Full wwPDB EM Validation Report ⓘ

May 1, 2024 – 04:20 pm BST

PDB ID	:	8QQM
EMDB ID	:	EMD-18596
Title	:	nicotinic acetylcholine receptor in intact synaptic membrane
Authors	:	Unwin, N.
Deposited on	:	2023-10-05
Resolution	:	4.70 Å(reported)
Based on initial model	:	7SMM

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:

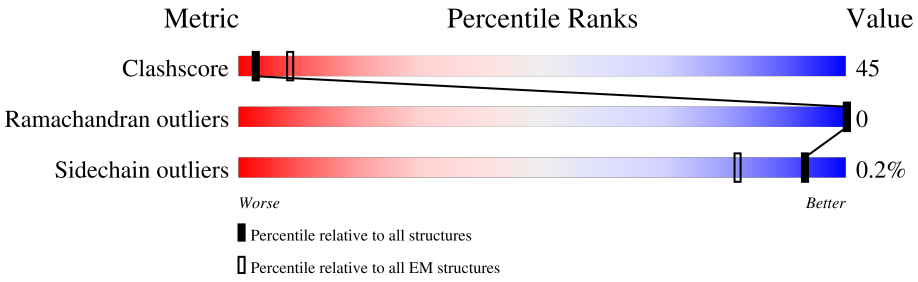
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	437	8% 24% 17% 58%
1	D	437	6% 25% 15% 58%
2	B	501	22% 13% 64%
3	C	469	7% 21% 14% 62%
4	E	489	19% 15% 65%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7118 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 Acetylcholine receptor subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	184	Total	C	N	O	S	0	0
			1450	964	221	253	12		
1	D	184	Total	C	N	O	S	0	0
			1450	964	221	253	12		

- Molecule 2 is a protein called Acetylcholine receptor subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	180	Total	C	N	O	S	0	0
			1420	937	226	248	9		

- Molecule 3 is a protein called Acetylcholine receptor subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	180	Total	C	N	O	S	0	0
			1455	980	220	248	7		

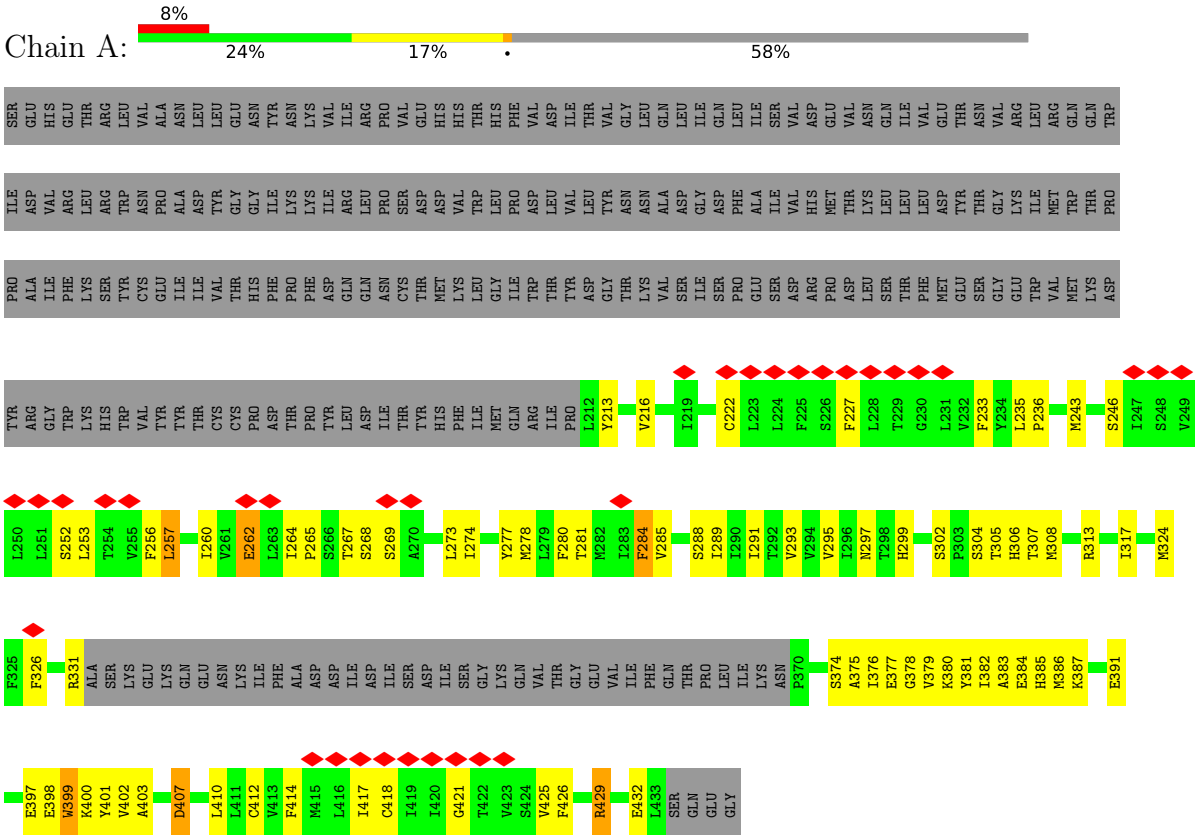
- Molecule 4 is a protein called Acetylcholine receptor subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	173	Total	C	N	O	S	0	0
			1343	896	208	230	9		

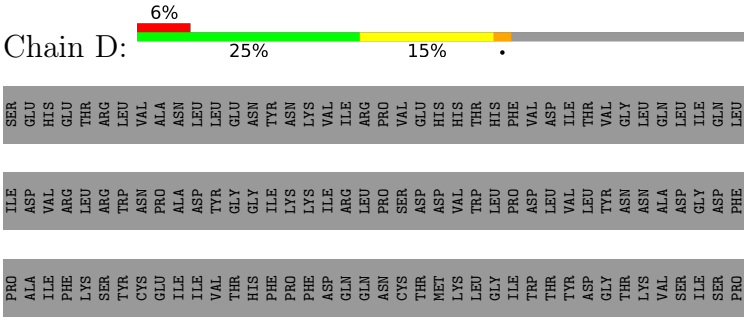
3 Residue-property plots (i)

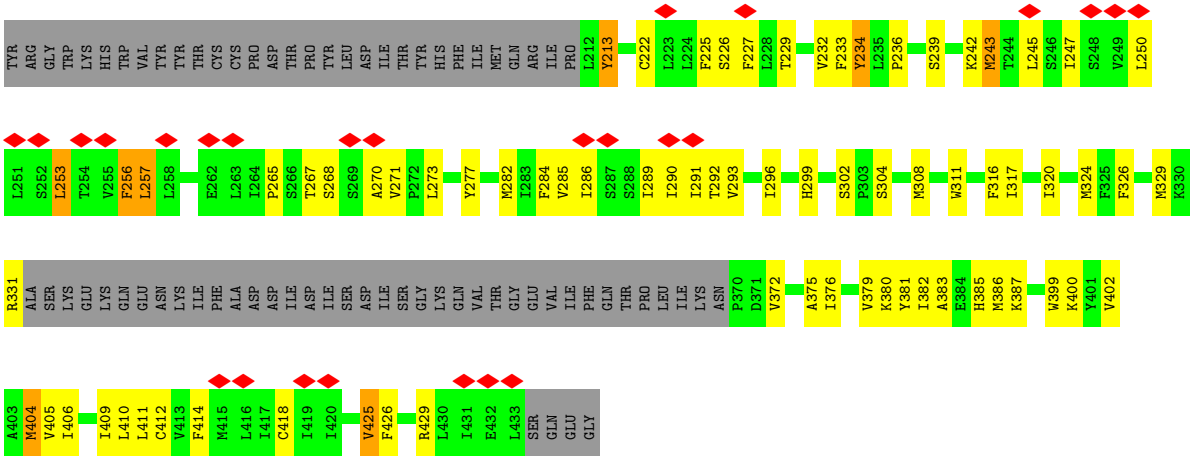
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



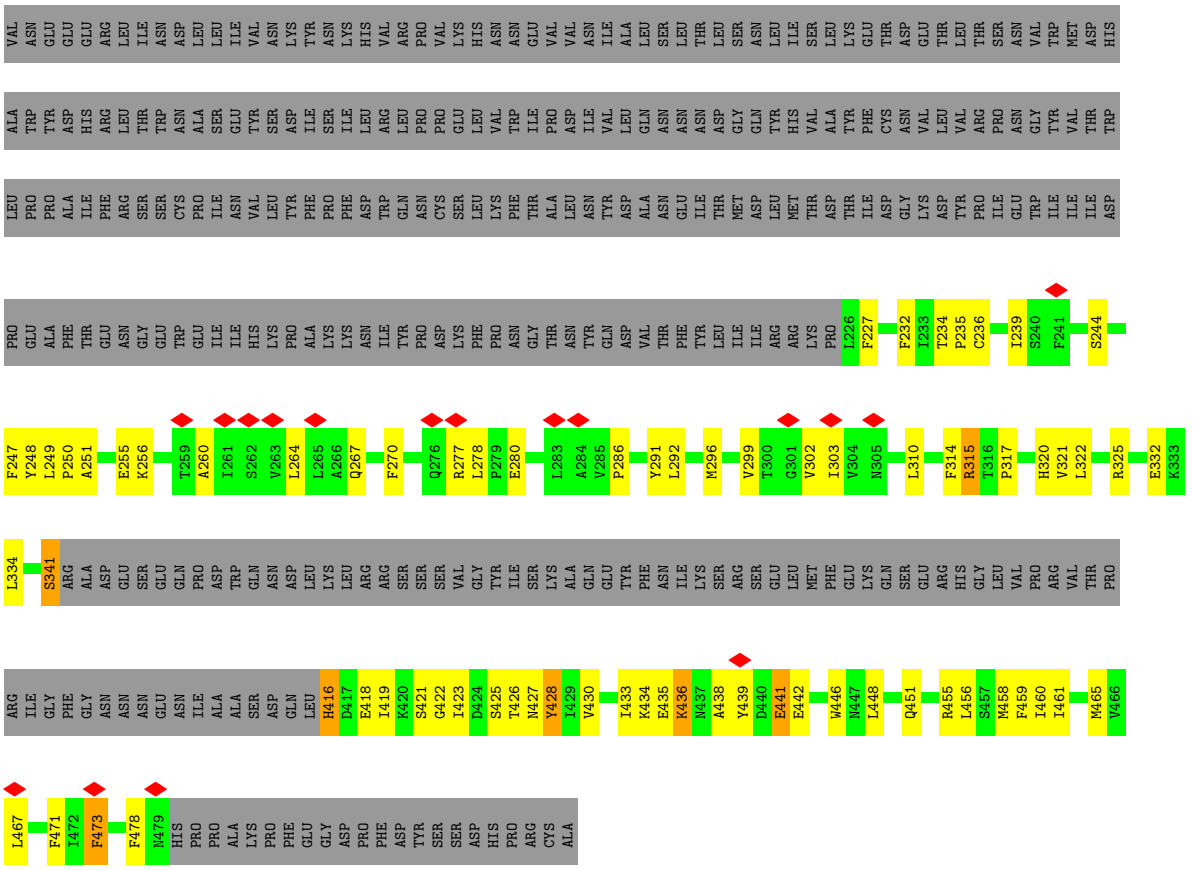
• Molecule 1: Acetylcholine receptor subunit alpha





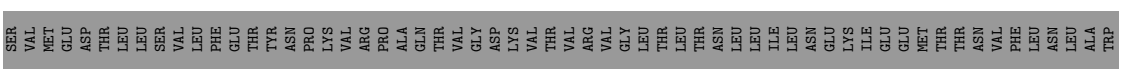
• Molecule 2: Acetylcholine receptor subunit delta

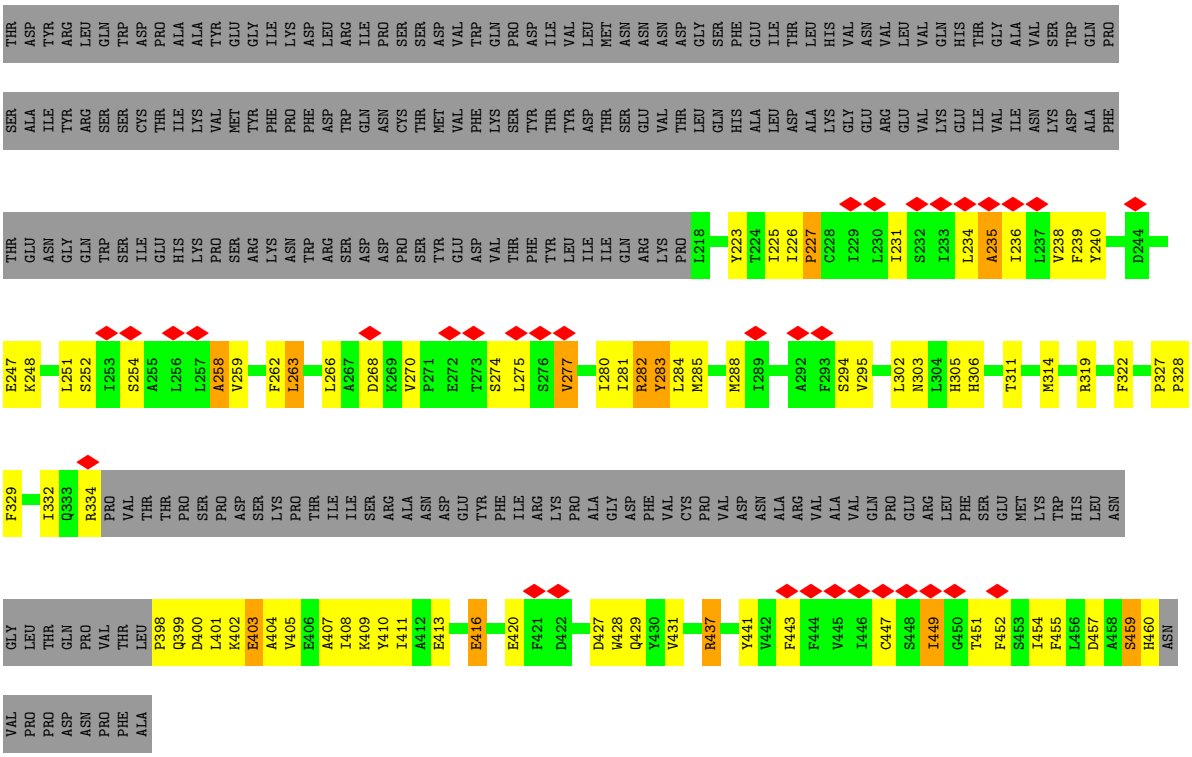
Chain B:



• Molecule 3: Acetylcholine receptor subunit beta

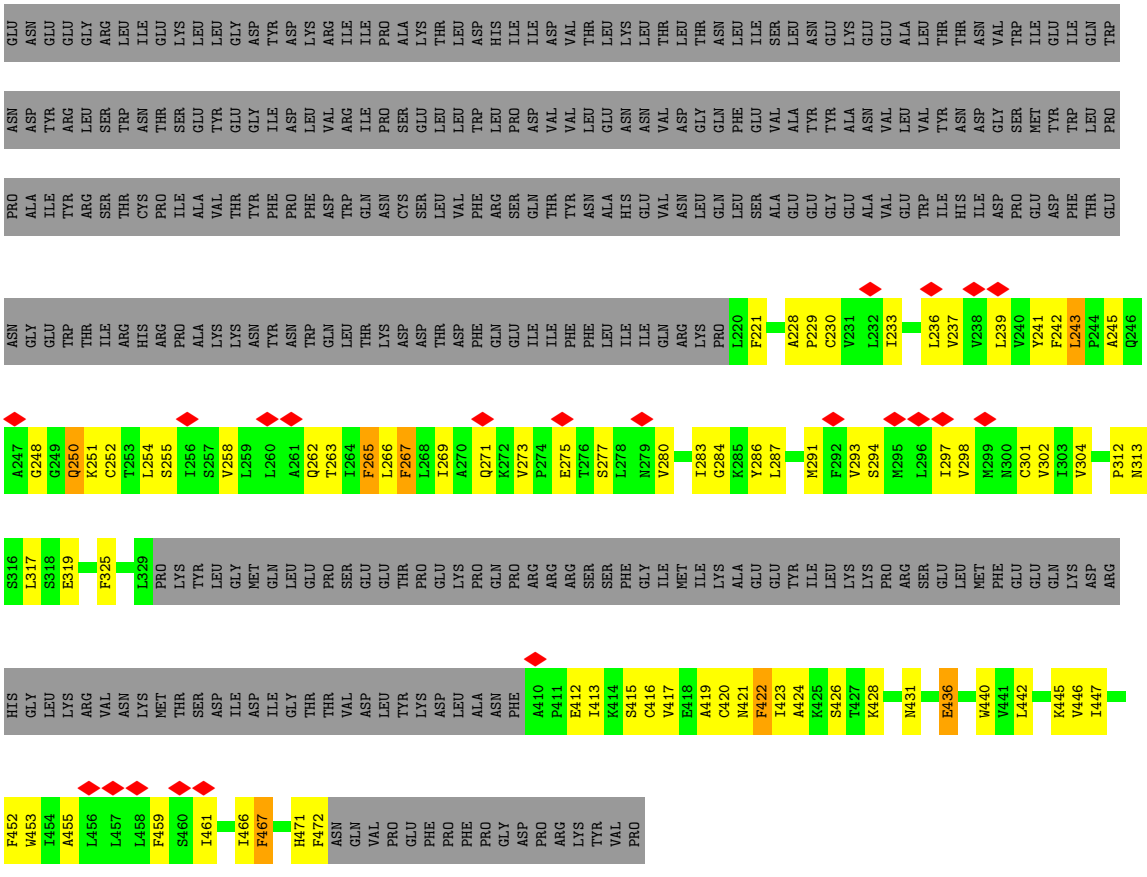
Chain C:





• Molecule 4: Acetylcholine receptor subunit gamma

Chain E:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	107524	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Correction performed by standard procedure in RELION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.001	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.0005	Depositor
Map size (Å)	268.0, 268.0, 268.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.58	2/1482 (0.1%)	1.60	23/2015 (1.1%)
1	D	1.53	0/1482	1.49	20/2015 (1.0%)
2	B	1.61	2/1449 (0.1%)	1.69	26/1966 (1.3%)
3	C	1.63	4/1493 (0.3%)	1.77	37/2037 (1.8%)
4	E	1.60	2/1370 (0.1%)	1.65	26/1861 (1.4%)
All	All	1.59	10/7276 (0.1%)	1.64	132/9894 (1.3%)

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	1
3	C	0	2
4	E	0	1
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	398	GLU	CD-OE1	-5.78	1.19	1.25
3	C	247	GLU	CD-OE2	-5.65	1.19	1.25
4	E	436	GLU	CD-OE1	-5.60	1.19	1.25
4	E	319	GLU	CD-OE2	-5.54	1.19	1.25
3	C	420	GLU	CD-OE1	-5.40	1.19	1.25
3	C	416	GLU	CD-OE1	-5.38	1.19	1.25
3	C	403	GLU	CD-OE1	-5.28	1.19	1.25
1	A	397	GLU	CD-OE1	5.27	1.31	1.25
2	B	435	GLU	CD-OE1	-5.22	1.20	1.25
2	B	441	GLU	CD-OE1	-5.03	1.20	1.25

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	282	ARG	NE-CZ-NH2	-17.22	111.69	120.30
3	C	437	ARG	NE-CZ-NH2	-15.21	112.69	120.30
2	B	471	PHE	CB-CG-CD1	14.58	131.01	120.80
2	B	315	ARG	NE-CZ-NH2	-14.57	113.01	120.30
2	B	280	GLU	OE1-CD-OE2	10.69	136.13	123.30
2	B	471	PHE	CG-CD1-CE1	10.55	132.40	120.80
3	C	437	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	A	326	PHE	CB-CG-CD2	-10.42	113.50	120.80
2	B	478	PHE	CB-CG-CD2	9.94	127.75	120.80
4	E	275	GLU	OE1-CD-OE2	9.80	135.06	123.30
3	C	452	PHE	CB-CG-CD2	-9.46	114.18	120.80
3	C	452	PHE	CB-CG-CD1	9.03	127.12	120.80
1	D	213	TYR	CG-CD2-CE2	-9.02	114.09	121.30
1	A	429	ARG	NE-CZ-NH2	8.79	124.69	120.30
1	A	313	ARG	NE-CZ-NH1	-8.06	116.27	120.30
2	B	315	ARG	NE-CZ-NH1	8.00	124.30	120.30
3	C	334	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	D	331	ARG	NE-CZ-NH2	-7.70	116.45	120.30
2	B	478	PHE	CG-CD2-CE2	7.69	129.26	120.80
3	C	223	TYR	CB-CG-CD1	-7.48	116.51	121.00
4	E	273	VAL	CA-CB-CG2	-7.45	99.72	110.90
1	D	425	VAL	CA-CB-CG2	-7.37	99.84	110.90
1	A	399	TRP	CE2-CD2-CG	-7.31	101.45	107.30
4	E	472	PHE	CG-CD1-CE1	7.31	128.84	120.80
3	C	413	GLU	OE1-CD-OE2	-7.21	114.65	123.30
1	A	313	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	A	377	GLU	OE1-CD-OE2	-7.18	114.68	123.30
3	C	277	VAL	CG1-CB-CG2	-7.17	99.44	110.90
1	D	265	PRO	O-C-N	7.14	134.12	122.70
1	D	225	PHE	CB-CG-CD1	7.01	125.71	120.80
2	B	473	PHE	CZ-CE2-CD2	7.00	128.51	120.10
2	B	455	ARG	NE-CZ-NH2	6.95	123.77	120.30
4	E	271	GLN	O-C-N	-6.86	111.73	122.70
1	A	331	ARG	NE-CZ-NH2	6.85	123.72	120.30
2	B	428	TYR	CB-CG-CD1	-6.77	116.94	121.00
4	E	459	PHE	CB-CG-CD2	-6.77	116.06	120.80
3	C	329	PHE	CB-CG-CD2	-6.71	116.10	120.80
3	C	227	PRO	CA-N-CD	6.60	120.94	111.70
4	E	319	GLU	CG-CD-OE2	6.60	131.49	118.30
4	E	453	TRP	CE2-CD2-CG	-6.56	102.05	107.30
3	C	268	ASP	O-C-N	-6.56	112.21	122.70
3	C	452	PHE	CG-CD1-CE1	6.55	128.00	120.80
4	E	472	PHE	CB-CG-CD2	6.54	125.38	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	478	PHE	CD1-CG-CD2	-6.53	109.81	118.30
1	D	331	ARG	NE-CZ-NH1	6.53	123.56	120.30
2	B	439	TYR	CB-CG-CD2	-6.53	117.08	121.00
4	E	453	TRP	CD1-CG-CD2	6.52	111.52	106.30
1	D	270	ALA	N-CA-CB	6.50	119.20	110.10
1	D	311	TRP	CD1-CG-CD2	-6.44	101.15	106.30
3	C	427	ASP	CB-CG-OD2	6.32	123.99	118.30
3	C	258	ALA	CB-CA-C	6.32	119.58	110.10
3	C	441	TYR	CG-CD2-CE2	-6.28	116.28	121.30
2	B	321	VAL	CG1-CB-CG2	-6.24	100.92	110.90
3	C	334	ARG	NH1-CZ-NH2	-6.21	112.58	119.40
1	D	257	LEU	CB-CG-CD2	-6.20	100.46	111.00
3	C	399	GLN	CG-CD-OE1	-6.19	109.21	121.60
3	C	235	ALA	N-CA-CB	-6.19	101.44	110.10
2	B	471	PHE	CB-CG-CD2	-6.19	116.47	120.80
4	E	284	GLY	O-C-N	-6.15	112.85	122.70
2	B	473	PHE	CG-CD2-CE2	-6.15	114.03	120.80
3	C	441	TYR	CZ-CE2-CD2	6.13	125.32	119.80
1	A	326	PHE	CG-CD2-CE2	-6.12	114.07	120.80
3	C	441	TYR	CG-CD1-CE1	6.11	126.19	121.30
1	D	225	PHE	CB-CG-CD2	-6.11	116.52	120.80
1	A	432	GLU	OE1-CD-OE2	-6.01	116.09	123.30
2	B	325	ARG	NE-CZ-NH1	5.99	123.30	120.30
2	B	314	PHE	CG-CD2-CE2	5.98	127.38	120.80
1	A	262	GLU	OE1-CD-OE2	5.96	130.45	123.30
4	E	248	GLY	O-C-N	5.88	133.20	123.20
3	C	223	TYR	CZ-CE2-CD2	-5.88	114.51	119.80
1	A	227	PHE	CB-CG-CD1	-5.87	116.69	120.80
1	D	267	THR	O-C-N	-5.87	113.31	122.70
4	E	248	GLY	C-N-CA	-5.84	110.03	122.30
2	B	332	GLU	OE1-CD-OE2	-5.83	116.31	123.30
4	E	472	PHE	CD1-CG-CD2	-5.77	110.80	118.30
1	D	213	TYR	CZ-CE2-CD2	5.71	124.94	119.80
3	C	334	ARG	NE-CZ-NH1	5.71	123.15	120.30
3	C	254	SER	O-C-N	-5.70	113.58	122.70
1	A	421	GLY	O-C-N	-5.69	113.59	122.70
2	B	459	PHE	CG-CD1-CE1	5.68	127.05	120.80
4	E	461	ILE	O-C-N	-5.65	113.60	123.20
1	A	280	PHE	CB-CG-CD1	5.64	124.75	120.80
2	B	428	TYR	CB-CG-CD2	5.64	124.38	121.00
3	C	457	ASP	CB-CG-OD1	5.63	123.36	118.30
4	E	293	VAL	O-C-N	-5.62	113.70	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	227	PHE	CB-CG-CD2	-5.61	116.88	120.80
4	E	422	PHE	CB-CG-CD1	5.58	124.71	120.80
3	C	270	VAL	CA-CB-CG2	-5.53	102.61	110.90
3	C	282	ARG	NE-CZ-NH1	5.52	123.06	120.30
4	E	263	THR	CA-CB-CG2	-5.50	104.70	112.40
4	E	265	PHE	CB-CG-CD2	-5.48	116.97	120.80
1	D	271	VAL	CA-CB-CG1	-5.46	102.72	110.90
1	D	253	LEU	O-C-N	-5.44	114.00	122.70
1	A	265	PRO	N-CA-CB	5.41	109.79	103.30
2	B	416	HIS	N-CA-CB	5.38	120.28	110.60
1	A	269	SER	N-CA-CB	-5.34	102.48	110.50
3	C	223	TYR	CG-CD1-CE1	-5.34	117.03	121.30
3	C	263	LEU	CB-CG-CD1	5.32	120.04	111.00
3	C	282	ARG	NH1-CZ-NH2	5.32	125.25	119.40
3	C	322	PHE	CB-CG-CD1	5.29	124.50	120.80
3	C	283	TYR	CB-CG-CD1	5.28	124.17	121.00
1	A	429	ARG	NE-CZ-NH1	-5.28	117.66	120.30
3	C	449	ILE	CA-CB-CG1	-5.25	101.02	111.00
4	E	471	HIS	CG-CD2-NE2	-5.25	99.22	109.20
4	E	275	GLU	CG-CD-OE2	-5.24	107.83	118.30
2	B	341	SER	CA-C-O	5.21	131.05	120.10
1	A	326	PHE	CB-CG-CD1	5.21	124.45	120.80
3	C	459	SER	CA-C-O	-5.20	109.19	120.10
2	B	280	GLU	CG-CD-OE2	-5.19	107.92	118.30
1	A	407	ASP	CB-CG-OD2	5.18	122.96	118.30
4	E	319	GLU	OE1-CD-OE2	-5.18	117.09	123.30
4	E	467	PHE	CB-CG-CD2	-5.17	117.18	120.80
1	A	401	TYR	CG-CD2-CE2	-5.17	117.17	121.30
2	B	467	LEU	O-C-N	-5.15	114.44	123.20
1	A	391	GLU	OE1-CD-OE2	5.12	129.45	123.30
1	A	257	LEU	CB-CG-CD1	5.12	119.70	111.00
1	D	311	TRP	CG-CD2-CE3	-5.12	129.29	133.90
4	E	250	GLN	O-C-N	5.12	130.88	122.70
1	D	243	MET	O-C-N	-5.11	114.52	122.70
1	A	284	PHE	CD1-CE1-CZ	5.08	126.20	120.10
3	C	452	PHE	CD1-CE1-CZ	-5.08	114.01	120.10
1	D	234	TYR	CG-CD2-CE2	-5.07	117.25	121.30
1	D	225	PHE	CG-CD2-CE2	-5.07	115.23	120.80
3	C	460	HIS	CG-ND1-CE1	5.05	115.28	108.20
4	E	243	LEU	CB-CG-CD1	-5.05	102.42	111.00
3	C	240	TYR	CD1-CE1-CZ	-5.04	115.26	119.80
4	E	266	LEU	N-CA-CB	-5.04	100.31	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	314	PHE	CZ-CE2-CD2	-5.04	114.06	120.10
1	A	252	SER	O-C-N	-5.03	114.66	122.70
2	B	478	PHE	N-CA-CB	-5.01	101.58	110.60
1	D	256	PHE	CG-CD2-CE2	-5.01	115.29	120.80
4	E	267	PHE	CG-CD2-CE2	5.01	126.31	120.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	267	THR	Mainchain
3	C	275	LEU	Mainchain
3	C	459	SER	Mainchain
4	E	315	HIS	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1450	0	1526	199	0
1	D	1450	0	1526	197	0
2	B	1420	0	1483	159	0
3	C	1455	0	1516	194	0
4	E	1343	0	1424	190	0
All	All	7118	0	7475	657	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 45.

All (657) 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)
3:C:231:ILE:HG13	3:C:262:PHE:CZ	1.72	1.22
1:A:216:VAL:HG21	4:E:280:VAL:CG2	1.69	1.21
4:E:255:SER:HB2	4:E:298:VAL:CG2	1.69	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:ILE:HD11	1:D:402:VAL:CG2	1.73	1.19
1:A:264:ILE:HG21	1:A:274:ILE:HD11	1.25	1.18
2:B:422:GLY:CA	3:C:405:VAL:HG13	1.73	1.18
1:A:376:ILE:HD13	4:E:412:GLU:C	1.65	1.17
4:E:255:SER:CB	4:E:298:VAL:HG22	1.74	1.17
3:C:259:VAL:HG12	3:C:288:MET:CE	1.74	1.15
2:B:422:GLY:HA3	3:C:405:VAL:HG13	1.29	1.14
4:E:286:TYR:CD1	4:E:466:ILE:HG21	1.80	1.14
1:D:253:LEU:HD22	1:D:285:VAL:HG21	1.25	1.14
4:E:312:PRO:HG3	4:E:436:GLU:CD	1.68	1.13
1:A:375:ALA:CB	2:B:423:ILE:HD12	1.78	1.12
1:A:381:TYR:CD2	2:B:430:VAL:HG13	1.85	1.11
1:A:257:LEU:HD13	1:A:278:MET:HE1	1.18	1.11
1:A:375:ALA:HB2	2:B:423:ILE:CG2	1.79	1.11
1:A:273:LEU:HD22	1:A:429:ARG:HG2	1.33	1.10
1:A:291:ILE:CG2	1:A:410:LEU:HD13	1.82	1.10
1:A:257:LEU:CD1	1:A:278:MET:HE1	1.79	1.10
1:A:257:LEU:HD13	1:A:278:MET:CE	1.81	1.09
3:C:259:VAL:HG12	3:C:288:MET:HE2	1.31	1.09
3:C:411:ILE:HG23	1:D:386:MET:CE	1.80	1.09
1:A:307:THR:HG22	2:B:341:SER:HB3	1.27	1.08
3:C:408:ILE:HG13	1:D:379:VAL:CG1	1.83	1.08
2:B:421:SER:HB2	3:C:409:LYS:NZ	1.70	1.07
4:E:269:ILE:HD13	4:E:287:LEU:HG	1.36	1.07
1:A:376:ILE:HD11	4:E:413:ILE:HD13	1.11	1.07
2:B:419:ILE:HA	3:C:405:VAL:HG21	1.09	1.07
3:C:408:ILE:HG13	1:D:379:VAL:HG11	1.34	1.07
1:A:386:MET:CE	4:E:423:ILE:HG23	1.84	1.06
1:A:386:MET:HE1	4:E:423:ILE:HG23	1.35	1.06
2:B:256:LYS:HD3	2:B:310:LEU:HD11	1.35	1.06
3:C:266:LEU:HD23	3:C:281:ILE:HD13	1.35	1.06
3:C:404:ALA:HB2	1:D:376:ILE:HG23	1.37	1.05
1:A:379:VAL:HG12	4:E:419:ALA:HB3	1.06	1.04
1:D:302:SER:CB	4:E:445:LYS:HE2	1.87	1.04
1:A:216:VAL:HG21	4:E:280:VAL:HG22	1.40	1.04
4:E:262:GLN:HB3	4:E:291:MET:HE3	1.38	1.04
3:C:283:TYR:CE2	3:C:455:PHE:HE1	1.74	1.03
1:D:299:HIS:NE2	1:D:400:LYS:HG2	1.73	1.03
1:A:378:GLY:CA	2:B:430:VAL:HG21	1.89	1.03
2:B:264:LEU:CD2	3:C:234:LEU:HD11	1.86	1.03
2:B:239:ILE:HD12	2:B:270:PHE:CE2	1.93	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:231:ILE:HG13	3:C:262:PHE:CE2	1.95	1.02
3:C:283:TYR:CD1	3:C:454:ILE:HG21	1.93	1.02
3:C:411:ILE:HG23	1:D:386:MET:HE1	1.05	1.01
1:A:375:ALA:CB	2:B:423:ILE:HG23	1.88	1.01
1:D:302:SER:HB2	4:E:445:LYS:HE2	1.02	1.01
1:A:291:ILE:HG21	1:A:410:LEU:HD13	1.36	1.01
1:A:379:VAL:HG12	4:E:419:ALA:CB	1.92	1.00
4:E:262:GLN:HB3	4:E:291:MET:CE	1.93	0.99
4:E:325:PHE:HD1	4:E:446:VAL:CG1	1.75	0.99
1:A:305:THR:HG22	2:B:448:LEU:HD22	1.46	0.98
3:C:283:TYR:HD1	3:C:454:ILE:HD13	1.27	0.98
1:D:302:SER:HB2	4:E:445:LYS:CE	1.93	0.98
1:A:273:LEU:CD2	1:A:429:ARG:HG2	1.94	0.97
4:E:262:GLN:C	4:E:291:MET:HE3	1.83	0.97
1:A:305:THR:CG2	2:B:448:LEU:HD22	1.93	0.97
2:B:334:LEU:HD13	2:B:456:LEU:HD22	1.45	0.97
4:E:237:VAL:HG12	4:E:258:VAL:HG11	1.43	0.97
1:A:222:CYS:HG	1:A:256:PHE:HE2	1.05	0.96
1:A:216:VAL:HG21	4:E:280:VAL:HG21	1.44	0.96
3:C:238:VAL:HA	3:C:251:LEU:CD2	1.94	0.96
1:D:232:VAL:HG23	1:D:245:LEU:HD23	1.48	0.96
4:E:269:ILE:CD1	4:E:287:LEU:HG	1.96	0.96
2:B:264:LEU:HD21	3:C:234:LEU:HD11	1.47	0.96
3:C:231:ILE:HG13	3:C:262:PHE:HZ	1.21	0.95
1:A:222:CYS:SG	1:A:256:PHE:HE2	1.89	0.95
2:B:418:GLU:HG3	3:C:402:LYS:HG3	1.47	0.95
2:B:421:SER:HB2	3:C:409:LYS:HZ3	1.23	0.95
2:B:247:PHE:CZ	2:B:461:ILE:HD13	2.01	0.94
1:D:253:LEU:CD2	1:D:285:VAL:HG21	1.98	0.94
4:E:286:TYR:HD1	4:E:466:ILE:HG21	1.30	0.94
1:D:273:LEU:CD2	1:D:429:ARG:HG2	1.97	0.93
2:B:418:GLU:O	3:C:405:VAL:HG11	1.69	0.93
4:E:317:LEU:HB2	4:E:440:TRP:CZ2	2.04	0.93
3:C:403:GLU:HB3	1:D:380:LYS:HD3	1.50	0.92
2:B:419:ILE:CA	3:C:405:VAL:HG21	1.98	0.92
3:C:238:VAL:HA	3:C:251:LEU:HD23	1.49	0.92
2:B:247:PHE:CE2	2:B:461:ILE:HD13	2.03	0.91
3:C:401:LEU:HD22	1:D:376:ILE:CD1	2.00	0.91
1:A:382:ILE:HG22	4:E:423:ILE:HG12	1.52	0.91
4:E:286:TYR:CE2	4:E:467:PHE:CZ	2.58	0.91
2:B:291:TYR:CZ	2:B:473:PHE:CZ	2.59	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:334:LEU:CD1	2:B:456:LEU:HD22	2.00	0.91
3:C:411:ILE:HD11	1:D:382:ILE:HG22	1.52	0.91
3:C:283:TYR:CE2	3:C:455:PHE:CE1	2.58	0.91
4:E:325:PHE:HD1	4:E:446:VAL:HG12	1.34	0.90
1:D:222:CYS:HG	1:D:256:PHE:HE2	1.15	0.90
3:C:283:TYR:OH	3:C:451:THR:HG23	1.73	0.89
4:E:262:GLN:CB	4:E:291:MET:HE3	2.02	0.89
1:D:277:TYR:CE1	1:D:426:PHE:CZ	2.60	0.89
1:D:317:ILE:HD11	1:D:402:VAL:HG23	1.51	0.89
1:A:264:ILE:HG21	1:A:274:ILE:CD1	2.02	0.89
2:B:291:TYR:CZ	2:B:473:PHE:HZ	1.91	0.89
1:A:304:SER:OG	2:B:448:LEU:HD21	1.74	0.88
2:B:422:GLY:HA3	3:C:405:VAL:CG1	2.04	0.88
2:B:232:PHE:HE2	2:B:277:ARG:HG3	1.39	0.88
1:A:264:ILE:CG2	1:A:274:ILE:HD11	2.03	0.87
4:E:242:PHE:CZ	4:E:452:PHE:CE1	2.63	0.87
4:E:237:VAL:CG1	4:E:258:VAL:HG11	2.04	0.87
3:C:259:VAL:HG12	3:C:288:MET:HE3	1.56	0.87
3:C:410:TYR:HE2	1:D:386:MET:CB	1.88	0.87
2:B:418:GLU:CG	3:C:402:LYS:HG3	2.05	0.87
2:B:422:GLY:N	3:C:405:VAL:HG13	1.90	0.86
1:D:273:LEU:HD22	1:D:429:ARG:HG2	1.55	0.86
1:D:222:CYS:SG	1:D:256:PHE:HE2	1.98	0.86
1:D:247:ILE:HD13	4:E:254:LEU:HD13	1.53	0.86
1:A:273:LEU:HD21	1:A:429:ARG:CB	2.05	0.86
1:A:387:LYS:HE3	4:E:422:PHE:CE1	2.10	0.86
1:A:307:THR:H	2:B:341:SER:CB	1.88	0.86
2:B:232:PHE:CE2	2:B:277:ARG:HG3	2.11	0.85
4:E:325:PHE:CD1	4:E:446:VAL:HG12	2.12	0.85
4:E:252:CYS:SG	4:E:302:VAL:HG22	2.17	0.85
1:D:253:LEU:HD22	1:D:285:VAL:CG2	2.05	0.85
3:C:408:ILE:CG1	1:D:379:VAL:HG11	2.07	0.85
3:C:411:ILE:CD1	1:D:382:ILE:HG22	2.06	0.85
2:B:322:LEU:HD13	2:B:446:TRP:CH2	2.11	0.85
3:C:407:ALA:HB1	1:D:383:ALA:CB	2.07	0.85
1:D:286:ILE:HD12	4:E:236:LEU:HD21	1.58	0.85
1:A:375:ALA:HB2	2:B:423:ILE:HG23	0.92	0.84
4:E:241:TYR:OH	4:E:297:ILE:HG12	1.77	0.84
3:C:311:THR:HG22	1:D:404:MET:SD	2.17	0.84
3:C:283:TYR:CD1	3:C:454:ILE:HD13	2.12	0.84
4:E:255:SER:HB2	4:E:298:VAL:HG22	0.88	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:ILE:HD13	4:E:254:LEU:CD1	2.06	0.84
1:A:387:LYS:HE3	4:E:422:PHE:CZ	2.13	0.84
1:A:277:TYR:CE2	1:A:426:PHE:CZ	2.66	0.83
1:A:293:VAL:HG13	2:B:249:LEU:HD13	1.59	0.83
2:B:256:LYS:HD3	2:B:310:LEU:CD1	2.08	0.83
2:B:239:ILE:CD1	2:B:270:PHE:HE2	1.91	0.83
1:D:233:PHE:CE2	1:D:414:PHE:CD2	2.66	0.83
1:D:375:ALA:HB2	4:E:417:VAL:HB	1.61	0.83
1:A:374:SER:HB3	2:B:427:ASN:HD21	1.41	0.83
1:A:291:ILE:HD12	1:A:414:PHE:CZ	2.14	0.83
4:E:286:TYR:CE2	4:E:467:PHE:CE2	2.66	0.83
1:D:320:ILE:CG2	1:D:409:ILE:HD11	2.08	0.83
1:A:381:TYR:HE2	2:B:433:ILE:HB	1.44	0.82
2:B:317:PRO:HG3	2:B:442:GLU:OE2	1.80	0.82
3:C:252:SER:HB2	3:C:295:VAL:HG22	1.60	0.82
3:C:410:TYR:OH	1:D:387:LYS:HA	1.79	0.82
2:B:239:ILE:CD1	2:B:270:PHE:CE2	2.62	0.82
3:C:410:TYR:CE2	1:D:386:MET:HB3	2.15	0.82
1:D:372:VAL:HA	4:E:417:VAL:HG11	1.62	0.82
4:E:241:TYR:CE2	4:E:455:ALA:CB	2.62	0.81
4:E:312:PRO:HG3	4:E:436:GLU:OE2	1.78	0.81
3:C:407:ALA:HB1	1:D:383:ALA:HB2	1.62	0.81
1:A:277:TYR:CE2	1:A:426:PHE:HZ	1.99	0.81
1:A:273:LEU:HD22	1:A:429:ARG:CG	2.10	0.81
1:D:320:ILE:CG2	1:D:409:ILE:CD1	2.59	0.81
2:B:264:LEU:CD2	3:C:234:LEU:CD1	2.59	0.81
1:D:375:ALA:HB2	4:E:417:VAL:CB	2.11	0.81
3:C:311:THR:HA	1:D:404:MET:SD	2.21	0.81
1:D:375:ALA:CB	4:E:417:VAL:HA	2.09	0.81
1:A:378:GLY:HA2	2:B:430:VAL:HG21	1.64	0.80
1:A:376:ILE:HD11	4:E:413:ILE:CD1	2.05	0.80
1:A:380:LYS:HE2	4:E:415:SER:OG	1.80	0.80
2:B:418:GLU:HG3	3:C:402:LYS:CG	2.09	0.80
3:C:266:LEU:HD23	3:C:281:ILE:CD1	2.12	0.80
1:A:277:TYR:CZ	1:A:426:PHE:CE2	2.69	0.80
2:B:239:ILE:HD12	2:B:270:PHE:CZ	2.16	0.80
3:C:408:ILE:CG1	1:D:379:VAL:CG1	2.60	0.80
4:E:230:CYS:HA	4:E:265:PHE:CE2	2.16	0.80
4:E:242:PHE:HZ	4:E:452:PHE:CE1	2.01	0.79
1:D:277:TYR:CD1	1:D:426:PHE:CZ	2.71	0.79
1:D:381:TYR:CZ	4:E:428:LYS:HE3	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:TYR:HD1	1:A:425:VAL:HG11	1.47	0.79
3:C:411:ILE:CG2	1:D:386:MET:HE1	2.00	0.79
1:A:375:ALA:HB1	2:B:423:ILE:HD12	1.64	0.78
2:B:247:PHE:CE2	2:B:461:ILE:HG21	2.19	0.78
2:B:419:ILE:HA	3:C:405:VAL:CG2	2.04	0.78
1:D:277:TYR:CE1	1:D:426:PHE:CE2	2.71	0.78
1:A:380:LYS:HE2	4:E:415:SER:CB	2.12	0.78
1:D:232:VAL:HG23	1:D:245:LEU:CD2	2.14	0.77
1:D:317:ILE:HD11	1:D:402:VAL:HG22	1.66	0.77
3:C:407:ALA:CA	1:D:383:ALA:CB	2.62	0.77
3:C:407:ALA:CA	1:D:383:ALA:HB2	2.14	0.77
3:C:283:TYR:CZ	3:C:455:PHE:CE1	2.72	0.77
1:A:379:VAL:O	4:E:419:ALA:HB1	1.84	0.76
1:D:375:ALA:HB2	4:E:417:VAL:CA	2.15	0.76
4:E:286:TYR:CZ	4:E:467:PHE:CE2	2.74	0.76
1:D:234:TYR:HD1	1:D:411:LEU:HD22	1.49	0.76
1:D:277:TYR:CZ	1:D:426:PHE:CZ	2.74	0.76
1:A:386:MET:HE3	4:E:423:ILE:HG23	1.67	0.76
1:A:387:LYS:CE	4:E:422:PHE:CE1	2.69	0.76
2:B:426:THR:HB	3:C:408:ILE:HG21	1.68	0.76
1:A:291:ILE:CG2	1:A:410:LEU:CD1	2.62	0.75
1:D:222:CYS:SG	1:D:256:PHE:CE2	2.77	0.75
3:C:401:LEU:CD2	1:D:376:ILE:HD11	2.17	0.75
3:C:407:ALA:CB	1:D:383:ALA:CB	2.64	0.75
4:E:317:LEU:HD13	4:E:440:TRP:CH2	2.22	0.75
1:A:273:LEU:CD2	1:A:429:ARG:CG	2.64	0.75
1:A:379:VAL:HG11	4:E:416:CYS:O	1.86	0.75
1:D:299:HIS:CE1	1:D:400:LYS:HG2	2.22	0.75
1:D:317:ILE:CD1	1:D:402:VAL:CG2	2.62	0.74
2:B:425:SER:CB	3:C:409:LYS:HA	2.16	0.74
3:C:407:ALA:HB2	1:D:380:LYS:HA	1.68	0.74
3:C:410:TYR:CE2	1:D:386:MET:CB	2.70	0.74
3:C:411:ILE:HD11	1:D:382:ILE:CG2	2.17	0.74
1:D:233:PHE:CE2	1:D:414:PHE:CE2	2.76	0.74
3:C:410:TYR:HE2	1:D:386:MET:HB3	1.51	0.74
2:B:291:TYR:CE2	2:B:473:PHE:HZ	2.06	0.74
3:C:401:LEU:HD22	1:D:376:ILE:HD11	1.69	0.74
1:D:277:TYR:CE2	1:D:426:PHE:HZ	2.05	0.74
1:A:381:TYR:CZ	2:B:434:LYS:HG3	2.22	0.73
1:A:381:TYR:CE1	2:B:434:LYS:HG3	2.23	0.73
1:A:273:LEU:HD21	1:A:429:ARG:HB3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:407:ALA:HA	1:D:383:ALA:CB	2.19	0.73
2:B:291:TYR:CE1	2:B:473:PHE:CZ	2.77	0.73
1:D:291:ILE:HD12	1:D:414:PHE:HZ	1.53	0.73
1:D:273:LEU:HD21	1:D:429:ARG:HG2	1.71	0.73
4:E:312:PRO:HD3	4:E:436:GLU:HG2	1.71	0.73
2:B:264:LEU:HD22	3:C:234:LEU:HD11	1.70	0.73
3:C:332:ILE:HD11	3:C:437:ARG:HG2	1.70	0.73
1:A:299:HIS:NE2	1:A:400:LYS:HG2	2.04	0.73
1:A:376:ILE:HA	4:E:416:CYS:HB2	1.69	0.72
3:C:225:ILE:HG23	3:C:455:PHE:CE2	2.24	0.72
3:C:236:ILE:HD11	3:C:447:CYS:SG	2.29	0.72
2:B:247:PHE:CZ	2:B:302:VAL:HG13	2.25	0.72
3:C:401:LEU:CD1	1:D:376:ILE:HD11	2.20	0.72
1:D:277:TYR:HD1	1:D:425:VAL:HG11	1.53	0.72
3:C:238:VAL:HA	3:C:251:LEU:HD21	1.69	0.72
1:D:242:LYS:HE2	1:D:292:THR:HG23	1.72	0.72
3:C:294:SER:CB	3:C:443:PHE:HE2	2.01	0.72
1:A:291:ILE:HG21	1:A:410:LEU:CD1	2.17	0.72
1:A:273:LEU:CD2	1:A:429:ARG:CB	2.68	0.71
1:A:374:SER:HB3	2:B:427:ASN:ND2	2.05	0.71
2:B:232:PHE:HZ	2:B:277:ARG:NE	1.87	0.71
1:A:305:THR:CG2	2:B:448:LEU:CD2	2.69	0.71
3:C:311:THR:CB	1:D:404:MET:SD	2.78	0.71
3:C:231:ILE:CG1	3:C:262:PHE:HZ	2.03	0.71
1:A:381:TYR:CG	2:B:430:VAL:HG13	2.25	0.71
1:A:277:TYR:CD1	1:A:425:VAL:HG11	2.25	0.71
1:A:277:TYR:CD2	1:A:426:PHE:CZ	2.79	0.71
3:C:411:ILE:CD1	1:D:382:ILE:CG2	2.68	0.71
1:A:374:SER:CB	2:B:427:ASN:HD21	2.04	0.70
2:B:317:PRO:HG3	2:B:442:GLU:CD	2.11	0.70
3:C:410:TYR:CE1	1:D:387:LYS:HD3	2.26	0.70
1:D:320:ILE:HG21	1:D:409:ILE:HG13	1.73	0.70
3:C:401:LEU:HD13	1:D:376:ILE:HD11	1.72	0.70
4:E:241:TYR:CZ	4:E:455:ALA:HB2	2.27	0.70
4:E:251:LYS:HB3	4:E:301:CYS:HB3	1.72	0.70
4:E:325:PHE:HD1	4:E:446:VAL:HG11	1.56	0.70
3:C:407:ALA:CB	1:D:380:LYS:HA	2.22	0.70
3:C:407:ALA:CB	1:D:383:ALA:HB2	2.20	0.69
1:D:234:TYR:CD1	1:D:411:LEU:HD22	2.27	0.69
1:A:324:MET:CE	1:A:412:CYS:SG	2.80	0.69
1:D:299:HIS:CD2	1:D:400:LYS:HA	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:TYR:CB	4:E:277:SER:HB2	2.23	0.69
1:A:324:MET:HE2	1:A:412:CYS:SG	2.32	0.69
1:A:382:ILE:HG22	4:E:423:ILE:CG1	2.23	0.69
1:D:316:PHE:O	1:D:405:VAL:HG11	1.93	0.69
4:E:262:GLN:CB	4:E:291:MET:CE	2.63	0.69
1:A:306:HIS:HA	2:B:341:SER:HB2	1.74	0.69
1:D:375:ALA:HA	4:E:421:ASN:OD1	1.92	0.69
1:A:379:VAL:CG1	4:E:419:ALA:HB3	2.02	0.68
3:C:407:ALA:C	1:D:383:ALA:HB2	2.14	0.68
1:D:277:TYR:CZ	1:D:426:PHE:HZ	2.08	0.68
3:C:403:GLU:CB	1:D:380:LYS:HD3	2.21	0.68
1:A:382:ILE:CG2	4:E:423:ILE:CD1	2.71	0.68
1:D:406:ILE:HG22	1:D:410:LEU:HD12	1.76	0.68
3:C:294:SER:HA	3:C:443:PHE:CE2	2.29	0.68
1:D:243:MET:HB2	4:E:250:GLN:OE1	1.93	0.68
1:A:233:PHE:CZ	1:A:288:SER:HB2	2.29	0.68
1:A:380:LYS:HE2	4:E:415:SER:HB2	1.74	0.67
4:E:230:CYS:HA	4:E:265:PHE:CZ	2.29	0.67
1:A:387:LYS:CE	4:E:422:PHE:CZ	2.77	0.67
2:B:247:PHE:CZ	2:B:461:ILE:CD1	2.76	0.67
1:A:386:MET:HE3	4:E:423:ILE:HG12	1.74	0.67
2:B:264:LEU:HD21	3:C:234:LEU:CD1	2.19	0.67
1:A:307:THR:H	2:B:341:SER:HB3	1.59	0.67
3:C:294:SER:CB	3:C:443:PHE:CE2	2.78	0.67
1:D:320:ILE:HG22	1:D:409:ILE:HD11	1.75	0.67
1:A:376:ILE:HD13	4:E:413:ILE:N	2.10	0.66
1:D:382:ILE:CD1	4:E:423:ILE:HG22	2.25	0.66
3:C:404:ALA:HB2	1:D:376:ILE:CG2	2.22	0.66
3:C:239:PHE:CE2	3:C:294:SER:HB2	2.30	0.66
3:C:311:THR:CG2	1:D:404:MET:SD	2.83	0.66
2:B:425:SER:OG	3:C:409:LYS:HA	1.95	0.66
1:D:375:ALA:HB1	4:E:417:VAL:HA	1.78	0.66
1:A:305:THR:HG21	2:B:451:GLN:OE1	1.95	0.66
3:C:238:VAL:HG23	3:C:251:LEU:HD23	1.78	0.66
1:A:291:ILE:HG22	1:A:410:LEU:HD13	1.75	0.65
3:C:294:SER:CA	3:C:443:PHE:CE2	2.79	0.65
1:A:307:THR:N	2:B:341:SER:CB	2.58	0.65
3:C:408:ILE:HG13	1:D:379:VAL:HG13	1.75	0.65
3:C:294:SER:CA	3:C:443:PHE:HE2	2.09	0.65
2:B:421:SER:HB2	3:C:409:LYS:HZ1	1.57	0.65
4:E:286:TYR:CD2	4:E:467:PHE:CZ	2.84	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:LEU:HD13	2:B:286:PRO:HG3	1.79	0.65
1:D:382:ILE:HD13	4:E:423:ILE:HG22	1.77	0.65
1:A:295:VAL:HG11	1:A:407:ASP:OD1	1.98	0.64
4:E:262:GLN:HE22	4:E:294:SER:CB	2.09	0.64
1:A:253:LEU:HD21	1:A:281:THR:HG22	1.80	0.64
3:C:266:LEU:CD2	3:C:281:ILE:HD13	2.20	0.64
1:D:243:MET:HE3	1:D:293:VAL:HG22	1.79	0.64
1:A:382:ILE:HB	4:E:423:ILE:HD11	1.79	0.64
4:E:241:TYR:CZ	4:E:455:ALA:CB	2.80	0.64
4:E:245:ALA:HB1	4:E:304:VAL:CG1	2.27	0.64
3:C:407:ALA:HB1	1:D:383:ALA:HB3	1.80	0.64
3:C:248:LYS:HB2	3:C:302:LEU:HD11	1.78	0.64
3:C:280:ILE:O	3:C:284:LEU:HD23	1.98	0.64
2:B:425:SER:HB3	3:C:409:LYS:HA	1.78	0.64
3:C:407:ALA:CB	1:D:383:ALA:HB3	2.28	0.64
4:E:230:CYS:CA	4:E:265:PHE:CE2	2.81	0.64
1:A:375:ALA:HB3	2:B:423:ILE:HD12	1.77	0.63
4:E:286:TYR:CD1	4:E:466:ILE:CG2	2.70	0.63
3:C:311:THR:O	1:D:329:MET:HA	1.98	0.63
1:D:247:ILE:CD1	4:E:254:LEU:CD1	2.77	0.63
1:A:304:SER:HG	2:B:448:LEU:HD21	1.61	0.63
4:E:312:PRO:HG3	4:E:436:GLU:CG	2.29	0.63
3:C:238:VAL:CA	3:C:251:LEU:CD2	2.76	0.63
3:C:411:ILE:HA	1:D:386:MET:SD	2.39	0.63
1:A:284:PHE:CZ	1:A:418:CYS:HB2	2.34	0.63
1:D:257:LEU:HD22	1:D:282:MET:CE	2.28	0.63
2:B:247:PHE:HE2	2:B:461:ILE:HG21	1.61	0.63
1:D:375:ALA:HB2	4:E:417:VAL:HA	1.76	0.63
1:A:375:ALA:HB1	2:B:423:ILE:CD1	2.29	0.63
1:A:378:GLY:HA3	2:B:430:VAL:HG21	1.80	0.62
1:A:375:ALA:CB	2:B:423:ILE:CD1	2.66	0.62
3:C:314:MET:HA	3:C:428:TRP:CZ2	2.35	0.62
1:A:381:TYR:CD1	2:B:434:LYS:HE3	2.35	0.62
2:B:260:ALA:HB1	2:B:303:ILE:HG12	1.82	0.62
1:A:257:LEU:HD13	1:A:278:MET:HE2	1.79	0.62
1:A:307:THR:HG22	2:B:341:SER:CB	2.16	0.62
4:E:245:ALA:HB1	4:E:304:VAL:HG12	1.82	0.62
3:C:294:SER:HB3	3:C:443:PHE:HE2	1.62	0.62
1:A:253:LEU:HD22	1:A:285:VAL:HG21	1.82	0.62
4:E:262:GLN:CA	4:E:291:MET:HE3	2.30	0.62
3:C:401:LEU:HD22	1:D:376:ILE:HD13	1.79	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:VAL:HG13	2:B:249:LEU:CD1	2.28	0.61
1:D:243:MET:CE	1:D:293:VAL:HG22	2.30	0.61
1:D:308:MET:CE	1:D:402:VAL:HG21	2.29	0.61
1:D:320:ILE:HG23	1:D:409:ILE:CD1	2.30	0.61
4:E:313:ASN:OD1	4:E:314:THR:N	2.33	0.61
1:A:216:VAL:HG11	4:E:280:VAL:HG21	1.81	0.61
4:E:283:ILE:O	4:E:287:LEU:HD23	1.99	0.61
3:C:231:ILE:CG1	3:C:262:PHE:CZ	2.67	0.61
1:D:324:MET:HE3	1:D:326:PHE:CE1	2.36	0.61
3:C:407:ALA:HB3	1:D:379:VAL:HG12	1.82	0.61
1:D:268:SER:HB3	4:E:221:PHE:HB2	1.82	0.61
1:A:375:ALA:HB2	2:B:423:ILE:HD12	1.75	0.61
1:D:317:ILE:CD1	1:D:402:VAL:HG22	2.27	0.61
4:E:262:GLN:C	4:E:291:MET:CE	2.63	0.61
1:A:376:ILE:CD1	4:E:412:GLU:HB3	2.30	0.60
3:C:403:GLU:HB3	1:D:380:LYS:CD	2.28	0.60
3:C:259:VAL:HG11	3:C:288:MET:HA	1.83	0.60
3:C:283:TYR:CG	3:C:454:ILE:HG21	2.34	0.60
1:D:375:ALA:CB	4:E:417:VAL:CB	2.79	0.60
1:D:326:PHE:CE1	1:D:412:CYS:SG	2.94	0.60
1:A:306:HIS:CA	2:B:341:SER:HB2	2.31	0.60
1:A:376:ILE:HG12	4:E:416:CYS:HB2	1.83	0.60
1:A:382:ILE:HG21	4:E:423:ILE:HD13	1.83	0.60
2:B:248:TYR:CD1	2:B:458:MET:CE	2.85	0.60
1:D:233:PHE:HE2	1:D:414:PHE:CD2	2.20	0.60
1:A:376:ILE:CD1	4:E:413:ILE:HD13	2.07	0.59
2:B:256:LYS:HD2	2:B:310:LEU:HD21	1.84	0.59
1:D:293:VAL:HG13	4:E:243:LEU:HD23	1.85	0.59
3:C:408:ILE:CD1	1:D:379:VAL:HG11	2.31	0.59
1:D:375:ALA:CB	4:E:417:VAL:CA	2.77	0.59
2:B:267:GLN:O	2:B:296:MET:HE3	2.02	0.59
3:C:311:THR:CA	1:D:404:MET:SD	2.90	0.59
3:C:239:PHE:HE2	3:C:294:SER:HB2	1.68	0.59
2:B:247:PHE:CE2	2:B:461:ILE:CD1	2.83	0.58
3:C:401:LEU:CD2	1:D:376:ILE:CD1	2.75	0.58
1:A:222:CYS:SG	1:A:256:PHE:CE2	2.75	0.58
1:A:216:VAL:CG2	4:E:280:VAL:HG21	2.27	0.58
1:A:284:PHE:HZ	1:A:418:CYS:HB2	1.67	0.58
1:A:381:TYR:OH	2:B:433:ILE:HG22	2.02	0.58
3:C:408:ILE:CG1	1:D:379:VAL:HG13	2.31	0.58
1:D:250:LEU:HD21	4:E:236:LEU:HD13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ILE:HG12	4:E:416:CYS:CB	2.33	0.58
3:C:407:ALA:O	1:D:383:ALA:HB2	2.04	0.58
1:A:277:TYR:CD2	1:A:426:PHE:HZ	2.21	0.58
1:A:378:GLY:C	2:B:430:VAL:HG21	2.24	0.58
3:C:311:THR:HB	1:D:404:MET:SD	2.44	0.58
4:E:269:ILE:HD13	4:E:287:LEU:CG	2.24	0.58
4:E:325:PHE:CD1	4:E:446:VAL:CG1	2.67	0.58
1:A:380:LYS:CE	4:E:415:SER:HB2	2.33	0.57
3:C:231:ILE:CG1	3:C:262:PHE:CE2	2.79	0.57
1:D:293:VAL:HG13	4:E:243:LEU:CD2	2.35	0.57
1:A:291:ILE:HD12	1:A:414:PHE:HZ	1.65	0.57
2:B:291:TYR:CZ	2:B:473:PHE:CE2	2.93	0.57
2:B:422:GLY:N	3:C:405:VAL:CG1	2.64	0.57
1:A:305:THR:HG23	2:B:448:LEU:CD2	2.35	0.57
1:A:273:LEU:HD21	1:A:429:ARG:HB2	1.86	0.57
1:A:277:TYR:CZ	1:A:426:PHE:HE2	2.20	0.57
1:A:297:ASN:OD1	2:B:250:PRO:HD3	2.05	0.56
1:A:284:PHE:CE1	1:A:417:ILE:HG22	2.40	0.56
3:C:231:ILE:HG21	3:C:262:PHE:HE2	1.71	0.56
1:A:243:MET:HB2	2:B:255:GLU:CD	2.26	0.56
1:A:288:SER:HA	1:A:414:PHE:CE2	2.41	0.56
2:B:422:GLY:HA3	3:C:405:VAL:CB	2.35	0.56
4:E:262:GLN:HB3	4:E:291:MET:HE2	1.82	0.56
2:B:256:LYS:HD3	2:B:310:LEU:CG	2.35	0.56
3:C:259:VAL:CG1	3:C:288:MET:HE3	2.34	0.56
1:D:372:VAL:HA	4:E:417:VAL:CG1	2.34	0.56
4:E:286:TYR:CE2	4:E:467:PHE:HZ	2.20	0.56
1:A:324:MET:HE1	1:A:412:CYS:SG	2.44	0.56
1:A:376:ILE:HG21	4:E:412:GLU:CA	2.35	0.56
1:A:308:MET:HE3	1:A:399:TRP:CZ3	2.41	0.56
1:A:381:TYR:CE2	2:B:433:ILE:HB	2.34	0.56
1:D:253:LEU:CD2	1:D:285:VAL:CG2	2.73	0.56
1:D:382:ILE:HD11	4:E:424:ALA:N	2.21	0.55
1:A:380:LYS:CE	4:E:415:SER:CB	2.83	0.55
1:D:277:TYR:CD2	1:D:426:PHE:HZ	2.24	0.55
1:A:383:ALA:O	4:E:422:PHE:CE2	2.60	0.55
1:D:277:TYR:CZ	1:D:426:PHE:CE2	2.94	0.55
1:D:277:TYR:CG	1:D:426:PHE:CZ	2.94	0.55
1:A:291:ILE:HD12	1:A:414:PHE:CE1	2.42	0.55
2:B:248:TYR:HD1	2:B:458:MET:HE2	1.72	0.55
3:C:231:ILE:CB	3:C:262:PHE:HE2	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:PHE:CZ	1:D:414:PHE:CE2	2.95	0.55
1:D:379:VAL:CG2	4:E:420:CYS:SG	2.94	0.55
2:B:239:ILE:HD13	2:B:270:PHE:HE2	1.67	0.55
1:D:253:LEU:HD22	1:D:285:VAL:HG11	1.88	0.55
2:B:418:GLU:HG2	3:C:402:LYS:HG3	1.87	0.54
3:C:411:ILE:CG2	1:D:386:MET:CE	2.71	0.54
2:B:248:TYR:CD1	2:B:458:MET:SD	3.00	0.54
1:D:326:PHE:CZ	1:D:412:CYS:SG	3.00	0.54
1:D:385:HIS:NE2	4:E:431:ASN:CG	2.61	0.54
4:E:237:VAL:HG12	4:E:258:VAL:CG1	2.27	0.54
1:A:307:THR:N	2:B:341:SER:HB3	2.23	0.54
3:C:408:ILE:HD11	1:D:379:VAL:HG21	1.88	0.54
1:A:305:THR:O	2:B:341:SER:HB2	2.07	0.54
1:D:320:ILE:HG23	1:D:409:ILE:HD11	1.85	0.54
3:C:314:MET:CA	3:C:428:TRP:CZ2	2.90	0.54
3:C:410:TYR:HE2	1:D:386:MET:HB2	1.71	0.54
1:D:375:ALA:CB	4:E:417:VAL:HB	2.37	0.54
2:B:267:GLN:HE22	2:B:299:VAL:HG11	1.72	0.54
1:D:242:LYS:HB2	1:D:296:ILE:HD11	1.90	0.54
1:A:257:LEU:CG	1:A:278:MET:HE1	2.35	0.54
4:E:245:ALA:CB	4:E:304:VAL:CG1	2.86	0.54
4:E:241:TYR:CE2	4:E:455:ALA:HB1	2.43	0.54
1:A:376:ILE:CG2	4:E:412:GLU:O	2.56	0.53
4:E:262:GLN:O	4:E:291:MET:HE3	2.07	0.53
1:A:277:TYR:CZ	1:A:426:PHE:CZ	2.95	0.53
2:B:291:TYR:CE1	2:B:473:PHE:CE2	2.97	0.53
1:A:386:MET:HB2	4:E:422:PHE:HE2	1.73	0.53
1:A:376:ILE:HD13	4:E:412:GLU:O	2.07	0.53
1:D:247:ILE:CD1	4:E:254:LEU:HD12	2.39	0.53
3:C:283:TYR:CD1	3:C:454:ILE:CD1	2.89	0.53
1:A:233:PHE:CE2	1:A:288:SER:HB2	2.44	0.52
3:C:314:MET:HB2	3:C:428:TRP:CZ2	2.44	0.52
1:A:376:ILE:HD13	4:E:412:GLU:CB	2.38	0.52
4:E:241:TYR:CE2	4:E:455:ALA:HB3	2.42	0.52
1:A:376:ILE:CA	4:E:416:CYS:HB2	2.39	0.52
3:C:238:VAL:CA	3:C:251:LEU:HD21	2.39	0.52
1:D:273:LEU:HD21	1:D:429:ARG:CG	2.38	0.52
2:B:422:GLY:H	3:C:405:VAL:CG1	2.23	0.52
1:A:305:THR:CG2	2:B:451:GLN:OE1	2.57	0.52
1:D:317:ILE:CG1	1:D:402:VAL:HG22	2.39	0.52
2:B:418:GLU:OE2	3:C:402:LYS:HE3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:THR:CG2	2:B:341:SER:HB3	2.19	0.52
1:A:385:HIS:CE1	2:B:436:LYS:HZ1	2.28	0.52
2:B:426:THR:CB	3:C:408:ILE:HG21	2.40	0.52
1:A:277:TYR:CE1	1:A:426:PHE:CE2	2.98	0.52
4:E:286:TYR:HD1	4:E:466:ILE:HD13	1.74	0.52
1:A:299:HIS:CE1	1:A:400:LYS:HG2	2.44	0.51
1:D:290:ILE:HG12	4:E:239:LEU:HD21	1.91	0.51
4:E:325:PHE:CZ	4:E:447:ILE:HG12	2.45	0.51
1:A:253:LEU:CD2	1:A:285:VAL:HG21	2.41	0.51
3:C:266:LEU:HD22	3:C:284:LEU:HG	1.92	0.51
1:A:383:ALA:HB1	4:E:422:PHE:CD2	2.45	0.51
1:A:382:ILE:HG13	2:B:430:VAL:HG22	1.92	0.51
1:D:257:LEU:HD22	1:D:282:MET:HE2	1.93	0.51
1:D:375:ALA:HB3	4:E:417:VAL:HG12	1.92	0.51
1:D:381:TYR:CZ	4:E:428:LYS:CE	2.90	0.51
4:E:269:ILE:CD1	4:E:287:LEU:CG	2.79	0.51
1:A:295:VAL:HG21	1:A:407:ASP:OD1	2.10	0.51
1:A:382:ILE:HG22	4:E:423:ILE:CD1	2.38	0.51
2:B:456:LEU:HG	2:B:460:ILE:HD12	1.92	0.51
1:D:234:TYR:CD1	1:D:411:LEU:CD2	2.93	0.51
1:A:256:PHE:O	1:A:260:ILE:HD12	2.10	0.51
1:A:376:ILE:CD1	4:E:412:GLU:CB	2.89	0.51
1:A:380:LYS:HA	4:E:419:ALA:HB2	1.93	0.50
1:D:250:LEU:HD13	1:D:289:ILE:CD1	2.40	0.50
4:E:242:PHE:HZ	4:E:452:PHE:HE1	1.58	0.50
2:B:234:THR:CG2	2:B:235:PRO:HD3	2.41	0.50
2:B:438:ALA:O	2:B:441:GLU:HG3	2.11	0.50
3:C:410:TYR:CE2	1:D:386:MET:HB2	2.47	0.50
1:D:324:MET:SD	1:D:409:ILE:HD13	2.51	0.50
3:C:410:TYR:CE2	1:D:387:LYS:N	2.80	0.50
1:A:213:TYR:CG	4:E:277:SER:CB	2.94	0.50
2:B:251:ALA:HB1	2:B:310:LEU:CD2	2.42	0.50
1:A:257:LEU:CB	1:A:278:MET:HE1	2.42	0.50
1:A:299:HIS:CD2	1:A:400:LYS:HG2	2.47	0.50
1:A:376:ILE:HD12	4:E:412:GLU:HB3	1.93	0.50
2:B:426:THR:N	3:C:408:ILE:CG2	2.75	0.50
3:C:283:TYR:OH	3:C:455:PHE:CE1	2.65	0.50
4:E:233:ILE:HD12	4:E:265:PHE:CZ	2.47	0.50
1:A:213:TYR:HB2	4:E:277:SER:HB2	1.94	0.49
3:C:398:PRO:N	3:C:402:LYS:HZ3	2.10	0.49
1:D:381:TYR:OH	4:E:428:LYS:CE	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:SER:HB2	1:A:289:ILE:HG12	1.92	0.49
1:A:297:ASN:HA	2:B:250:PRO:HG3	1.94	0.49
3:C:411:ILE:HG12	1:D:386:MET:HE3	1.94	0.49
1:D:320:ILE:CG2	1:D:409:ILE:HG13	2.42	0.49
4:E:237:VAL:CG1	4:E:258:VAL:CG1	2.85	0.49
1:D:253:LEU:HD22	1:D:285:VAL:CB	2.42	0.49
4:E:237:VAL:HG11	4:E:294:SER:OG	2.11	0.49
1:D:239:SER:O	1:D:239:SER:OG	2.25	0.49
1:D:308:MET:HE2	1:D:402:VAL:HG21	1.93	0.49
1:A:302:SER:CB	2:B:451:GLN:HE22	2.26	0.49
1:A:382:ILE:CB	4:E:423:ILE:HD11	2.42	0.49
3:C:411:ILE:HD13	1:D:382:ILE:CG2	2.43	0.49
2:B:248:TYR:CE1	2:B:458:MET:HE1	2.48	0.49
1:A:386:MET:SD	4:E:426:SER:HB2	2.53	0.49
3:C:226:ILE:HB	3:C:227:PRO:HD3	1.94	0.49
3:C:235:ALA:O	3:C:238:VAL:HG12	2.13	0.49
1:D:257:LEU:HD22	1:D:282:MET:HE3	1.93	0.49
2:B:248:TYR:CD1	2:B:458:MET:HE2	2.48	0.48
3:C:225:ILE:HG23	3:C:455:PHE:CZ	2.48	0.48
1:D:232:VAL:HA	1:D:245:LEU:HD21	1.95	0.48
1:A:317:ILE:HD11	1:A:402:VAL:CG2	2.43	0.48
3:C:225:ILE:CG2	3:C:455:PHE:CE2	2.95	0.48
1:A:381:TYR:OH	2:B:434:LYS:HG3	2.13	0.48
1:D:308:MET:HE1	1:D:402:VAL:HG21	1.95	0.48
4:E:243:LEU:HD11	4:E:254:LEU:HD23	1.95	0.48
1:D:302:SER:CB	4:E:445:LYS:CE	2.70	0.48
2:B:317:PRO:CG	2:B:442:GLU:CD	2.81	0.48
1:A:213:TYR:CG	4:E:277:SER:HB3	2.49	0.48
3:C:238:VAL:CA	3:C:251:LEU:HD23	2.33	0.48
1:A:262:GLU:OE2	4:E:267:PHE:CE1	2.67	0.48
2:B:256:LYS:CD	2:B:310:LEU:HD21	2.43	0.48
4:E:312:PRO:CD	4:E:436:GLU:HG2	2.43	0.47
1:A:243:MET:HB2	2:B:255:GLU:OE1	2.13	0.47
1:A:383:ALA:O	4:E:422:PHE:HE2	1.97	0.47
3:C:231:ILE:HD12	3:C:258:ALA:HB1	1.95	0.47
4:E:242:PHE:CZ	4:E:452:PHE:HE1	2.29	0.47
4:E:312:PRO:CG	4:E:436:GLU:OE2	2.57	0.47
2:B:267:GLN:NE2	2:B:299:VAL:HG11	2.29	0.47
1:D:299:HIS:NE2	1:D:400:LYS:CG	2.63	0.47
1:D:381:TYR:OH	4:E:428:LYS:HE3	2.14	0.47
4:E:230:CYS:CB	4:E:265:PHE:CE2	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:GLY:O	2:B:430:VAL:CG2	2.63	0.47
3:C:248:LYS:HD2	3:C:302:LEU:HG	1.96	0.47
3:C:314:MET:CB	3:C:428:TRP:CZ2	2.97	0.47
1:A:376:ILE:HG21	4:E:412:GLU:HB3	1.96	0.47
2:B:315:ARG:HD3	2:B:320:HIS:CD2	2.50	0.47
1:A:268:SER:OG	2:B:227:PHE:CD1	2.56	0.47
2:B:260:ALA:HB1	2:B:303:ILE:HG23	1.97	0.47
3:C:238:VAL:HG23	3:C:251:LEU:HB3	1.96	0.47
3:C:407:ALA:HA	1:D:383:ALA:HB1	1.95	0.47
1:D:382:ILE:HD13	4:E:423:ILE:CG2	2.43	0.47
3:C:263:LEU:HD21	3:C:285:MET:HE1	1.97	0.47
1:D:291:ILE:HD12	1:D:414:PHE:CZ	2.41	0.47
4:E:325:PHE:CD1	4:E:446:VAL:HG11	2.45	0.47
2:B:426:THR:HB	3:C:408:ILE:CG2	2.43	0.46
2:B:418:GLU:HG3	3:C:402:LYS:HG2	1.96	0.46
3:C:239:PHE:CE2	3:C:443:PHE:CD2	3.04	0.46
3:C:231:ILE:CG2	3:C:262:PHE:HE2	2.28	0.46
4:E:262:GLN:CB	4:E:291:MET:HE2	2.43	0.46
2:B:244:SER:OG	2:B:465:MET:CE	2.64	0.46
4:E:317:LEU:HD13	4:E:440:TRP:CZ3	2.51	0.46
3:C:294:SER:HB3	3:C:443:PHE:CE2	2.45	0.46
3:C:314:MET:HB2	3:C:428:TRP:CE2	2.51	0.46
3:C:410:TYR:OH	1:D:387:LYS:CA	2.58	0.46
1:A:376:ILE:HD13	4:E:412:GLU:CA	2.42	0.46
1:A:376:ILE:HG21	4:E:412:GLU:HA	1.97	0.46
1:A:213:TYR:HB3	4:E:277:SER:HB2	1.97	0.45
1:D:320:ILE:CG2	1:D:409:ILE:CG1	2.94	0.45
2:B:248:TYR:CE1	2:B:458:MET:CE	3.00	0.45
2:B:428:TYR:OH	3:C:416:GLU:HG3	2.16	0.45
3:C:274:SER:HB3	1:D:213:TYR:HB2	1.98	0.45
1:D:382:ILE:HD11	4:E:423:ILE:HG22	1.97	0.45
1:A:381:TYR:OH	2:B:434:LYS:HA	2.16	0.45
1:A:381:TYR:OH	2:B:434:LYS:CA	2.64	0.45
3:C:314:MET:HE2	3:C:319:ARG:HB2	1.98	0.45
1:D:324:MET:HE3	1:D:326:PHE:HE1	1.80	0.45
2:B:267:GLN:HB3	2:B:296:MET:HE3	1.99	0.45
3:C:410:TYR:CE2	1:D:387:LYS:HG2	2.52	0.45
1:D:308:MET:HE3	1:D:399:TRP:CZ3	2.52	0.45
1:D:284:PHE:HZ	1:D:418:CYS:HB2	1.81	0.45
1:A:233:PHE:HZ	1:A:288:SER:HB2	1.79	0.44
1:A:268:SER:OG	2:B:227:PHE:CE1	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:MET:HB2	4:E:422:PHE:CE2	2.52	0.44
4:E:243:LEU:HD11	4:E:254:LEU:CD2	2.48	0.44
3:C:236:ILE:HD11	3:C:447:CYS:CB	2.48	0.44
1:D:304:SER:OG	4:E:442:LEU:CD2	2.65	0.44
2:B:423:ILE:HA	2:B:426:THR:HG22	2.00	0.44
4:E:228:ALA:HB3	4:E:229:PRO:HD3	1.99	0.44
4:E:241:TYR:OH	4:E:455:ALA:HB2	2.17	0.44
1:A:299:HIS:HB2	1:A:403:ALA:CB	2.47	0.44
2:B:248:TYR:HD1	2:B:458:MET:CE	2.25	0.44
2:B:291:TYR:HH	2:B:473:PHE:HE2	1.66	0.44
1:A:381:TYR:CE1	2:B:434:LYS:HE3	2.53	0.44
3:C:238:VAL:HG23	3:C:251:LEU:CD2	2.45	0.43
3:C:238:VAL:HB	3:C:251:LEU:HG	2.01	0.43
1:A:384:GLU:O	1:A:387:LYS:HB2	2.17	0.43
3:C:407:ALA:HB1	1:D:379:VAL:O	2.19	0.43
1:D:226:SER:O	1:D:229:THR:HG22	2.18	0.43
3:C:226:ILE:N	3:C:227:PRO:CD	2.81	0.43
3:C:238:VAL:HG23	3:C:251:LEU:CG	2.48	0.43
2:B:416:HIS:O	2:B:416:HIS:ND1	2.52	0.43
2:B:236:CYS:SG	2:B:292:LEU:HD21	2.59	0.43
2:B:426:THR:N	3:C:408:ILE:HG21	2.33	0.43
4:E:237:VAL:HG13	4:E:258:VAL:HG11	1.97	0.43
3:C:306:HIS:CD2	1:D:239:SER:HB3	2.54	0.42
1:D:284:PHE:CZ	1:D:418:CYS:HB2	2.54	0.42
1:D:317:ILE:HG13	1:D:402:VAL:HG22	1.99	0.42
3:C:283:TYR:CD1	3:C:454:ILE:CG2	2.84	0.42
3:C:303:ASN:ND2	1:D:236:PRO:HD3	2.34	0.42
1:D:277:TYR:CD2	1:D:426:PHE:CZ	3.06	0.42
1:D:317:ILE:HD11	1:D:402:VAL:HG21	1.86	0.42
1:A:264:ILE:CG2	1:A:274:ILE:CD1	2.80	0.42
3:C:239:PHE:HZ	3:C:294:SER:HA	1.84	0.42
3:C:327:PRO:N	3:C:328:PRO:HD2	2.34	0.42
4:E:269:ILE:HG22	4:E:269:ILE:O	2.18	0.42
1:A:308:MET:CE	1:A:402:VAL:HG21	2.50	0.42
2:B:421:SER:CB	3:C:409:LYS:NZ	2.61	0.42
3:C:305:HIS:O	3:C:429:GLN:HG2	2.20	0.42
4:E:286:TYR:CD1	4:E:466:ILE:HD13	2.52	0.42
1:A:306:HIS:HA	2:B:341:SER:CB	2.45	0.42
3:C:410:TYR:CZ	1:D:387:LYS:HA	2.55	0.42
3:C:411:ILE:HD13	1:D:382:ILE:HG21	2.01	0.42
1:A:380:LYS:HA	4:E:419:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:TYR:OH	2:B:434:LYS:N	2.53	0.42
3:C:277:VAL:O	3:C:282:ARG:NH1	2.53	0.42
3:C:231:ILE:HG21	3:C:262:PHE:CE2	2.52	0.41
3:C:263:LEU:HD11	3:C:285:MET:HE2	2.02	0.41
1:A:273:LEU:CD2	1:A:429:ARG:HB2	2.47	0.41
3:C:314:MET:HE3	3:C:431:VAL:HG21	2.02	0.41
1:D:406:ILE:HG22	1:D:410:LEU:CD1	2.48	0.41
1:A:383:ALA:CB	4:E:422:PHE:HD2	2.33	0.41
3:C:410:TYR:CZ	1:D:387:LYS:HG2	2.54	0.41
1:A:213:TYR:CB	4:E:277:SER:CB	2.94	0.41
1:A:260:ILE:HD12	1:A:260:ILE:H	1.86	0.41
1:A:376:ILE:HG21	4:E:412:GLU:CB	2.50	0.41
1:A:376:ILE:HG21	4:E:412:GLU:O	2.20	0.41
1:A:381:TYR:CZ	2:B:433:ILE:HG22	2.55	0.41
1:A:385:HIS:CE1	2:B:436:LYS:NZ	2.88	0.41
1:A:308:MET:HE3	1:A:399:TRP:CH2	2.54	0.41
1:A:376:ILE:HG23	4:E:412:GLU:O	2.21	0.41
3:C:400:ASP:O	1:D:376:ILE:HG21	2.21	0.41
1:A:376:ILE:HD13	4:E:412:GLU:HB3	2.00	0.41
1:D:253:LEU:CD2	1:D:285:VAL:CB	2.99	0.41
4:E:286:TYR:CD2	4:E:467:PHE:HZ	2.35	0.41
3:C:238:VAL:CG2	3:C:251:LEU:HD23	2.50	0.41
3:C:283:TYR:HH	3:C:451:THR:HG23	1.80	0.41
2:B:418:GLU:OE2	3:C:402:LYS:CE	2.69	0.41
1:D:253:LEU:HD22	1:D:285:VAL:CG1	2.51	0.41
1:D:375:ALA:CB	4:E:417:VAL:HG12	2.51	0.41
2:B:232:PHE:CZ	2:B:277:ARG:NE	2.79	0.41
2:B:256:LYS:HB2	2:B:310:LEU:HD11	2.02	0.41
2:B:267:GLN:HB3	2:B:296:MET:CE	2.51	0.41
2:B:278:LEU:CD1	2:B:286:PRO:HG3	2.49	0.41
1:D:326:PHE:HE1	1:D:412:CYS:SG	2.43	0.40
3:C:449:ILE:HD12	3:C:449:ILE:HG23	1.93	0.40
4:E:251:LYS:HD3	4:E:301:CYS:HB3	2.03	0.40
4:E:255:SER:OG	4:E:298:VAL:HG13	2.20	0.40
2:B:418:GLU:CG	3:C:402:LYS:CG	2.83	0.40
3:C:231:ILE:HB	3:C:262:PHE:HE2	1.87	0.40
3:C:303:ASN:ND2	1:D:234:TYR:O	2.55	0.40
3:C:449:ILE:HD13	3:C:449:ILE:HA	1.83	0.40
1:A:235:LEU:HD12	1:A:236:PRO:HD2	2.03	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	180/437 (41%)	173 (96%)	7 (4%)	0	100	100
1	D	180/437 (41%)	174 (97%)	6 (3%)	0	100	100
2	B	176/501 (35%)	173 (98%)	3 (2%)	0	100	100
3	C	176/469 (38%)	170 (97%)	6 (3%)	0	100	100
4	E	169/489 (35%)	167 (99%)	2 (1%)	0	100	100
All	All	881/2333 (38%)	857 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	171/405 (42%)	171 (100%)	0	100	100
1	D	171/405 (42%)	170 (99%)	1 (1%)	86	92
2	B	162/458 (35%)	161 (99%)	1 (1%)	86	92
3	C	165/431 (38%)	165 (100%)	0	100	100
4	E	154/446 (34%)	154 (100%)	0	100	100
All	All	823/2145 (38%)	821 (100%)	2 (0%)	93	96

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

Mol	Chain	Res	Type
2	B	436	LYS
1	D	404	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	267	GLN
3	C	306	HIS
1	D	408	HIS
4	E	262	GLN
4	E	300	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

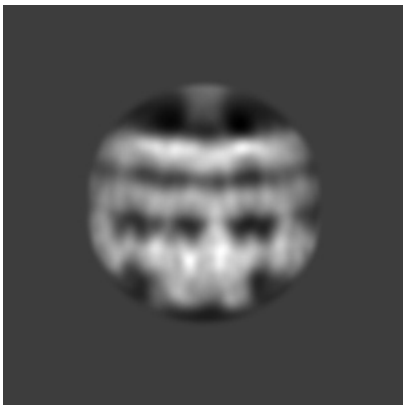
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18596. 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

6.1.1 Primary map

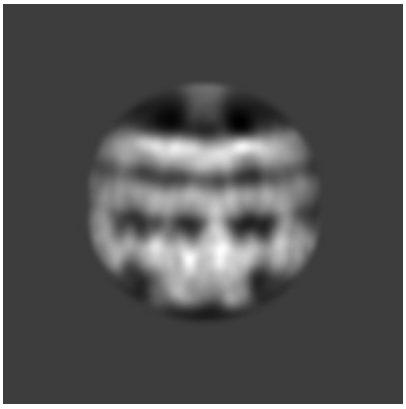


X

Y

Z

6.1.2 Raw map



X

Y

Z

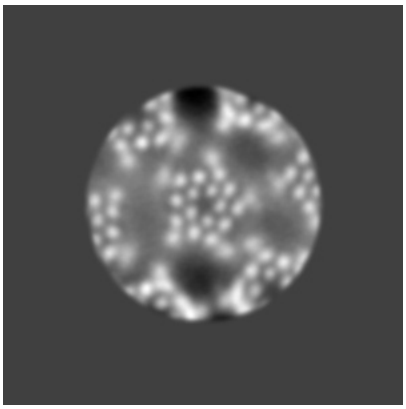
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

X Index: 100

Y Index: 100

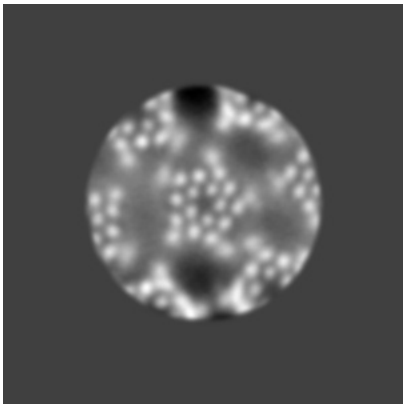


Z Index: 100

6.2.2 Raw map

X Index: 100

Y Index: 100

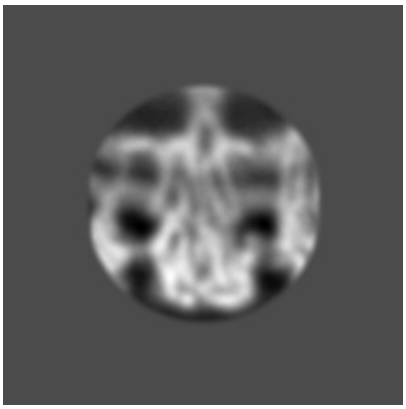


Z Index: 100

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

6.3 Largest variance slices (i)

6.3.1 Primary map

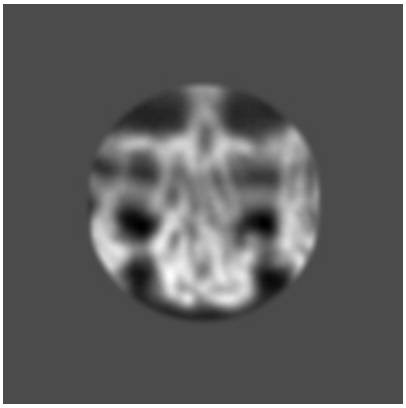


X Index: 111

Y Index: 112

Z Index: 76

6.3.2 Raw map



X Index: 111

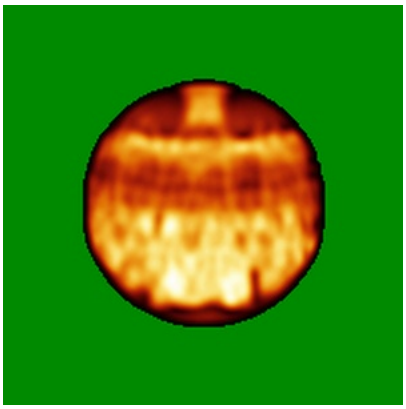
Y Index: 112

Z Index: 76

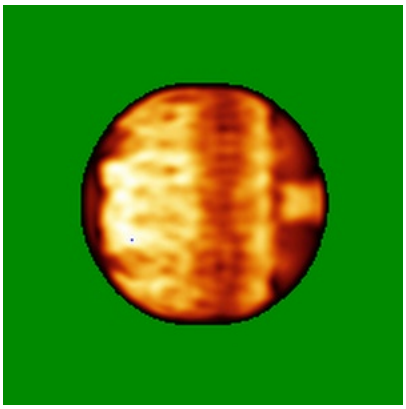
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

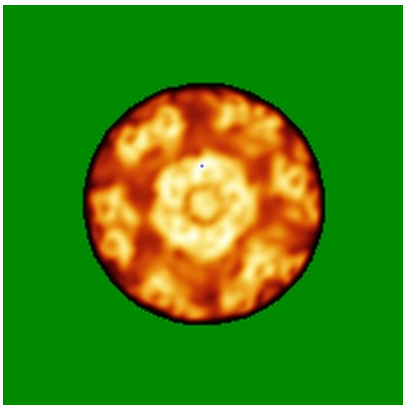
6.4.1 Primary map



X

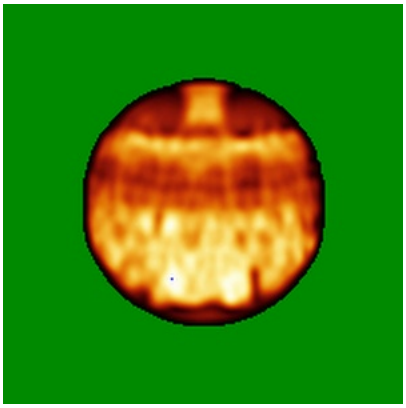


Y

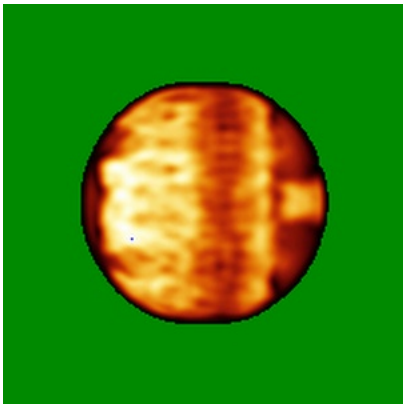


Z

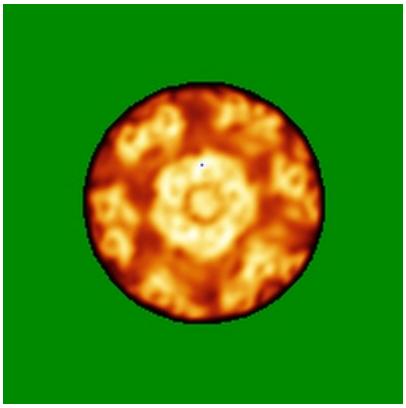
6.4.2 Raw map



X



Y

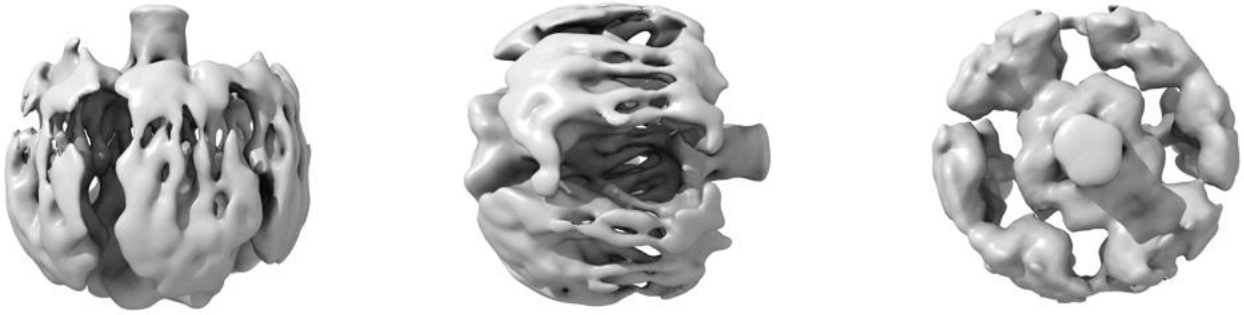


Z

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)

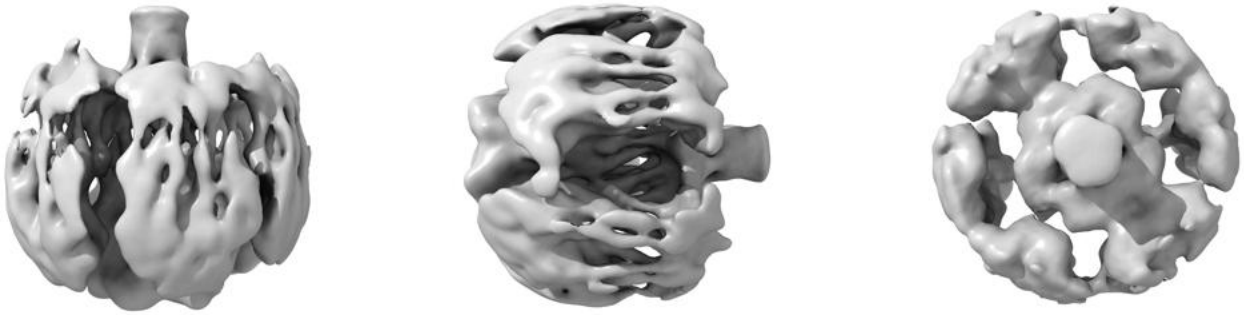
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0005. 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



X Y Z

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.

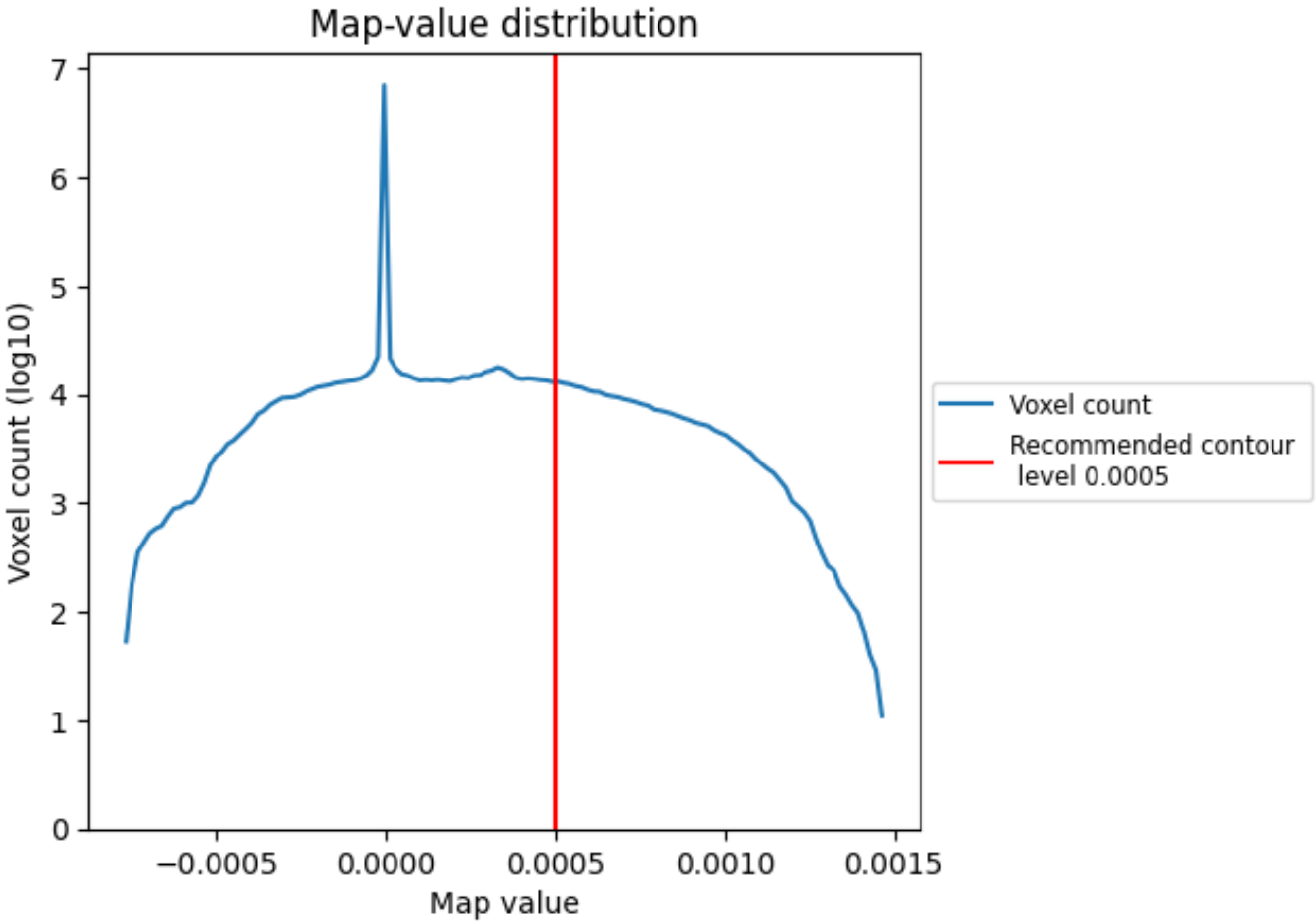
6.6 Mask visualisation (i)

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

7 Map analysis

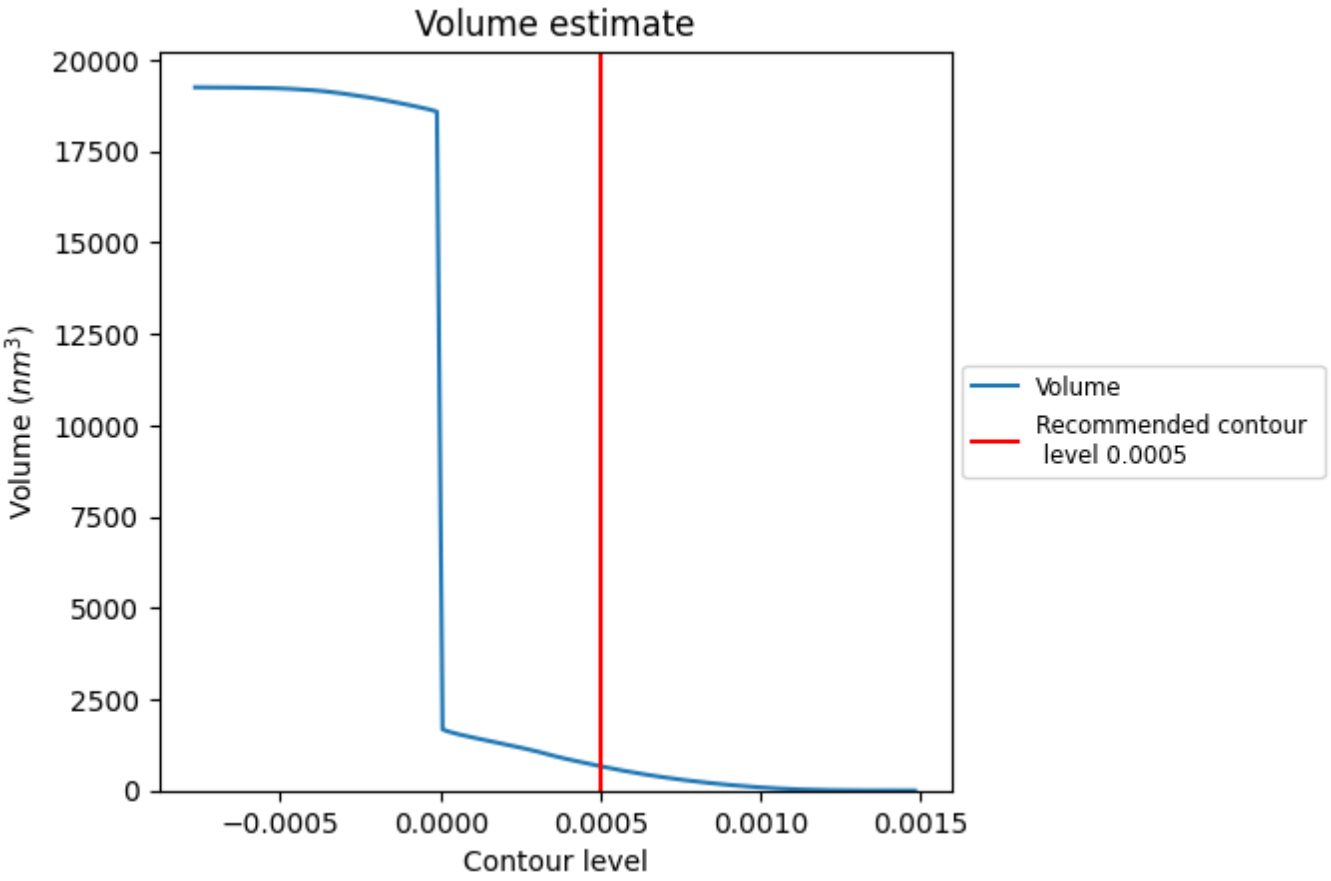
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

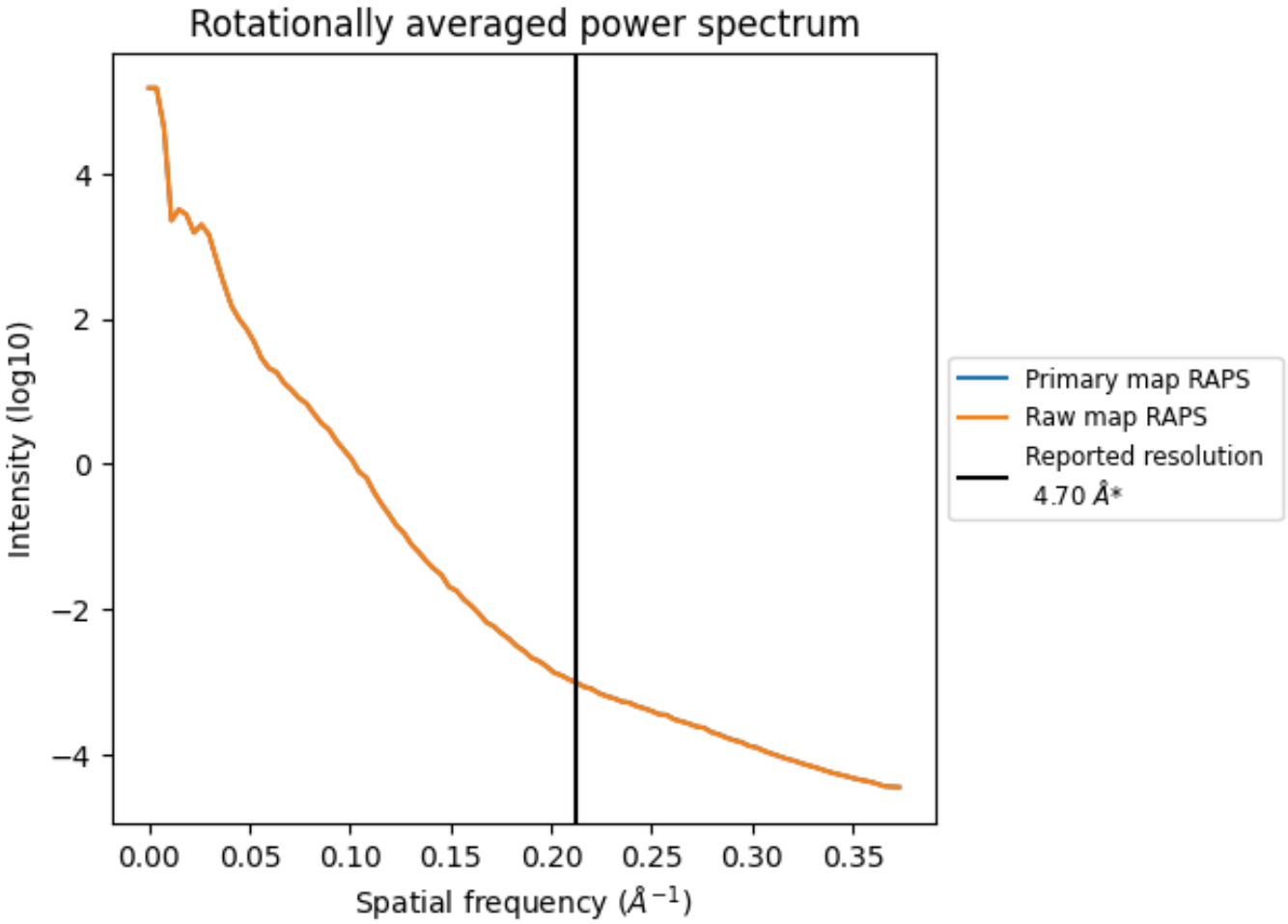
7.2 Volume estimate



The volume at the recommended contour level is 666 nm^3; this corresponds to an approximate mass of 602 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 (i)

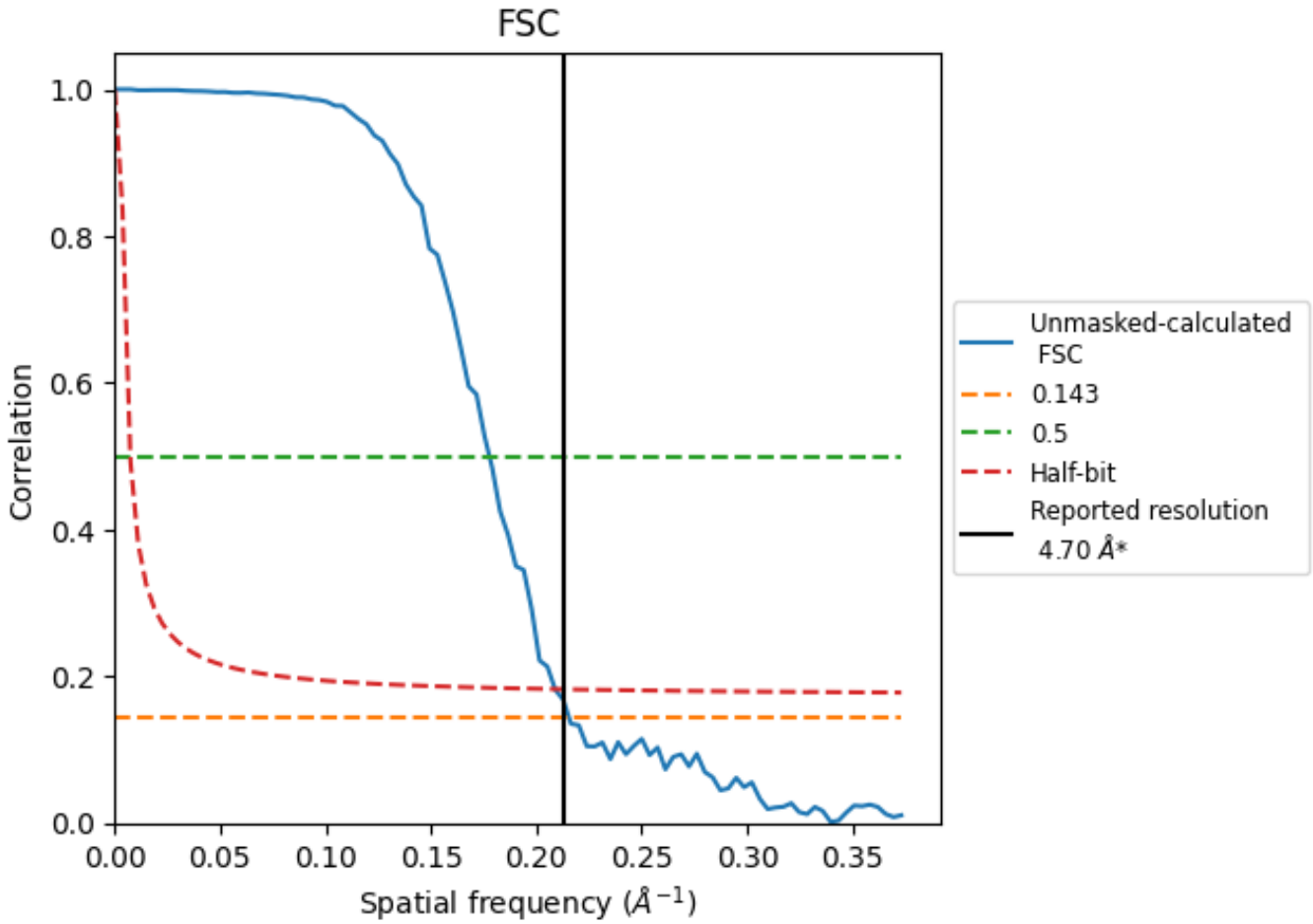


*Reported resolution corresponds to spatial frequency of 0.213 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.213 Å^{-1}

8.2 Resolution estimates (i)

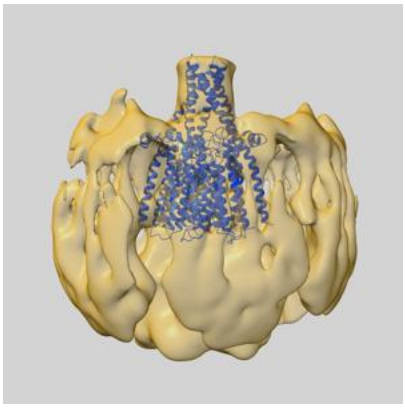
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.64	5.63	4.79

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

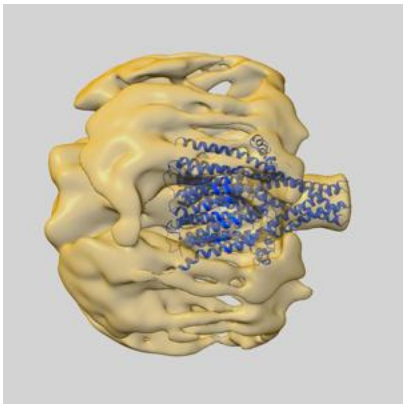
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18596 and PDB model 8QQM. Per-residue inclusion information can be found in section 3 on page 4.

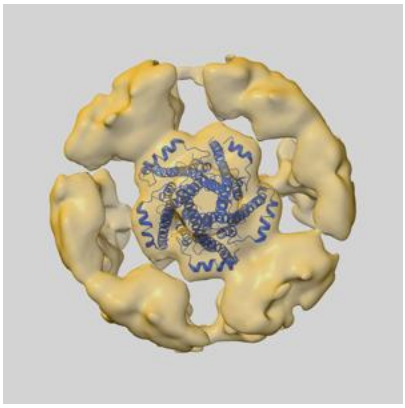
9.1 Map-model overlay



X



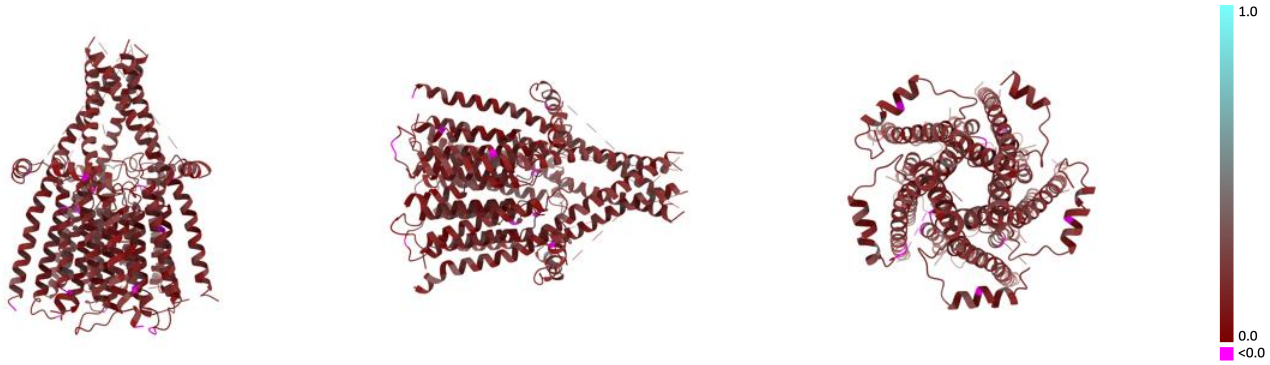
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0005 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.

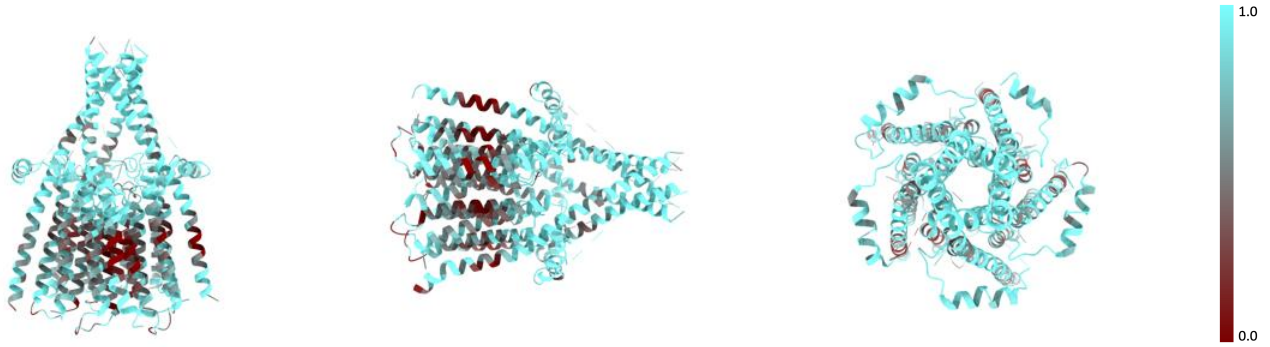
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

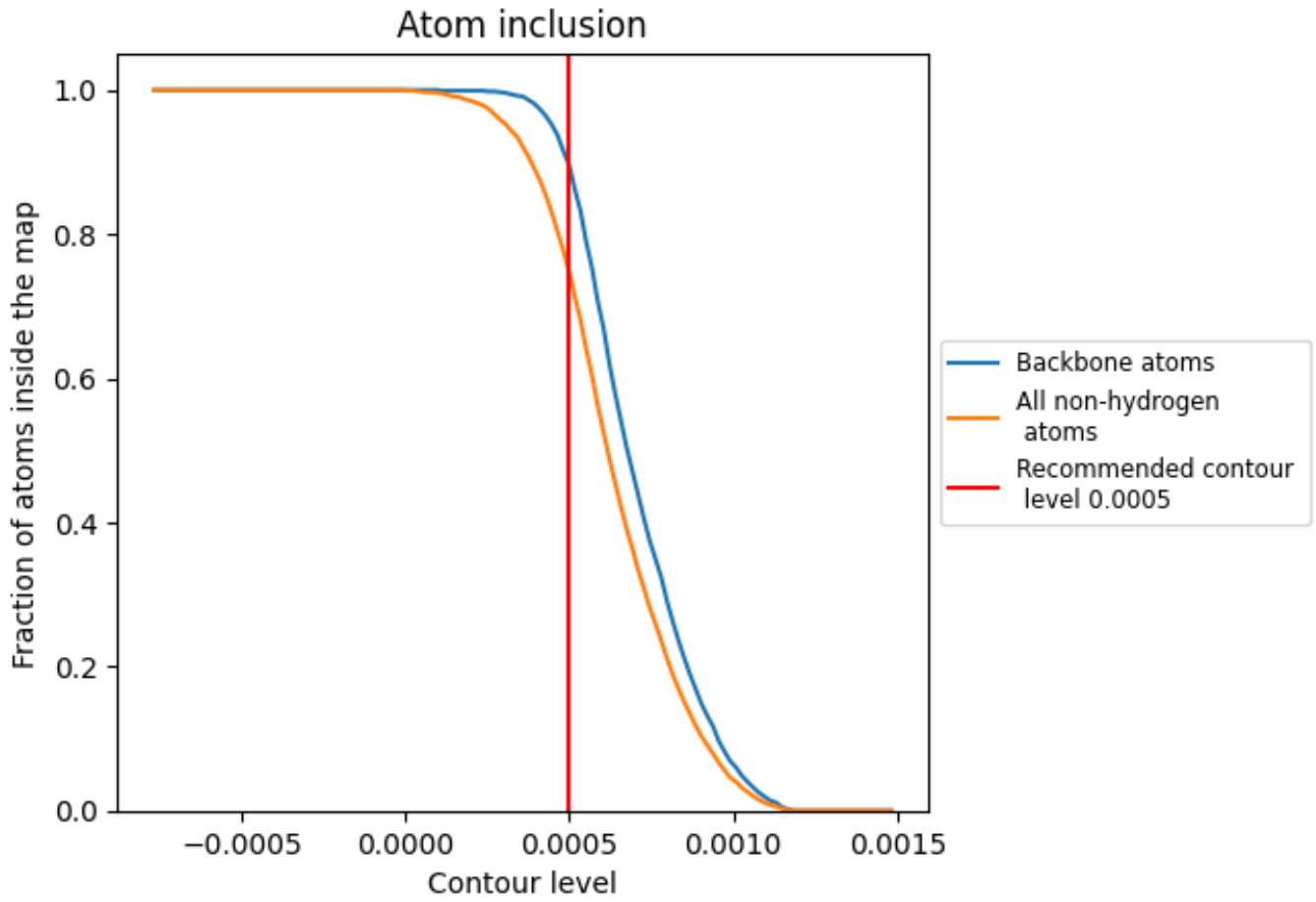
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0005).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 75% 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 (0.0005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7470	0.1560
A	0.7290	0.1580
B	0.7740	0.1590
C	0.7210	0.1530
D	0.7530	0.1550
E	0.7600	0.1540