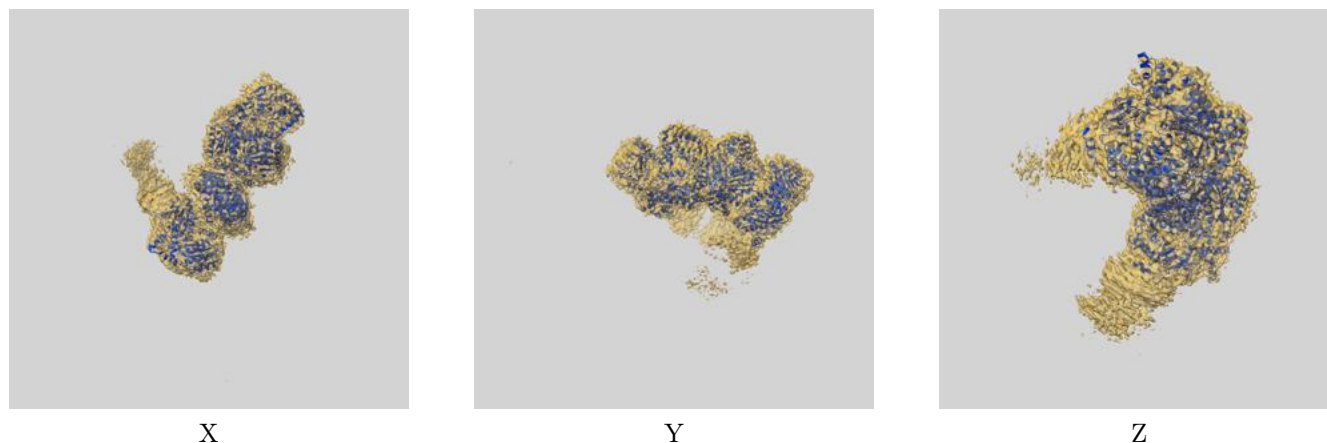
## 8 Fourier-Shell correlation ⓘ

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 EMDB map EMD-24760 and PDB model 7RZH. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

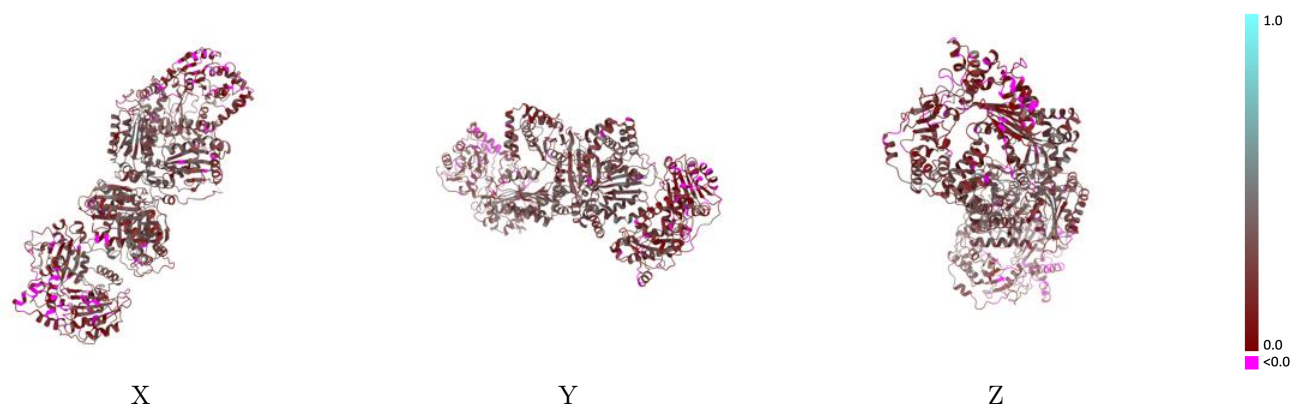
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

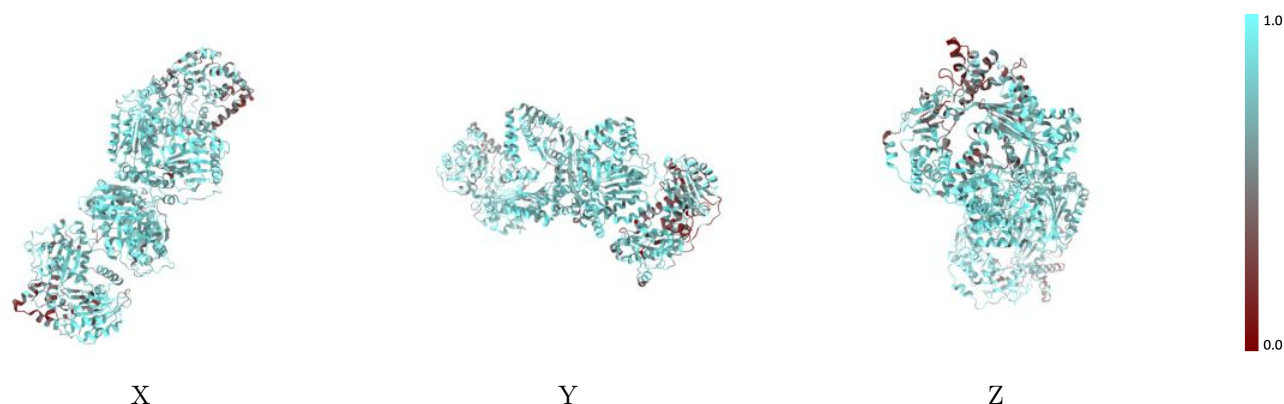


## 9.2 Q-score mapped to coordinate model [i](#)



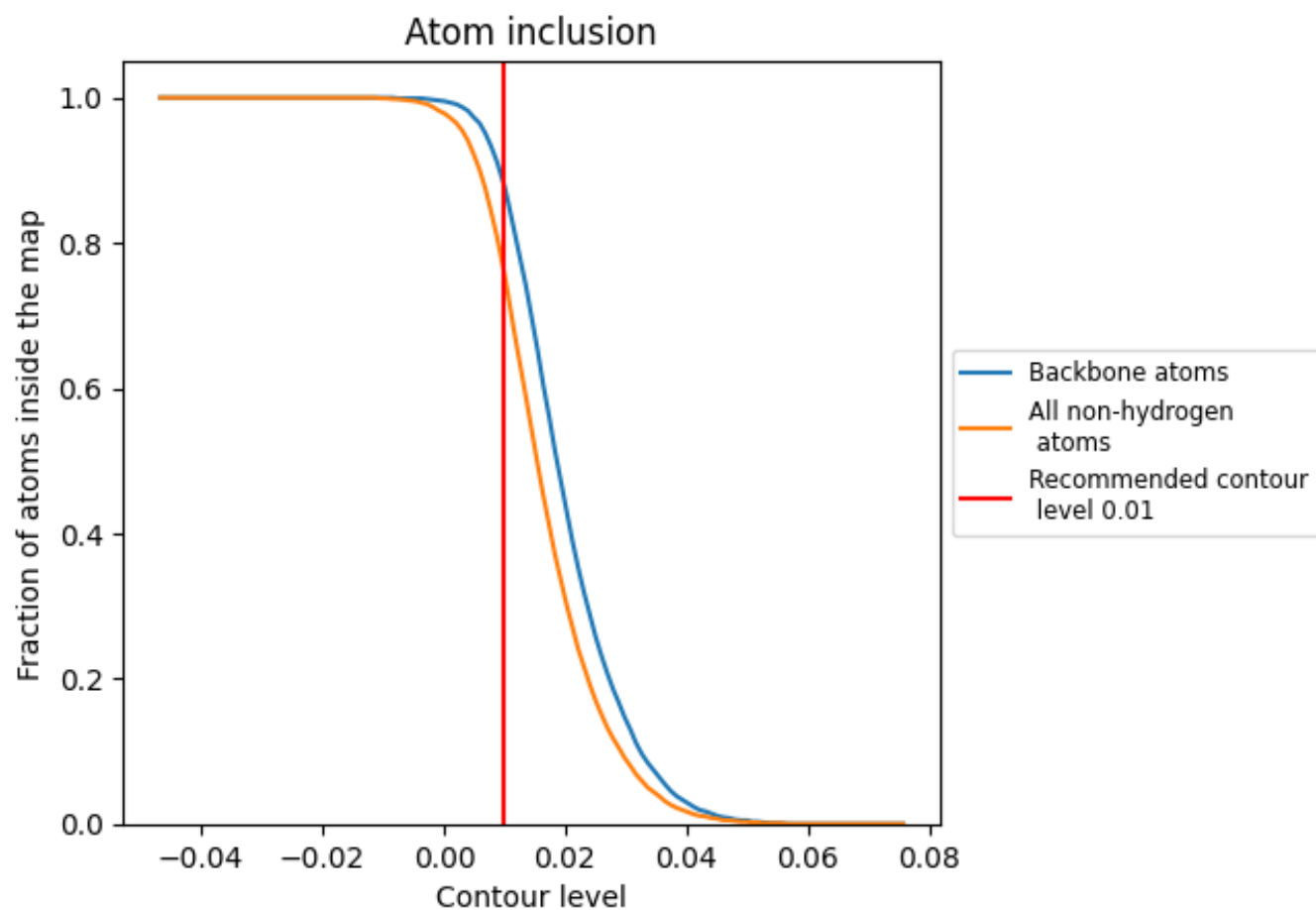
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 76% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7570	<div></div> 0.2340
A	<div></div> 0.7370	<div></div> 0.2320
B	<div></div> 0.7770	<div></div> 0.2350

