



## Full wwPDB EM Validation Report ⓘ

Jun 28, 2025 – 11:06 pm BST

PDB ID : 7Z1H / pdb\_00007z1h  
EMDB ID : EMD-14446  
Title : VAR2CSA APO  
Authors : Raghavan, S.S.R.; Wang, K.T.  
Deposited on : 2022-02-24  
Resolution : 3.12 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) : 2.44

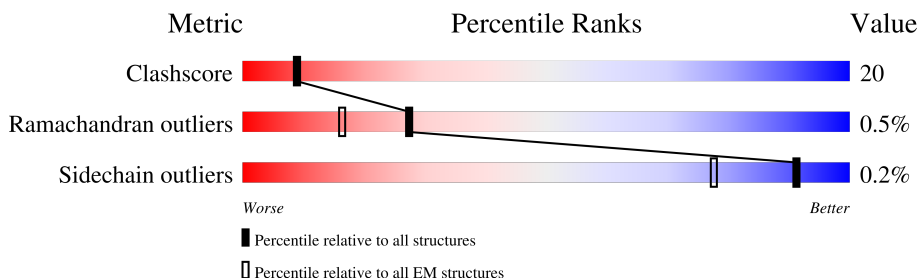
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.12 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	2040	<div> <div>22%</div> <div>61%</div> <div>28%</div> <div>• 9%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15032 atoms, of which 0 are hydrogens and 0 are deuteriums.

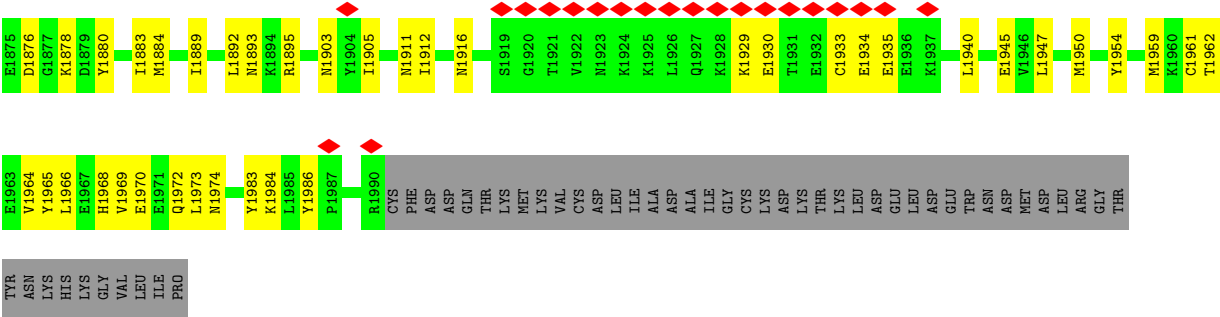
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VAR2CSA APO.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1848	15032	9381	2590	2962	99	0	0







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	207129	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.154	Depositor
Minimum map value	-1.063	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	366.08002, 366.08002, 366.08002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.76	49/15330 (0.3%)	0.67	58/20612 (0.3%)

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	7

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	374	PHE	CE2-CZ	28.17	2.23	1.38
1	A	374	PHE	CD2-CE2	28.10	2.23	1.38
1	A	374	PHE	CE1-CZ	27.14	2.20	1.38
1	A	374	PHE	CD1-CE1	27.00	2.19	1.38
1	A	374	PHE	CG-CD1	20.23	1.81	1.38
1	A	374	PHE	CG-CD2	19.55	1.79	1.38
1	A	1381	GLU	C-N	19.07	1.60	1.33
1	A	356	ASN	C-N	18.37	1.56	1.33
1	A	1375	ASP	CA-C	18.34	1.71	1.52
1	A	343	GLN	C-N	17.70	1.60	1.33
1	A	357	LYS	N-CA	16.72	1.67	1.46
1	A	337	LYS	CA-C	16.07	1.70	1.52
1	A	1381	GLU	CA-C	14.08	1.66	1.53
1	A	1382	LYS	N-CA	13.06	1.62	1.46
1	A	337	LYS	C-N	12.38	1.52	1.33
1	A	341	GLU	C-N	10.96	1.49	1.33
1	A	343	GLN	N-CA	10.29	1.61	1.46
1	A	339	GLU	CA-C	10.15	1.66	1.52
1	A	338	THR	CA-C	10.00	1.66	1.52
1	A	1377	LYS	CA-C	9.85	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	344	GLU	N-CA	9.78	1.59	1.47
1	A	1380	ILE	CA-C	9.49	1.66	1.52
1	A	338	THR	N-CA	9.03	1.58	1.46
1	A	1381	GLU	N-CA	9.01	1.60	1.46
1	A	343	GLN	CA-C	8.97	1.62	1.53
1	A	1377	LYS	C-N	8.96	1.45	1.33
1	A	341	GLU	CA-C	8.83	1.64	1.52
1	A	338	THR	C-N	8.52	1.46	1.33
1	A	1376	ILE	CA-C	8.36	1.63	1.52
1	A	1379	ILE	CA-C	7.96	1.62	1.52
1	A	1376	ILE	C-N	7.92	1.45	1.33
1	A	1379	ILE	N-CA	7.86	1.56	1.46
1	A	339	GLU	C-N	7.78	1.44	1.33
1	A	1377	LYS	N-CA	7.75	1.56	1.46
1	A	1376	ILE	N-CA	7.41	1.55	1.46
1	A	1375	ASP	C-N	7.28	1.43	1.33
1	A	341	GLU	N-CA	7.22	1.55	1.46
1	A	339	GLU	N-CA	7.20	1.55	1.46
1	A	342	ASN	C-N	7.14	1.43	1.33
1	A	340	TRP	N-CA	6.97	1.54	1.46
1	A	1380	ILE	C-N	6.83	1.41	1.33
1	A	342	ASN	N-CA	6.80	1.54	1.46
1	A	1378	LYS	C-N	6.70	1.42	1.33
1	A	1378	LYS	CA-C	6.60	1.58	1.52
1	A	1379	ILE	C-N	6.52	1.41	1.33
1	A	342	ASN	CA-C	6.24	1.61	1.52
1	A	1378	LYS	N-CA	6.19	1.53	1.46
1	A	340	TRP	C-N	5.96	1.42	1.33
1	A	1380	ILE	N-CA	5.91	1.53	1.46

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1381	GLU	CA-C-N	21.31	150.76	122.42
1	A	1381	GLU	C-N-CA	21.31	150.76	122.42
1	A	356	ASN	CA-C-N	20.11	153.59	122.42
1	A	356	ASN	C-N-CA	20.11	153.59	122.42
1	A	343	GLN	CA-C-N	18.75	147.78	121.71
1	A	343	GLN	C-N-CA	18.75	147.78	121.71
1	A	341	GLU	CA-C-N	13.06	146.49	121.54
1	A	341	GLU	C-N-CA	13.06	146.49	121.54
1	A	1380	ILE	N-CA-C	11.15	123.61	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	THR	CA-C-N	10.98	140.91	121.92
1	A	338	THR	C-N-CA	10.98	140.91	121.92
1	A	1375	ASP	CA-C-N	9.57	139.20	121.97
1	A	1375	ASP	C-N-CA	9.57	139.20	121.97
1	A	340	TRP	CA-C-N	9.48	138.01	121.52
1	A	340	TRP	C-N-CA	9.48	138.01	121.52
1	A	1375	ASP	N-CA-C	9.38	124.73	112.72
1	A	337	LYS	CA-C-N	9.31	140.56	121.94
1	A	337	LYS	C-N-CA	9.31	140.56	121.94
1	A	340	TRP	N-CA-C	8.78	123.89	112.12
1	A	1376	ILE	CA-C-N	8.63	137.19	122.26
1	A	1376	ILE	C-N-CA	8.63	137.19	122.26
1	A	1375	ASP	N-CA-CB	-8.29	96.01	110.44
1	A	1377	LYS	CA-C-N	8.16	134.73	122.17
1	A	1377	LYS	C-N-CA	8.16	134.73	122.17
1	A	344	GLU	CB-CA-C	-8.03	97.63	112.00
1	A	1380	ILE	CA-C-N	8.02	133.54	122.79
1	A	1380	ILE	C-N-CA	8.02	133.54	122.79
1	A	337	LYS	N-CA-CB	-8.01	95.14	111.07
1	A	1378	LYS	N-CA-C	7.97	122.80	112.12
1	A	337	LYS	N-CA-C	7.94	126.61	113.50
1	A	1375	ASP	O-C-N	-7.81	112.48	122.09
1	A	1375	ASP	CA-C-O	-7.64	110.87	119.81
1	A	1378	LYS	CA-C-N	7.55	135.55	121.97
1	A	1378	LYS	C-N-CA	7.55	135.55	121.97
1	A	344	GLU	N-CA-C	7.47	125.05	110.56
1	A	1375	ASP	CB-CA-C	7.39	122.48	110.37
1	A	342	ASN	CA-C-N	6.81	131.52	122.06
1	A	342	ASN	C-N-CA	6.81	131.52	122.06
1	A	337	LYS	O-C-N	-6.67	113.96	121.84
1	A	1382	LYS	N-CA-C	6.67	119.15	108.41
1	A	1376	ILE	N-CA-C	5.98	121.77	109.34
1	A	341	GLU	N-CA-C	5.96	122.26	114.75
1	A	1379	ILE	CA-C-N	5.92	131.51	122.69
1	A	1379	ILE	C-N-CA	5.92	131.51	122.69
1	A	356	ASN	CA-C-O	-5.91	113.12	120.57
1	A	337	LYS	CB-CA-C	5.75	122.52	110.45
1	A	1203	LYS	CA-C-N	5.75	132.04	121.70
1	A	1203	LYS	C-N-CA	5.75	132.04	121.70
1	A	1382	LYS	CB-CA-C	-5.73	101.36	110.81
1	A	1377	LYS	N-CA-C	5.50	120.14	113.38
1	A	339	GLU	CA-C-N	5.33	130.38	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	GLU	C-N-CA	5.33	130.38	122.17
1	A	357	LYS	N-CA-C	5.33	119.48	111.96
1	A	339	GLU	N-CA-C	5.30	120.02	113.50
1	A	1379	ILE	N-CA-C	5.26	120.27	109.34
1	A	357	LYS	CB-CA-C	-5.16	101.75	110.88
1	A	1381	GLU	N-CA-C	5.04	116.27	109.11
1	A	338	THR	N-CA-C	5.04	119.30	113.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ASN	Peptide
1	A	1375	ASP	Peptide
1	A	1376	ILE	Peptide
1	A	1380	ILE	Peptide
1	A	337	LYS	Peptide
1	A	338	THR	Peptide
1	A	342	ASN	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	15032	0	14596	605	0
All	All	15032	0	14596	605	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (605) 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:374:PHE:CD2	1:A:374:PHE:CG	1.79	1.70
1:A:374:PHE:CG	1:A:374:PHE:CD1	1.81	1.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:LYS:N	1:A:357:LYS:CA	1.67	1.54
1:A:357:LYS:N	1:A:374:PHE:CE2	1.94	1.36
1:A:357:LYS:N	1:A:374:PHE:CZ	1.90	1.35
1:A:374:PHE:CD1	1:A:374:PHE:CE1	2.19	1.31
1:A:374:PHE:CZ	1:A:374:PHE:CE1	2.20	1.29
1:A:374:PHE:CD2	1:A:374:PHE:CE2	2.22	1.26
1:A:374:PHE:CE2	1:A:374:PHE:CZ	2.23	1.26
1:A:357:LYS:N	1:A:374:PHE:CE1	2.03	1.25
1:A:338:THR:N	1:A:344:GLU:H	1.34	1.25
1:A:1376:ILE:H	1:A:1380:ILE:C	1.49	1.21
1:A:357:LYS:HA	1:A:374:PHE:CG	1.78	1.19
1:A:337:LYS:C	1:A:344:GLU:H	1.55	1.15
1:A:357:LYS:N	1:A:374:PHE:CD2	2.14	1.15
1:A:337:LYS:C	1:A:344:GLU:N	2.05	1.14
1:A:1376:ILE:CA	1:A:1382:LYS:H	1.63	1.12
1:A:1375:ASP:O	1:A:1379:ILE:N	1.83	1.11
1:A:1376:ILE:N	1:A:1382:LYS:H	1.47	1.11
1:A:1375:ASP:HB3	1:A:1380:ILE:N	1.65	1.11
1:A:1375:ASP:C	1:A:1382:LYS:N	2.09	1.10
1:A:338:THR:H	1:A:342:ASN:C	1.61	1.07
1:A:1375:ASP:HA	1:A:1379:ILE:H	0.95	1.06
1:A:340:TRP:N	1:A:344:GLU:HA	1.70	1.05
1:A:357:LYS:N	1:A:374:PHE:CD1	2.25	1.05
1:A:1377:LYS:N	1:A:1381:GLU:C	2.15	1.05
1:A:339:GLU:N	1:A:343:GLN:C	2.16	1.04
1:A:338:THR:N	1:A:344:GLU:N	2.03	1.03
1:A:337:LYS:H	1:A:343:GLN:N	1.57	1.03
1:A:1375:ASP:O	1:A:1382:LYS:N	1.92	1.02
1:A:1375:ASP:HB3	1:A:1380:ILE:H	0.85	1.02
1:A:1375:ASP:CB	1:A:1380:ILE:H	1.73	1.01
1:A:337:LYS:CB	1:A:342:ASN:H	1.72	1.00
1:A:1375:ASP:HA	1:A:1379:ILE:N	1.76	1.00
1:A:1375:ASP:C	1:A:1381:GLU:C	2.30	0.99
1:A:1377:LYS:N	1:A:1382:LYS:N	2.11	0.99
1:A:357:LYS:N	1:A:374:PHE:CG	2.32	0.97
1:A:337:LYS:CA	1:A:341:GLU:H	1.78	0.96
1:A:1378:LYS:H	1:A:1381:GLU:C	1.72	0.96
1:A:1378:LYS:N	1:A:1382:LYS:HA	1.79	0.95
1:A:337:LYS:HG3	1:A:342:ASN:HB3	1.48	0.95
1:A:339:GLU:H	1:A:343:GLN:C	1.72	0.95
1:A:339:GLU:C	1:A:344:GLU:HA	1.89	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1378:LYS:N	1:A:1381:GLU:O	2.00	0.95
1:A:338:THR:N	1:A:343:GLN:CA	2.30	0.94
1:A:356:ASN:C	1:A:374:PHE:CD1	2.46	0.93
1:A:357:LYS:CA	1:A:374:PHE:CD1	2.53	0.92
1:A:1376:ILE:N	1:A:1381:GLU:CA	2.33	0.92
1:A:1376:ILE:N	1:A:1381:GLU:N	2.17	0.92
1:A:339:GLU:N	1:A:344:GLU:N	2.18	0.91
1:A:1376:ILE:CA	1:A:1382:LYS:N	2.33	0.91
1:A:356:ASN:C	1:A:374:PHE:CE1	2.48	0.91
1:A:357:LYS:CA	1:A:374:PHE:CG	2.54	0.91
1:A:1376:ILE:N	1:A:1380:ILE:C	2.29	0.91
1:A:1376:ILE:N	1:A:1382:LYS:N	2.15	0.91
1:A:337:LYS:C	1:A:342:ASN:N	2.29	0.90
1:A:356:ASN:C	1:A:374:PHE:CD2	2.49	0.90
1:A:1376:ILE:H	1:A:1381:GLU:N	1.68	0.90
1:A:1377:LYS:H	1:A:1381:GLU:C	1.79	0.90
1:A:337:LYS:H	1:A:343:GLN:H	0.91	0.89
1:A:338:THR:CA	1:A:344:GLU:H	1.85	0.89
1:A:1375:ASP:CA	1:A:1379:ILE:H	1.84	0.89
1:A:338:THR:N	1:A:342:ASN:C	2.30	0.88
1:A:356:ASN:C	1:A:374:PHE:CG	2.51	0.88
1:A:338:THR:CA	1:A:344:GLU:N	2.37	0.88
1:A:356:ASN:O	1:A:374:PHE:CG	2.27	0.87
1:A:1376:ILE:C	1:A:1382:LYS:N	2.32	0.87
1:A:338:THR:H	1:A:343:GLN:N	1.71	0.87
1:A:1375:ASP:C	1:A:1382:LYS:H	1.76	0.87
1:A:337:LYS:N	1:A:343:GLN:H	1.72	0.86
1:A:340:TRP:H	1:A:343:GLN:C	1.84	0.86
1:A:357:LYS:HA	1:A:374:PHE:CD1	2.12	0.84
1:A:337:LYS:HB2	1:A:342:ASN:H	1.43	0.84
1:A:340:TRP:N	1:A:343:GLN:O	2.10	0.84
1:A:356:ASN:O	1:A:374:PHE:CD1	2.30	0.84
1:A:337:LYS:N	1:A:343:GLN:N	2.26	0.83
1:A:983:ASN:HA	1:A:991:ARG:HG2	1.61	0.83
1:A:1377:LYS:C	1:A:1382:LYS:HA	2.03	0.83
1:A:357:LYS:CA	1:A:374:PHE:CD2	2.62	0.82
1:A:356:ASN:HA	1:A:374:PHE:CZ	2.15	0.81
1:A:1143:ASN:HB3	1:A:1973:LEU:HD21	1.62	0.80
1:A:337:LYS:HA	1:A:341:GLU:H	1.46	0.80
1:A:991:ARG:HA	1:A:1106:LYS:HZ3	1.47	0.80
1:A:337:LYS:CB	1:A:341:GLU:H	1.95	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ASN:C	1:A:374:PHE:CE2	2.59	0.79
1:A:1375:ASP:C	1:A:1381:GLU:N	2.41	0.79
1:A:337:LYS:O	1:A:341:GLU:N	2.15	0.79
1:A:85:ASN:ND2	1:A:91:GLY:O	2.15	0.79
1:A:1375:ASP:C	1:A:1380:ILE:N	2.40	0.79
1:A:338:THR:N	1:A:343:GLN:C	2.41	0.79
1:A:231:ARG:HE	1:A:232:SER:H	1.27	0.79
1:A:338:THR:N	1:A:343:GLN:N	2.29	0.79
1:A:1378:LYS:N	1:A:1382:LYS:N	2.31	0.78
1:A:338:THR:C	1:A:344:GLU:N	2.41	0.78
1:A:337:LYS:C	1:A:343:GLN:C	2.51	0.78
1:A:167:ARG:HH12	1:A:211:ARG:HG3	1.50	0.75
1:A:1374:GLU:O	1:A:1378:LYS:HB3	1.85	0.75
1:A:356:ASN:C	1:A:374:PHE:CZ	2.64	0.75
1:A:256:CYS:SG	1:A:257:ARG:NH1	2.60	0.75
1:A:1968:HIS:O	1:A:1972:GLN:NE2	2.19	0.75
1:A:1138:VAL:HG11	1:A:1966:LEU:HD22	1.68	0.75
1:A:1376:ILE:N	1:A:1381:GLU:C	2.45	0.75
1:A:1206:GLU:H	1:A:1207:SER:HA	1.52	0.74
1:A:337:LYS:O	1:A:341:GLU:CA	2.36	0.73
1:A:965:GLN:HE22	1:A:967:LYS:HE3	1.53	0.73
1:A:337:LYS:O	1:A:344:GLU:HB2	1.87	0.73
1:A:1376:ILE:HA	1:A:1382:LYS:HG2	1.69	0.73
1:A:1339:LEU:HD12	1:A:1436:GLU:HA	1.70	0.73
1:A:1003:GLU:O	1:A:1117:ASN:ND2	2.20	0.73
1:A:1041:GLU:HB2	1:A:1853:ARG:HH22	1.53	0.73
1:A:337:LYS:CA	1:A:342:ASN:H	2.00	0.73
1:A:337:LYS:O	1:A:341:GLU:C	2.32	0.73
1:A:337:LYS:HB2	1:A:342:ASN:N	2.04	0.73
1:A:629:LYS:HB2	1:A:727:ALA:HB1	1.69	0.73
1:A:1378:LYS:N	1:A:1381:GLU:C	2.43	0.73
1:A:337:LYS:CA	1:A:343:GLN:C	2.62	0.72
1:A:1375:ASP:CA	1:A:1381:GLU:N	2.51	0.72
1:A:340:TRP:N	1:A:344:GLU:N	2.38	0.72
1:A:527:CYS:SG	1:A:528:GLN:N	2.63	0.72
1:A:357:LYS:CA	1:A:374:PHE:CE1	2.72	0.72
1:A:951:SER:O	1:A:953:LEU:N	2.22	0.71
1:A:1219:CYS:HB3	1:A:1422:LYS:HE2	1.71	0.71
1:A:1375:ASP:H	1:A:1381:GLU:H	1.36	0.71
1:A:338:THR:H	1:A:343:GLN:CA	2.00	0.71
1:A:302:ARG:HH22	1:A:319:CYS:HB3	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:GLN:OE1	1:A:991:ARG:NE	2.22	0.71
1:A:1371:LYS:O	1:A:1375:ASP:HB2	1.90	0.71
1:A:206:LYS:HD2	1:A:209:LYS:HD3	1.73	0.71
1:A:357:LYS:C	1:A:374:PHE:CE1	2.69	0.71
1:A:1375:ASP:O	1:A:1379:ILE:CA	2.39	0.71
1:A:1323:SER:O	1:A:1330:GLN:NE2	2.24	0.70
1:A:340:TRP:N	1:A:344:GLU:CA	2.53	0.70
1:A:1378:LYS:N	1:A:1382:LYS:CA	2.55	0.70
1:A:587:LEU:HD13	1:A:655:TYR:HE1	1.56	0.70
1:A:1880:TYR:HB3	1:A:1883:ILE:HD12	1.74	0.69
1:A:338:THR:N	1:A:343:GLN:HA	2.08	0.69
1:A:519:CYS:SG	1:A:520:ASP:N	2.65	0.69
1:A:1970:GLU:O	1:A:1974:ASN:ND2	2.26	0.69
1:A:990:ALA:O	1:A:1106:LYS:NZ	2.23	0.68
1:A:583:ARG:NH1	1:A:654:ASP:OD2	2.25	0.68
1:A:139:ILE:HD11	1:A:154:ALA:HB1	1.75	0.68
1:A:986:SER:OG	1:A:1008:ASN:OD1	2.09	0.68
1:A:1377:LYS:HB3	1:A:1381:GLU:CD	2.19	0.68
1:A:339:GLU:C	1:A:344:GLU:CA	2.67	0.67
1:A:357:LYS:CA	1:A:357:LYS:H	2.00	0.67
1:A:1375:ASP:C	1:A:1379:ILE:C	2.62	0.67
1:A:63:LYS:HA	1:A:110:LEU:HD13	1.77	0.66
1:A:337:LYS:HB2	1:A:341:GLU:CA	2.25	0.66
1:A:1375:ASP:N	1:A:1381:GLU:H	1.93	0.66
1:A:1312:TYR:OH	1:A:1427:ASN:ND2	2.28	0.66
1:A:957:PRO:HG2	1:A:960:TYR:HB2	1.76	0.66
1:A:1699:GLU:OE1	1:A:1757:ARG:NH1	2.29	0.66
1:A:1603:MET:HE1	1:A:1630:GLN:HB3	1.77	0.66
1:A:1377:LYS:C	1:A:1382:LYS:CA	2.69	0.66
1:A:1488:ASN:O	1:A:1498:GLN:NE2	2.27	0.66
1:A:337:LYS:HA	1:A:341:GLU:N	2.11	0.66
1:A:258:LYS:HD3	1:A:259:CYS:H	1.62	0.65
1:A:337:LYS:CA	1:A:343:GLN:N	2.59	0.65
1:A:1378:LYS:CA	1:A:1382:LYS:HA	2.26	0.65
1:A:1142:SER:OG	1:A:1187:GLY:N	2.29	0.65
1:A:1376:ILE:HA	1:A:1382:LYS:H	1.60	0.65
1:A:336:TRP:O	1:A:340:TRP:HB3	1.97	0.65
1:A:50:ASN:O	1:A:50:ASN:ND2	2.28	0.65
1:A:187:PHE:HA	1:A:190:ILE:HG22	1.79	0.65
1:A:356:ASN:CA	1:A:374:PHE:CZ	2.79	0.65
1:A:357:LYS:HA	1:A:374:PHE:CD2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LYS:C	1:A:343:GLN:N	2.56	0.64
1:A:337:LYS:CA	1:A:341:GLU:N	2.56	0.64
1:A:357:LYS:N	1:A:357:LYS:HA	1.99	0.64
1:A:1279:ASP:HB2	1:A:1287:ASN:HD21	1.63	0.64
1:A:340:TRP:N	1:A:343:GLN:C	2.53	0.64
1:A:1375:ASP:CG	1:A:1379:ILE:HB	2.23	0.64
1:A:1378:LYS:C	1:A:1382:LYS:HB3	2.23	0.64
1:A:676:ASN:O	1:A:680:ASN:ND2	2.30	0.64
1:A:1375:ASP:CB	1:A:1380:ILE:N	2.45	0.63
1:A:357:LYS:CA	1:A:374:PHE:CE2	2.81	0.63
1:A:1375:ASP:CA	1:A:1381:GLU:H	2.11	0.63
1:A:1674:ASN:ND2	1:A:1684:ASN:OD1	2.31	0.63
1:A:338:THR:HG22	1:A:343:GLN:HA	1.80	0.63
1:A:340:TRP:CA	1:A:344:GLU:HA	2.28	0.63
1:A:794:LYS:NZ	1:A:797:THR:OG1	2.31	0.63
1:A:1096:LYS:HA	1:A:1100:TYR:HB3	1.81	0.63
1:A:1206:GLU:N	1:A:1207:SER:HA	2.13	0.63
1:A:1933:CYS:HB2	1:A:1935:GLU:HA	1.80	0.62
1:A:337:LYS:HB2	1:A:341:GLU:C	2.24	0.62
1:A:1310:LEU:O	1:A:1314:TYR:N	2.29	0.62
1:A:357:LYS:CB	1:A:374:PHE:CE2	2.82	0.62
1:A:337:LYS:N	1:A:343:GLN:CA	2.63	0.62
1:A:1377:LYS:HA	1:A:1383:GLY:N	2.15	0.62
1:A:336:TRP:HA	1:A:343:GLN:HB3	1.81	0.61
1:A:1375:ASP:C	1:A:1381:GLU:CA	2.72	0.61
1:A:81:LYS:HB3	1:A:92:LYS:H	1.64	0.61
1:A:587:LEU:HD12	1:A:590:GLY:H	1.64	0.61
1:A:894:LEU:HD11	1:A:903:ASN:HD22	1.64	0.61
1:A:1863:TYR:HA	1:A:1866:ILE:HG22	1.82	0.61
1:A:753:ILE:HA	1:A:756:ILE:HD12	1.82	0.61
1:A:30:ALA:HB3	1:A:125:LEU:HD22	1.81	0.61
1:A:1892:LEU:HB3	1:A:1940:LEU:HD21	1.83	0.61
1:A:249:ARG:NH2	1:A:256:CYS:SG	2.68	0.60
1:A:712:TRP:O	1:A:716:LYS:HB3	2.01	0.60
1:A:799:CYS:SG	1:A:804:LYS:NZ	2.74	0.60
1:A:648:LEU:HD12	1:A:723:MET:HG2	1.84	0.60
1:A:992:THR:H	1:A:1106:LYS:HD3	1.66	0.60
1:A:1839:LYS:HA	1:A:1964:VAL:HG11	1.83	0.60
1:A:1375:ASP:O	1:A:1382:LYS:CB	2.50	0.60
1:A:1376:ILE:HA	1:A:1382:LYS:CG	2.32	0.60
1:A:1540:LYS:HA	1:A:1546:CYS:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ASP:O	1:A:173:LYS:NZ	2.32	0.59
1:A:573:GLU:O	1:A:841:ARG:NH1	2.35	0.59
1:A:637:ASN:ND2	1:A:640:ASN:O	2.34	0.59
1:A:1013:LYS:H	1:A:1950:MET:HE1	1.66	0.59
1:A:1792:LYS:O	1:A:1797:ARG:NH1	2.35	0.59
1:A:337:LYS:HG3	1:A:342:ASN:CB	2.28	0.59
1:A:1375:ASP:C	1:A:1379:ILE:N	2.57	0.59
1:A:1375:ASP:O	1:A:1382:LYS:CA	2.51	0.59
1:A:175:THR:O	1:A:178:ASN:ND2	2.34	0.59
1:A:1013:LYS:HE3	1:A:1018:ARG:HH21	1.67	0.59
1:A:1375:ASP:O	1:A:1382:LYS:HB3	2.02	0.59
1:A:1758:GLN:NE2	1:A:1786:GLU:O	2.32	0.59
1:A:337:LYS:O	1:A:344:GLU:CB	2.50	0.59
1:A:102:ARG:NH2	1:A:282:GLU:OE2	2.36	0.58
1:A:1371:LYS:HG2	1:A:1375:ASP:OD2	2.04	0.58
1:A:587:LEU:HD13	1:A:655:TYR:CE1	2.37	0.58
1:A:1164:LYS:HD3	1:A:1972:GLN:HG2	1.86	0.58
1:A:1370:GLY:O	1:A:1373:GLN:N	2.36	0.58
1:A:33:SER:HB3	1:A:48:LYS:HD2	1.84	0.58
1:A:1376:ILE:N	1:A:1380:ILE:CA	2.66	0.58
1:A:357:LYS:CA	1:A:374:PHE:CZ	2.86	0.57
1:A:1744:ASN:OD1	1:A:1746:THR:OG1	2.22	0.57
1:A:192:GLU:HA	1:A:198:GLN:HE22	1.69	0.57
1:A:1107:ILE:HD12	1:A:1110:GLN:HB3	1.87	0.57
1:A:1256:ILE:HG13	1:A:1257:HIS:CD2	2.39	0.57
1:A:1984:LYS:O	1:A:1986:TYR:N	2.35	0.57
1:A:1423:ILE:HA	1:A:1426:LYS:HZ1	1.69	0.57
1:A:1368:HIS:O	1:A:1368:HIS:ND1	2.38	0.57
1:A:37:TYR:HB2	1:A:42:GLY:HA3	1.85	0.57
1:A:525:ASP:O	1:A:610:LYS:NZ	2.38	0.57
1:A:1375:ASP:H	1:A:1381:GLU:N	2.01	0.57
1:A:1635:GLU:OE2	1:A:1664:ARG:NH1	2.37	0.57
1:A:1138:VAL:HG21	1:A:1966:LEU:HD13	1.87	0.57
1:A:337:LYS:O	1:A:342:ASN:N	2.38	0.56
1:A:1204:GLU:N	1:A:1205:ASN:HA	2.19	0.56
1:A:853:ARG:HH22	1:A:866:THR:HG23	1.69	0.56
1:A:8:ALA:HA	1:A:12:GLU:HB2	1.87	0.56
1:A:800:LYS:HG3	1:A:801:THR:H	1.69	0.56
1:A:1315:HIS:HD2	1:A:1343:PHE:HB3	1.70	0.56
1:A:1375:ASP:O	1:A:1379:ILE:C	2.48	0.56
1:A:1199:GLU:HG3	1:A:1200:LYS:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LYS:C	1:A:342:ASN:C	2.73	0.56
1:A:1375:ASP:O	1:A:1378:LYS:C	2.46	0.56
1:A:239:ARG:O	1:A:257:ARG:NE	2.37	0.56
1:A:1250:ILE:HB	1:A:1265:ILE:HB	1.86	0.56
1:A:356:ASN:CA	1:A:374:PHE:CE2	2.88	0.56
1:A:560:TRP:HH2	1:A:838:ILE:HD11	1.71	0.56
1:A:1757:ARG:HH21	1:A:1788:ILE:HG23	1.72	0.55
1:A:1794:GLN:H	1:A:1878:LYS:NZ	2.04	0.55
1:A:340:TRP:C	1:A:344:GLU:HB2	2.31	0.55
1:A:1628:ARG:HH22	1:A:1713:THR:HG21	1.71	0.55
1:A:1954:TYR:HH	1:A:1961:CYS:HG	1.52	0.55
1:A:328:LYS:HB2	1:A:332:CYS:HB2	1.87	0.55
1:A:1202:CYS:N	1:A:1203:LYS:HB2	2.22	0.55
1:A:1375:ASP:CA	1:A:1381:GLU:C	2.80	0.55
1:A:1488:ASN:OD1	1:A:1490:LYS:NZ	2.40	0.55
1:A:337:LYS:N	1:A:343:GLN:C	2.65	0.55
1:A:984:GLN:HB3	1:A:1007:TYR:CE1	2.42	0.55
1:A:856:GLY:N	1:A:858:LYS:HZ3	2.05	0.55
1:A:1376:ILE:H	1:A:1380:ILE:CA	2.18	0.55
1:A:1755:THR:HG23	1:A:1758:GLN:H	1.72	0.55
1:A:1911:ASN:HB3	1:A:1916:ASN:HA	1.88	0.54
1:A:1120:LYS:O	1:A:1124:LYS:NZ	2.41	0.54
1:A:337:LYS:H	1:A:343:GLN:CA	2.21	0.54
1:A:1377:LYS:H	1:A:1381:GLU:CA	2.20	0.54
1:A:583:ARG:NH2	1:A:650:TYR:HB3	2.22	0.54
1:A:127:ASP:OD1	1:A:128:VAL:N	2.41	0.54
1:A:1700:ASP:OD2	1:A:1797:ARG:NH2	2.37	0.54
1:A:125:LEU:HG	1:A:129:LEU:HD13	1.90	0.54
1:A:1239:ILE:HA	1:A:1319:THR:HG21	1.90	0.54
1:A:1423:ILE:HA	1:A:1426:LYS:NZ	2.22	0.54
1:A:279:TRP:NE1	1:A:282:GLU:OE1	2.40	0.53
1:A:1380:ILE:HG12	1:A:1380:ILE:O	2.08	0.53
1:A:1468:TYR:O	1:A:1472:ILE:HG12	2.08	0.53
1:A:511:ARG:NH1	1:A:514:SER:H	2.07	0.53
1:A:1103:TRP:HA	1:A:1106:LYS:HE3	1.91	0.53
1:A:1233:LYS:H	1:A:1310:LEU:HD22	1.74	0.53
1:A:1375:ASP:N	1:A:1381:GLU:N	2.56	0.53
1:A:1414:ASP:OD1	1:A:1415:ALA:N	2.41	0.53
1:A:1497:ILE:HG13	1:A:1502:LYS:HB2	1.90	0.53
1:A:54:ILE:HD13	1:A:129:LEU:HB3	1.90	0.53
1:A:804:LYS:HG3	1:A:965:GLN:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1633:LEU:HD11	1:A:1712:TYR:HB3	1.91	0.53
1:A:338:THR:C	1:A:345:ASN:N	2.66	0.53
1:A:338:THR:CG2	1:A:343:GLN:HA	2.38	0.53
1:A:1419:ALA:O	1:A:1423:ILE:HG12	2.09	0.53
1:A:304:GLU:HB3	1:A:314:GLU:HB3	1.90	0.52
1:A:786:LYS:HD2	1:A:790:GLU:HA	1.90	0.52
1:A:985:TRP:HB2	1:A:989:SER:HB3	1.91	0.52
1:A:850:LYS:HD2	1:A:864:SER:O	2.09	0.52
1:A:1682:ASP:OD1	1:A:1682:ASP:N	2.42	0.52
1:A:256:CYS:HA	1:A:257:ARG:HD2	1.92	0.52
1:A:1374:GLU:HA	1:A:1381:GLU:OE1	2.10	0.52
1:A:1125:GLN:HB2	1:A:1129:ALA:HB2	1.92	0.52
1:A:841:ARG:HE	1:A:845:HIS:CD2	2.28	0.52
1:A:1227:ILE:HD11	1:A:1302:ASN:HD21	1.75	0.52
1:A:145:ASP:OD1	1:A:146:THR:N	2.41	0.52
1:A:337:LYS:CB	1:A:342:ASN:N	2.54	0.52
1:A:1306:LYS:O	1:A:1309:GLU:HG3	2.10	0.52
1:A:338:THR:CA	1:A:343:GLN:HA	2.40	0.52
1:A:1800:GLU:OE2	1:A:1895:ARG:NE	2.43	0.52
1:A:1325:ASN:OD1	1:A:1330:GLN:NE2	2.43	0.51
1:A:1252:LYS:HB2	1:A:1260:THR:O	2.10	0.51
1:A:526:GLU:HA	1:A:610:LYS:HD2	1.92	0.51
1:A:337:LYS:HA	1:A:343:GLN:C	2.35	0.51
1:A:357:LYS:HB2	1:A:374:PHE:CE2	2.46	0.51
1:A:1377:LYS:CA	1:A:1381:GLU:C	2.83	0.51
1:A:45:ASP:OD1	1:A:46:TYR:N	2.43	0.51
1:A:1143:ASN:HB3	1:A:1973:LEU:CD2	2.38	0.51
1:A:1375:ASP:CA	1:A:1380:ILE:N	2.73	0.51
1:A:1853:ARG:HA	1:A:1947:LEU:HD13	1.93	0.51
1:A:775:GLN:HA	1:A:778:VAL:HG12	1.92	0.51
1:A:1202:CYS:HA	1:A:1203:LYS:C	2.35	0.51
1:A:1377:LYS:HA	1:A:1382:LYS:C	2.35	0.51
1:A:511:ARG:HD2	1:A:513:SER:H	1.76	0.51
1:A:856:GLY:H	1:A:858:LYS:HZ3	1.59	0.51
1:A:1203:LYS:HB3	1:A:1204:GLU:C	2.36	0.51
1:A:1569:ASP:N	1:A:1569:ASP:OD1	2.43	0.51
1:A:374:PHE:CD1	1:A:374:PHE:CB	2.82	0.51
1:A:990:ALA:HB2	1:A:1107:ILE:HD13	1.93	0.51
1:A:1720:LEU:HD22	1:A:1724:PHE:HE2	1.76	0.51
1:A:615:ALA:O	1:A:619:ILE:HG12	2.11	0.50
1:A:799:CYS:HB2	1:A:803:CYS:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:940:SER:HB2	1:A:943:THR:HG23	1.92	0.50
1:A:1376:ILE:HG12	1:A:1376:ILE:O	2.12	0.50
1:A:1666:ALA:HB2	1:A:1764:MET:HG2	1.91	0.50
1:A:68:GLU:HG3	1:A:110:LEU:HA	1.93	0.50
1:A:1933:CYS:HB2	1:A:1934:GLU:HA	1.93	0.50
1:A:1138:VAL:HG12	1:A:1139:VAL:H	1.76	0.50
1:A:1376:ILE:N	1:A:1381:GLU:HA	2.24	0.50
1:A:1945:GLU:HG3	1:A:1950:MET:HB2	1.93	0.50
1:A:1502:LYS:HA	1:A:1505:CYS:SG	2.52	0.50
1:A:337:LYS:HB3	1:A:340:TRP:HE3	1.76	0.50
1:A:1519:TRP:CZ2	1:A:1523:LYS:HD3	2.47	0.50
1:A:1272:LEU:HD21	1:A:1354:TYR:HE1	1.77	0.49
1:A:1874:SER:OG	1:A:1876:ASP:O	2.22	0.49
1:A:1377:LYS:CA	1:A:1382:LYS:N	2.75	0.49
1:A:221:LYS:O	1:A:225:VAL:HG23	2.13	0.49
1:A:1335:ASP:OD2	1:A:1341:LYS:N	2.44	0.49
1:A:522:LYS:NZ	1:A:713:ASN:O	2.33	0.49
1:A:337:LYS:C	1:A:342:ASN:CA	2.85	0.49
1:A:337:LYS:CG	1:A:342:ASN:H	2.24	0.49
1:A:1564:TYR:CD2	1:A:1594:SER:HA	2.48	0.49
1:A:511:ARG:HD2	1:A:512:GLY:N	2.28	0.49
1:A:939:GLN:HG2	1:A:940:SER:N	2.28	0.49
1:A:1422:LYS:HD2	1:A:1426:LYS:NZ	2.28	0.49
1:A:653:ALA:HB2	1:A:753:ILE:HG23	1.94	0.49
1:A:1719:LYS:O	1:A:1723:ILE:HG12	2.12	0.49
1:A:1636:LEU:HD12	1:A:1661:VAL:HG21	1.94	0.49
1:A:337:LYS:C	1:A:341:GLU:N	2.70	0.48
1:A:582:PRO:HA	1:A:585:GLN:HE21	1.77	0.48
1:A:1747:ILE:HG21	1:A:1759:LEU:HD11	1.95	0.48
1:A:1349:ARG:NH2	1:A:1543:TYR:OH	2.46	0.48
1:A:1611:LYS:HD2	1:A:1707:LEU:HA	1.95	0.48
1:A:1375:ASP:C	1:A:1380:ILE:CA	2.87	0.48
1:A:339:GLU:CA	1:A:343:GLN:C	2.87	0.48
1:A:1357:MET:HG2	1:A:1369:ILE:HD12	1.95	0.48
1:A:1794:GLN:H	1:A:1878:LYS:HZ1	1.61	0.48
1:A:532:GLU:HG3	1:A:533:LYS:HG3	1.96	0.48
1:A:72:PRO:HB2	1:A:75:ASP:OD2	2.14	0.48
1:A:1136:LYS:HD2	1:A:1139:VAL:HA	1.95	0.48
1:A:1571:SER:O	1:A:1575:SER:OG	2.29	0.48
1:A:1662:ALA:HB1	1:A:1764:MET:HG3	1.96	0.48
1:A:1768:VAL:HG21	1:A:1783:MET:HE3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1209:ASP:HA	1:A:1210:THR:HA	1.61	0.47
1:A:991:ARG:HA	1:A:1106:LYS:NZ	2.24	0.47
1:A:1122:ARG:HD3	1:A:1140:SER:HA	1.96	0.47
1:A:1134:GLN:NE2	1:A:1136:LYS:HB2	2.29	0.47
1:A:1138:VAL:HG12	1:A:1139:VAL:N	2.28	0.47
1:A:1581:TYR:N	1:A:1656:GLU:OE1	2.38	0.47
1:A:358:THR:N	1:A:374:PHE:CE1	2.83	0.47
1:A:700:SER:OG	1:A:701:TYR:N	2.47	0.47
1:A:659:ILE:HD11	1:A:712:TRP:CE3	2.49	0.47
1:A:1516:LYS:NZ	1:A:1555:PHE:O	2.46	0.47
1:A:1475:ALA:HA	1:A:1478:ILE:HG22	1.96	0.47
1:A:338:THR:HA	1:A:345:ASN:H	1.79	0.47
1:A:1029:VAL:HG21	1:A:1959:MET:SD	2.54	0.47
1:A:1161:ASP:HB3	1:A:1847:ASN:ND2	2.29	0.47
1:A:1233:LYS:H	1:A:1310:LEU:CD2	2.28	0.47
1:A:1252:LYS:HE3	1:A:1521:LYS:HB3	1.96	0.47
1:A:1375:ASP:N	1:A:1381:GLU:CA	2.78	0.47
1:A:1933:CYS:H	1:A:1934:GLU:HB2	1.80	0.47
1:A:287:PHE:HA	1:A:290:GLU:HG2	1.97	0.47
1:A:1667:TYR:OH	1:A:1671:LYS:NZ	2.46	0.47
1:A:208:THR:HA	1:A:211:ARG:HG2	1.97	0.47
1:A:522:LYS:HG3	1:A:524:GLN:OE1	2.15	0.47
1:A:1375:ASP:HB3	1:A:1380:ILE:CA	2.42	0.47
1:A:1377:LYS:C	1:A:1381:GLU:O	2.58	0.47
1:A:258:LYS:HD3	1:A:259:CYS:N	2.27	0.46
1:A:580:LEU:HD12	1:A:581:PRO:HD2	1.97	0.46
1:A:794:LYS:HD2	1:A:796:LYS:HE3	1.95	0.46
1:A:339:GLU:C	1:A:343:GLN:O	2.58	0.46
1:A:523:ASN:HB2	1:A:710:SER:OG	2.15	0.46
1:A:832:SER:OG	1:A:948:ASN:ND2	2.42	0.46
1:A:1457:TRP:CH2	1:A:1519:TRP:HB2	2.51	0.46
1:A:179:LEU:HA	1:A:182:ASN:HB3	1.98	0.46
1:A:338:THR:C	1:A:345:ASN:H	2.24	0.46
1:A:624:GLU:OE1	1:A:655:TYR:OH	2.21	0.46
1:A:1106:LYS:HE3	1:A:1106:LYS:HB3	1.68	0.46
1:A:1349:ARG:HE	1:A:1456:GLU:HB2	1.81	0.46
1:A:1376:ILE:HG22	1:A:1381:GLU:HA	1.97	0.46
1:A:1628:ARG:NH2	1:A:1706:ASP:OD2	2.38	0.46
1:A:31:ASP:O	1:A:33:SER:N	2.49	0.46
1:A:161:ASP:O	1:A:165:ILE:HG12	2.15	0.46
1:A:337:LYS:CB	1:A:341:GLU:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1155:GLN:OE1	1:A:1161:ASP:N	2.49	0.46
1:A:1687:ALA:O	1:A:1691:ILE:HG13	2.16	0.46
1:A:25:ASP:HA	1:A:28:LEU:HB2	1.98	0.46
1:A:121:ASN:CG	1:A:214:TRP:HE1	2.24	0.46
1:A:561:LYS:HG2	1:A:562:LYS:H	1.80	0.46
1:A:582:PRO:HA	1:A:585:GLN:HG2	1.98	0.46
1:A:724:LYS:HG3	1:A:729:MET:HG2	1.98	0.46
1:A:858:LYS:HD2	1:A:878:VAL:HG12	1.98	0.46
1:A:1307:GLU:O	1:A:1311:LEU:HG	2.15	0.46
1:A:1377:LYS:C	1:A:1382:LYS:N	2.73	0.46
1:A:177:SER:O	1:A:181:LYS:HG2	2.16	0.46
1:A:203:LYS:O	1:A:206:LYS:NZ	2.48	0.46
1:A:1147:PHE:CE2	1:A:1969:VAL:HG22	2.51	0.46
1:A:1632:CYS:SG	1:A:1664:ARG:NH2	2.89	0.46
1:A:1761:TRP:NE1	1:A:1785:VAL:O	2.39	0.46
1:A:337:LYS:O	1:A:344:GLU:N	2.44	0.46
1:A:338:THR:H	1:A:343:GLN:HA	1.74	0.46
1:A:1058:ILE:HB	1:A:1059:ASP:HB3	1.98	0.46
1:A:901:LEU:HA	1:A:904:VAL:HG22	1.96	0.46
1:A:1038:TRP:O	1:A:1042:ILE:HG12	2.16	0.46
1:A:1376:ILE:CA	1:A:1381:GLU:HA	2.46	0.46
1:A:1058:ILE:HA	1:A:1059:ASP:HA	1.76	0.45
1:A:1200:LYS:C	1:A:1203:LYS:HE2	2.41	0.45
1:A:1326:ASP:OD1	1:A:1327:LYS:N	2.49	0.45
1:A:385:GLU:HB3	1:A:387:TYR:HD1	1.81	0.45
1:A:788:CYS:HB2	1:A:794:LYS:HE3	1.97	0.45
1:A:1304:ILE:HG22	1:A:1354:TYR:HE2	1.81	0.45
1:A:1508:TYR:O	1:A:1512:ILE:HG12	2.17	0.45
1:A:1903:ASN:O	1:A:1905:ILE:N	2.47	0.45
1:A:633:PRO:HA	1:A:634:GLN:HA	1.54	0.45
1:A:805:ASP:OD1	1:A:806:GLU:N	2.50	0.45
1:A:1035:PHE:CZ	1:A:1141:LEU:HD11	2.52	0.45
1:A:1375:ASP:H	1:A:1381:GLU:CA	2.29	0.45
1:A:1828:ASP:OD1	1:A:1833:ASN:ND2	2.38	0.45
1:A:338:THR:C	1:A:344:GLU:C	2.85	0.45
1:A:932:GLU:OE2	1:A:939:GLN:NE2	2.41	0.45
1:A:1133:SER:HA	1:A:1134:GLN:HA	1.46	0.45
1:A:1965:TYR:O	1:A:1969:VAL:HG23	2.16	0.45
1:A:106:CYS:SG	1:A:134:ASN:HB3	2.57	0.45
1:A:1203:LYS:HB3	1:A:1204:GLU:CA	2.47	0.45
1:A:1636:LEU:O	1:A:1640:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1655:LEU:HD13	1:A:1756:ILE:HG23	1.98	0.45
1:A:143:HIS:O	1:A:692:ASN:ND2	2.50	0.45
1:A:786:LYS:NZ	1:A:960:TYR:OH	2.36	0.45
1:A:1203:LYS:CB	1:A:1204:GLU:HA	2.46	0.45
1:A:1314:TYR:CD2	1:A:1320:ALA:HB2	2.52	0.45
1:A:188:ALA:O	1:A:192:GLU:HG2	2.17	0.45
1:A:256:CYS:HA	1:A:257:ARG:HA	1.63	0.45
1:A:356:ASN:OD1	1:A:374:PHE:CE1	2.70	0.45
1:A:1372:LEU:O	1:A:1381:GLU:HB2	2.17	0.45
1:A:1929:LYS:HA	1:A:1930:GLU:HA	1.55	0.45
1:A:1950:MET:HE3	1:A:1950:MET:HB3	1.77	0.45
1:A:1635:GLU:O	1:A:1638:PRO:HD2	2.16	0.44
1:A:113:LEU:O	1:A:179:LEU:HD21	2.18	0.44
1:A:600:GLU:O	1:A:603:LYS:NZ	2.42	0.44
1:A:1375:ASP:N	1:A:1381:GLU:C	2.75	0.44
1:A:184:LYS:NZ	1:A:211:ARG:HH22	2.14	0.44
1:A:337:LYS:HB3	1:A:340:TRP:CE3	2.52	0.44
1:A:725:HIS:O	1:A:730:ASN:ND2	2.51	0.44
1:A:570:LEU:HA	1:A:665:TRP:HA	2.00	0.44
1:A:990:ALA:C	1:A:991:ARG:HD2	2.43	0.44
1:A:1376:ILE:C	1:A:1382:LYS:C	2.85	0.44
1:A:1695:PHE:HB2	1:A:1764:MET:SD	2.56	0.44
1:A:1889:ILE:O	1:A:1893:ASN:ND2	2.49	0.44
1:A:1386:GLN:HE22	1:A:1404:TRP:HB3	1.82	0.44
1:A:1657:THR:HA	1:A:1660:ILE:HG22	1.99	0.44
1:A:337:LYS:CA	1:A:342:ASN:N	2.69	0.44
1:A:339:GLU:H	1:A:343:GLN:CA	2.30	0.44
1:A:391:ASP:HB3	1:A:392:PRO:HD3	1.99	0.44
1:A:782:ILE:HG13	1:A:912:ALA:HB3	1.98	0.44
1:A:915:ALA:HB1	1:A:952:PRO:HB3	2.00	0.44
1:A:1457:TRP:CZ2	1:A:1515:LYS:HD2	2.53	0.44
1:A:1469:GLU:O	1:A:1473:ARG:HG2	2.18	0.43
1:A:1473:ARG:HH22	1:A:1645:GLU:H	1.64	0.43
1:A:200:LYS:HD2	1:A:205:GLN:HG2	2.00	0.43
1:A:201:TYR:N	1:A:202:PRO:HD2	2.33	0.43
1:A:385:GLU:HG2	1:A:386:ASN:H	1.84	0.43
1:A:1375:ASP:HB3	1:A:1380:ILE:HG22	1.98	0.43
1:A:1526:TYR:CZ	1:A:1538:LEU:HD22	2.53	0.43
1:A:1515:LYS:HD3	1:A:1515:LYS:HA	1.80	0.43
1:A:499:LEU:HD23	1:A:499:LEU:HA	1.84	0.43
1:A:523:ASN:O	1:A:524:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1708:VAL:HG23	1:A:1798:TRP:HH2	1.84	0.43
1:A:1933:CYS:N	1:A:1934:GLU:HB2	2.34	0.43
1:A:521:ASN:OD1	1:A:522:LYS:N	2.51	0.43
1:A:644:LEU:O	1:A:648:LEU:HD23	2.19	0.43
1:A:1026:GLY:O	1:A:1030:THR:HG23	2.19	0.43
1:A:357:LYS:C	1:A:374:PHE:CD1	2.96	0.43
1:A:846:ILE:HG23	1:A:890:ILE:HD11	2.00	0.43
1:A:923:TYR:OH	1:A:948:ASN:ND2	2.52	0.43
1:A:1836:ILE:HD12	1:A:1839:LYS:HD2	2.01	0.43
1:A:335:LYS:C	1:A:337:LYS:HG2	2.44	0.43
1:A:723:MET:HE3	1:A:723:MET:HB2	1.94	0.43
1:A:724:LYS:O	1:A:729:MET:HB3	2.17	0.43
1:A:1056:SER:OG	1:A:1201:LYS:NZ	2.31	0.43
1:A:1352:ILE:HG12	1:A:1446:ASP:HB2	2.01	0.43
1:A:1497:ILE:HD12	1:A:1498:GLN:H	1.83	0.43
1:A:54:ILE:HG13	1:A:58:HIS:NE2	2.33	0.43
1:A:285:GLU:N	1:A:285:GLU:OE1	2.52	0.43
1:A:935:LYS:HG2	1:A:936:SER:H	1.83	0.43
1:A:1118:TYR:CG	1:A:1141:LEU:HD13	2.53	0.43
1:A:1003:GLU:HB3	1:A:1113:LYS:HE2	2.00	0.42
1:A:66:PRO:HA	1:A:111:GLU:HB2	2.02	0.42
1:A:1934:GLU:HA	1:A:1935:GLU:HA	1.69	0.42
1:A:150:ASN:HB3	1:A:289:ARG:NH1	2.34	0.42
1:A:660:LYS:HD3	1:A:712:TRP:CD1	2.54	0.42
1:A:203:LYS:HA	1:A:204:ASP:HA	1.74	0.42
1:A:846:ILE:O	1:A:850:LYS:HG3	2.20	0.42
1:A:1519:TRP:CH2	1:A:1523:LYS:HD3	2.54	0.42
1:A:719:ILE:HD12	1:A:719:ILE:H	1.84	0.42
1:A:1741:TRP:CD1	1:A:1746:THR:HG21	2.55	0.42
1:A:652:PHE:CZ	1:A:720:TRP:HB2	2.54	0.42
1:A:683:LYS:HE3	1:A:683:LYS:HB2	1.85	0.42
1:A:691:LYS:HB3	1:A:702:SER:HA	2.02	0.42
1:A:1304:ILE:HA	1:A:1307:GLU:HG3	2.01	0.42
1:A:220:GLN:O	1:A:223:TRP:N	2.52	0.42
1:A:228:CYS:SG	1:A:229:GLY:N	2.93	0.42
1:A:1465:ARG:HH11	1:A:1554:ILE:HD11	1.85	0.42
1:A:256:CYS:CA	1:A:257:ARG:HD2	2.49	0.42
1:A:701:TYR:HD2	1:A:707:LEU:HD12	1.84	0.42
1:A:1377:LYS:CA	1:A:1382:LYS:C	2.93	0.42
1:A:1487:ILE:O	1:A:1487:ILE:HG22	2.20	0.42
1:A:1626:PRO:HA	1:A:1629:GLN:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:CYS:HB2	1:A:329:TYR:CD1	2.55	0.41
1:A:528:GLN:O	1:A:529:LYS:HB2	2.20	0.41
1:A:1278:TRP:HZ3	1:A:1284:GLY:HA2	1.85	0.41
1:A:9:ASN:ND2	1:A:385:GLU:OE1	2.52	0.41
1:A:339:GLU:HB2	1:A:343:GLN:HG2	2.02	0.41
1:A:1174:GLU:OE2	1:A:1983:TYR:OH	2.34	0.41
1:A:1804:ASN:O	1:A:1808:GLU:HG3	2.20	0.41
1:A:995:ARG:NH2	1:A:1004:LEU:HB2	2.35	0.41
1:A:1688:CYS:SG	1:A:1783:MET:HE2	2.60	0.41
1:A:235:LEU:HD13	1:A:258:LYS:HB2	2.02	0.41
1:A:842:TYR:O	1:A:846:ILE:HG12	2.20	0.41
1:A:1334:ASN:OD1	1:A:1335:ASP:N	2.54	0.41
1:A:1377:LYS:H	1:A:1381:GLU:HA	1.86	0.41
1:A:1450:SER:HB3	1:A:1525:LYS:NZ	2.36	0.41
1:A:1647:MET:C	1:A:1649:LYS:H	2.29	0.41
1:A:1745:GLU:HG3	1:A:1753:ARG:HB3	2.02	0.41
1:A:67:CYS:HB3	1:A:107:THR:C	2.46	0.41
1:A:1056:SER:HB3	1:A:1094:LYS:HD3	2.03	0.41
1:A:1599:LYS:NZ	1:A:1665:GLU:OE2	2.47	0.41
1:A:1632:CYS:HB3	1:A:1665:GLU:OE1	2.21	0.41
1:A:1697:ASP:O	1:A:1701:ILE:HG13	2.21	0.41
1:A:1862:TYR:O	1:A:1865:LYS:HG2	2.19	0.41
1:A:951:SER:O	1:A:952:PRO:C	2.63	0.41
1:A:1029:VAL:HG13	1:A:1962:THR:HG21	2.01	0.41
1:A:1056:SER:HB2	1:A:1057:CYS:HB3	2.02	0.41
1:A:1293:LYS:O	1:A:1296:LEU:HG	2.20	0.41
1:A:1339:LEU:HD23	1:A:1339:LEU:HA	1.90	0.41
1:A:337:LYS:C	1:A:343:GLN:CA	2.90	0.41
1:A:337:LYS:HB2	1:A:341:GLU:H	1.82	0.41
1:A:685:PHE:HB3	1:A:707:LEU:HD11	2.02	0.41
1:A:897:PRO:O	1:A:901:LEU:HD23	2.21	0.41
1:A:1094:LYS:HE2	1:A:1094:LYS:HB2	1.80	0.41
1:A:1266:PRO:O	1:A:1269:THR:OG1	2.33	0.41
1:A:1452:SER:HA	1:A:1455:LYS:HE2	2.03	0.41
1:A:1466:LEU:HD23	1:A:1466:LEU:HA	1.89	0.41
1:A:1605:TRP:CH2	1:A:1802:TRP:HB2	2.56	0.41
1:A:1606:SER:OG	1:A:1629:GLN:NE2	2.41	0.41
1:A:1710:ASP:HB2	1:A:1711:GLU:OE2	2.21	0.41
1:A:101:ARG:HD2	1:A:282:GLU:HG2	2.02	0.41
1:A:1001:ASN:HB3	1:A:1002:TYR:HB2	2.03	0.41
1:A:1294:GLU:HA	1:A:1297:LYS:HZ1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1478:ILE:C	1:A:1480:GLY:H	2.29	0.41
1:A:1013:LYS:N	1:A:1950:MET:HE1	2.34	0.40
1:A:189:LYS:HE3	1:A:189:LYS:HB2	1.91	0.40
1:A:506:CYS:HB2	1:A:517:ASP:HB3	2.03	0.40
1:A:841:ARG:HA	1:A:841:ARG:HD2	1.93	0.40
1:A:1150:TRP:O	1:A:1154:ILE:HG12	2.21	0.40
1:A:1430:SER:HB3	1:A:1432:PHE:HE2	1.87	0.40
1:A:1585:ASN:OD1	1:A:1586:ASN:ND2	2.55	0.40
1:A:1627:ARG:NH1	1:A:1697:ASP:OD2	2.30	0.40
1:A:1810:TYR:CD2	1:A:1912:ILE:HG13	2.56	0.40
1:A:530:LYS:HD2	1:A:530:LYS:HA	1.85	0.40
1:A:1200:LYS:HD2	1:A:1200:LYS:HA	1.85	0.40
1:A:1215:SER:HB2	1:A:1216:GLU:HB3	2.04	0.40
1:A:1280:LYS:HD2	1:A:1280:LYS:HA	1.98	0.40
1:A:1431:ILE:O	1:A:1431:ILE:HG23	2.22	0.40
1:A:1558:ASN:CG	1:A:1560:GLU:HG2	2.46	0.40
1:A:1749:ASN:H	1:A:1753:ARG:HH21	1.68	0.40
1:A:136:GLY:HA2	1:A:139:ILE:HG22	2.02	0.40
1:A:711:TRP:O	1:A:714:THR:OG1	2.23	0.40
1:A:1382:LYS:HG3	1:A:1382:LYS:O	2.21	0.40
1:A:1560:GLU:HB2	1:A:1564:TYR:CE2	2.57	0.40
1:A:1884:MET:HE3	1:A:1884:MET:HB2	1.94	0.40
1:A:357:LYS:HB2	1:A:374:PHE:CD2	2.56	0.40
1:A:659:ILE:HB	1:A:711:TRP:HZ3	1.87	0.40
1:A:754:ASP:OD1	1:A:755:LEU:N	2.54	0.40
1:A:1154:ILE:HG21	1:A:1164:LYS:HG2	2.04	0.40
1:A:1201:LYS:HD2	1:A:1201:LYS:HA	1.89	0.40
1:A:1473:ARG:HH12	1:A:1644:GLU:HB3	1.87	0.40
1:A:1823:PRO:HA	1:A:1824:PRO:HD3	1.90	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	1836/2040 (90%)	1628 (89%)	199 (11%)	9 (0%)	25 56

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	529	LYS
1	A	907	ASP
1	A	952	PRO
1	A	793	ASN
1	A	1366	TYR
1	A	1531	VAL
1	A	237	ILE
1	A	537	SER
1	A	1055	ILE

### 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	1670/1839 (91%)	1667 (100%)	3 (0%)	92 96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	1107	ILE
1	A	1365	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	112	ASN
1	A	176	ASN
1	A	198	GLN

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Mol	Chain	Res	Type
1	A	386	ASN
1	A	606	ASN
1	A	623	HIS
1	A	637	ASN
1	A	692	ASN
1	A	713	ASN
1	A	730	ASN
1	A	764	GLN
1	A	784	ASN
1	A	903	ASN
1	A	965	GLN
1	A	1043	GLN
1	A	1114	GLN
1	A	1125	GLN
1	A	1134	GLN
1	A	1305	HIS
1	A	1330	GLN
1	A	1356	ASN
1	A	1427	ASN
1	A	1470	GLN
1	A	1586	ASN
1	A	1629	GLN
1	A	1674	ASN
1	A	1776	ASN
1	A	1847	ASN
1	A	1972	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	343:GLN	C	344:GLU	N	1.60
1	A	1381:GLU	C	1382:LYS	N	1.60

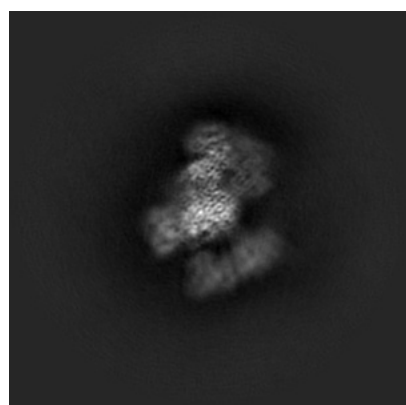
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14446. These allow visual inspection of the internal detail of the map and identification of artifacts.

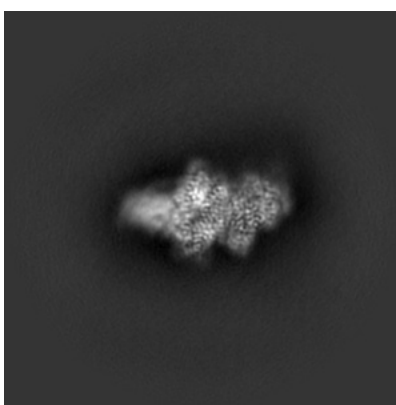
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

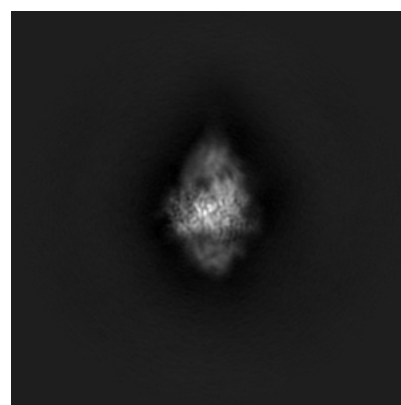
#### 6.1.1 Primary map



X



Y

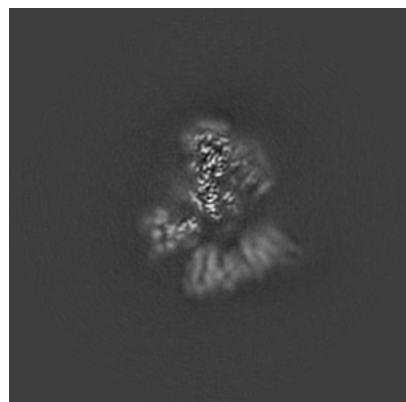


Z

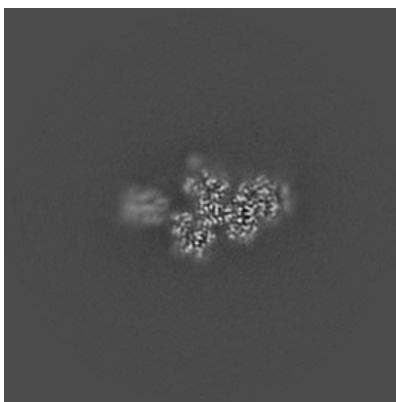
The images above show the map projected in three orthogonal directions.

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

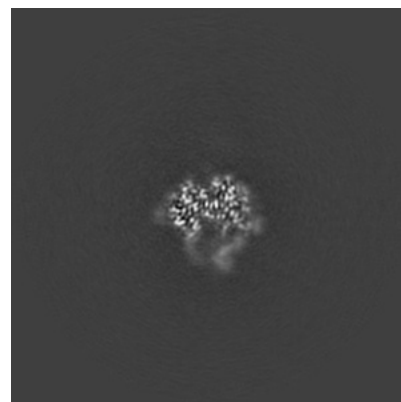
#### 6.2.1 Primary map



X Index: 220



Y Index: 220

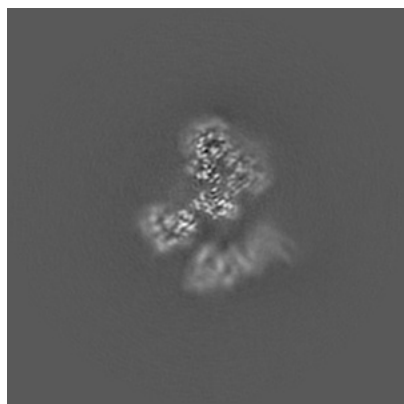


Z Index: 220

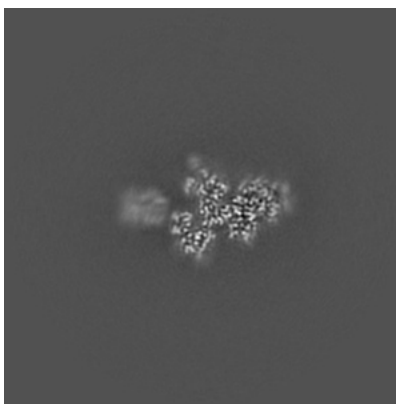
The images above show central slices of the map in three orthogonal directions.

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

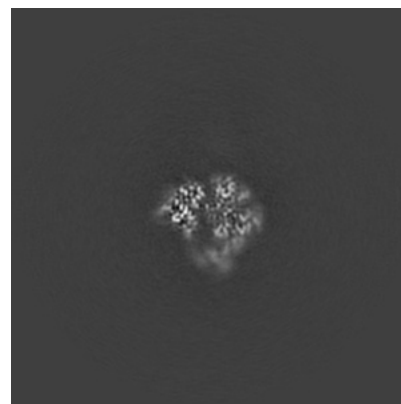
### 6.3.1 Primary map



X Index: 227



Y Index: 218

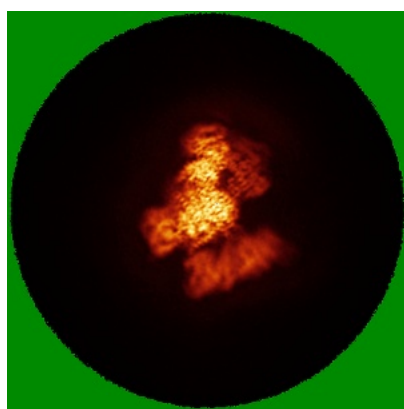


Z Index: 215

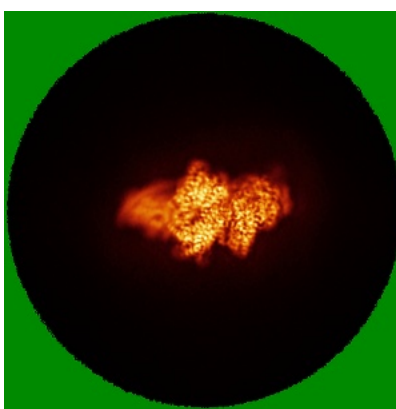
The images above show the largest variance slices of the map in three orthogonal directions.

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

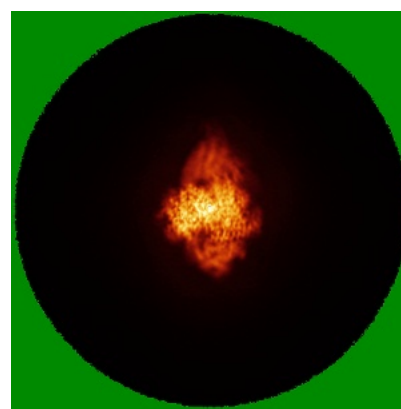
### 6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

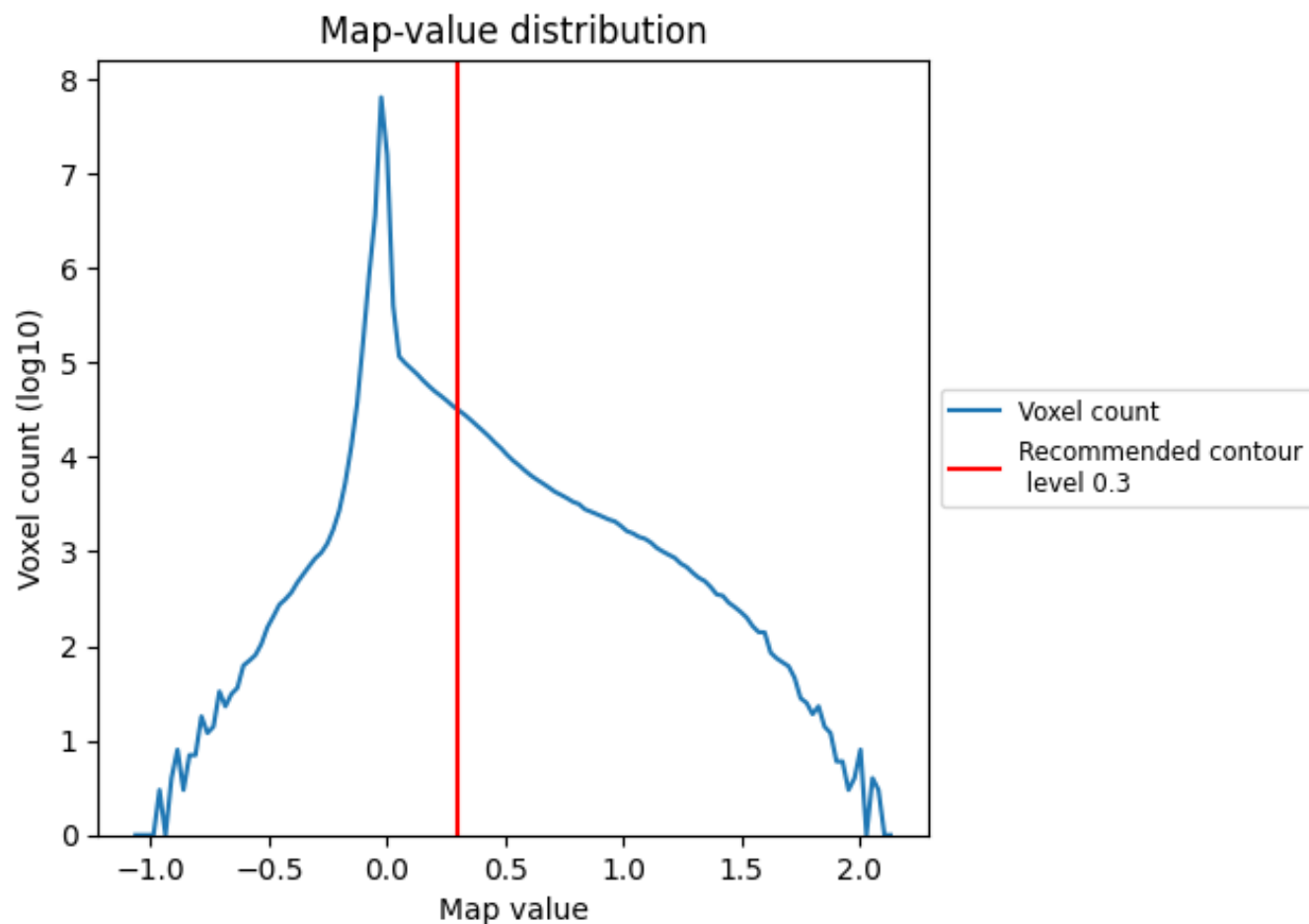
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

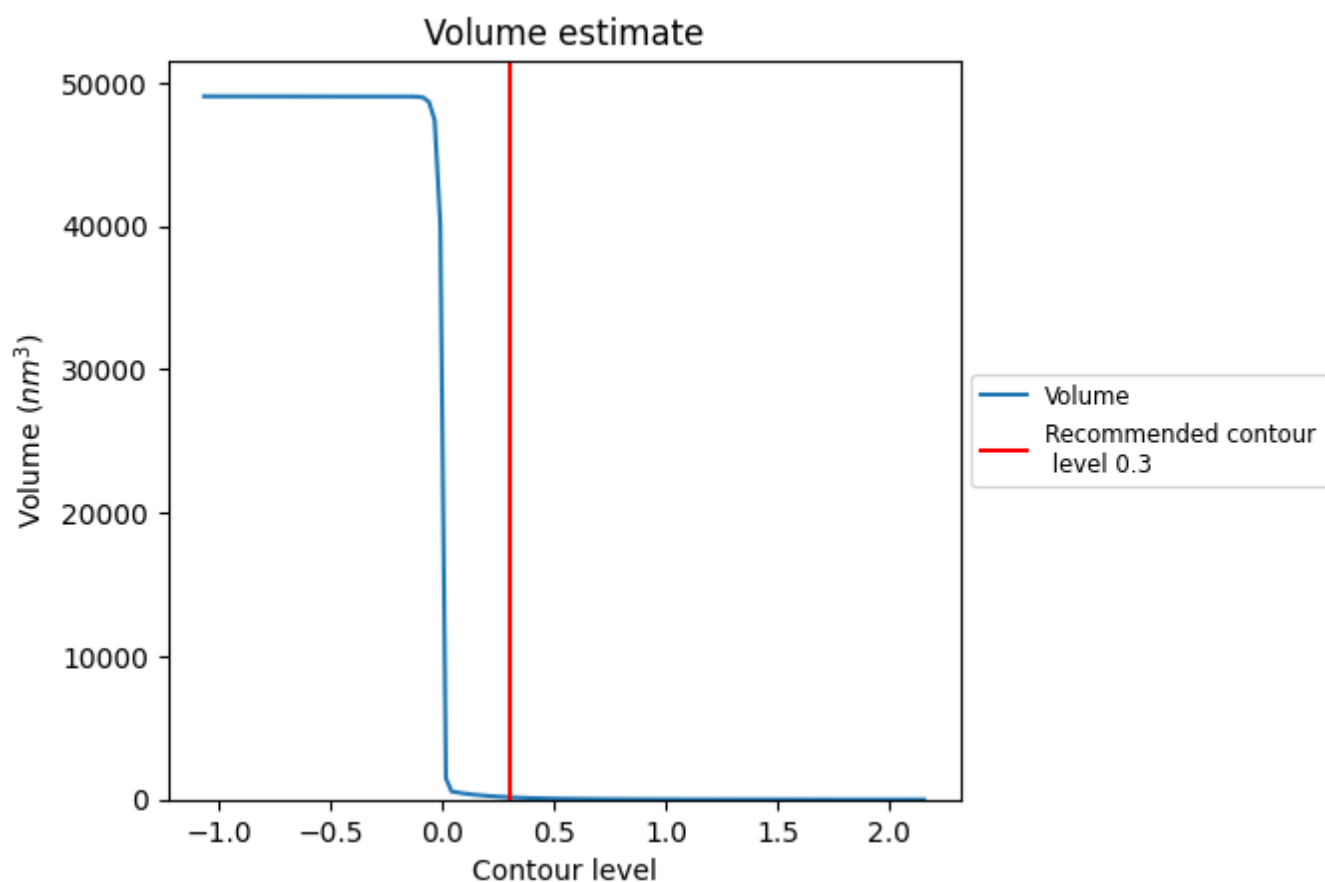
This section contains the results of statistical analysis of the map.

### 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.

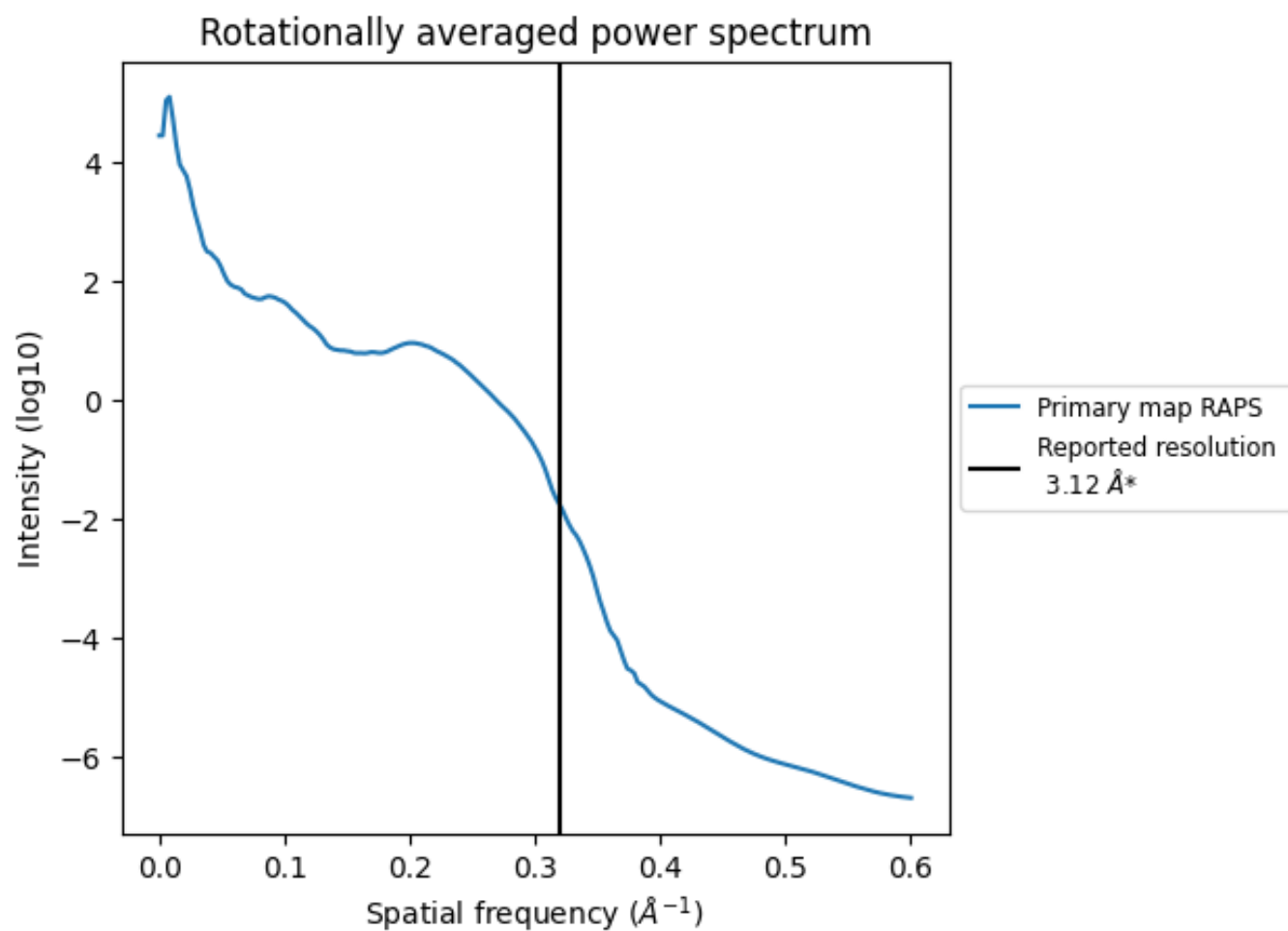
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 162 nm<sup>3</sup>; this corresponds to an approximate mass of 146 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 ⓘ

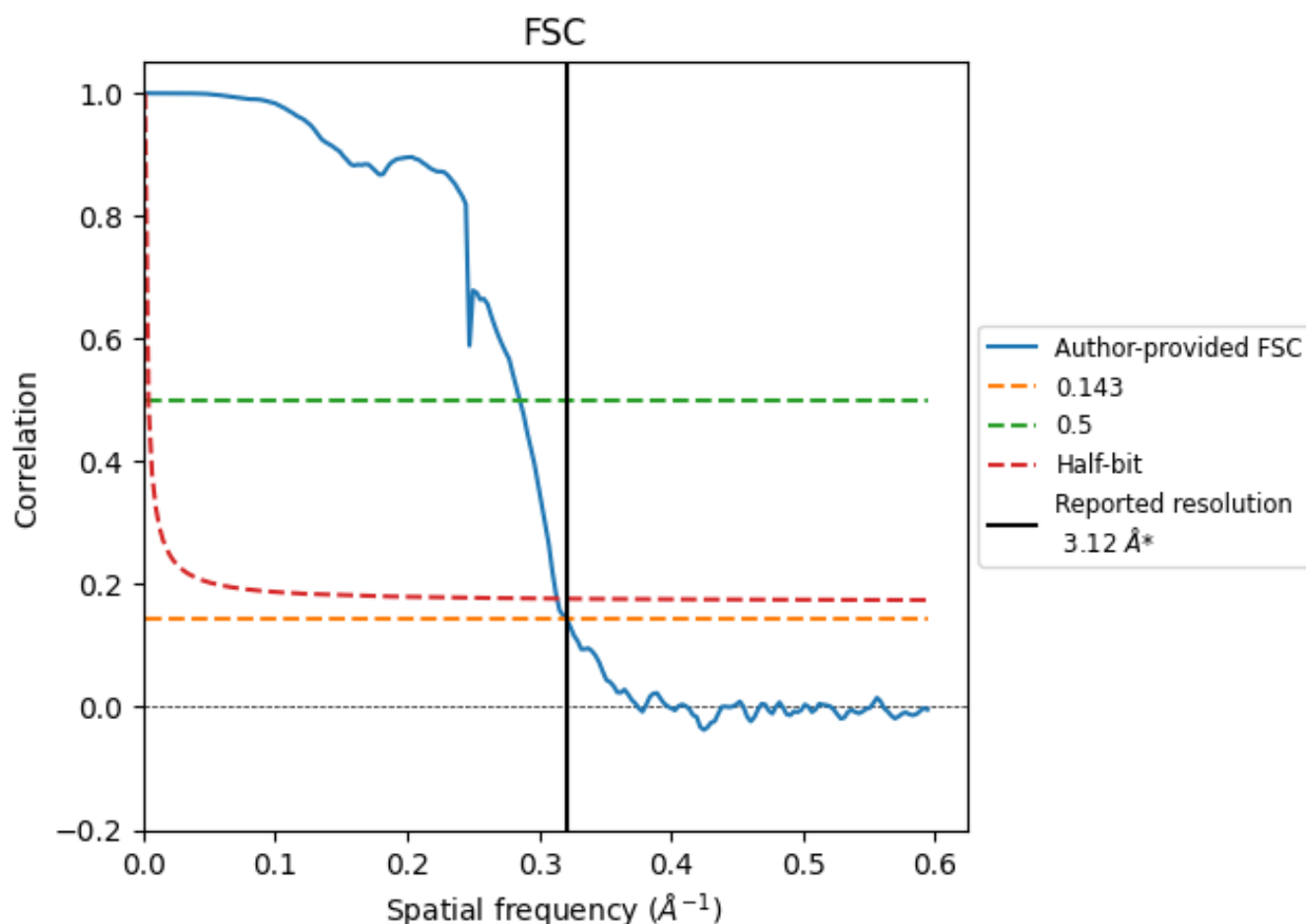


\*Reported resolution corresponds to spatial frequency of 0.321  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.321 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

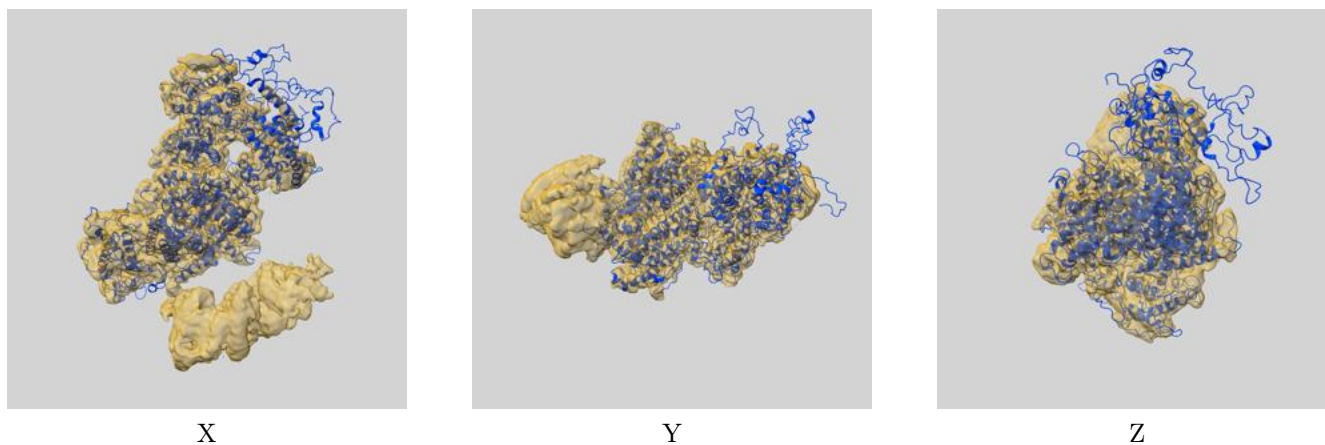
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.12	-	-
Author-provided FSC curve	3.12	3.50	3.19
Unmasked-calculated*	-	-	-

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

## 9 Map-model fit [i](#)

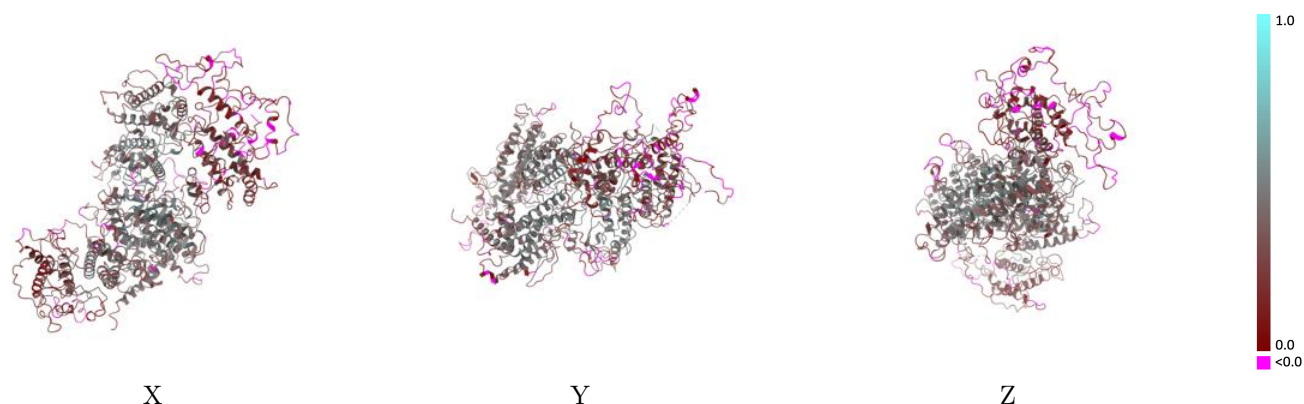
This section contains information regarding the fit between EMDB map EMD-14446 and PDB model 7Z1H. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

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



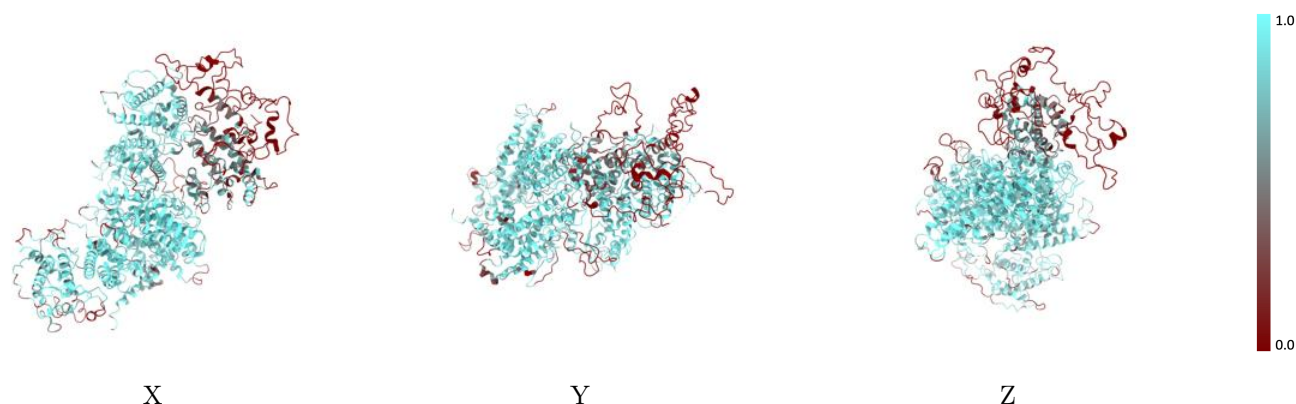
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



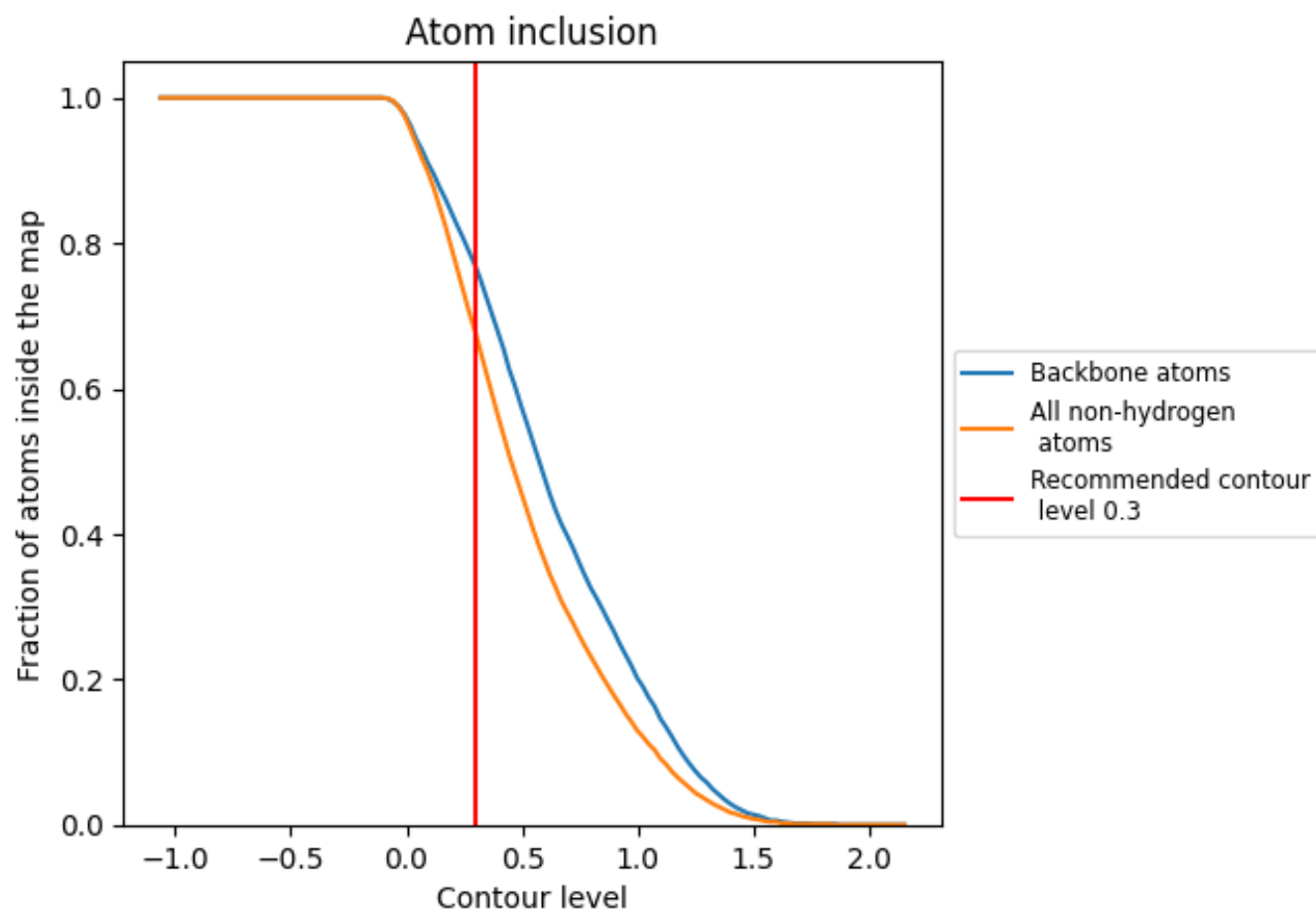
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 68% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6750	<div></div> 0.3150
A	<div></div> 0.6750	<div></div> 0.3150

