



Full wwPDB EM Validation Report ⓘ

Jul 8, 2025 – 10:10 am BST

PDB ID : 8RIA / pdb_00008ria
EMDB ID : EMD-19185
Title : BmrA E504-100uMATPMg-IF
Authors : Gobet, A.; Zarkadas, E.; Schoehn, G.; Falson, P.; Chaptal, V.
Deposited on : 2023-12-18
Resolution : 4.40 Å(reported)
Based on initial model : 6r81

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.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

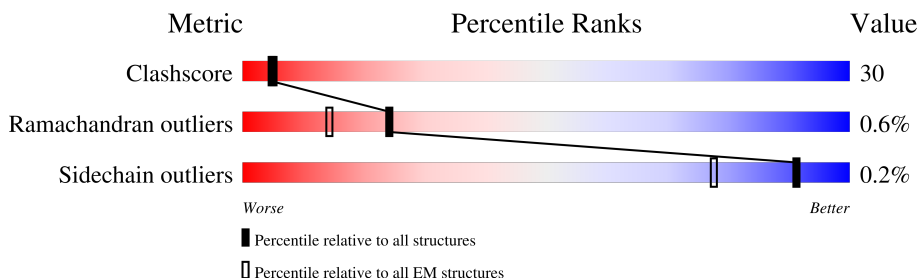
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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 ≥ 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	599	<div> <div>43%</div> <div>44%</div> <div>47%</div> <div>5%</div> </div>
1	B	599	<div> <div>41%</div> <div>44%</div> <div>46%</div> <div>5%</div> <div>5%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8786 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 Multidrug resistance ABC transporter ATP-binding/permease protein BmrA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	571	Total	C	N	O	S	0	0
			4393	2821	732	822	18		
1	B	571	Total	C	N	O	S	0	0
			4393	2821	732	822	18		

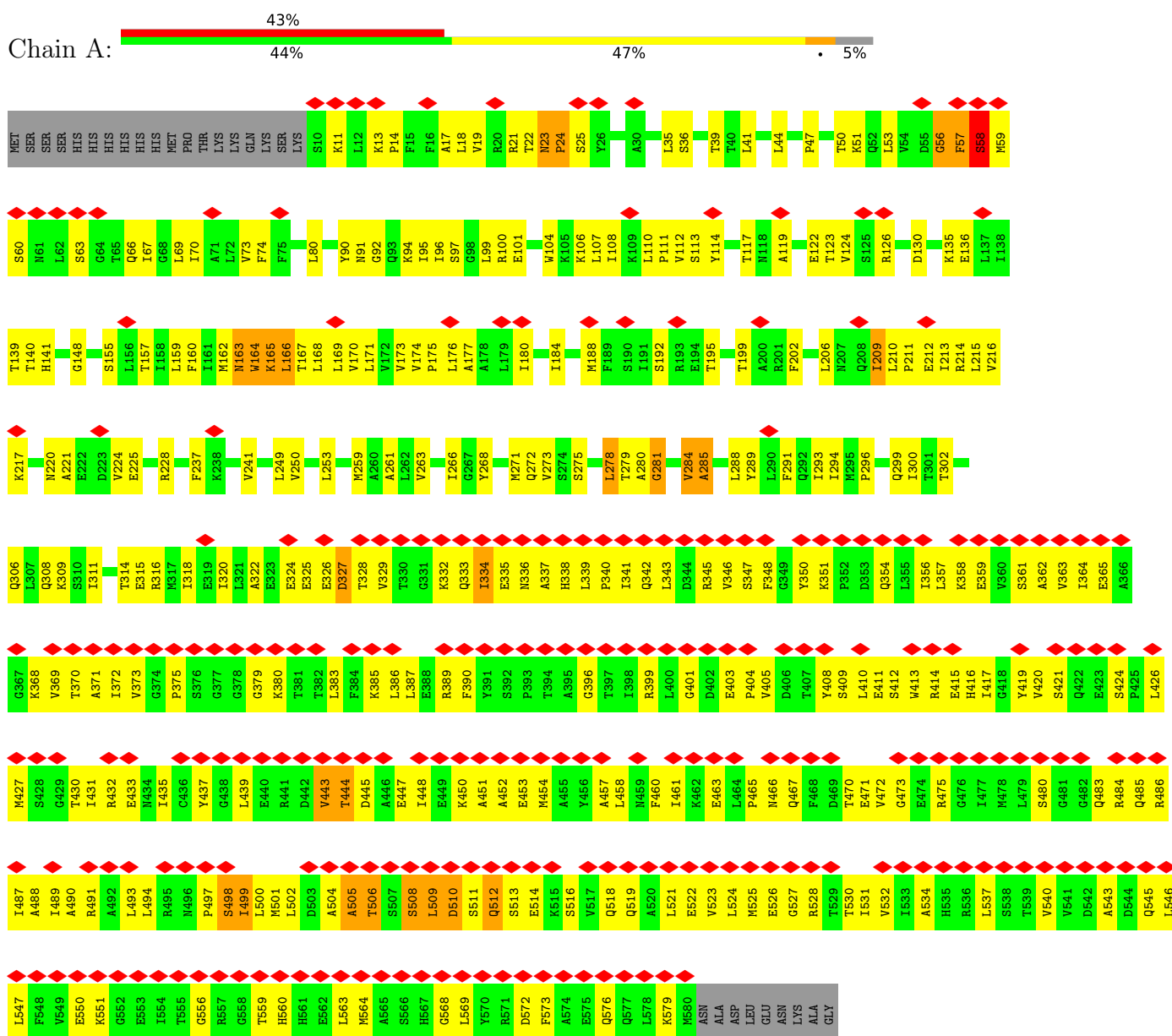
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP O06967
A	-8	SER	-	expression tag	UNP O06967
A	-7	SER	-	expression tag	UNP O06967
A	-6	SER	-	expression tag	UNP O06967
A	-5	HIS	-	expression tag	UNP O06967
A	-4	HIS	-	expression tag	UNP O06967
A	-3	HIS	-	expression tag	UNP O06967
A	-2	HIS	-	expression tag	UNP O06967
A	-1	HIS	-	expression tag	UNP O06967
A	0	HIS	-	expression tag	UNP O06967
A	504	ALA	GLU	engineered mutation	UNP O06967
B	-9	MET	-	initiating methionine	UNP O06967
B	-8	SER	-	expression tag	UNP O06967
B	-7	SER	-	expression tag	UNP O06967
B	-6	SER	-	expression tag	UNP O06967
B	-5	HIS	-	expression tag	UNP O06967
B	-4	HIS	-	expression tag	UNP O06967
B	-3	HIS	-	expression tag	UNP O06967
B	-2	HIS	-	expression tag	UNP O06967
B	-1	HIS	-	expression tag	UNP O06967
B	0	HIS	-	expression tag	UNP O06967
B	504	ALA	GLU	engineered mutation	UNP O06967

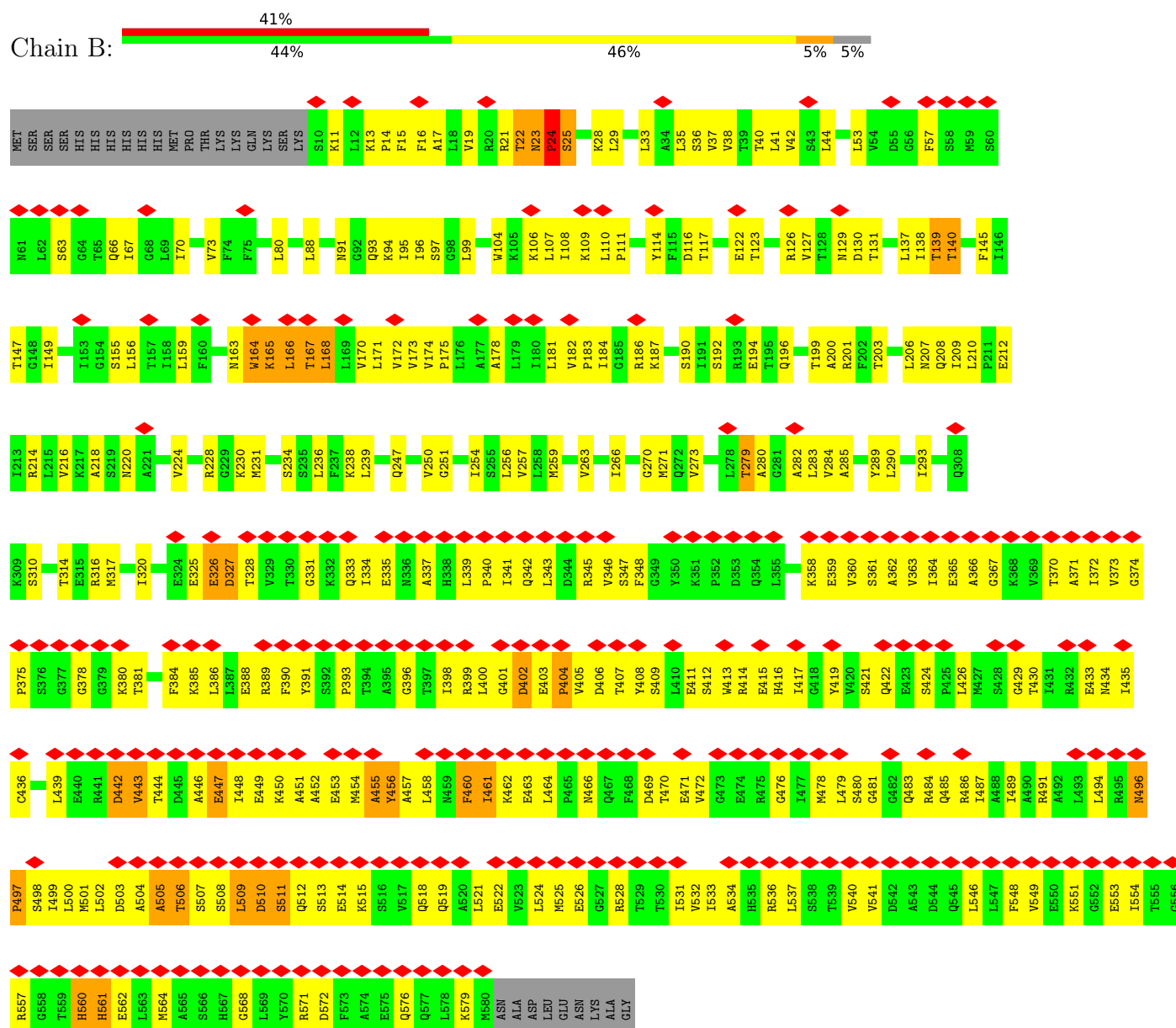
3 Residue-property plots

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: Multidrug resistance ABC transporter ATP-binding/permease protein BmrA



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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	418416	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.831	Depositor
Minimum map value	-0.511	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.218	Depositor
Map size (Å)	229.0, 229.0, 229.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.145, 1.145, 1.145	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	0.29	0/4460	1.19	61/6036 (1.0%)
1	B	0.33	1/4460 (0.0%)	1.27	69/6036 (1.1%)
All	All	0.31	1/8920 (0.0%)	1.23	130/12072 (1.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	497	PRO	N-CD	9.72	1.61	1.47

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	460	PHE	N-CA-C	30.16	150.29	112.89
1	A	163	ASN	N-CA-C	-20.60	74.83	109.24
1	A	57	PHE	N-CA-C	18.85	151.77	113.31
1	B	22	THR	CB-CA-C	-18.27	81.16	111.68
1	A	164	TRP	N-CA-C	16.71	136.11	112.04
1	B	23	ASN	N-CA-C	16.25	145.73	109.81
1	B	455	ALA	CB-CA-C	-16.07	83.01	110.81
1	B	23	ASN	N-CA-CB	-16.01	81.87	110.37
1	B	560	HIS	N-CA-C	15.67	130.28	112.57
1	B	327	ASP	N-CA-C	14.43	132.37	113.18
1	B	165	LYS	N-CA-CB	14.29	134.64	110.49
1	A	334	ILE	CB-CA-C	-14.02	93.80	111.88
1	B	562	GLU	N-CA-C	-13.69	96.19	113.43
1	B	561	HIS	N-CA-C	13.54	130.05	113.12
1	A	335	GLU	N-CA-C	13.46	133.91	114.39
1	B	461	ILE	N-CA-CB	-13.41	89.10	111.23
1	A	164	TRP	N-CA-CB	-13.41	89.41	110.19
1	A	163	ASN	CB-CA-C	13.39	135.87	109.35
1	A	58	SER	N-CA-C	-13.12	82.85	110.80
1	A	278	LEU	N-CA-C	-12.88	85.30	107.20
1	B	165	LYS	N-CA-C	-12.60	83.97	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	LEU	N-CA-CB	12.33	129.85	110.86
1	A	165	LYS	N-CA-CB	12.20	128.96	111.15
1	B	167	THR	CB-CA-C	-12.17	90.52	111.45
1	A	165	LYS	N-CA-C	-12.11	99.50	114.75
1	B	167	THR	N-CA-C	-12.03	95.49	110.88
1	A	509	LEU	N-CA-C	-11.94	95.08	111.56
1	A	380	LYS	N-CA-C	-11.85	98.50	113.43
1	A	334	ILE	N-CA-C	11.57	124.86	107.15
1	B	460	PHE	CB-CA-C	-11.52	85.91	109.99
1	A	510	ASP	N-CA-C	11.49	125.77	108.31
1	A	335	GLU	N-CA-CB	-11.48	95.82	110.98
1	B	509	LEU	N-CA-C	-11.35	93.83	110.06
1	B	25	SER	N-CA-CB	-11.30	91.39	110.49
1	A	327	ASP	N-CA-C	11.30	134.86	110.80
1	B	510	ASP	CB-CA-C	11.28	129.71	116.63
1	A	25	SER	N-CA-CB	-11.14	96.27	110.98
1	B	511	SER	N-CA-C	-10.76	98.23	114.16
1	A	509	LEU	CB-CA-C	-10.70	94.48	111.18
1	A	328	THR	N-CA-C	-10.66	97.57	114.09
1	B	455	ALA	N-CA-C	10.65	124.86	112.93
1	A	57	PHE	CB-CA-C	-10.64	87.57	110.76
1	A	497	PRO	N-CA-C	10.48	126.62	112.48
1	A	506	THR	N-CA-C	-10.12	92.91	109.40
1	B	328	THR	N-CA-C	-10.03	101.17	113.50
1	B	511	SER	CB-CA-C	-10.03	94.93	110.37
1	B	510	ASP	N-CA-C	9.95	124.89	108.08
1	B	456	TYR	N-CA-C	9.84	127.87	113.40
1	B	326	GLU	CB-CA-C	-9.82	93.91	109.72
1	B	139	THR	N-CA-C	9.74	121.90	111.28
1	B	166	LEU	N-CA-C	9.50	123.12	108.30
1	A	139	THR	N-CA-C	9.39	121.60	111.36
1	B	164	TRP	N-CA-C	9.23	130.46	110.80
1	B	457	ALA	N-CA-C	-9.23	100.40	112.68
1	B	168	LEU	N-CA-C	-9.06	91.51	110.80
1	B	512	GLN	N-CA-C	-8.95	99.34	111.96
1	B	24	PRO	N-CA-C	8.75	130.50	112.47
1	B	561	HIS	CB-CA-C	-8.63	95.32	109.56
1	B	167	THR	N-CA-CB	8.53	124.13	111.51
1	B	456	TYR	CB-CA-C	-8.53	95.45	111.06
1	A	511	SER	N-CA-CB	8.49	122.19	110.90
1	A	24	PRO	N-CA-C	8.41	128.06	112.33
1	A	510	ASP	CB-CA-C	8.34	126.14	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	506	THR	CB-CA-C	-8.33	100.32	111.82
1	A	280	ALA	N-CA-C	8.27	128.41	110.80
1	B	280	ALA	N-CA-C	7.99	122.30	112.23
1	B	498	SER	N-CA-C	7.99	121.14	111.40
1	A	24	PRO	CB-CA-C	-7.84	102.42	113.09
1	A	329	VAL	N-CA-C	-7.84	102.33	113.07
1	A	511	SER	N-CA-C	-7.77	104.28	114.31
1	A	166	LEU	N-CA-C	-7.65	99.86	111.56
1	A	505	ALA	CB-CA-C	-7.57	99.09	111.50
1	A	499	ILE	CB-CA-C	7.55	121.99	111.19
1	A	505	ALA	N-CA-C	-7.31	95.27	108.58
1	B	22	THR	N-CA-C	-7.28	93.45	107.57
1	B	279	THR	N-CA-C	7.21	121.78	112.41
1	A	140	THR	N-CA-C	-7.20	101.68	112.04
1	B	447	GLU	N-CA-C	-7.11	104.22	113.17
1	A	285	ALA	N-CA-C	-7.08	101.84	112.04
1	B	511	SER	N-CA-CB	7.02	124.08	110.88
1	A	165	LYS	CB-CA-C	-7.01	100.12	109.16
1	B	404	PRO	CA-N-CD	-7.00	102.20	112.00
1	A	335	GLU	CB-CA-C	-6.91	97.94	109.27
1	A	328	THR	CB-CA-C	-6.90	98.69	109.80
1	A	284	VAL	CB-CA-C	-6.89	99.98	111.29
1	B	140	THR	N-CA-C	-6.79	102.27	112.04
1	B	279	THR	N-CA-CB	-6.76	100.04	111.20
1	A	281	GLY	N-CA-C	-6.72	97.25	113.18
1	B	168	LEU	N-CA-CB	6.67	121.76	110.49
1	B	280	ALA	CB-CA-C	-6.65	96.81	110.38
1	A	336	ASN	N-CA-C	-6.59	96.75	110.80
1	A	379	GLY	N-CA-C	-6.58	97.59	113.18
1	B	139	THR	CB-CA-C	-6.54	99.93	110.79
1	B	509	LEU	CB-CA-C	-6.53	98.98	111.97
1	A	56	GLY	N-CA-C	-6.52	104.60	112.49
1	A	508	SER	N-CA-C	-6.51	97.19	108.52
1	B	25	SER	N-CA-C	6.51	124.66	110.80
1	B	505	ALA	N-CA-C	-6.50	96.95	110.80
1	B	446	ALA	N-CA-C	-6.46	102.77	111.87
1	B	496	ASN	CB-CA-C	6.43	122.85	110.17
1	A	508	SER	CB-CA-C	-6.42	101.56	111.83
1	B	327	ASP	CB-CA-C	-6.39	98.99	110.23
1	B	442	ASP	CB-CA-C	6.36	122.14	110.88
1	B	496	ASN	N-CA-C	-6.12	96.27	109.81
1	B	505	ALA	CB-CA-C	-6.08	98.32	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	498	SER	N-CA-CB	-6.06	100.25	110.49
1	B	442	ASP	N-CA-C	-6.05	103.42	111.96
1	A	139	THR	CB-CA-C	-6.03	100.61	110.85
1	B	404	PRO	N-CA-C	-5.93	100.26	112.47
1	B	403	GLU	CB-CA-C	-5.91	98.53	110.17
1	A	280	ALA	CB-CA-C	-5.90	98.69	110.42
1	A	209	ILE	CA-C-N	-5.90	113.28	119.83
1	A	209	ILE	C-N-CA	-5.90	113.28	119.83
1	A	512	GLN	N-CA-C	-5.84	102.62	111.56
1	A	499	ILE	N-CA-C	-5.82	100.19	109.20
1	B	402	ASP	N-CA-C	-5.79	104.13	110.91
1	A	572	ASP	N-CA-C	5.73	119.09	111.75
1	B	327	ASP	N-CA-CB	-5.71	97.35	110.83
1	B	507	SER	N-CA-CB	-5.68	101.67	111.22
1	A	328	THR	N-CA-CB	5.64	119.82	111.01
1	B	404	PRO	N-CA-CB	5.64	109.17	103.25
1	A	511	SER	CB-CA-C	-5.49	99.80	109.02
1	B	497	PRO	N-CA-CB	5.38	108.90	103.25
1	A	25	SER	N-CA-C	5.28	122.05	114.39
1	A	336	ASN	N-CA-CB	5.27	119.40	110.49
1	B	446	ALA	CB-CA-C	-5.25	102.99	111.28
1	B	23	ASN	CA-C-N	-5.23	113.31	119.84
1	B	23	ASN	C-N-CA	-5.23	113.31	119.84
1	A	58	SER	N-CA-CB	5.21	119.29	110.49
1	B	560	HIS	CB-CA-C	-5.11	103.14	111.06

There are no chirality outliers.

There are no planarity outliers.

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	4393	0	4567	268	0
1	B	4393	0	4567	284	0
All	All	8786	0	9134	529	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 30.

All (529) 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:B:478:MET:O	1:B:479:LEU:HD22	1.47	1.15
1:B:560:HIS:O	1:B:560:HIS:CG	1.92	1.13
1:B:560:HIS:O	1:B:560:HIS:CD2	2.03	1.11
1:A:334:ILE:O	1:A:334:ILE:CG2	1.96	1.10
1:B:167:THR:HG23	1:B:167:THR:O	1.47	1.10
1:B:456:TYR:CG	1:B:456:TYR:O	2.03	1.05
1:B:456:TYR:O	1:B:456:TYR:CD2	2.09	1.04
1:A:334:ILE:O	1:A:334:ILE:HG23	1.21	1.01
1:B:460:PHE:CG	1:B:460:PHE:O	2.15	0.99
1:B:442:ASP:O	1:B:443:VAL:HG12	1.63	0.97
1:B:96:ILE:HD11	1:B:131:THR:HB	1.49	0.94
1:A:347:SER:HB3	1:A:359:GLU:H	1.38	0.89
1:A:410:LEU:HD21	1:A:414:ARG:HH21	1.35	0.89
1:B:167:THR:O	1:B:167:THR:CG2	2.14	0.88
1:B:326:GLU:O	1:B:326:GLU:CD	2.19	0.85
1:A:499:ILE:O	1:A:500:LEU:HD23	1.76	0.85
1:B:460:PHE:O	1:B:460:PHE:CD2	2.31	0.83
1:A:556:GLY:O	1:A:564:MET:HE1	1.77	0.83
1:B:506:THR:O	1:B:536:ARG:NH1	2.12	0.82
1:A:23:ASN:HB3	1:A:24:PRO:HD3	1.59	0.82
1:A:345:ARG:HE	1:A:359:GLU:HB2	1.46	0.81
1:A:333:GLN:HB3	1:A:408:TYR:HB3	1.63	0.80
1:B:35:LEU:HD11	1:B:80:LEU:HD12	1.64	0.80
1:A:340:PRO:HB3	1:A:365:GLU:HA	1.63	0.79
1:B:358:LYS:NZ	1:B:551:LYS:O	2.16	0.78
1:B:568:GLY:HA2	1:B:572:ASP:HB3	1.64	0.78
1:A:272:GLN:NE2	1:A:278:LEU:O	2.16	0.78
1:B:422:GLN:HB3	1:B:505:ALA:HA	1.66	0.78
1:A:159:LEU:O	1:A:163:ASN:O	2.02	0.77
1:B:345:ARG:O	1:B:345:ARG:NH1	2.17	0.77
1:A:346:VAL:HG12	1:A:357:LEU:HD21	1.65	0.77
1:B:541:VAL:HG12	1:B:560:HIS:HE2	1.48	0.77
1:B:399:ARG:NH2	1:B:402:ASP:OD1	2.19	0.76
1:A:368:LYS:NZ	1:A:545:GLN:OE1	2.19	0.75
1:B:448:ILE:HG13	1:B:449:GLU:H	1.50	0.75
1:B:19:VAL:O	1:B:22:THR:O	2.05	0.75
1:B:515:LYS:O	1:B:519:GLN:NE2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:VAL:HA	1:A:396:GLY:HA3	1.67	0.74
1:A:343:LEU:O	1:A:361:SER:HA	1.88	0.74
1:A:364:ILE:HG23	1:A:368:LYS:HZ1	1.51	0.74
1:A:339:LEU:HD22	1:A:401:GLY:H	1.53	0.73
1:A:101:GLU:OE1	1:B:230:LYS:NZ	2.21	0.73
1:A:358:LYS:NZ	1:A:551:LYS:O	2.22	0.72
1:A:272:GLN:HE21	1:A:279:THR:HG22	1.56	0.70
1:B:460:PHE:HE2	1:B:483:GLN:HG2	1.56	0.70
1:B:502:LEU:HD12	1:B:532:VAL:HG22	1.72	0.70
1:B:290:LEU:HA	1:B:293:ILE:HD12	1.73	0.70
1:A:510:ASP:O	1:A:514:GLU:CG	2.40	0.69
1:A:564:MET:HB3	1:A:569:LEU:HB2	1.73	0.69
1:B:478:MET:O	1:B:478:MET:HG2	1.92	0.69
1:A:206:LEU:HD22	1:B:104:TRP:CZ3	2.28	0.69
1:A:460:PHE:HE2	1:A:486:ARG:HD3	1.57	0.69
1:A:369:VAL:HG22	1:A:525:MET:HE1	1.76	0.68
1:B:25:SER:O	1:B:29:LEU:HG	1.94	0.68
1:A:67:ILE:HA	1:A:70:ILE:HD12	1.76	0.67
1:A:188:MET:HG3	1:A:250:VAL:HG11	1.75	0.67
1:A:510:ASP:O	1:A:514:GLU:HG3	1.95	0.67
1:B:88:LEU:HD21	1:B:139:THR:O	1.95	0.67
1:B:110:LEU:HD13	1:B:325:GLU:H	1.59	0.67
1:B:279:THR:HA	1:B:282:ALA:HB3	1.76	0.67
1:B:346:VAL:HA	1:B:396:GLY:HA3	1.77	0.67
1:A:414:ARG:HH11	1:B:218:ALA:HA	1.60	0.67
1:A:475:ARG:HH21	1:B:208:GLN:HB2	1.60	0.66
1:A:421:SER:O	1:A:424:SER:OG	2.14	0.66
1:B:540:VAL:HG23	1:B:560:HIS:CE1	2.30	0.66
1:B:415:GLU:OE2	1:B:496:ASN:ND2	2.29	0.66
1:B:502:LEU:N	1:B:531:ILE:O	2.29	0.66
1:A:91:ASN:O	1:A:95:ILE:HD12	1.97	0.65
1:A:385:LYS:HE3	1:B:214:ARG:HH22	1.61	0.65
1:B:16:PHE:HA	1:B:19:VAL:HG12	1.77	0.65
1:B:561:HIS:H	1:B:561:HIS:CD2	2.13	0.65
1:A:155:SER:HA	1:A:289:TYR:CE2	2.32	0.65
1:B:155:SER:HA	1:B:289:TYR:OH	1.97	0.65
1:B:360:VAL:HG13	1:B:554:ILE:HG12	1.76	0.65
1:B:194:GLU:HG2	1:B:239:LEU:HD11	1.78	0.65
1:A:171:LEU:O	1:A:175:PRO:HD2	1.96	0.64
1:B:122:GLU:OE1	1:B:126:ARG:NH1	2.30	0.64
1:B:22:THR:HG21	1:B:95:ILE:HD12	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:LEU:HD12	1:A:362:ALA:HB3	1.78	0.64
1:B:129:ASN:OD1	1:B:130:ASP:N	2.31	0.64
1:A:348:PHE:H	1:A:357:LEU:HD23	1.61	0.64
1:B:388:GLU:HG3	1:B:390:PHE:CD2	2.31	0.64
1:B:114:TYR:O	1:B:117:THR:HB	1.97	0.64
1:A:177:ALA:HA	1:A:180:ILE:HD12	1.79	0.63
1:A:559:THR:HG22	1:A:563:LEU:HD23	1.80	0.63
1:A:308:GLN:O	1:A:311:ILE:HG22	1.99	0.63
1:B:347:SER:HB3	1:B:359:GLU:H	1.62	0.63
1:A:435:ILE:HD12	1:A:448:ILE:HD12	1.81	0.62
1:B:171:LEU:O	1:B:175:PRO:HD3	1.99	0.62
1:B:435:ILE:HG21	1:B:448:ILE:HG22	1.81	0.62
1:A:35:LEU:HD11	1:A:80:LEU:HD22	1.81	0.62
1:B:341:ILE:HG13	1:B:364:ILE:HB	1.81	0.62
1:B:170:VAL:O	1:B:174:VAL:HG23	2.00	0.62
1:B:326:GLU:CD	1:B:326:GLU:C	2.68	0.62
1:B:361:SER:O	1:B:557:ARG:NH2	2.33	0.61
1:A:22:THR:O	1:A:23:ASN:HB3	2.01	0.61
1:B:345:ARG:HH12	1:B:396:GLY:HA2	1.65	0.61
1:A:273:VAL:HA	1:A:279:THR:HG21	1.83	0.61
1:B:91:ASN:O	1:B:95:ILE:HG12	1.99	0.61
1:A:56:GLY:O	1:A:57:PHE:CD2	2.53	0.61
1:B:212:GLU:N	1:B:212:GLU:OE2	2.33	0.60
1:B:434:ASN:HB3	1:B:491:ARG:HE	1.64	0.60
1:A:417:ILE:HG22	1:A:499:ILE:HB	1.82	0.60
1:B:455:ALA:O	1:B:456:TYR:HB3	2.00	0.60
1:B:419:TYR:HA	1:B:501:MET:SD	2.40	0.60
1:A:288:LEU:HD11	1:B:263:VAL:HG22	1.83	0.60
1:A:53:LEU:HD13	1:A:66:GLN:HB3	1.83	0.60
1:A:500:LEU:HD12	1:A:525:MET:HB3	1.83	0.60
1:A:136:GLU:HG2	1:A:141:HIS:HE1	1.66	0.59
1:A:560:HIS:O	1:A:564:MET:HB2	2.02	0.59
1:B:519:GLN:HA	1:B:522:GLU:HG2	1.84	0.59
1:B:541:VAL:HG12	1:B:560:HIS:NE2	2.17	0.59
1:A:480:SER:N	1:A:483:GLN:HE21	2.00	0.59
1:A:483:GLN:HA	1:A:486:ARG:HG2	1.84	0.59
1:B:444:THR:HG21	1:B:494:LEU:HD21	1.85	0.59
1:B:371:ALA:HB3	1:B:546:LEU:HD12	1.85	0.59
1:B:466:ASN:HD22	1:B:469:ASP:HB2	1.67	0.59
1:B:486:ARG:HA	1:B:489:ILE:HG22	1.84	0.59
1:B:560:HIS:ND1	1:B:564:MET:HB2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:HD13	1:A:324:GLU:HA	1.85	0.59
1:B:374:GLY:HA3	1:B:380:LYS:HB3	1.84	0.59
1:A:266:ILE:HG22	1:B:284:VAL:HG23	1.85	0.58
1:B:346:VAL:O	1:B:360:VAL:N	2.36	0.58
1:B:156:LEU:HD23	1:B:159:LEU:HD12	1.86	0.58
1:A:508:SER:O	1:A:508:SER:OG	2.10	0.58
1:B:13:LYS:HB2	1:B:14:PRO:HD3	1.86	0.58
1:A:164:TRP:CD1	1:A:165:LYS:HZ1	2.22	0.58
1:A:155:SER:HA	1:A:289:TYR:HE2	1.68	0.58
1:B:500:LEU:HD22	1:B:525:MET:HG2	1.86	0.58
1:A:216:VAL:O	1:A:220:ASN:N	2.36	0.58
1:B:375:PRO:HG2	1:B:378:GLY:HA3	1.84	0.58
1:A:500:LEU:O	1:A:530:THR:HA	2.04	0.58
1:A:165:LYS:HG3	1:A:166:LEU:HD22	1.85	0.57
1:B:364:ILE:HG12	1:B:370:THR:HG21	1.85	0.57
1:B:381:THR:O	1:B:385:LYS:HG3	2.03	0.57
1:A:332:LYS:HE2	1:A:334:ILE:HG22	1.85	0.57
1:B:466:ASN:O	1:B:470:THR:OG1	2.22	0.57
1:A:22:THR:HG21	1:A:95:ILE:HG13	1.86	0.57
1:A:389:ARG:HH12	1:A:408:TYR:HE1	1.52	0.57
1:A:480:SER:H	1:A:483:GLN:HE21	1.53	0.57
1:A:184:ILE:HG22	1:A:250:VAL:HG23	1.87	0.57
1:A:466:ASN:N	1:A:470:THR:OG1	2.38	0.57
1:B:360:VAL:HG22	1:B:553:GLU:HA	1.86	0.57
1:B:373:VAL:HB	1:B:548:PHE:HD1	1.69	0.57
1:B:515:LYS:HB3	1:B:519:GLN:HE22	1.70	0.57
1:A:399:ARG:HB2	1:A:403:GLU:H	1.71	0.56
1:A:419:TYR:HA	1:A:501:MET:O	2.05	0.56
1:B:163:ASN:ND2	1:B:167:THR:HG22	2.20	0.56
1:A:113:SER:O	1:A:117:THR:HG23	2.05	0.56
1:B:504:ALA:HB3	1:B:534:ALA:HB2	1.86	0.56
1:A:351:LYS:HZ2	1:A:354:GLN:HG2	1.70	0.56
1:B:212:GLU:O	1:B:216:VAL:HG23	2.05	0.56
1:A:337:ALA:HB1	1:A:499:ILE:HD11	1.87	0.56
1:A:409:SER:HB2	1:A:411:GLU:OE1	2.05	0.56
1:B:126:ARG:O	1:B:130:ASP:HB2	2.06	0.56
1:B:346:VAL:HG11	1:B:386:LEU:HD21	1.88	0.56
1:B:421:SER:OG	1:B:424:SER:OG	2.23	0.56
1:B:63:SER:O	1:B:67:ILE:HG12	2.06	0.55
1:B:326:GLU:O	1:B:326:GLU:CG	2.53	0.55
1:A:427:MET:HE3	1:A:437:TYR:CD2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:THR:H	1:A:433:GLU:HG2	1.71	0.55
1:B:156:LEU:HA	1:B:159:LEU:HD12	1.87	0.55
1:A:504:ALA:HB3	1:A:534:ALA:HB2	1.88	0.55
1:B:270:GLY:HA2	1:B:273:VAL:HG12	1.87	0.55
1:A:522:GLU:HA	1:A:525:MET:HG3	1.88	0.55
1:B:23:ASN:HB3	1:B:24:PRO:HD3	1.89	0.55
1:A:281:GLY:O	1:A:284:VAL:HB	2.07	0.55
1:B:341:ILE:HA	1:B:400:LEU:HD21	1.88	0.55
1:B:541:VAL:HA	1:B:560:HIS:CD2	2.42	0.55
1:B:181:LEU:HD13	1:B:257:VAL:HG11	1.89	0.54
1:B:373:VAL:HG23	1:B:546:LEU:HD21	1.89	0.54
1:A:512:GLN:HG2	1:A:513:SER:N	2.22	0.54
1:B:485:GLN:OE1	1:B:509:LEU:HD11	2.08	0.54
1:B:448:ILE:HG13	1:B:449:GLU:N	2.22	0.54
1:B:484:ARG:HA	1:B:487:ILE:HD12	1.90	0.54
1:B:371:ALA:HB2	1:B:532:VAL:HB	1.90	0.54
1:B:414:ARG:HA	1:B:417:ILE:HG13	1.89	0.53
1:B:426:LEU:HD11	1:B:484:ARG:HB3	1.89	0.53
1:A:284:VAL:HG13	1:B:266:ILE:HG22	1.88	0.53
1:A:390:PHE:HE2	1:B:214:ARG:HD3	1.74	0.53
1:A:512:GLN:HG2	1:A:513:SER:H	1.72	0.53
1:A:444:THR:O	1:A:445:ASP:OD1	2.25	0.53
1:A:47:PRO:O	1:A:50:THR:OG1	2.22	0.53
1:A:452:ALA:HB1	1:A:457:ALA:HB3	1.91	0.53
1:A:210:LEU:HB3	1:A:211:PRO:HD3	1.91	0.53
1:A:451:ALA:HB1	1:A:494:LEU:HD13	1.91	0.53
1:B:385:LYS:HA	1:B:388:GLU:OE1	2.09	0.53
1:A:170:VAL:O	1:A:174:VAL:HG23	2.09	0.53
1:A:249:LEU:O	1:A:253:LEU:HD23	2.09	0.53
1:B:416:HIS:HB3	1:B:499:ILE:HD13	1.92	0.53
1:B:93:GLN:HA	1:B:96:ILE:HG22	1.91	0.52
1:A:414:ARG:HA	1:A:417:ILE:HG12	1.90	0.52
1:A:11:LYS:HB3	1:A:311:ILE:HD11	1.90	0.52
1:A:166:LEU:HD12	1:A:268:TYR:CE1	2.44	0.52
1:B:381:THR:C	1:B:385:LYS:HZ2	2.18	0.52
1:B:15:PHE:HD1	1:B:314:THR:HG21	1.74	0.52
1:B:289:TYR:O	1:B:293:ILE:HG13	2.09	0.52
1:A:57:PHE:CD1	1:A:57:PHE:C	2.88	0.52
1:A:92:GLY:O	1:A:96:ILE:HG12	2.10	0.52
1:B:234:SER:OG	1:B:238:LYS:NZ	2.41	0.52
1:A:342:GLN:OE1	1:A:363:VAL:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:VAL:HA	1:B:408:TYR:CZ	2.46	0.51
1:B:502:LEU:HB2	1:B:532:VAL:HA	1.92	0.51
1:A:112:VAL:HB	1:A:114:TYR:CE1	2.44	0.51
1:A:443:VAL:HG12	1:A:443:VAL:O	2.10	0.51
1:A:148:GLY:HA2	1:A:296:PRO:HB3	1.93	0.51
1:B:33:LEU:O	1:B:36:SER:OG	2.26	0.51
1:A:22:THR:O	1:A:23:ASN:CB	2.58	0.51
1:A:466:ASN:N	1:A:470:THR:HG1	2.08	0.51
1:A:453:GLU:HB2	1:A:458:LEU:HD13	1.92	0.51
1:A:471:GLU:CD	1:A:473:GLY:H	2.18	0.51
1:A:532:VAL:HG12	1:A:534:ALA:H	1.75	0.51
1:A:271:MET:SD	1:B:57:PHE:HA	2.51	0.51
1:B:279:THR:O	1:B:283:LEU:N	2.44	0.51
1:B:375:PRO:HD3	1:B:549:VAL:O	2.10	0.51
1:A:69:LEU:O	1:A:73:VAL:HG23	2.11	0.51
1:B:413:TRP:CZ3	1:B:417:ILE:HD11	2.46	0.51
1:A:502:LEU:HG	1:A:504:ALA:H	1.76	0.51
1:B:340:PRO:HG3	1:B:366:ALA:H	1.75	0.51
1:B:401:GLY:O	1:B:404:PRO:HD3	2.11	0.51
1:B:335:GLU:HG2	1:B:337:ALA:H	1.75	0.51
1:A:110:LEU:HB3	1:A:325:GLU:HB3	1.92	0.51
1:B:250:VAL:O	1:B:254:ILE:HG13	2.10	0.51
1:A:19:VAL:O	1:A:22:THR:HB	2.12	0.50
1:B:524:LEU:O	1:B:528:ARG:NH2	2.44	0.50
1:A:96:ILE:HD11	1:A:135:LYS:HB2	1.93	0.50
1:A:389:ARG:NH2	1:A:408:TYR:OH	2.41	0.50
1:A:475:ARG:NH2	1:B:208:GLN:HB2	2.25	0.50
1:A:273:VAL:HG22	1:A:279:THR:HB	1.94	0.50
1:B:549:VAL:HG22	1:B:554:ILE:HD13	1.94	0.50
1:A:107:LEU:O	1:A:111:PRO:HD2	2.11	0.50
1:A:318:ILE:O	1:A:322:ALA:N	2.45	0.50
1:B:508:SER:O	1:B:508:SER:OG	2.29	0.50
1:A:130:ASP:CG	1:A:316:ARG:HH21	2.19	0.50
1:B:348:PHE:HE2	1:B:391:TYR:HB3	1.76	0.50
1:A:18:LEU:HD21	1:A:99:LEU:HD11	1.94	0.50
1:A:209:ILE:O	1:A:212:GLU:HB2	2.12	0.50
1:B:145:PHE:O	1:B:149:ILE:HG22	2.11	0.50
1:A:159:LEU:C	1:A:168:LEU:HD11	2.37	0.50
1:B:67:ILE:HA	1:B:70:ILE:HG12	1.93	0.50
1:A:327:ASP:OD1	1:A:327:ASP:C	2.55	0.49
1:A:576:GLN:HA	1:A:579:LYS:HE2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:GLY:C	1:B:472:VAL:HG22	2.37	0.49
1:A:104:TRP:CZ3	1:B:206:LEU:HD22	2.46	0.49
1:A:458:LEU:HG	1:A:461:ILE:HB	1.93	0.49
1:A:420:VAL:HG11	1:A:489:ILE:HG22	1.94	0.49
1:B:17:ALA:O	1:B:21:ARG:HG2	2.11	0.49
1:B:53:LEU:HA	1:B:66:GLN:OE1	2.12	0.49
1:A:516:SER:O	1:A:519:GLN:HG2	2.12	0.49
1:B:109:LYS:HG3	1:B:110:LEU:HD23	1.94	0.49
1:A:107:LEU:HD21	1:B:210:LEU:HD11	1.94	0.49
1:B:130:ASP:HB3	1:B:317:MET:HE2	1.94	0.49
1:B:316:ARG:O	1:B:320:ILE:HG12	2.13	0.49
1:B:576:GLN:HA	1:B:579:LYS:HE2	1.95	0.49
1:A:114:TYR:O	1:A:117:THR:OG1	2.29	0.49
1:A:112:VAL:HG23	1:A:325:GLU:HG3	1.95	0.48
1:A:509:LEU:O	1:A:513:SER:HB2	2.13	0.48
1:A:104:TRP:CH2	1:A:108:ILE:HD11	2.48	0.48
1:B:402:ASP:C	1:B:404:PRO:HD3	2.38	0.48
1:B:522:GLU:O	1:B:526:GLU:HB2	2.14	0.48
1:B:106:LYS:O	1:B:111:PRO:HD3	2.14	0.48
1:B:430:THR:HG22	1:B:471:GLU:HA	1.96	0.48
1:A:315:GLU:O	1:A:318:ILE:HG22	2.13	0.48
1:A:540:VAL:HB	1:A:546:LEU:HD21	1.95	0.48
1:B:224:VAL:O	1:B:228:ARG:HG3	2.14	0.48
1:A:339:LEU:HD22	1:A:401:GLY:N	2.25	0.48
1:A:546:LEU:HD22	1:A:564:MET:HG3	1.96	0.48
1:B:199:THR:O	1:B:203:THR:HG23	2.14	0.48
1:A:458:LEU:HA	1:A:461:ILE:HD12	1.94	0.48
1:A:523:VAL:HA	1:A:526:GLU:OE2	2.13	0.48
1:B:388:GLU:HG3	1:B:390:PHE:CE2	2.49	0.48
1:A:163:ASN:ND2	1:A:167:THR:OG1	2.46	0.48
1:A:405:VAL:HA	1:A:408:TYR:CZ	2.49	0.48
1:B:165:LYS:O	1:B:166:LEU:HD22	2.13	0.48
1:B:511:SER:O	1:B:515:LYS:HD2	2.13	0.48
1:B:537:LEU:O	1:B:540:VAL:HG22	2.13	0.48
1:B:340:PRO:HB3	1:B:365:GLU:HA	1.95	0.48
1:B:123:THR:O	1:B:127:VAL:HG23	2.14	0.48
1:B:187:LYS:O	1:B:190:SER:OG	2.25	0.48
1:A:350:TYR:H	1:A:356:ILE:HD12	1.79	0.47
1:A:17:ALA:O	1:A:21:ARG:HG2	2.14	0.47
1:A:387:LEU:O	1:A:413:TRP:HH2	1.98	0.47
1:A:545:GLN:CD	1:A:547:LEU:HD11	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:MET:O	1:A:569:LEU:N	2.45	0.47
1:B:331:GLY:O	1:B:409:SER:HB2	2.14	0.47
1:A:259:MET:O	1:A:263:VAL:HG23	2.14	0.47
1:B:28:LYS:HB2	1:B:91:ASN:HD21	1.80	0.47
1:B:456:TYR:OH	1:B:486:ARG:NH1	2.48	0.47
1:A:414:ARG:HD2	1:B:220:ASN:OD1	2.14	0.47
1:B:94:LYS:O	1:B:97:SER:OG	2.24	0.47
1:B:462:LYS:HD3	1:B:483:GLN:NE2	2.29	0.47
1:A:13:LYS:HB3	1:A:14:PRO:HD3	1.97	0.47
1:A:96:ILE:CD1	1:A:135:LYS:HB2	2.44	0.47
1:A:383:LEU:O	1:A:387:LEU:HD23	2.14	0.47
1:A:399:ARG:HD2	1:A:399:ARG:O	2.15	0.47
1:A:404:PRO:HB2	1:A:408:TYR:HD2	1.78	0.47
1:A:447:GLU:HG2	1:A:450:LYS:HD3	1.96	0.47
1:A:463:GLU:HG2	1:A:465:PRO:HD3	1.97	0.47
1:B:348:PHE:CD2	1:B:393:PRO:HA	2.49	0.47
1:B:362:ALA:HA	1:B:557:ARG:HH12	1.79	0.47
1:B:401:GLY:C	1:B:404:PRO:HD3	2.40	0.47
1:B:426:LEU:HD22	1:B:472:VAL:HB	1.97	0.47
1:A:23:ASN:CB	1:A:24:PRO:HD3	2.40	0.47
1:A:202:PHE:HE1	1:A:206:LEU:HD11	1.80	0.47
1:A:411:GLU:O	1:A:415:GLU:OE1	2.33	0.47
1:B:155:SER:O	1:B:159:LEU:HG	2.14	0.47
1:B:41:LEU:HD13	1:B:44:LEU:HD12	1.97	0.47
1:B:371:ALA:HA	1:B:532:VAL:O	2.14	0.47
1:A:431:ILE:HD12	1:A:431:ILE:H	1.80	0.47
1:B:104:TRP:CH2	1:B:108:ILE:HD11	2.49	0.47
1:A:60:SER:HA	1:A:63:SER:HB2	1.97	0.46
1:B:483:GLN:O	1:B:487:ILE:HG13	2.14	0.46
1:A:57:PHE:CD1	1:A:57:PHE:O	2.68	0.46
1:A:296:PRO:O	1:A:300:ILE:HD12	2.15	0.46
1:A:311:ILE:O	1:A:314:THR:HB	2.14	0.46
1:A:527:GLY:C	1:A:528:ARG:HD3	2.40	0.46
1:B:400:LEU:O	1:B:404:PRO:HD2	2.15	0.46
1:A:41:LEU:HD23	1:A:44:LEU:HD12	1.98	0.46
1:A:486:ARG:HA	1:A:489:ILE:HG12	1.98	0.46
1:B:93:GLN:O	1:B:96:ILE:HG22	2.14	0.46
1:B:372:ILE:HG22	1:B:533:ILE:HG13	1.98	0.46
1:B:389:ARG:HB2	1:B:413:TRP:CZ3	2.49	0.46
1:A:284:VAL:O	1:A:284:VAL:HG12	2.15	0.46
1:B:95:ILE:O	1:B:99:LEU:HD23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:VAL:CG2	1:B:560:HIS:CE1	2.98	0.46
1:A:435:ILE:HA	1:A:491:ARG:HG3	1.98	0.46
1:B:175:PRO:HA	1:B:178:ALA:HB3	1.98	0.46
1:A:74:PHE:HD2	1:B:256:LEU:HD12	1.80	0.46
1:A:124:VAL:HG21	1:B:207:ASN:OD1	2.16	0.46
1:A:272:GLN:HG2	1:A:279:THR:CG2	2.45	0.46
1:A:389:ARG:CZ	1:A:405:VAL:HG13	2.46	0.46
1:B:184:ILE:HG22	1:B:250:VAL:HG23	1.97	0.46
1:B:170:VAL:HA	1:B:173:VAL:HG12	1.97	0.46
1:B:504:ALA:O	1:B:506:THR:N	2.45	0.46
1:A:372:ILE:HD13	1:A:547:LEU:HB2	1.97	0.46
1:B:172:VAL:O	1:B:175:PRO:HD2	2.15	0.46
1:B:540:VAL:HG23	1:B:560:HIS:NE2	2.30	0.46
1:A:439:LEU:HG	1:A:443:VAL:HA	1.97	0.46
1:B:183:PRO:HA	1:B:186:ARG:HG2	1.97	0.46
1:B:325:GLU:CD	1:B:326:GLU:H	2.24	0.46
1:B:455:ALA:O	1:B:456:TYR:CB	2.63	0.46
1:B:460:PHE:CD2	1:B:486:ARG:HD2	2.51	0.46
1:B:480:SER:N	1:B:483:GLN:OE1	2.29	0.46
1:B:560:HIS:ND1	1:B:564:MET:CB	2.79	0.46
1:A:164:TRP:HE1	1:A:165:LYS:HE3	1.80	0.46
1:B:327:ASP:CG	1:B:411:GLU:HB2	2.41	0.46
1:A:35:LEU:O	1:A:39:THR:HG23	2.17	0.45
1:A:416:HIS:O	1:A:498:SER:HB2	2.17	0.45
1:A:126:ARG:HG2	1:A:320:ILE:HD11	1.98	0.45
1:B:11:LYS:H	1:B:11:LYS:HD2	1.81	0.45
1:B:192:SER:O	1:B:196:GLN:OE1	2.34	0.45
1:B:345:ARG:O	1:B:345:ARG:HG2	2.16	0.45
1:A:466:ASN:H	1:A:470:THR:HG1	1.62	0.45
1:A:36:SER:O	1:A:39:THR:OG1	2.30	0.45
1:A:504:ALA:O	1:A:506:THR:N	2.50	0.45
1:B:442:ASP:O	1:B:443:VAL:CG1	2.50	0.45
1:A:426:LEU:HD11	1:A:472:VAL:HG21	1.99	0.45
1:B:70:ILE:HA	1:B:73:VAL:HG12	1.99	0.45
1:A:58:SER:N	1:B:271:MET:HE1	2.31	0.45
1:B:509:LEU:HB3	1:B:513:SER:HB2	1.98	0.45
1:A:160:PHE:CD1	1:A:168:LEU:HD22	2.52	0.45
1:A:370:THR:HB	1:A:531:ILE:HA	1.99	0.45
1:A:493:LEU:HB3	1:A:524:LEU:HG	1.99	0.45
1:A:521:LEU:O	1:A:525:MET:HG3	2.16	0.45
1:B:481:GLY:HA2	1:B:484:ARG:NE	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ALA:HB1	1:A:540:VAL:HG12	1.99	0.45
1:B:38:VAL:O	1:B:42:VAL:HG23	2.17	0.45
1:A:51:LYS:NZ	1:A:162:MET:SD	2.87	0.45
1:A:237:PHE:O	1:A:241:VAL:HG23	2.16	0.45
1:B:165:LYS:C	1:B:166:LEU:HD22	2.42	0.45
1:B:452:ALA:C	1:B:458:LEU:HB2	2.43	0.45
1:B:478:MET:O	1:B:479:LEU:CD2	2.41	0.44
1:B:548:PHE:HE2	1:B:571:ARG:HH12	1.65	0.44
1:B:164:TRP:HE1	1:B:165:LYS:NZ	2.15	0.44
1:A:272:GLN:O	1:A:275:SER:HB3	2.18	0.44
1:A:365:GLU:OE2	1:A:368:LYS:HB2	2.17	0.44
1:B:341:ILE:HG22	1:B:400:LEU:HD21	1.99	0.44
1:B:342:GLN:O	1:B:399:ARG:N	2.50	0.44
1:B:342:GLN:OE1	1:B:363:VAL:HG22	2.17	0.44
1:B:400:LEU:HD12	1:B:405:VAL:HG23	2.00	0.44
1:A:174:VAL:HG13	1:A:261:ALA:HB1	1.98	0.44
1:A:291:PHE:O	1:A:294:ILE:HG22	2.18	0.44
1:B:486:ARG:O	1:B:489:ILE:HG22	2.18	0.44
1:A:225:GLU:OE1	1:A:228:ARG:HD3	2.17	0.44
1:B:444:THR:O	1:B:447:GLU:HB3	2.17	0.44
1:A:213:ILE:HG21	1:B:116:ASP:OD2	2.18	0.44
1:A:299:GLN:O	1:A:302:THR:OG1	2.22	0.44
1:B:398:ILE:O	1:B:405:VAL:HG21	2.17	0.44
1:B:400:LEU:HB2	1:B:405:VAL:HG23	1.99	0.44
1:A:213:ILE:HA	1:A:216:VAL:HG12	1.99	0.44
1:B:33:LEU:O	1:B:37:VAL:HG23	2.18	0.44
1:B:234:SER:O	1:B:238:LYS:HG2	2.18	0.44
1:A:421:SER:O	1:A:505:ALA:HB2	2.18	0.43
1:A:537:LEU:HA	1:A:540:VAL:HG22	2.00	0.43
1:B:439:LEU:HD12	1:B:443:VAL:HG23	1.99	0.43
1:A:173:VAL:O	1:A:176:LEU:HB3	2.18	0.43
1:B:178:ALA:O	1:B:181:LEU:HB3	2.18	0.43
1:B:310:SER:O	1:B:314:THR:HG23	2.18	0.43
1:A:293:ILE:C	1:A:296:PRO:HD2	2.42	0.43
1:A:372:ILE:N	1:A:532:VAL:O	2.48	0.43
1:B:414:ARG:HA	1:B:417:ILE:CG1	2.48	0.43
1:A:112:VAL:HG12	1:A:113:SER:N	2.34	0.43
1:A:195:THR:O	1:A:199:THR:HG23	2.18	0.43
1:A:383:LEU:O	1:A:386:LEU:HG	2.17	0.43
1:A:126:ARG:NH1	1:A:316:ARG:HB3	2.34	0.43
1:A:325:GLU:CD	1:A:326:GLU:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:SER:HA	1:A:415:GLU:OE1	2.18	0.43
1:A:432:ARG:NH1	1:A:467:GLN:HE22	2.16	0.43
1:A:487:ILE:HG13	1:A:488:ALA:N	2.33	0.43
1:A:136:GLU:HG2	1:A:141:HIS:CE1	2.49	0.43
1:A:546:LEU:HD13	1:A:560:HIS:HB3	2.00	0.43
1:B:367:GLY:HA2	1:B:528:ARG:C	2.44	0.43
1:B:389:ARG:HD3	1:B:413:TRP:CH2	2.53	0.43
1:B:510:ASP:O	1:B:514:GLU:HG2	2.18	0.43
1:A:341:ILE:HG22	1:A:364:ILE:HB	2.01	0.43
1:A:485:GLN:O	1:A:489:ILE:HG12	2.19	0.43
1:A:540:VAL:O	1:A:546:LEU:HD11	2.19	0.43
1:B:339:LEU:C	1:B:366:ALA:HB2	2.44	0.43
1:A:112:VAL:HG12	1:A:113:SER:H	1.83	0.42
1:A:123:THR:O	1:A:126:ARG:HB3	2.19	0.42
1:A:339:LEU:HD13	1:A:401:GLY:HA2	2.00	0.42
1:A:499:ILE:O	1:A:500:LEU:CD2	2.60	0.42
1:B:345:ARG:HH22	1:B:396:GLY:HA2	1.84	0.42
1:B:417:ILE:HG22	1:B:419:TYR:H	1.84	0.42
1:B:447:GLU:HA	1:B:450:LYS:HB3	2.01	0.42
1:B:447:GLU:HG2	1:B:450:LYS:HD3	2.01	0.42
1:B:453:GLU:HG3	1:B:454:MET:HE2	2.01	0.42
1:A:119:ALA:HB3	1:A:122:GLU:OE2	2.19	0.42
1:A:126:ARG:NE	1:A:316:ARG:HD2	2.34	0.42
1:B:201:ARG:HB3	1:B:201:ARG:CZ	2.50	0.42
1:B:430:THR:H	1:B:433:GLU:CD	2.26	0.42
1:A:537:LEU:HD21	1:A:573:PHE:CZ	2.54	0.42
1:B:389:ARG:HD3	1:B:413:TRP:CZ3	2.55	0.42
1:B:518:GLN:O	1:B:521:LEU:HG	2.19	0.42
1:A:460:PHE:CE2	1:A:486:ARG:HD3	2.45	0.42
1:B:504:ALA:C	1:B:506:THR:N	2.77	0.42
1:B:40:THR:OG1	1:B:147:THR:OG1	2.27	0.42
1:B:57:PHE:CD1	1:B:57:PHE:C	2.98	0.42
1:A:97:SER:O	1:A:101:GLU:HG3	2.20	0.42
1:A:399:ARG:HB3	1:A:403:GLU:OE2	2.19	0.42
1:B:447:GLU:OE2	1:B:451:ALA:HB2	2.18	0.42
1:B:450:LYS:O	1:B:454:MET:HG2	2.18	0.42
1:B:506:THR:O	1:B:506:THR:OG1	2.37	0.42
1:A:58:SER:OG	1:A:59:MET:N	2.51	0.42
1:A:221:ALA:HB1	1:A:224:VAL:HB	2.00	0.42
1:A:300:ILE:HD12	1:A:300:ILE:H	1.84	0.42
1:A:432:ARG:HD2	1:A:435:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ALA:O	1:A:494:LEU:HG	2.20	0.42
1:B:421:SER:HA	1:B:503:ASP:HB3	2.01	0.42
1:B:483:GLN:O	1:B:486:ARG:HG2	2.19	0.42
1:A:453:GLU:HG3	1:A:454:MET:HE2	2.01	0.42
1:B:19:VAL:O	1:B:22:THR:HB	2.19	0.42
1:B:247:GLN:HA	1:B:250:VAL:HG12	2.00	0.42
1:B:333:GLN:HB2	1:B:408:TYR:HB3	2.01	0.42
1:B:537:LEU:HA	1:B:540:VAL:HG22	2.02	0.42
1:A:100:ARG:NH1	1:B:236:LEU:HD23	2.35	0.42
1:A:165:LYS:CG	1:A:166:LEU:HD22	2.50	0.42
1:A:214:ARG:HG3	1:A:215:LEU:N	2.35	0.42
1:A:365:GLU:H	1:A:368:LYS:HE3	1.85	0.42
1:B:171:LEU:HD13	1:B:290:LEU:HD11	2.00	0.42
1:B:404:PRO:O	1:B:407:THR:N	2.53	0.42
1:A:57:PHE:O	1:A:57:PHE:HD1	2.03	0.42
1:A:165:LYS:O	1:A:169:LEU:HB2	2.20	0.42
1:A:518:GLN:O	1:A:521:LEU:HG	2.20	0.42
1:A:211:PRO:O	1:A:214:ARG:HG2	2.19	0.41
1:B:384:PHE:CD1	1:B:533:ILE:HG21	2.55	0.41
1:B:509:LEU:O	1:B:513:SER:HB2	2.20	0.41
1:A:414:ARG:HD3	1:B:218:ALA:HA	2.02	0.41
1:B:285:ALA:O	1:B:289:TYR:HB2	2.20	0.41
1:A:390:PHE:HE2	1:B:214:ARG:CD	2.32	0.41
1:A:525:MET:HA	1:A:528:ARG:HB2	2.02	0.41
1:B:22:THR:HG21	1:B:95:ILE:HG23	2.02	0.41
1:B:127:VAL:O	1:B:131:THR:HG23	2.20	0.41
1:B:230:LYS:HG3	1:B:231:MET:HE2	2.01	0.41
1:B:259:MET:O	1:B:263:VAL:HG23	2.20	0.41
1:B:334:ILE:HG12	1:B:412:SER:HB3	2.02	0.41
1:A:489:ILE:HG13	1:A:490:ALA:N	2.34	0.41
1:B:96:ILE:HD12	1:B:96:ILE:HA	1.89	0.41
1:B:137:LEU:O	1:B:138:ILE:C	2.63	0.41
1:B:340:PRO:N	1:B:366:ALA:HB2	2.36	0.41
1:B:460:PHE:CD2	1:B:460:PHE:C	2.87	0.41
1:B:500:LEU:HD21	1:B:502:LEU:HD21	2.02	0.41
1:A:491:ARG:HE	1:A:491:ARG:HB3	1.65	0.41
1:A:545:GLN:C	1:A:546:LEU:HD12	2.46	0.41
1:B:110:LEU:HD22	1:B:325:GLU:O	2.21	0.41
1:B:250:VAL:HG13	1:B:251:GLY:N	2.36	0.41
1:B:343:LEU:HD23	1:B:398:ILE:HG23	2.02	0.41
1:A:217:LYS:HE2	1:B:414:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:MET:SD	1:B:501:MET:C	3.04	0.41
1:B:159:LEU:HD11	1:B:293:ILE:HD11	2.03	0.41
1:B:337:ALA:O	1:B:499:ILE:HD11	2.21	0.41
1:B:114:TYR:HA	1:B:117:THR:OG1	2.20	0.41
1:B:463:GLU:C	1:B:464:LEU:HD23	2.45	0.41
1:A:110:LEU:HD22	1:A:325:GLU:C	2.46	0.41
1:A:119:ALA:HB3	1:A:122:GLU:CD	2.46	0.41
1:A:157:THR:O	1:A:160:PHE:HB2	2.21	0.41
1:A:192:SER:O	1:A:195:THR:HB	2.20	0.41
1:A:334:ILE:CG2	1:A:412:SER:HB3	2.51	0.41
1:A:373:VAL:N	1:A:547:LEU:O	2.48	0.41
1:A:458:LEU:O	1:A:458:LEU:HD23	2.21	0.41
1:A:500:LEU:HB2	1:A:530:THR:HG22	2.03	0.41
1:B:178:ALA:O	1:B:182:VAL:HG23	2.21	0.41
1:B:209:ILE:HD13	1:B:209:ILE:HA	1.90	0.41
1:B:259:MET:HE2	1:B:259:MET:HB2	1.81	0.41
1:B:506:THR:OG1	1:B:536:ARG:NH1	2.47	0.41
1:A:432:ARG:HH11	1:A:467:GLN:HE22	1.68	0.41
1:B:200:ALA:O	1:B:203:THR:OG1	2.32	0.41
1:B:405:VAL:HG13	1:B:406:ASP:N	2.36	0.41
1:A:160:PHE:O	1:A:163:ASN:O	2.38	0.40
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.97	0.40
1:A:369:VAL:HB	1:A:543:ALA:HA	2.02	0.40
1:A:385:LYS:HE3	1:B:214:ARG:NH2	2.31	0.40
1:A:106:LYS:CD	1:A:110:LEU:HD12	2.50	0.40
1:A:341:ILE:CG2	1:A:364:ILE:HB	2.52	0.40
1:A:516:SER:HA	1:A:519:GLN:NE2	2.36	0.40
1:B:472:VAL:O	1:B:476:GLY:HA2	2.22	0.40
1:A:306:GLN:O	1:A:309:LYS:HB3	2.21	0.40
1:A:564:MET:SD	1:A:568:GLY:HA3	2.61	0.40
1:B:168:LEU:O	1:B:172:VAL:HG23	2.22	0.40
1:B:456:TYR:HE2	1:B:486:ARG:HD3	1.86	0.40
1:A:11:LYS:O	1:A:14:PRO:HD2	2.21	0.40
1:A:368:LYS:HG2	1:A:369:VAL:O	2.22	0.40
1:A:375:PRO:HG3	1:A:550:GLU:OE1	2.21	0.40
1:A:480:SER:O	1:A:484:ARG:HG3	2.22	0.40
1:B:107:LEU:HD11	1:B:123:THR:CG2	2.51	0.40
1:A:90:TYR:O	1:A:94:LYS:HG2	2.20	0.40
1:A:281:GLY:O	1:A:285:ALA:N	2.54	0.40
1:B:433:GLU:HA	1:B:436:CYS:HB2	2.04	0.40
1:B:461:ILE:H	1:B:461:ILE:HG12	1.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	569/599 (95%)	506 (89%)	59 (10%)	4 (1%)	19	56
1	B	569/599 (95%)	508 (89%)	58 (10%)	3 (0%)	25	63
All	All	1138/1198 (95%)	1014 (89%)	117 (10%)	7 (1%)	24	59

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	443	VAL
1	B	443	VAL
1	A	58	SER
1	A	444	THR
1	B	497	PRO
1	B	24	PRO

5.3.2 Protein sidechains [i](#)

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	481/506 (95%)	480 (100%)	1 (0%)	92	94
1	B	481/506 (95%)	480 (100%)	1 (0%)	92	94
All	All	962/1012 (95%)	960 (100%)	2 (0%)	91	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	338	HIS
1	B	140	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	141	HIS
1	A	163	ASN
1	A	354	GLN
1	A	416	HIS
1	A	422	GLN
1	A	434	ASN
1	A	467	GLN
1	A	483	GLN
1	A	561	HIS
1	B	519	GLN
1	B	561	HIS
1	B	577	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

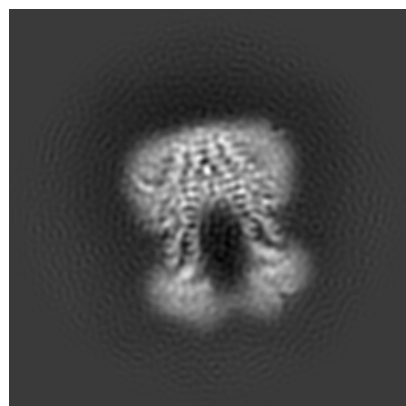
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19185. These allow visual inspection of the internal detail of the map and identification of artifacts.

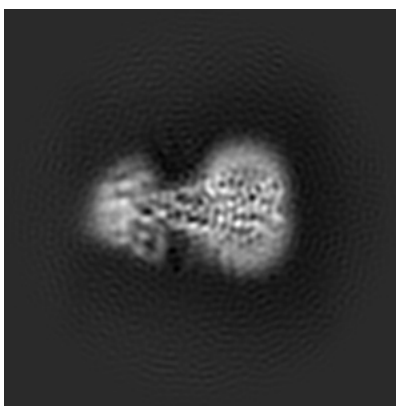
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

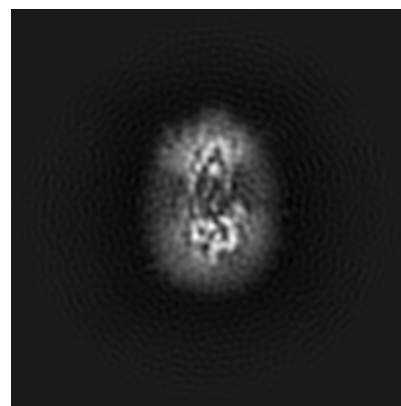
6.1.1 Primary map



X

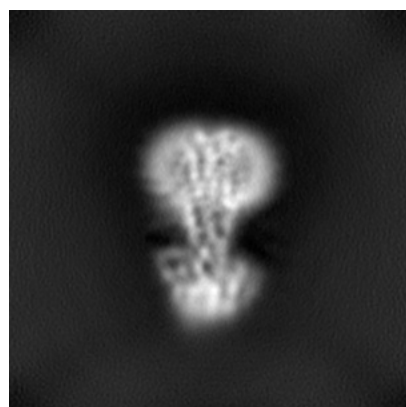


Y

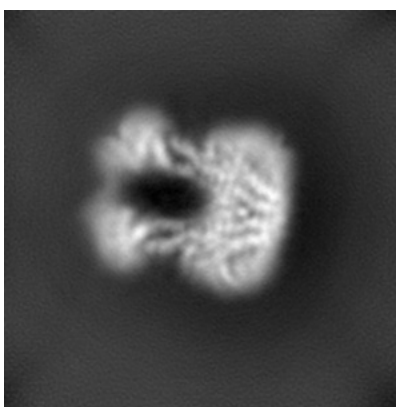


Z

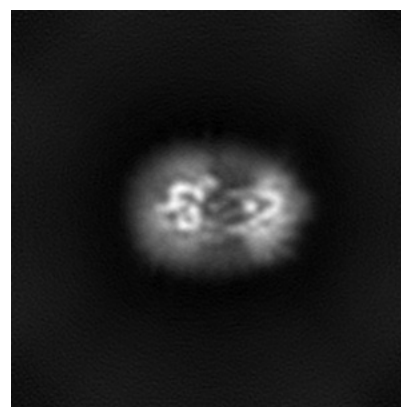
6.1.2 Raw map



X



Y

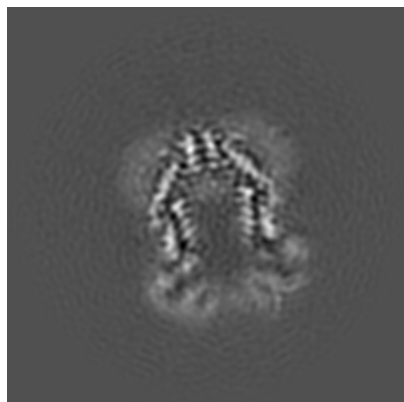


Z

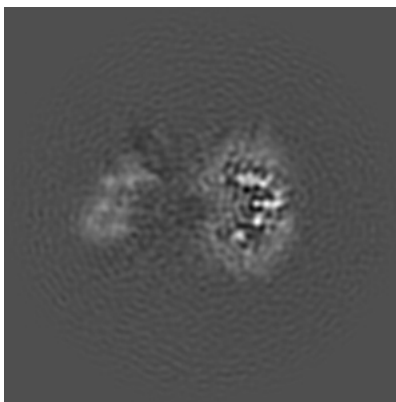
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

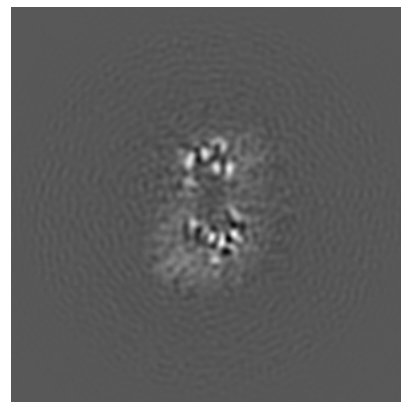
6.2.1 Primary map



X Index: 100

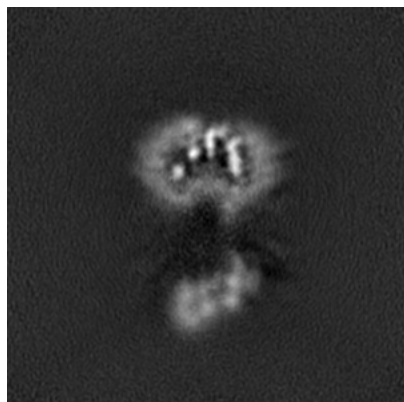


Y Index: 100

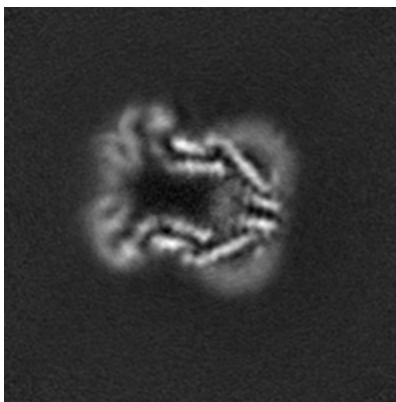


Z Index: 100

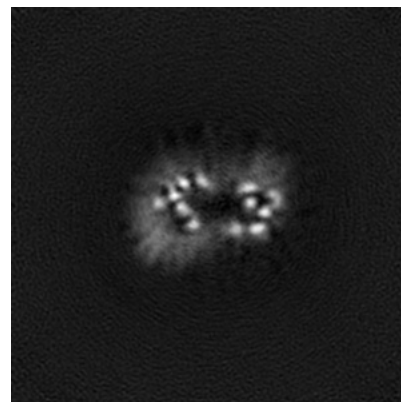
6.2.2 Raw map



X Index: 100



Y Index: 100

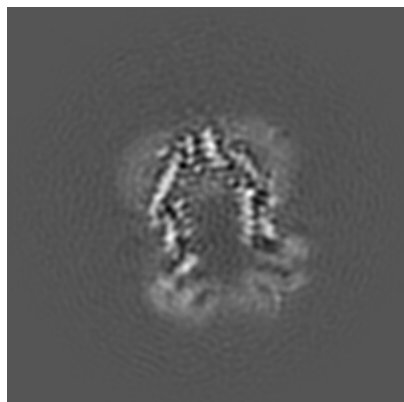


Z Index: 100

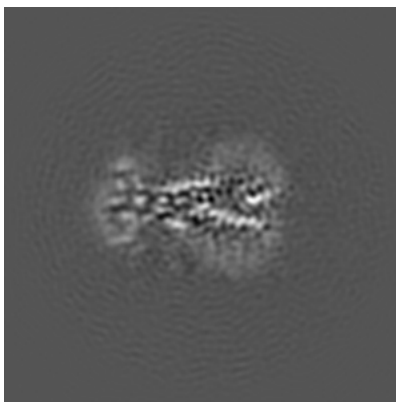
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

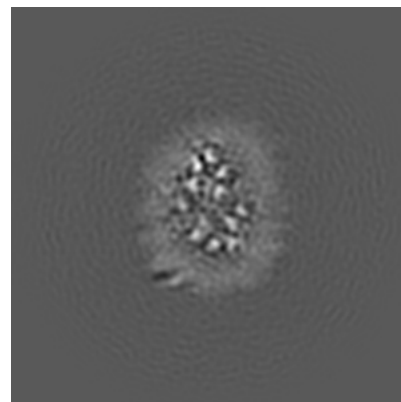
6.3.1 Primary map



X Index: 101

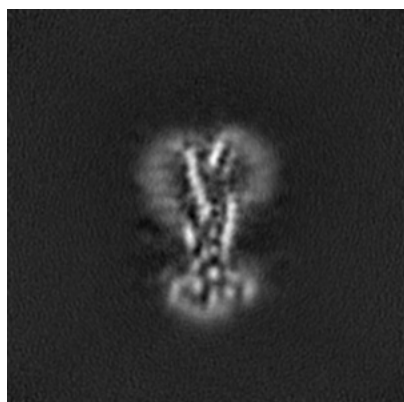


Y Index: 85

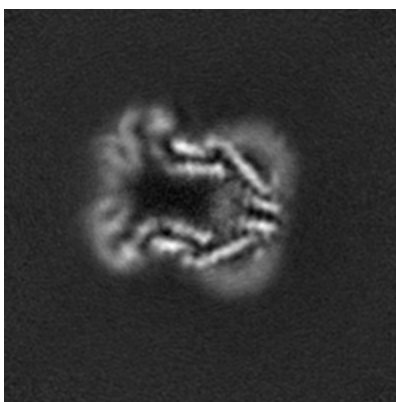


Z Index: 116

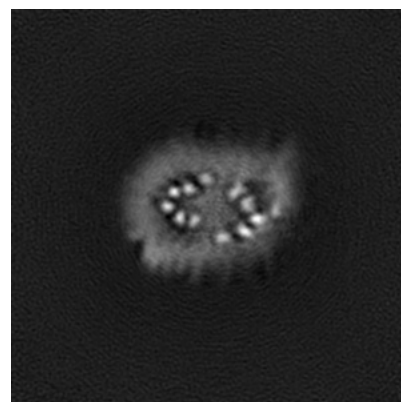
6.3.2 Raw map



X Index: 85



Y Index: 100

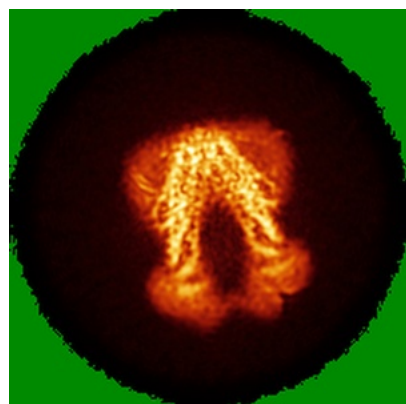


Z Index: 109

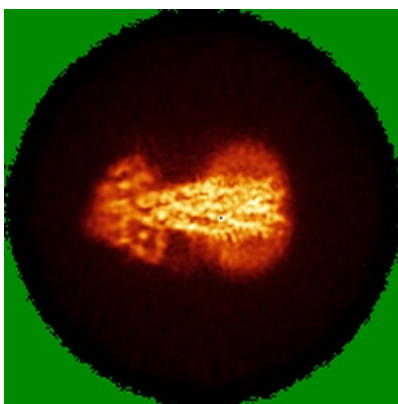
The images above show the largest variance slices of the map in three orthogonal directions.

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

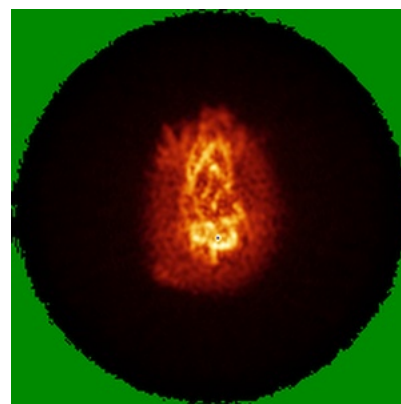
6.4.1 Primary map



X



Y

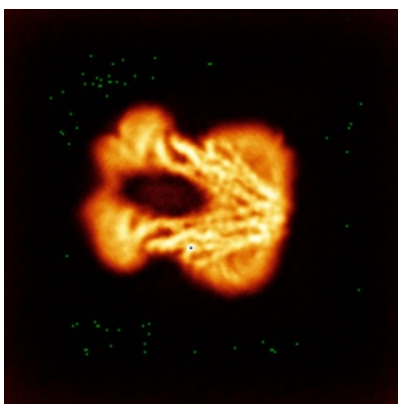


Z

6.4.2 Raw map



X



Y

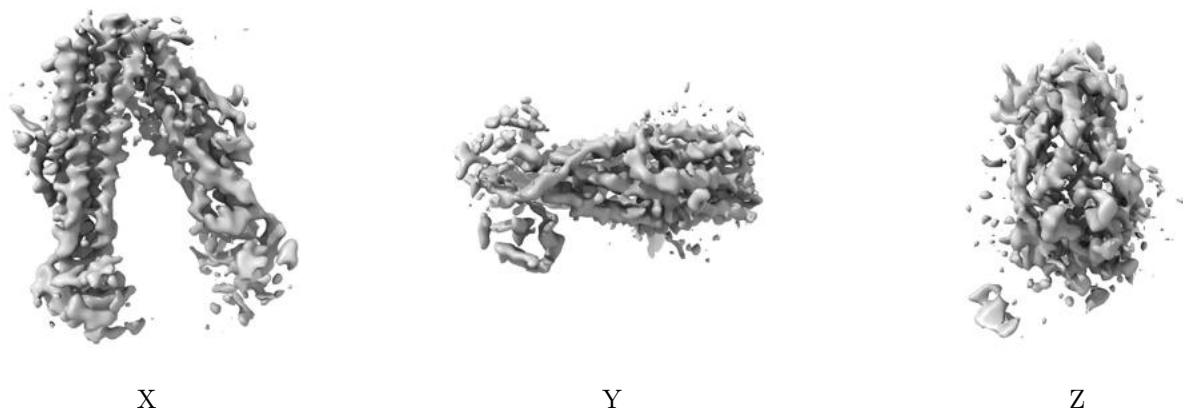


Z

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

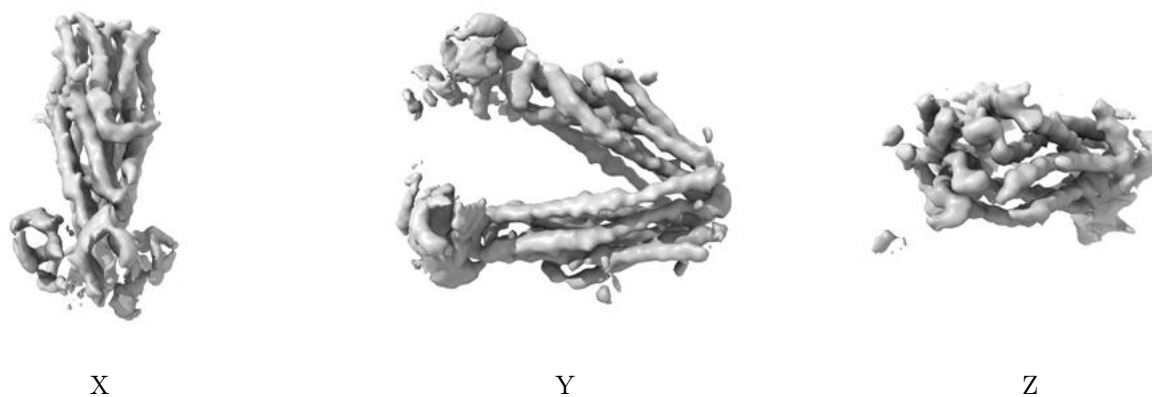
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.218. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

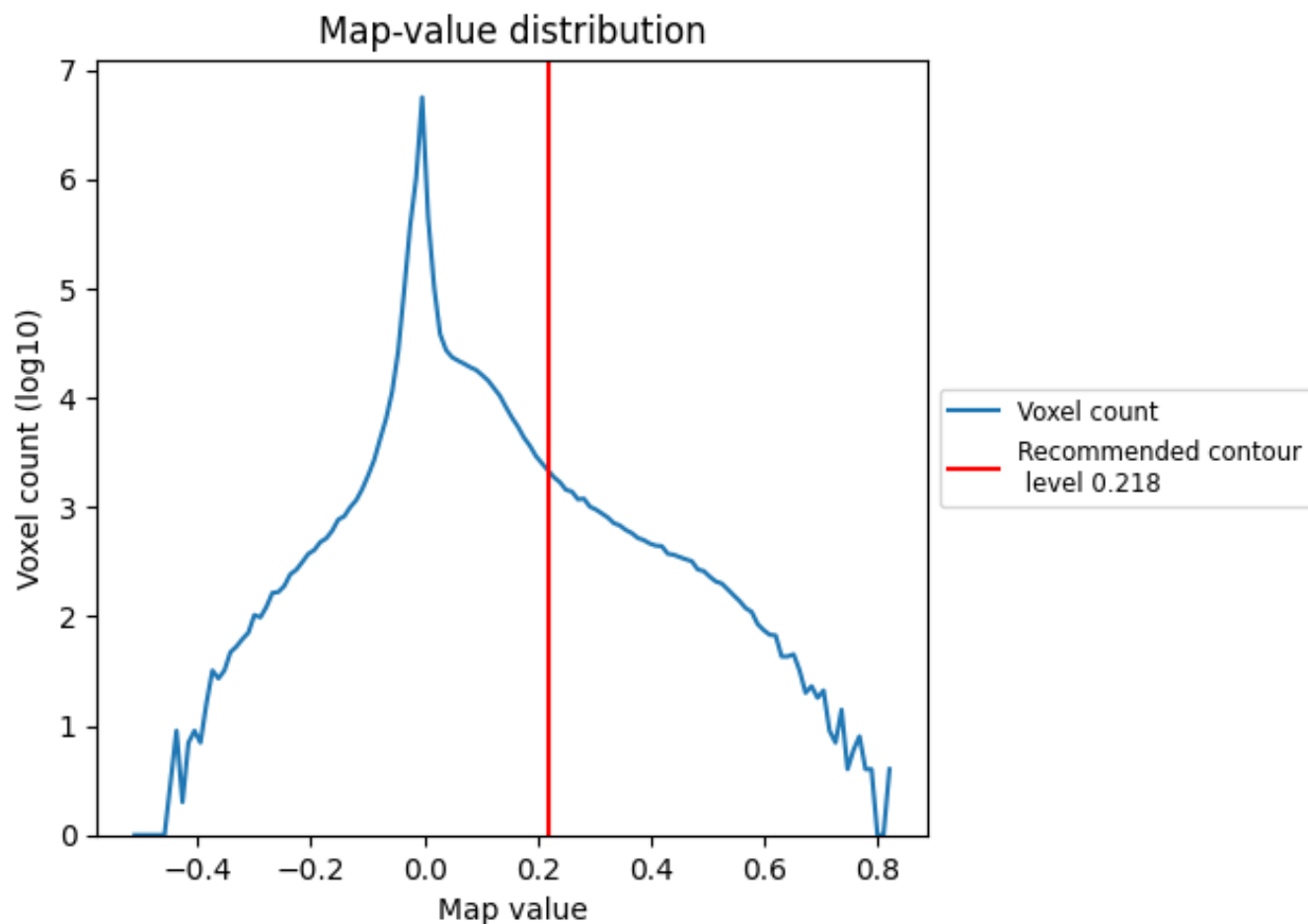
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

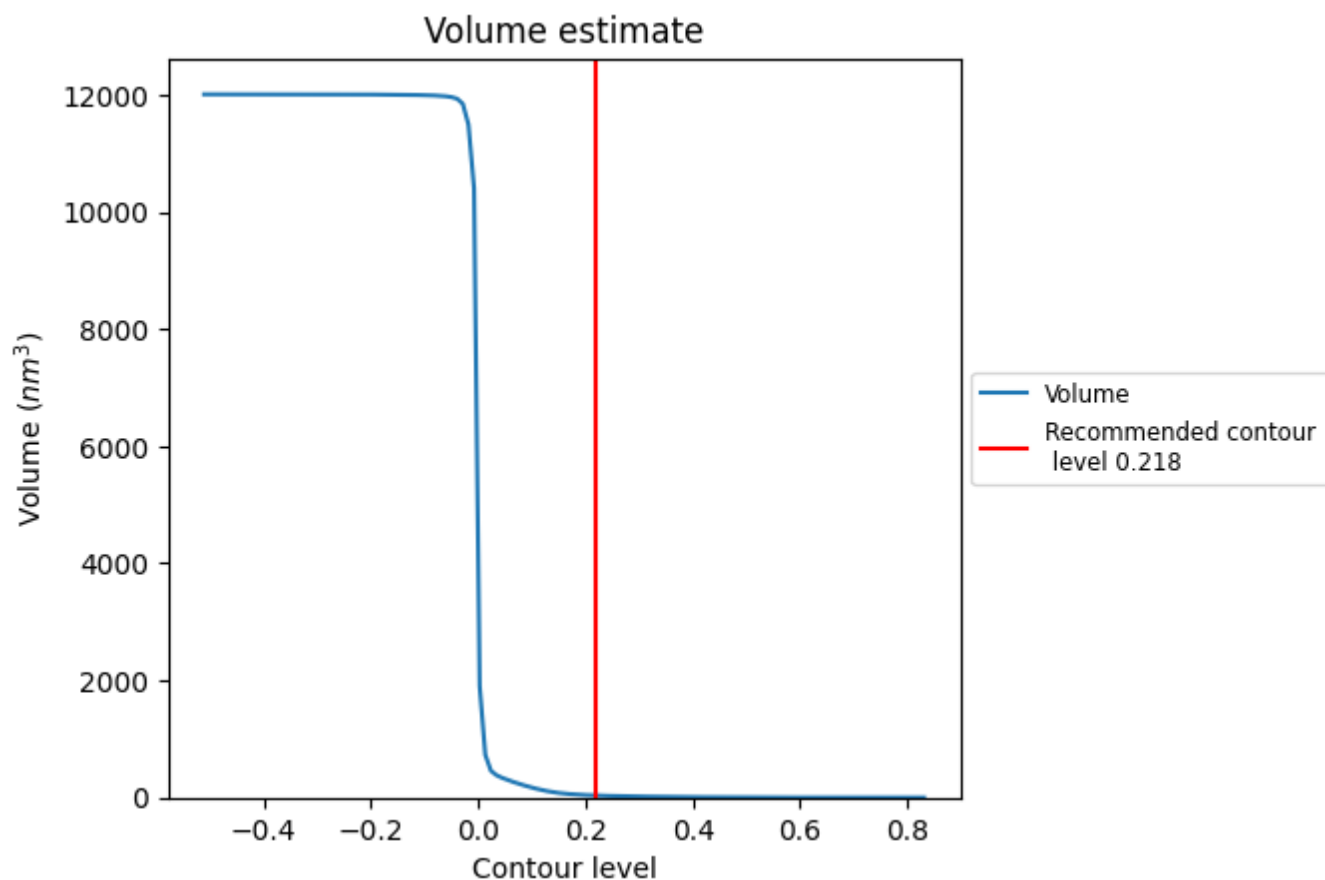
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

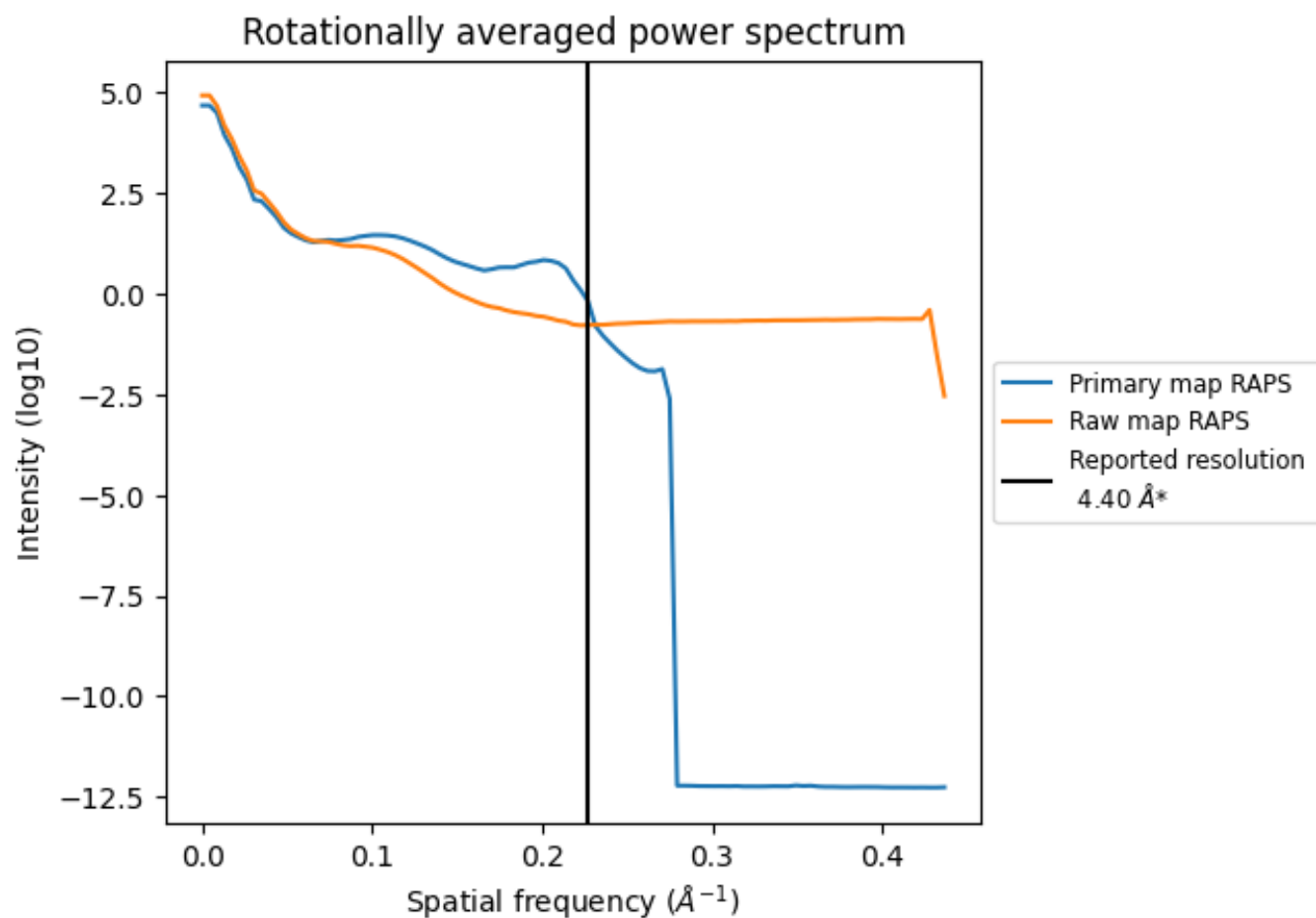
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 36 nm³; this corresponds to an approximate mass of 32 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 ⓘ

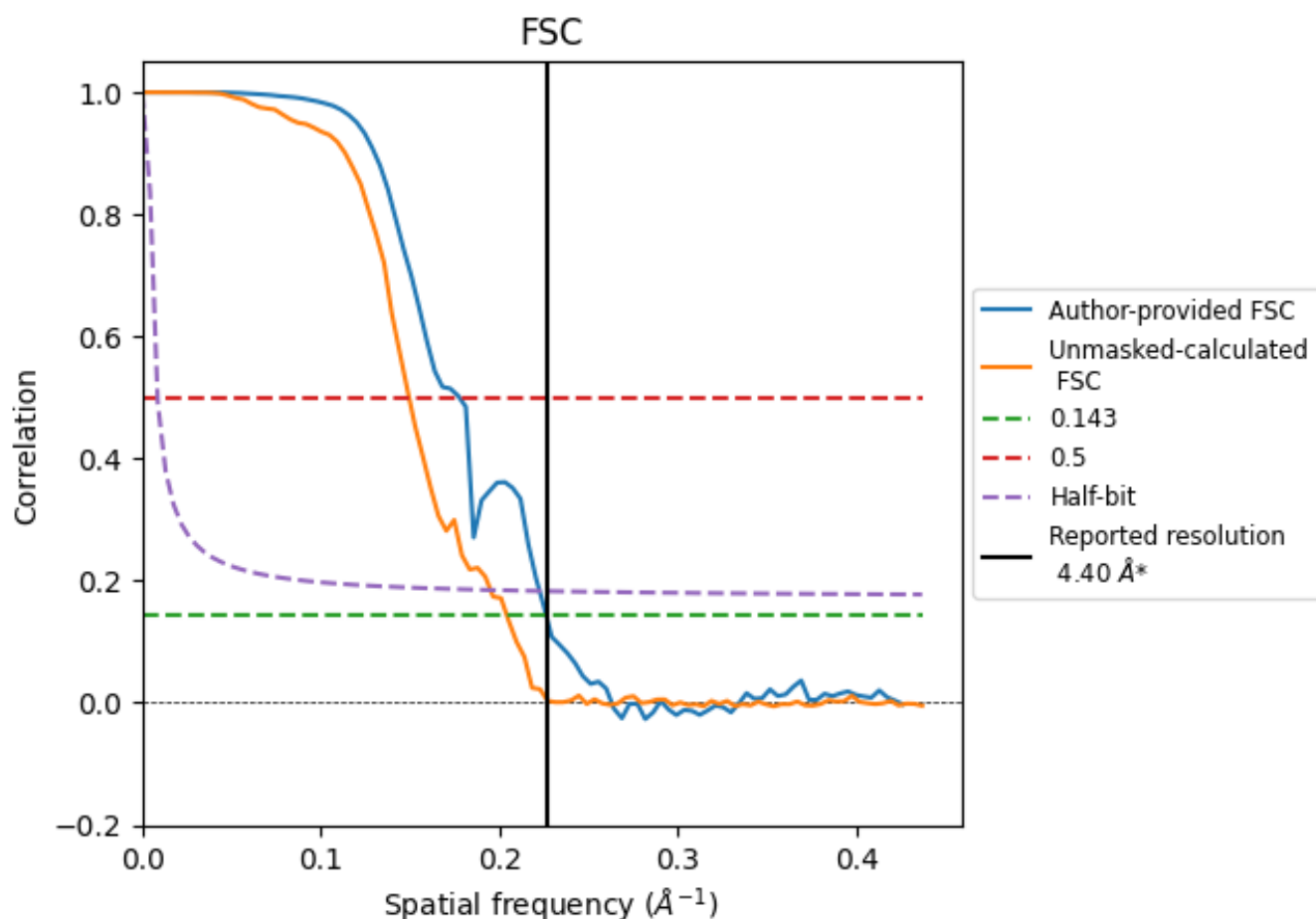


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 \AA^{-1}

8.2 Resolution estimates [i](#)

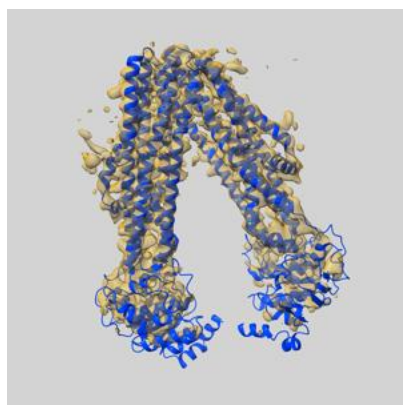
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.42	5.63	4.49
Unmasked-calculated*	4.90	6.69	5.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.90 differs from the reported value 4.4 by more than 10 %

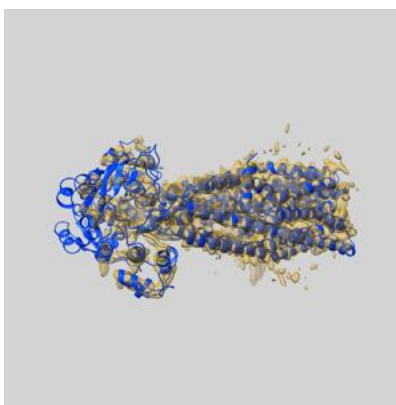
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19185 and PDB model 8RIA. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

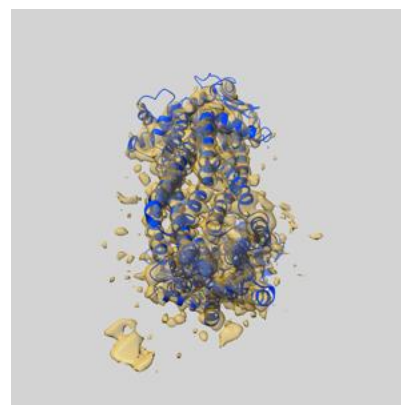
9.1 Map-model overlay [i](#)



X



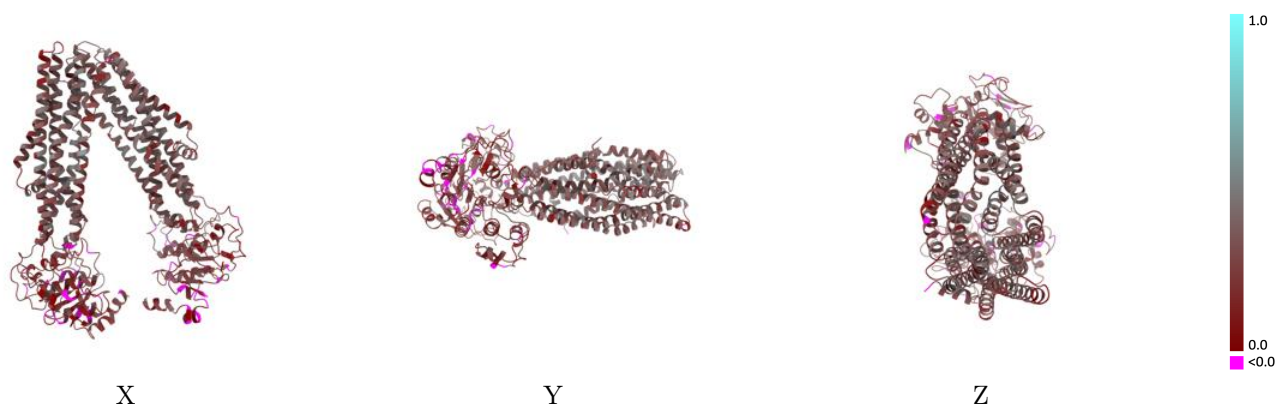
Y



Z

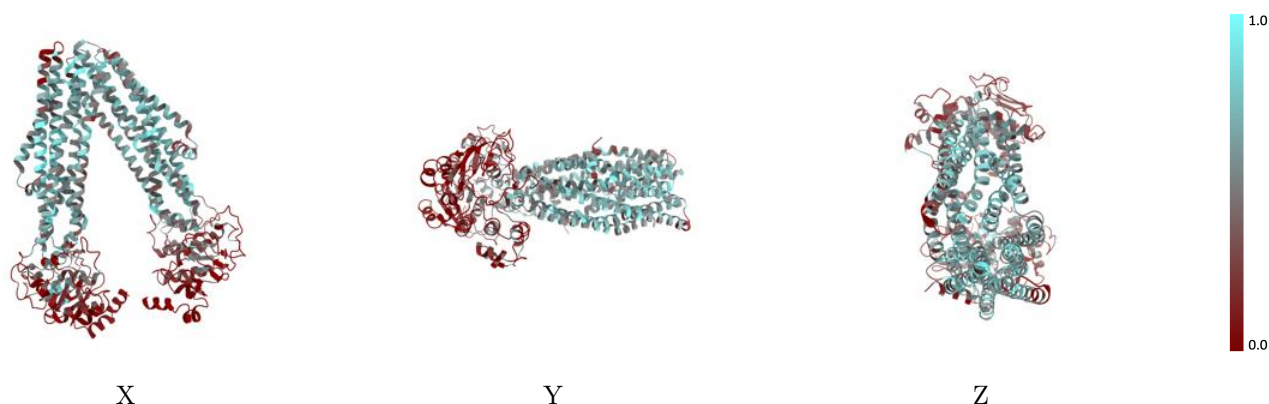
The images above show the 3D surface view of the map at the recommended contour level 0.218 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



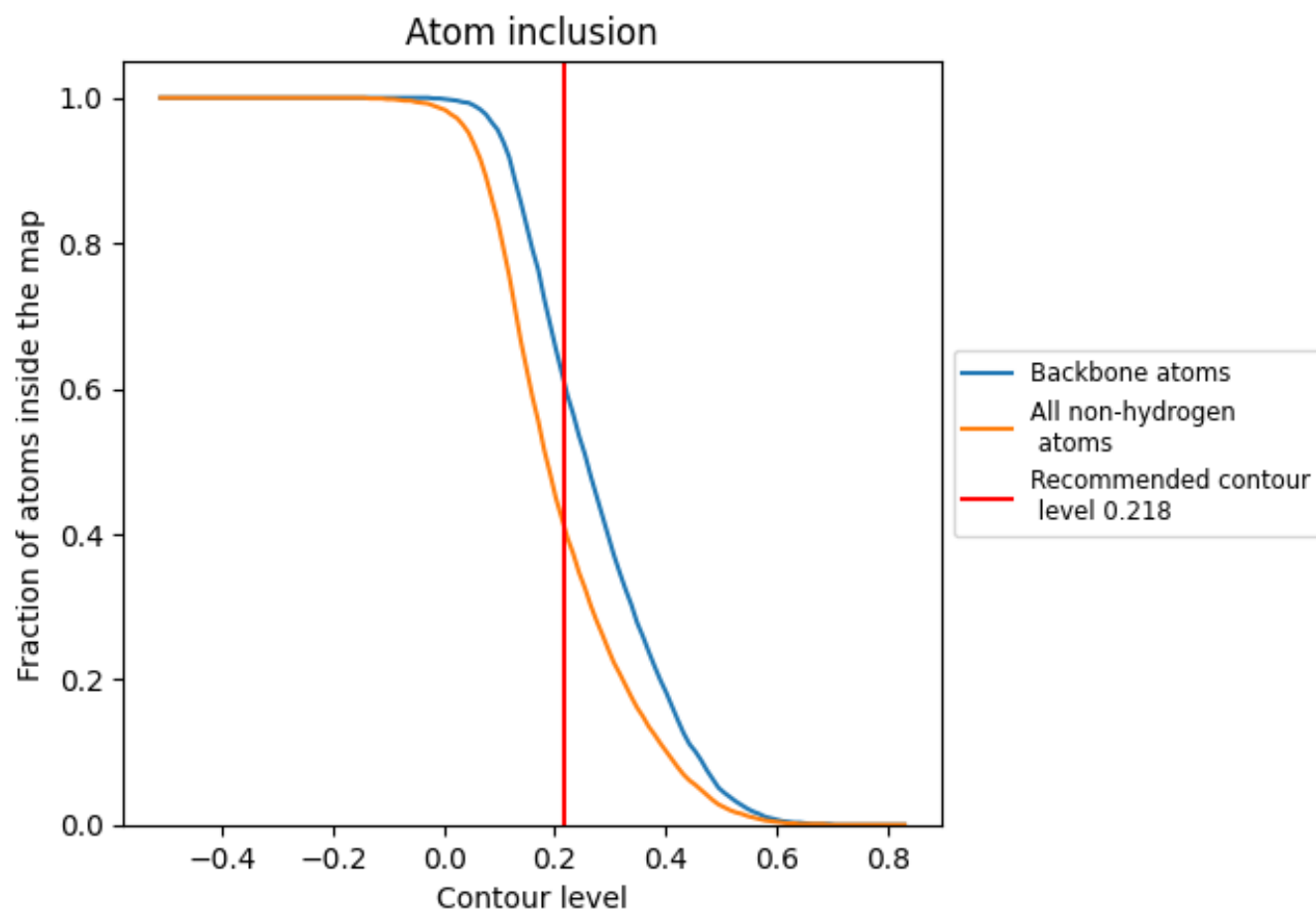
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.218).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 41% 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 (0.218) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4090	<div></div> 0.2670
A	<div></div> 0.4060	<div></div> 0.2690
B	<div></div> 0.4110	<div></div> 0.2660

