



Full wwPDB EM Validation Report ⓘ

Jan 27, 2025 – 12:35 PM JST

PDB ID : 8XLL
EMDB ID : EMD-38452
Title : Structure of the native 2-oxoglutarate dehydrogenase complex (OGDHC) in the adult cortex and hippocampus
Authors : Zhang, M.; Feng, J.; Li, Y.; Zhu, S.
Deposited on : 2023-12-26
Resolution : 3.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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:

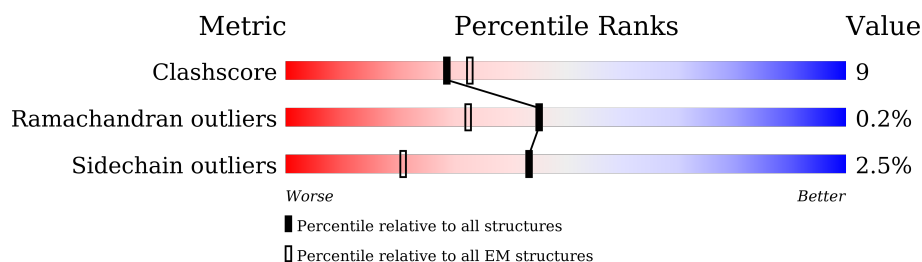
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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	216	
1	B	216	
1	C	216	
1	D	216	
1	E	216	
1	F	216	
1	G	216	
1	H	216	

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Mol	Chain	Length	Quality of chain
1	I	216	
1	J	216	
1	K	216	
1	L	216	
1	M	216	
1	N	216	
1	O	216	
1	P	216	
1	R	216	
1	S	216	
1	T	216	
1	U	216	
1	V	216	
1	W	216	
1	X	216	
1	Y	216	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 39478 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 Dihydrolipoyllysine-residue succinyltransferase component of 2-oxoglutarate dehydrogenase complex, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	213	Total	C	N	O	S	0	0
			1653	1048	287	308	10		
1	B	212	Total	C	N	O	S	0	0
			1648	1045	286	307	10		
1	C	215	Total	C	N	O	S	0	0
			1671	1059	290	312	10		
1	D	211	Total	C	N	O	S	0	0
			1639	1040	284	305	10		
1	E	213	Total	C	N	O	S	0	0
			1653	1048	287	308	10		
1	F	210	Total	C	N	O	S	0	0
			1631	1036	282	303	10		
1	G	216	Total	C	N	O	S	0	0
			1679	1065	291	313	10		
1	H	210	Total	C	N	O	S	0	0
			1631	1036	282	303	10		
1	I	214	Total	C	N	O	S	0	0
			1662	1053	288	311	10		
1	J	208	Total	C	N	O	S	0	0
			1618	1029	280	300	9		
1	K	211	Total	C	N	O	S	0	0
			1639	1040	284	305	10		
1	L	209	Total	C	N	O	S	0	0
			1624	1032	281	301	10		
1	M	212	Total	C	N	O	S	0	0
			1648	1045	286	307	10		
1	N	215	Total	C	N	O	S	0	0
			1671	1059	290	312	10		
1	O	208	Total	C	N	O	S	0	0
			1618	1029	280	300	9		
1	P	216	Total	C	N	O	S	0	0
			1679	1065	291	313	10		

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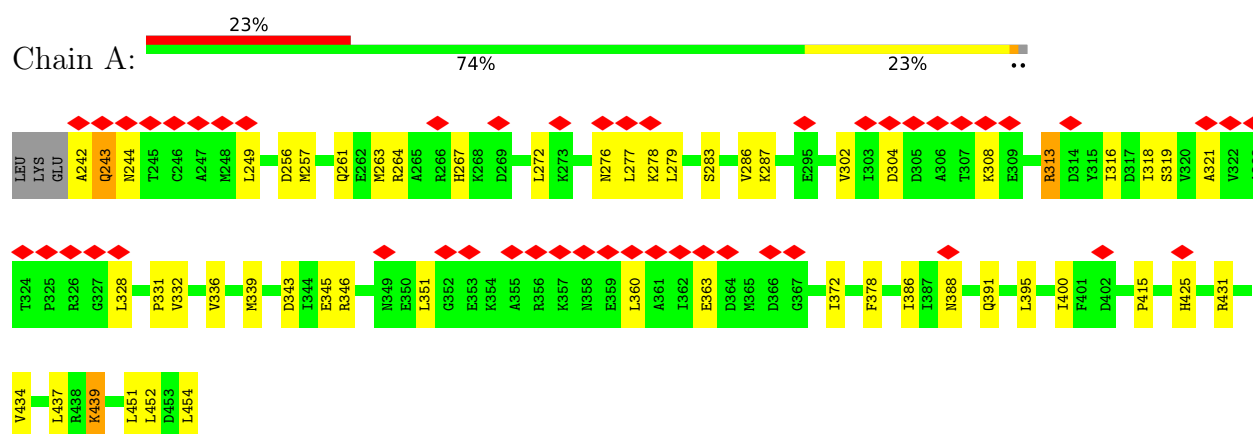
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	212	Total	C	N	O	S	0	0
			1648	1045	286	307	10		
1	S	212	Total	C	N	O	S	0	0
			1648	1045	286	307	10		
1	T	210	Total	C	N	O	S	0	0
			1631	1036	282	303	10		
1	U	211	Total	C	N	O	S	0	0
			1639	1040	284	305	10		
1	V	213	Total	C	N	O	S	0	0
			1653	1048	287	308	10		
1	W	209	Total	C	N	O	S	0	0
			1624	1032	281	301	10		
1	X	209	Total	C	N	O	S	0	0
			1624	1032	281	301	10		
1	Y	212	Total	C	N	O	S	0	0
			1647	1045	286	306	10		

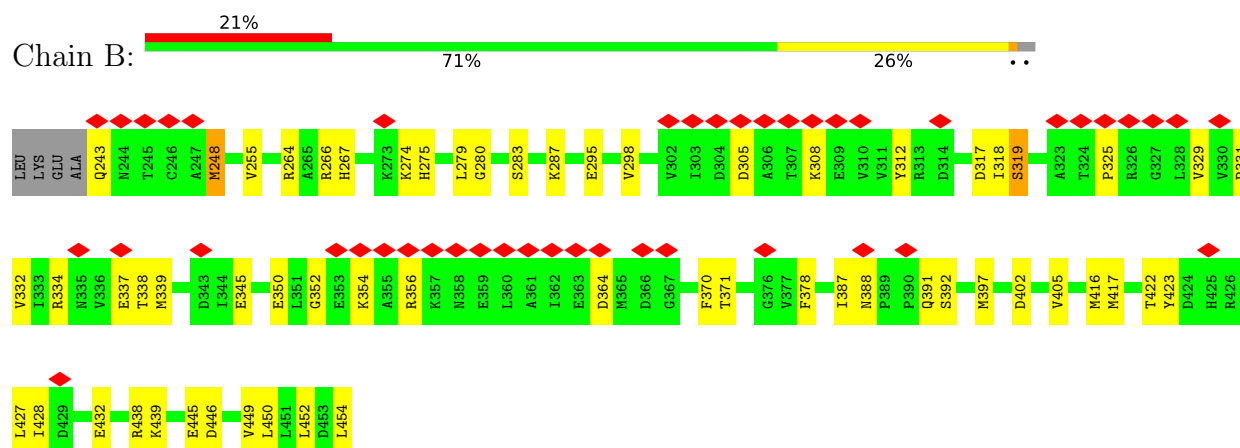
3 Residue-property plots

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: Dihydrolipoyllysine-residue succinyltransferase component of 2-oxoglutarate dehydrogenase complex, mitochondrial

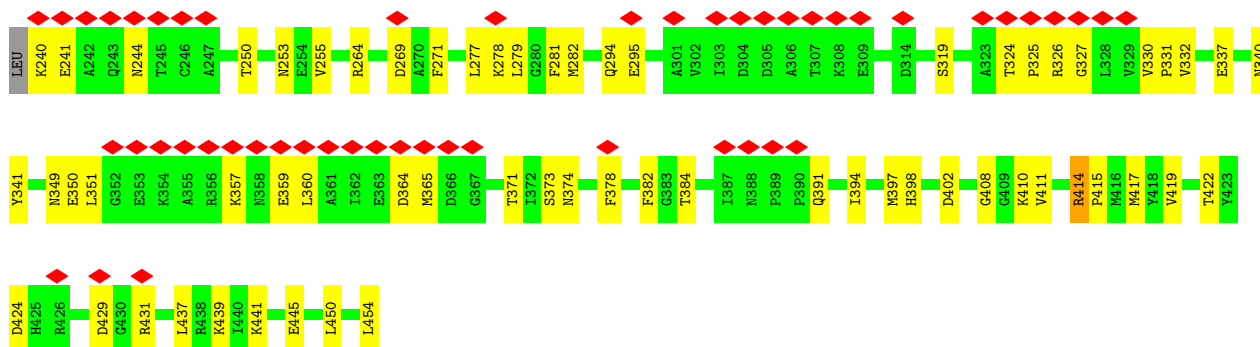


- Molecule 1: Dihydrolipoyllysine-residue succinyltransferase component of 2-oxoglutarate dehydrogenase complex, mitochondrial

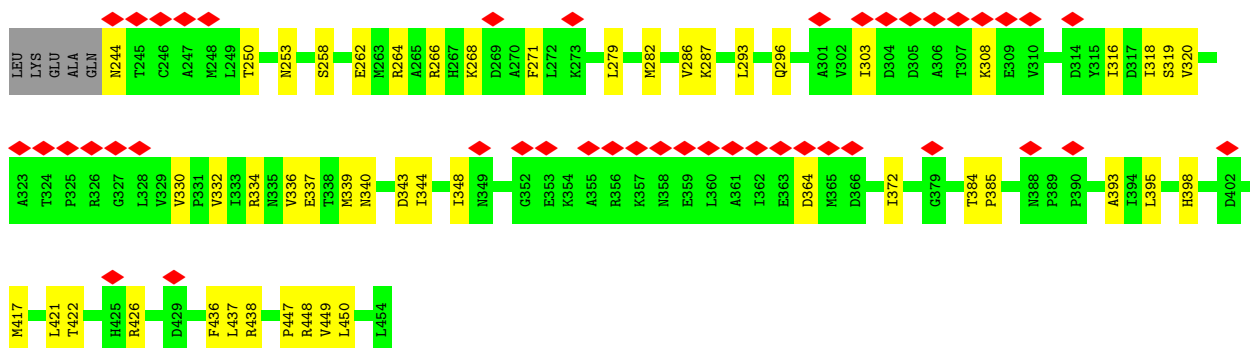
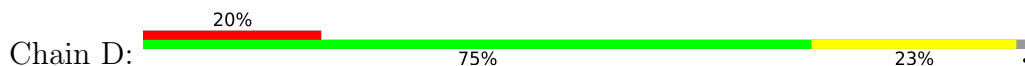


- Molecule 1: Dihydrolipoyllysine-residue succinyltransferase component of 2-oxoglutarate dehydrogenase complex, mitochondrial

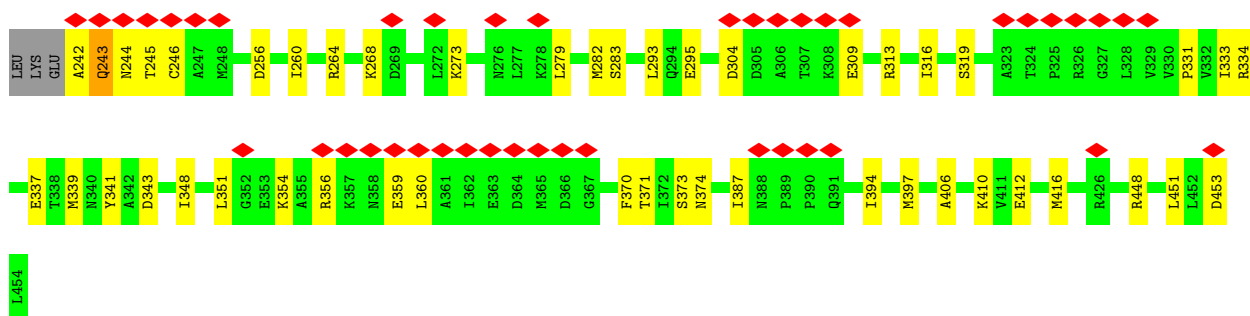
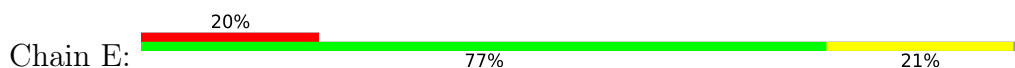




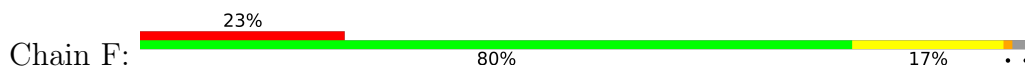
- Molecule 1: Dihydrolipoyllysine-residue succinyltransferase component of 2-oxoglutarate dehydrogenase complex, mitochondrial

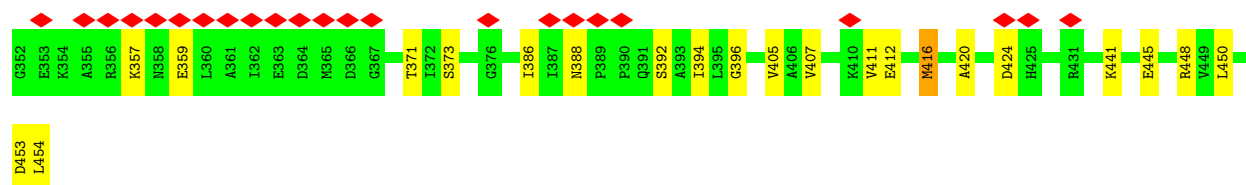


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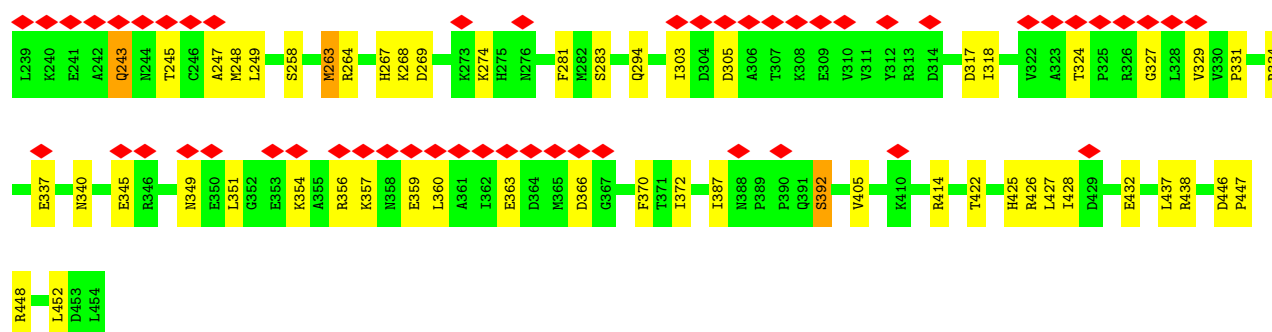
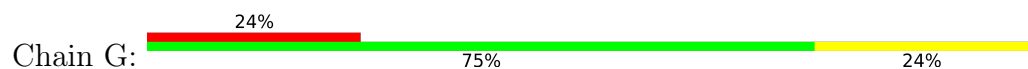


- Molecule 1: Dihydrolipoyllysine-residue succinyltransferase component of 2-oxoglutarate dehydrogenase complex, mitochondrial

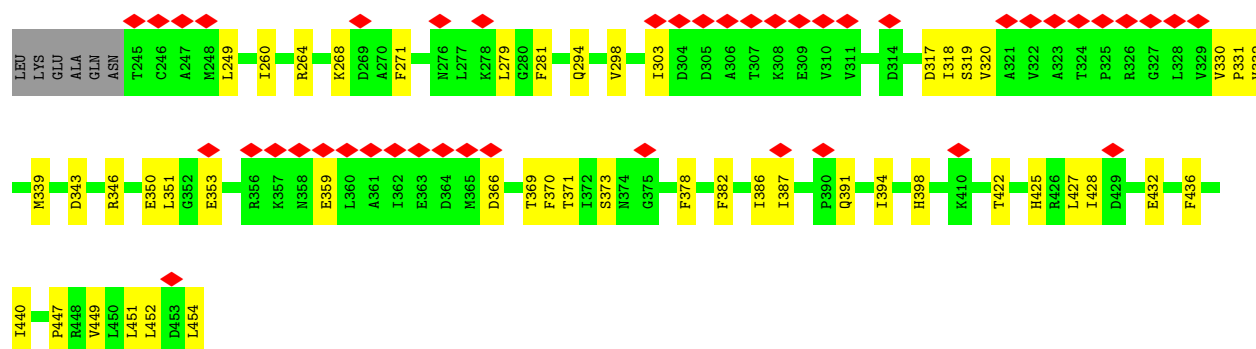
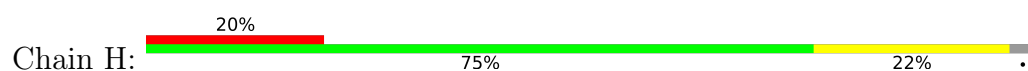




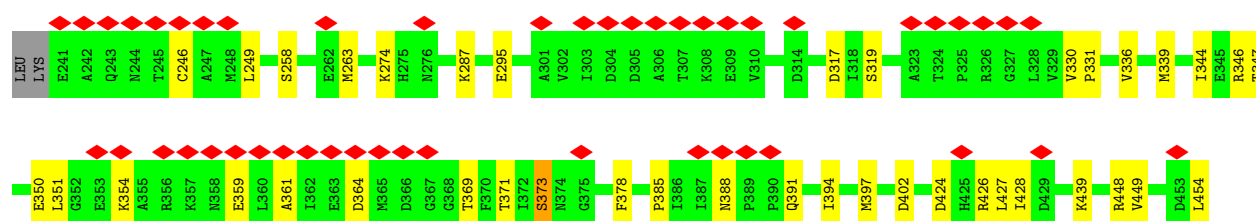
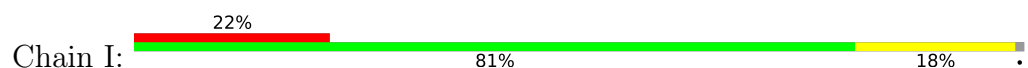
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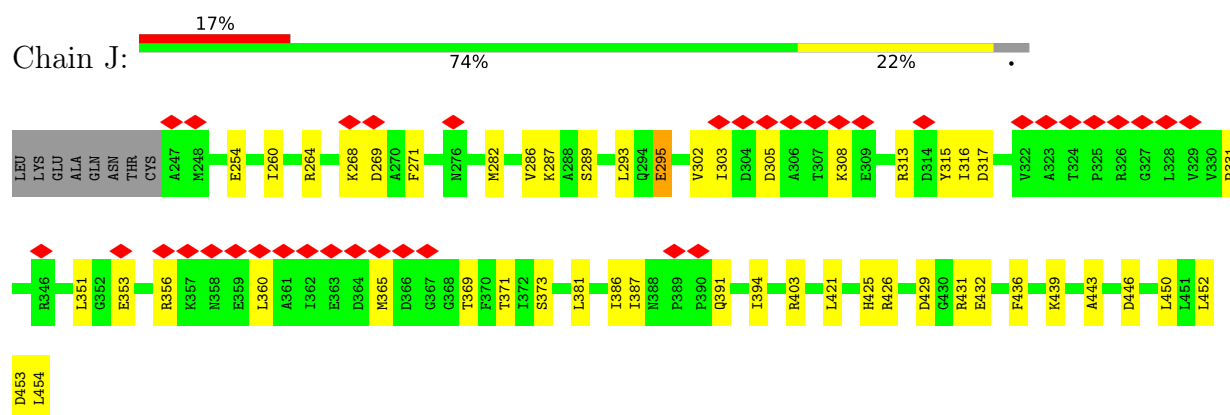
- Molecule 1: Dihydrolipoyllysine-residue succinyltransferase component of 2-oxoglutarate dehydrogenase complex, mitochondrial



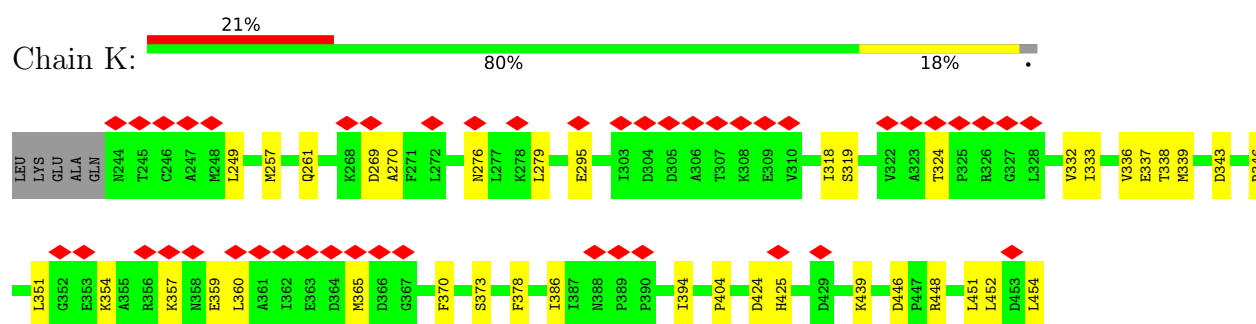
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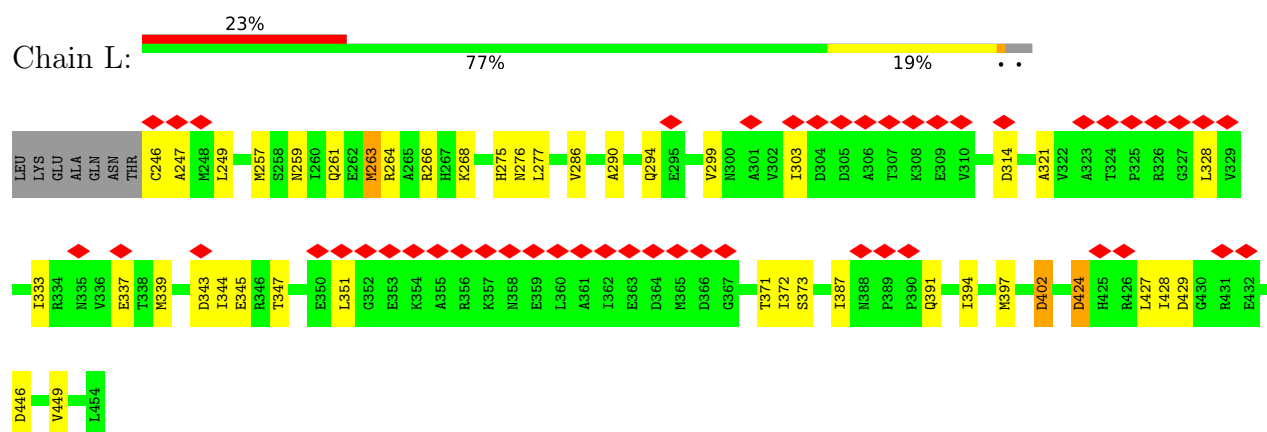
- Molecule 1: Dihydrolipoyllysine-residue succinyltransferase component of 2-oxoglutarate dehydrogenase complex, mitochondrial



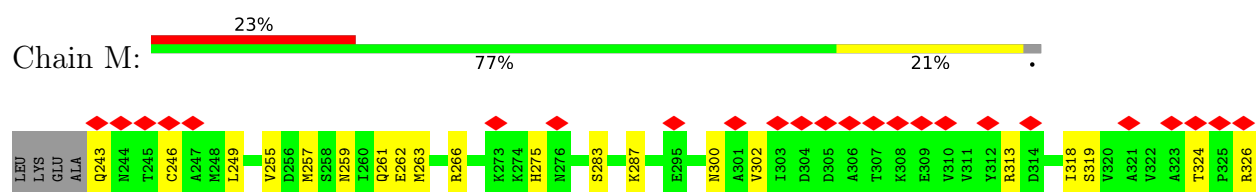
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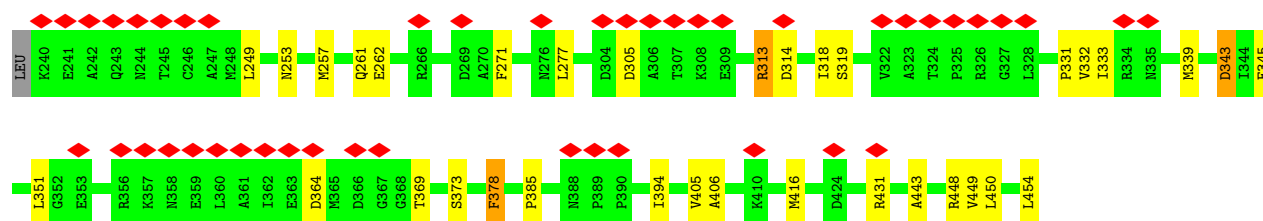
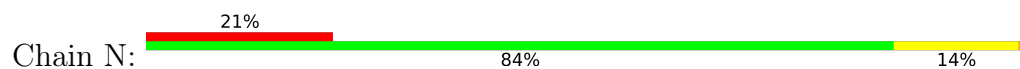


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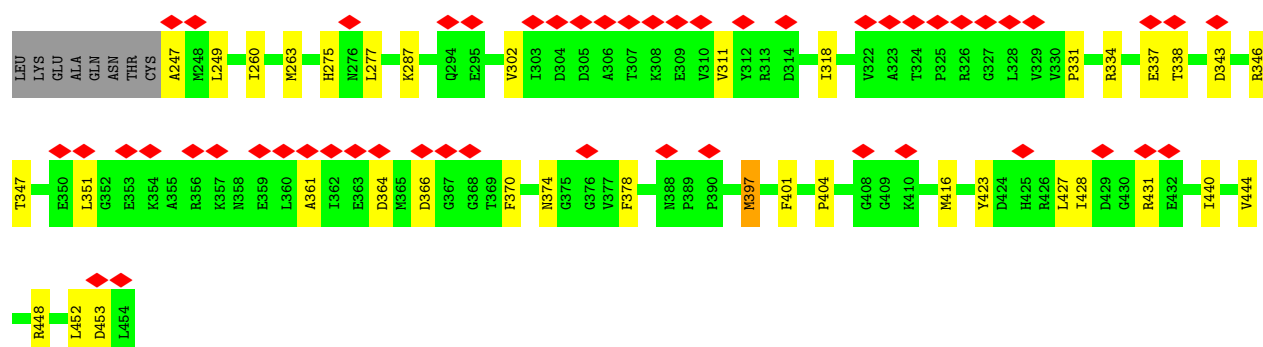
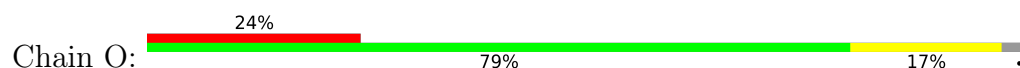




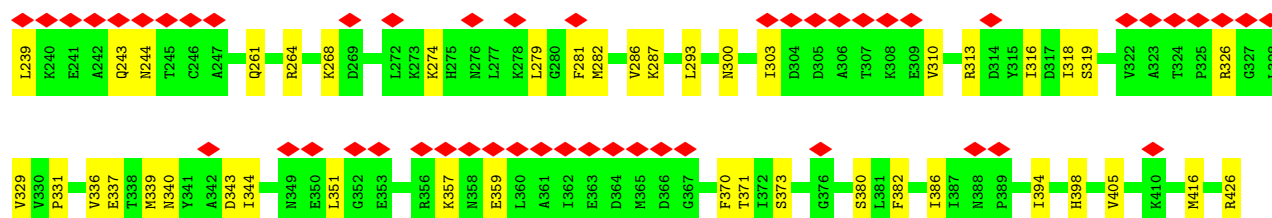
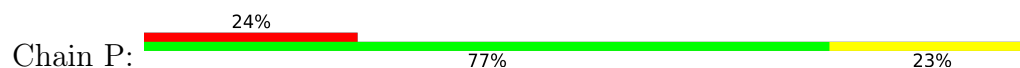
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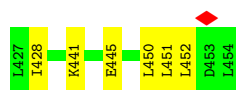


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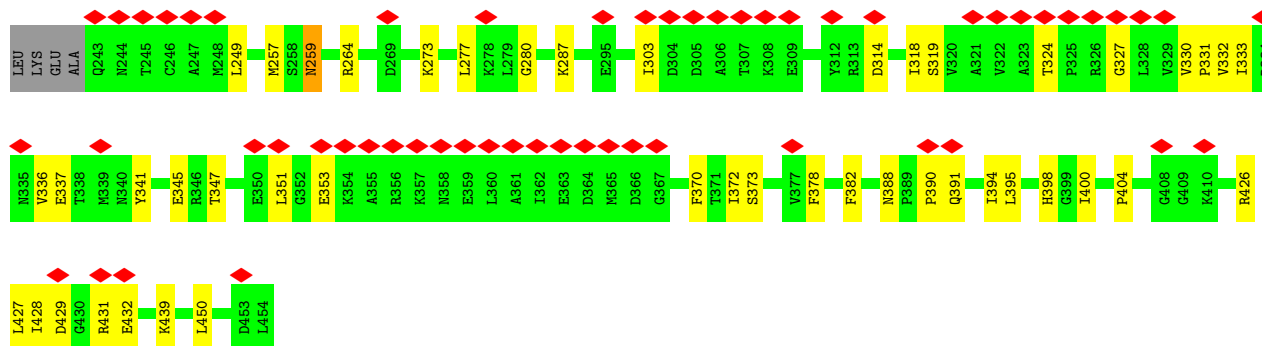
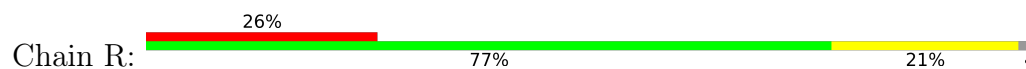


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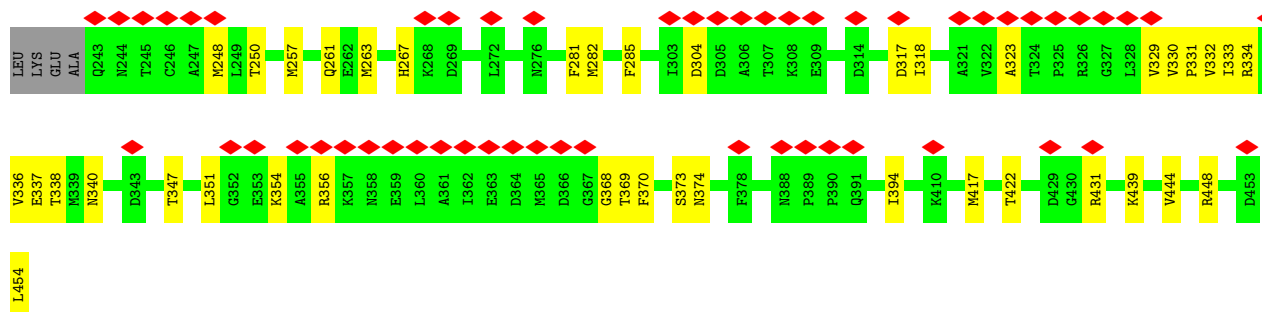




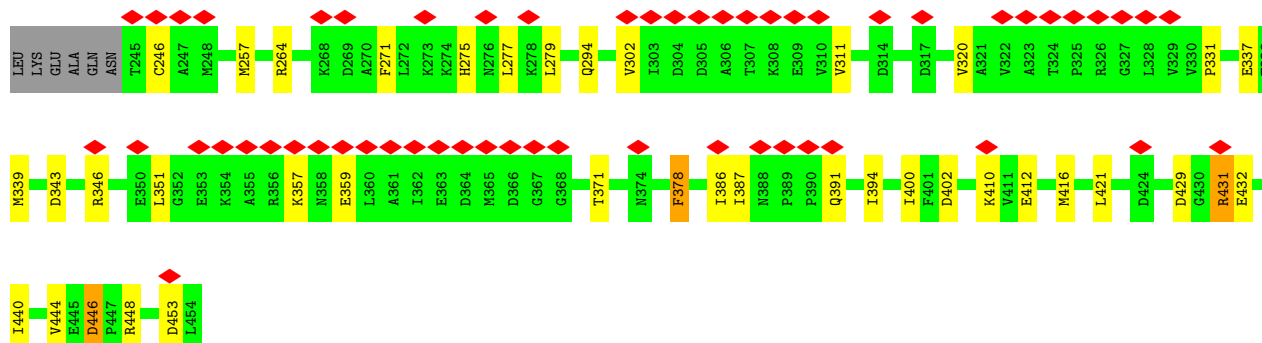
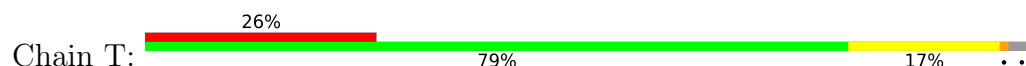
- Molecule 1: Dihydrolipoyllysine-residue succinyltransferase component of 2-oxoglutarate dehydrogenase complex, mitochondrial



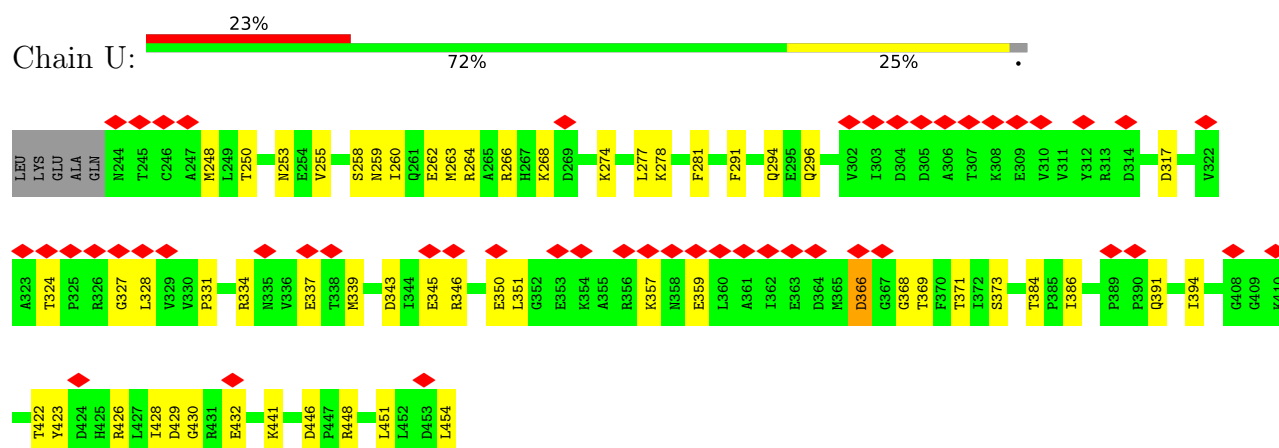
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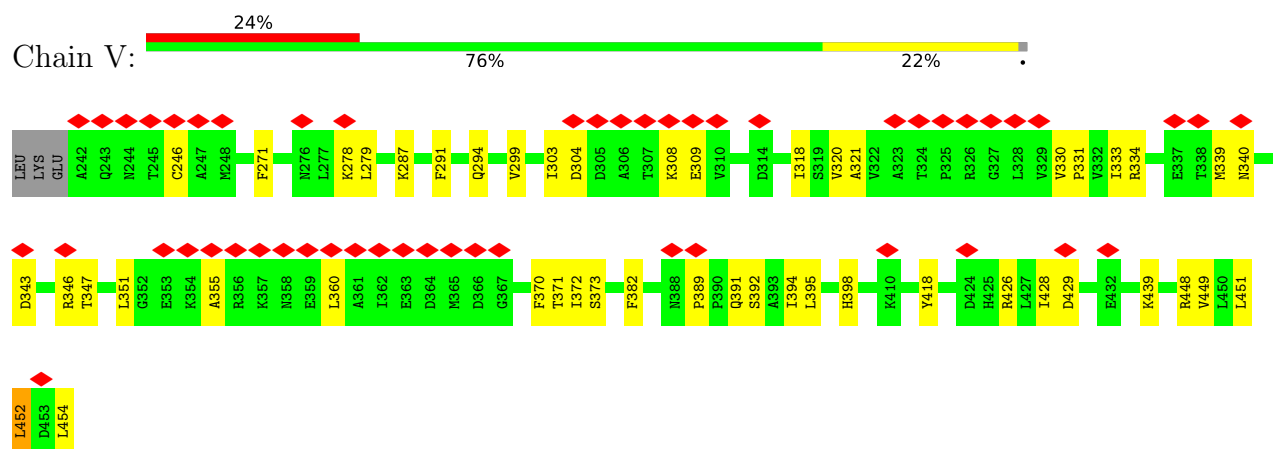
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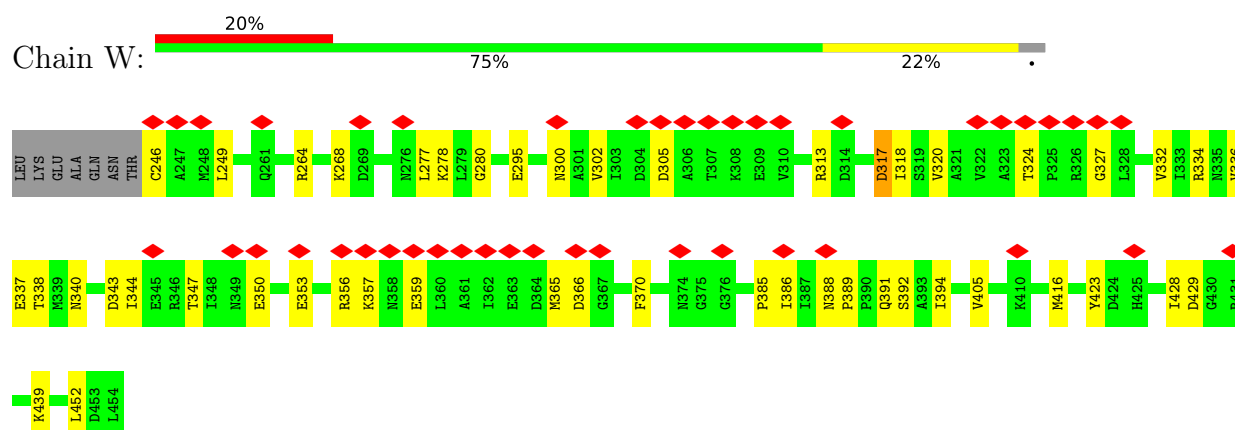
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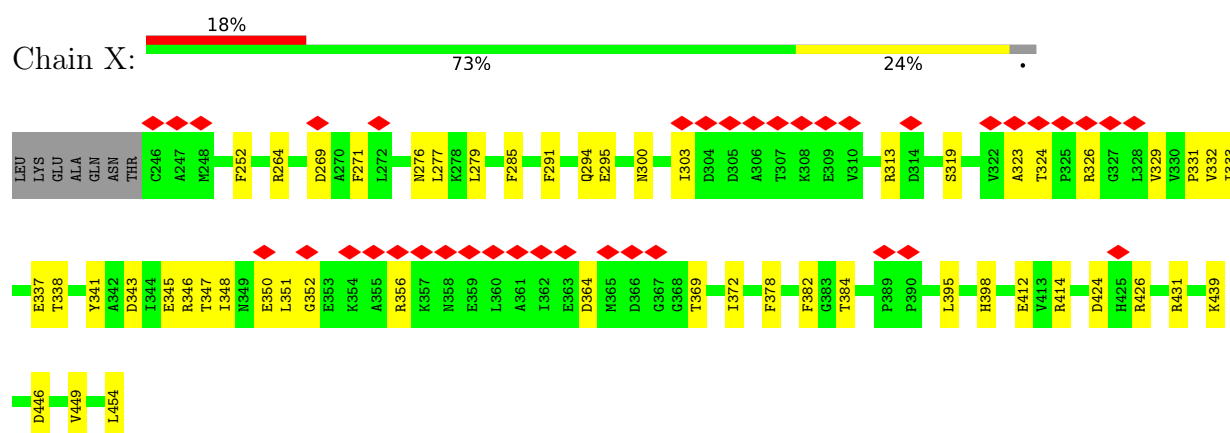
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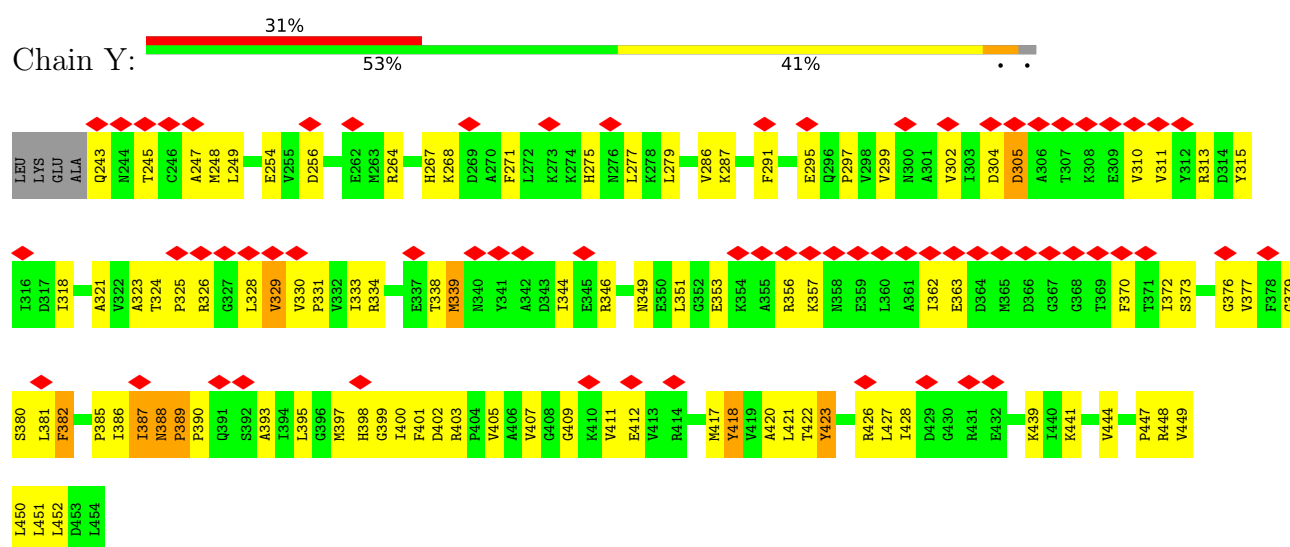
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	268960	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-10 (5k x 4k)	Depositor
Maximum map value	1.418	Depositor
Minimum map value	-0.933	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.288	Depositor
Map size (\AA)	460.53, 460.53, 460.53	wwPDB
Map dimensions	430, 430, 430	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.071, 1.071, 1.071	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/1680	0.57	0/2272
1	B	0.28	0/1675	0.52	0/2265
1	C	0.27	0/1698	0.53	0/2295
1	D	0.29	0/1666	0.54	0/2253
1	E	0.27	0/1680	0.52	0/2272
1	F	0.27	0/1658	0.53	0/2242
1	G	0.28	0/1706	0.54	0/2306
1	H	0.26	0/1658	0.51	0/2242
1	I	0.26	0/1689	0.51	0/2284
1	J	0.28	0/1645	0.54	0/2224
1	K	0.26	0/1666	0.51	0/2253
1	L	0.27	0/1651	0.51	0/2232
1	M	0.27	0/1675	0.52	0/2265
1	N	0.27	0/1698	0.52	0/2295
1	O	0.28	0/1645	0.53	0/2224
1	P	0.26	0/1706	0.51	0/2306
1	R	0.27	0/1675	0.52	0/2265
1	S	0.26	0/1675	0.51	0/2265
1	T	0.28	0/1658	0.55	0/2242
1	U	0.28	0/1666	0.53	0/2253
1	V	0.27	0/1680	0.53	0/2272
1	W	0.28	0/1651	0.53	0/2232
1	X	0.27	0/1651	0.50	0/2232
1	Y	0.34	0/1674	0.68	1/2265 (0.0%)
All	All	0.28	0/40126	0.53	1/54256 (0.0%)

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	W	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	386	ILE	N-CA-C	-5.09	97.26	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	W	389	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1653	0	1679	37	0
1	B	1648	0	1674	41	0
1	C	1671	0	1698	48	0
1	D	1639	0	1666	35	0
1	E	1653	0	1679	34	0
1	F	1631	0	1660	26	0
1	G	1679	0	1709	38	0
1	H	1631	0	1660	32	0
1	I	1662	0	1685	24	0
1	J	1618	0	1648	36	0
1	K	1639	0	1666	27	0
1	L	1624	0	1653	29	0
1	M	1648	0	1674	34	0
1	N	1671	0	1698	21	0
1	O	1618	0	1648	28	0
1	P	1679	0	1709	31	0
1	R	1648	0	1674	29	0
1	S	1648	0	1674	24	0
1	T	1631	0	1660	26	0
1	U	1639	0	1666	35	0
1	V	1653	0	1679	34	0
1	W	1624	0	1653	33	0
1	X	1624	0	1653	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	1647	0	1674	90	0
All	All	39478	0	40139	735	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 9.

All (735) 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:R:331:PRO:HB3	1:R:351:LEU:HD12	1.59	0.84
1:O:331:PRO:HB2	1:O:351:LEU:HD23	1.59	0.83
1:V:339:MET:HB2	1:V:343:ASP:HB2	1.61	0.82
1:W:385:PRO:HB2	1:W:394:ILE:HD11	1.65	0.78
1:D:339:MET:HB3	1:D:343:ASP:HB3	1.65	0.78
1:A:339:MET:HB3	1:A:343:ASP:HB2	1.64	0.77
1:M:334:ARG:NH2	1:M:363:GLU:O	2.18	0.77
1:E:448:ARG:NH1	1:M:259:ASN:OD1	2.18	0.76
1:A:386:ILE:HB	1:W:249:LEU:HD21	1.68	0.75
1:J:386:ILE:HB	1:Y:249:LEU:HD21	1.67	0.74
1:S:317:ASP:HB2	1:S:369:THR:HG23	1.69	0.74
1:F:331:PRO:HB2	1:F:351:LEU:HD13	1.70	0.74
1:X:324:THR:HG22	1:X:326:ARG:H	1.53	0.74
1:K:295:GLU:HG3	1:K:439:LYS:HE3	1.70	0.73
1:W:452:LEU:HA	1:X:341:TYR:HB2	1.69	0.72
1:C:244:ASN:HB3	1:O:247:ALA:HA	1.70	0.72
1:W:264:ARG:HH11	1:W:280:GLY:HA2	1.54	0.72
1:Y:310:VAL:HG12	1:Y:311:VAL:HG23	1.72	0.72
1:P:339:MET:HB2	1:P:343:ASP:HB2	1.72	0.71
1:A:249:LEU:HD21	1:M:386:ILE:HB	1.72	0.71
1:R:373:SER:HB3	1:R:394:ILE:HD11	1.74	0.70
1:Y:256:ASP:HB2	1:Y:447:PRO:HB3	1.75	0.69
1:Y:326:ARG:HE	1:Y:331:PRO:HG3	1.58	0.69
1:M:353:GLU:HG2	1:M:356:ARG:HH22	1.57	0.69
1:S:250:THR:HG1	1:S:422:THR:HG1	1.41	0.69
1:T:331:PRO:HG2	1:T:351:LEU:HD13	1.74	0.69
1:J:331:PRO:HB2	1:J:351:LEU:HD13	1.75	0.69
1:F:262:GLU:OE1	1:U:448:ARG:NH1	2.26	0.68
1:N:331:PRO:HB2	1:N:351:LEU:HD13	1.74	0.68
1:U:371:THR:OG1	1:U:391:GLN:OE1	2.11	0.68
1:K:386:ILE:HB	1:N:249:LEU:HD11	1.76	0.68
1:Y:387:ILE:HG23	1:Y:398:HIS:CE1	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:300:ASN:O	1:M:313:ARG:NH2	2.28	0.67
1:J:303:ILE:HG21	1:J:426:ARG:HH12	1.58	0.67
1:F:329:VAL:HG12	1:F:331:PRO:HD3	1.76	0.67
1:P:371:THR:HB	1:P:394:ILE:HG13	1.77	0.66
1:E:374:ASN:HA	1:E:397:MET:HB2	1.77	0.66
1:I:361:ALA:HB3	1:I:364:ASP:HB2	1.78	0.66
1:K:339:MET:HB3	1:K:343:ASP:HB2	1.77	0.66
1:D:250:THR:HG22	1:D:422:THR:HB	1.78	0.66
1:W:324:THR:OG1	1:W:327:GLY:O	2.12	0.66
1:D:244:ASN:O	1:G:243:GLN:NE2	2.29	0.66
1:G:331:PRO:HG3	1:G:360:LEU:HD11	1.77	0.65
1:L:266:ARG:NH2	1:T:446:ASP:OD2	2.29	0.65
1:C:371:THR:OG1	1:C:391:GLN:OE1	2.15	0.65
1:P:318:ILE:HG12	1:P:336:VAL:HG21	1.78	0.65
1:Y:423:TYR:HB2	1:Y:439:LYS:HD3	1.78	0.65
1:M:331:PRO:HB2	1:M:351:LEU:HD13	1.78	0.65
1:X:264:ARG:HG2	1:X:279:LEU:HG	1.79	0.65
1:B:423:TYR:HB2	1:B:428:ILE:HD11	1.78	0.64
1:C:319:SER:HA	1:C:332:VAL:HA	1.80	0.64
1:B:337:GLU:HG2	1:B:338:THR:HG23	1.80	0.64
1:B:427:LEU:HG	1:B:428:ILE:HG23	1.78	0.64
1:V:331:PRO:HB2	1:V:351:LEU:HD13	1.79	0.64
1:Y:299:VAL:HG12	1:Y:372:ILE:HD11	1.77	0.64
1:B:325:PRO:HD2	1:B:356:ARG:HH12	1.62	0.64
1:C:360:LEU:HB3	1:C:365:MET:HE3	1.80	0.64
1:E:319:SER:HB2	1:E:371:THR:HG23	1.79	0.64
1:I:274:LYS:NZ	1:N:454:LEU:OXT	2.31	0.64
1:J:254:GLU:OE1	1:J:403:ARG:NH1	2.31	0.64
1:Y:395:LEU:HD22	1:Y:423:TYR:CD1	2.32	0.64
1:Y:395:LEU:HD22	1:Y:423:TYR:HD1	1.61	0.64
1:H:331:PRO:HB2	1:H:351:LEU:HD13	1.78	0.64
1:G:329:VAL:HG23	1:G:331:PRO:HD3	1.80	0.64
1:H:339:MET:HB2	1:H:343:ASP:HB2	1.79	0.63
1:E:339:MET:HB3	1:E:343:ASP:HB2	1.81	0.63
1:D:250:THR:HG21	1:D:384:THR:HB	1.80	0.63
1:U:337:GLU:OE2	1:U:337:GLU:N	2.22	0.63
1:A:278:LYS:HE3	1:A:278:LYS:HA	1.81	0.63
1:E:453:ASP:O	1:M:275:HIS:NE2	2.31	0.63
1:B:371:THR:OG1	1:B:391:GLN:NE2	2.32	0.63
1:H:319:SER:HB3	1:H:332:VAL:HG22	1.80	0.63
1:S:331:PRO:HB2	1:S:351:LEU:HD13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:371:THR:OG1	1:T:391:GLN:OE1	2.15	0.63
1:Y:385:PRO:HD3	1:Y:400:ILE:HD11	1.80	0.62
1:A:372:ILE:HG23	1:A:395:LEU:HB3	1.81	0.62
1:V:398:HIS:ND1	1:V:418:TYR:O	2.30	0.62
1:P:339:MET:HG3	1:P:344:ILE:HG13	1.80	0.62
1:P:326:ARG:O	1:P:326:ARG:NH1	2.26	0.62
1:U:331:PRO:HB2	1:U:351:LEU:HD11	1.81	0.62
1:E:243:GLN:HG3	1:E:244:ASN:H	1.64	0.62
1:D:264:ARG:NH1	1:D:279:LEU:O	2.32	0.62
1:C:282:MET:HE1	1:C:374:ASN:HB2	1.81	0.61
1:G:354:LYS:HG3	1:G:359:GLU:HB3	1.82	0.61
1:G:428:ILE:HG23	1:G:432:GLU:HB2	1.81	0.61
1:D:385:PRO:HG2	1:D:422:THR:HG22	1.82	0.61
1:L:246:CYS:SG	1:L:247:ALA:N	2.73	0.61
1:R:388:ASN:O	1:R:391:GLN:HB2	2.00	0.61
1:G:447:PRO:HG2	1:K:448:ARG:HD3	1.83	0.61
1:J:371:THR:OG1	1:J:391:GLN:OE1	2.16	0.61
1:B:405:VAL:HG11	1:B:416:MET:SD	2.40	0.61
1:H:271:PHE:HB3	1:H:279:LEU:HD11	1.82	0.61
1:X:431:ARG:HH11	1:Y:380:SER:HB2	1.65	0.61
1:Y:387:ILE:HG23	1:Y:398:HIS:HE1	1.65	0.61
1:A:434:VAL:HG11	1:M:378:PHE:HB3	1.83	0.60
1:F:386:ILE:HD12	1:H:249:LEU:HD11	1.82	0.60
1:S:282:MET:SD	1:S:374:ASN:ND2	2.72	0.60
1:E:245:THR:OG1	1:E:246:CYS:N	2.28	0.60
1:B:295:GLU:HG3	1:B:439:LYS:HE2	1.83	0.60
1:U:339:MET:HB2	1:U:343:ASP:HB2	1.83	0.60
1:O:302:VAL:HG12	1:O:311:VAL:HG22	1.83	0.60
1:B:274:LYS:NZ	1:J:295:GLU:OE1	2.35	0.60
1:P:331:PRO:HB2	1:P:351:LEU:HD13	1.84	0.59
1:A:277:LEU:O	1:A:278:LYS:HD2	2.02	0.59
1:G:334:ARG:NH2	1:G:366:ASP:O	2.35	0.59
1:L:371:THR:OG1	1:L:391:GLN:OE1	2.20	0.59
1:H:451:LEU:HD21	1:Y:449:VAL:HG12	1.83	0.59
1:M:319:SER:HA	1:M:332:VAL:HA	1.84	0.59
1:A:257:MET:HG3	1:A:400:ILE:HD13	1.82	0.59
1:P:293:LEU:HD22	1:P:300:ASN:HB2	1.84	0.59
1:Y:357:LYS:HG2	1:Y:362:ILE:HG12	1.84	0.59
1:B:275:HIS:NE2	1:J:453:ASP:O	2.35	0.59
1:U:264:ARG:HE	1:U:281:PHE:HE1	1.51	0.59
1:P:319:SER:HB2	1:P:371:THR:HG23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:277:LEU:HD22	1:F:345:GLU:HG3	1.85	0.58
1:H:249:LEU:HD13	1:H:425:HIS:HB2	1.84	0.58
1:M:326:ARG:NH2	1:M:327:GLY:HA3	2.18	0.58
1:Y:379:GLY:N	1:Y:401:PHE:HZ	2.01	0.58
1:K:337:GLU:HG2	1:K:338:THR:HG23	1.85	0.58
1:X:333:ILE:HG23	1:X:347:THR:HG21	1.86	0.58
1:Y:325:PRO:HA	1:Y:330:VAL:HG22	1.84	0.58
1:F:373:SER:HB2	1:F:394:ILE:HD11	1.86	0.58
1:C:349:ASN:ND2	1:C:350:GLU:OE1	2.37	0.58
1:N:449:VAL:HG13	1:N:454:LEU:HB2	1.86	0.58
1:X:431:ARG:NH1	1:Y:380:SER:HB2	2.18	0.58
1:L:347:THR:O	1:L:351:LEU:HG	2.03	0.58
1:S:323:ALA:O	1:S:356:ARG:NH2	2.37	0.58
1:P:405:VAL:HG11	1:P:416:MET:HG3	1.86	0.57
1:Y:395:LEU:HD13	1:Y:423:TYR:CE1	2.38	0.57
1:A:431:ARG:HG3	1:M:378:PHE:CZ	2.39	0.57
1:I:336:VAL:HA	1:I:339:MET:HE3	1.86	0.57
1:L:337:GLU:OE2	1:L:337:GLU:N	2.36	0.57
1:V:371:THR:OG1	1:V:391:GLN:OE1	2.20	0.57
1:C:429:ASP:OD1	1:C:429:ASP:N	2.36	0.57
1:K:249:LEU:HD22	1:K:425:HIS:HD2	1.69	0.57
1:L:263:MET:HB2	1:T:448:ARG:NE	2.20	0.57
1:L:299:VAL:HG23	1:L:428:ILE:HD13	1.86	0.57
1:M:318:ILE:HD13	1:M:370:PHE:HB3	1.87	0.57
1:P:300:ASN:ND2	1:P:313:ARG:O	2.37	0.57
1:Y:264:ARG:NH2	1:Y:279:LEU:O	2.37	0.57
1:L:387:ILE:HG13	1:L:394:ILE:HG22	1.87	0.57
1:O:452:LEU:HD12	1:S:267:HIS:HD2	1.70	0.57
1:A:318:ILE:HG12	1:A:336:VAL:HG21	1.87	0.56
1:Y:395:LEU:HB3	1:Y:423:TYR:HE1	1.69	0.56
1:C:253:ASN:ND2	1:C:441:LYS:HD2	2.20	0.56
1:G:247:ALA:HA	1:P:243:GLN:HG2	1.87	0.56
1:A:331:PRO:HB2	1:A:351:LEU:HD13	1.87	0.56
1:L:303:ILE:HG23	1:L:427:LEU:HD22	1.86	0.56
1:L:339:MET:HG2	1:L:343:ASP:HB3	1.87	0.56
1:U:343:ASP:OD1	1:U:346:ARG:NH2	2.38	0.56
1:X:343:ASP:O	1:X:345:GLU:N	2.34	0.56
1:X:352:GLY:O	1:X:356:ARG:HG2	2.06	0.56
1:B:446:ASP:O	1:B:449:VAL:HG22	2.06	0.56
1:H:447:PRO:HB2	1:Y:450:LEU:HD22	1.86	0.56
1:T:359:GLU:OE2	1:T:359:GLU:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:372:ILE:HG22	1:V:372:ILE:O	2.05	0.56
1:O:337:GLU:HG2	1:O:338:THR:HG23	1.87	0.56
1:M:429:ASP:OD1	1:M:429:ASP:N	2.38	0.56
1:P:428:ILE:H	1:P:428:ILE:HD12	1.70	0.56
1:C:330:VAL:HG23	1:C:330:VAL:O	2.06	0.56
1:U:277:LEU:HD12	1:U:278:LYS:H	1.69	0.56
1:A:283:SER:OG	1:A:345:GLU:OE2	2.25	0.55
1:O:453:ASP:OD2	1:S:340:ASN:ND2	2.31	0.55
1:Y:256:ASP:HA	1:Y:418:TYR:CE1	2.41	0.55
1:G:363:GLU:N	1:G:363:GLU:OE2	2.34	0.55
1:D:320:VAL:HG22	1:D:372:ILE:HD11	1.88	0.55
1:L:286:VAL:HG23	1:L:344:ILE:HD13	1.89	0.55
1:X:372:ILE:HG13	1:X:395:LEU:HD23	1.88	0.55
1:E:316:ILE:HD12	1:E:337:GLU:HB3	1.88	0.55
1:A:439:LYS:NZ	1:A:454:LEU:O	2.38	0.55
1:J:317:ASP:H	1:J:369:THR:HG22	1.70	0.55
1:P:264:ARG:NH2	1:P:279:LEU:O	2.30	0.55
1:A:388:ASN:O	1:A:391:GLN:HB2	2.07	0.55
1:C:408:GLY:O	1:C:410:LYS:NZ	2.39	0.55
1:M:283:SER:HB3	1:M:345:GLU:HG2	1.87	0.55
1:B:449:VAL:HG12	1:B:454:LEU:HD12	1.87	0.55
1:X:412:GLU:OE1	1:X:414:ARG:NH1	2.40	0.55
1:E:341:TYR:HB2	1:M:452:LEU:HA	1.89	0.54
1:J:353:GLU:HA	1:J:356:ARG:HH12	1.71	0.54
1:C:331:PRO:HB2	1:C:351:LEU:HD22	1.88	0.54
1:T:275:HIS:HB3	1:T:277:LEU:HD12	1.88	0.54
1:R:259:ASN:OD1	1:V:448:ARG:NH1	2.40	0.54
1:C:271:PHE:HE1	1:C:277:LEU:HB2	1.71	0.54
1:F:388:ASN:OD1	1:F:388:ASN:N	2.39	0.54
1:I:385:PRO:HB2	1:I:394:ILE:HD13	1.90	0.54
1:X:252:PHE:HZ	1:X:384:THR:HG22	1.73	0.54
1:G:245:THR:O	1:G:426:ARG:NH1	2.41	0.54
1:I:319:SER:HB3	1:I:330:VAL:HG12	1.90	0.54
1:M:255:VAL:HG12	1:M:441:LYS:HB2	1.90	0.54
1:N:319:SER:HB3	1:N:332:VAL:HG22	1.90	0.54
1:R:333:ILE:HG23	1:R:347:THR:HG21	1.90	0.54
1:D:286:VAL:HG12	1:D:336:VAL:HG11	1.90	0.54
1:D:319:SER:HB2	1:D:332:VAL:HG22	1.88	0.54
1:A:263:MET:O	1:A:267:HIS:HB2	2.08	0.54
1:S:257:MET:HG3	1:S:417:MET:HG3	1.90	0.53
1:U:250:THR:HG21	1:U:384:THR:HB	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:317:ASP:HB3	1:W:334:ARG:HA	1.90	0.53
1:P:357:LYS:HG3	1:P:359:GLU:HG3	1.89	0.53
1:X:449:VAL:HG12	1:X:454:LEU:HD12	1.89	0.53
1:B:305:ASP:OD1	1:B:305:ASP:N	2.41	0.53
1:O:343:ASP:O	1:O:347:THR:HG22	2.08	0.53
1:D:293:LEU:HD12	1:D:436:PHE:HZ	1.73	0.53
1:Y:321:ALA:HB3	1:Y:373:SER:HA	1.90	0.53
1:Y:304:ASP:OD2	1:Y:313:ARG:NH1	2.41	0.53
1:B:298:VAL:HA	1:B:312:TYR:HE1	1.74	0.53
1:L:264:ARG:O	1:L:268:LYS:HB3	2.08	0.53
1:W:295:GLU:OE1	1:W:439:LYS:HE2	2.08	0.53
1:W:423:TYR:HB2	1:W:428:ILE:HD12	1.90	0.53
1:Y:349:ASN:O	1:Y:353:GLU:HB3	2.09	0.53
1:B:319:SER:HB2	1:B:332:VAL:HG22	1.91	0.53
1:H:427:LEU:HG	1:H:428:ILE:HG13	1.90	0.53
1:K:257:MET:O	1:K:261:GLN:HG2	2.09	0.53
1:N:313:ARG:NH2	1:N:369:THR:HA	2.24	0.53
1:L:249:LEU:HD21	1:U:386:ILE:HD12	1.90	0.53
1:Y:398:HIS:HD2	1:Y:422:THR:HG23	1.73	0.53
1:V:320:VAL:O	1:V:331:PRO:HD2	2.09	0.52
1:Y:304:ASP:O	1:Y:305:ASP:HB2	2.09	0.52
1:A:286:VAL:HG22	1:A:318:ILE:HG21	1.90	0.52
1:R:427:LEU:HG	1:R:428:ILE:HG13	1.90	0.52
1:S:333:ILE:HG23	1:S:347:THR:HG21	1.92	0.52
1:A:321:ALA:HB1	1:A:328:LEU:HD21	1.91	0.52
1:I:317:ASP:HB2	1:I:369:THR:HG23	1.92	0.52
1:J:387:ILE:HG12	1:J:394:ILE:HG22	1.90	0.52
1:Y:304:ASP:HB2	1:Y:313:ARG:HD2	1.91	0.52
1:R:330:VAL:HG23	1:R:330:VAL:O	2.10	0.52
1:U:366:ASP:OD1	1:U:366:ASP:N	2.43	0.52
1:F:405:VAL:HG11	1:F:416:MET:SD	2.50	0.52
1:H:298:VAL:HG21	1:H:432:GLU:OE1	2.10	0.52
1:H:378:PHE:CZ	1:R:431:ARG:HG3	2.45	0.52
1:K:354:LYS:HB3	1:K:360:LEU:HG	1.92	0.52
1:W:347:THR:HA	1:W:350:GLU:HG2	1.92	0.52
1:D:293:LEU:HD22	1:D:316:ILE:HG23	1.91	0.52
1:R:382:PHE:HA	1:R:398:HIS:CD2	2.44	0.52
1:Y:407:VAL:HG11	1:Y:418:TYR:CE2	2.45	0.52
1:B:298:VAL:HB	1:B:432:GLU:OE2	2.09	0.51
1:C:441:LYS:HZ2	1:C:445:GLU:CD	2.13	0.51
1:M:249:LEU:HD11	1:W:386:ILE:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:429:ASP:OD1	1:R:432:GLU:HG3	2.09	0.51
1:X:382:PHE:HA	1:X:398:HIS:CD2	2.44	0.51
1:L:286:VAL:HG12	1:L:372:ILE:HD12	1.92	0.51
1:L:333:ILE:HG23	1:L:347:THR:HG21	1.92	0.51
1:R:337:GLU:OE1	1:R:337:GLU:N	2.30	0.51
1:X:424:ASP:OD1	1:X:424:ASP:N	2.37	0.51
1:V:318:ILE:HD13	1:V:370:PHE:HB3	1.90	0.51
1:Y:286:VAL:HG12	1:Y:346:ARG:HH11	1.74	0.51
1:F:448:ARG:NH1	1:U:259:ASN:OD1	2.42	0.51
1:J:452:LEU:HB3	1:J:454:LEU:HD23	1.92	0.51
1:S:373:SER:HB3	1:S:394:ILE:HD11	1.91	0.51
1:W:305:ASP:N	1:W:305:ASP:OD1	2.39	0.51
1:W:334:ARG:NH2	1:W:366:ASP:O	2.43	0.51
1:C:253:ASN:HD21	1:C:441:LYS:HD2	1.75	0.51
1:D:282:MET:O	1:D:286:VAL:HG23	2.11	0.51
1:E:448:ARG:NH2	1:M:266:ARG:HH21	2.09	0.51
1:J:429:ASP:HB2	1:J:432:GLU:HG3	1.92	0.51
1:U:357:LYS:HB2	1:U:359:GLU:HG3	1.92	0.51
1:W:405:VAL:HG11	1:W:416:MET:SD	2.51	0.51
1:Y:291:PHE:CD2	1:Y:452:LEU:HD22	2.46	0.51
1:H:386:ILE:HD13	1:R:249:LEU:HD21	1.93	0.51
1:K:373:SER:HB3	1:K:394:ILE:HD11	1.92	0.51
1:B:267:HIS:NE2	1:J:446:ASP:OD2	2.37	0.51
1:F:396:GLY:HA3	1:F:420:ALA:HB3	1.93	0.51
1:Y:381:LEU:HA	1:Y:401:PHE:CG	2.45	0.51
1:C:294:GLN:NE2	1:C:337:GLU:HB2	2.26	0.51
1:I:331:PRO:HB2	1:I:351:LEU:HD23	1.92	0.51
1:S:332:VAL:HG12	1:S:334:ARG:HD3	1.93	0.50
1:B:283:SER:HB3	1:B:345:GLU:OE1	2.11	0.50
1:W:429:ASP:OD1	1:W:429:ASP:N	2.39	0.50
1:T:277:LEU:HD11	1:T:346:ARG:HD3	1.91	0.50
1:W:300:ASN:ND2	1:W:313:ARG:O	2.41	0.50
1:A:287:LYS:HE3	1:A:339:MET:O	2.11	0.50
1:B:452:LEU:HB3	1:J:271:PHE:HE1	1.76	0.50
1:W:336:VAL:HG13	1:W:344:ILE:HD11	1.92	0.50
1:O:334:ARG:NH1	1:O:366:ASP:O	2.41	0.50
1:X:319:SER:HB3	1:X:332:VAL:HG22	1.94	0.50
1:G:318:ILE:HD13	1:G:370:PHE:HB3	1.94	0.50
1:J:269:ASP:OD1	1:J:269:ASP:N	2.41	0.50
1:X:294:GLN:NE2	1:X:337:GLU:HB2	2.26	0.50
1:Y:402:ASP:HB3	1:Y:417:MET:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:339:MET:HB2	1:N:343:ASP:HB2	1.93	0.50
1:P:282:MET:O	1:P:286:VAL:HG23	2.11	0.50
1:Y:395:LEU:HD13	1:Y:423:TYR:CD1	2.47	0.50
1:B:388:ASN:O	1:B:391:GLN:HG2	2.12	0.49
1:B:438:ARG:NH1	1:N:378:PHE:O	2.44	0.49
1:D:316:ILE:HD13	1:D:337:GLU:HB3	1.94	0.49
1:V:389:PRO:HA	1:V:391:GLN:H	1.76	0.49
1:E:448:ARG:HD2	1:M:263:MET:SD	2.52	0.49
1:I:246:CYS:HA	1:I:426:ARG:HH21	1.77	0.49
1:Y:318:ILE:HB	1:Y:339:MET:HG2	1.95	0.49
1:B:266:ARG:HB3	1:B:267:HIS:CD2	2.47	0.49
1:F:450:LEU:HB2	1:U:451:LEU:HD11	1.94	0.49
1:A:304:ASP:O	1:A:308:LYS:N	2.45	0.49
1:C:332:VAL:HG12	1:C:364:ASP:O	2.13	0.49
1:D:303:ILE:HG12	1:D:426:ARG:HD3	1.95	0.49
1:U:345:GLU:HA	1:U:345:GLU:OE1	2.11	0.49
1:W:318:ILE:HD12	1:W:370:PHE:HB3	1.93	0.49
1:B:318:ILE:HG12	1:B:370:PHE:HB3	1.95	0.49
1:D:372:ILE:HG22	1:D:395:LEU:HB3	1.94	0.49
1:V:372:ILE:HD13	1:V:395:LEU:HB3	1.94	0.49
1:J:295:GLU:OE1	1:J:439:LYS:NZ	2.37	0.49
1:V:439:LYS:NZ	1:V:454:LEU:O	2.42	0.49
1:Y:382:PHE:CZ	1:Y:385:PRO:HG3	2.48	0.49
1:C:424:ASP:OD1	1:C:424:ASP:N	2.40	0.49
1:I:347:THR:O	1:I:351:LEU:HD13	2.13	0.49
1:O:440:ILE:O	1:O:444:VAL:HG12	2.12	0.49
1:R:318:ILE:HG12	1:R:336:VAL:HG11	1.93	0.49
1:C:281:PHE:HE1	1:C:374:ASN:HD21	1.59	0.49
1:D:332:VAL:N	1:D:364:ASP:O	2.46	0.49
1:R:450:LEU:HB2	1:V:451:LEU:HD11	1.94	0.49
1:A:319:SER:HA	1:A:332:VAL:HA	1.94	0.49
1:E:331:PRO:HB2	1:E:351:LEU:HD13	1.95	0.49
1:G:331:PRO:HB3	1:G:351:LEU:HD13	1.94	0.49
1:K:324:THR:O	1:N:431:ARG:NH2	2.46	0.49
1:T:257:MET:HG3	1:T:400:ILE:HD13	1.94	0.49
1:O:431:ARG:HG3	1:T:378:PHE:CE1	2.48	0.48
1:T:302:VAL:HG13	1:T:311:VAL:HB	1.95	0.48
1:F:291:PHE:HZ	1:F:453:ASP:HA	1.78	0.48
1:W:359:GLU:N	1:W:359:GLU:OE1	2.46	0.48
1:Y:247:ALA:HB1	1:Y:427:LEU:HB2	1.94	0.48
1:Y:264:ARG:O	1:Y:268:LYS:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:LEU:O	1:D:340:ASN:HB2	2.13	0.48
1:I:371:THR:HG23	1:I:394:ILE:HG13	1.96	0.48
1:W:277:LEU:HD12	1:W:278:LYS:H	1.79	0.48
1:H:452:LEU:HD22	1:Y:271:PHE:CZ	2.47	0.48
1:V:449:VAL:HG13	1:V:454:LEU:HB2	1.95	0.48
1:B:387:ILE:HG13	1:B:422:THR:OG1	2.13	0.48
1:A:267:HIS:CE1	1:D:449:VAL:HG22	2.48	0.48
1:S:317:ASP:HB3	1:S:368:GLY:HA2	1.96	0.48
1:Y:395:LEU:HB3	1:Y:423:TYR:CE1	2.47	0.48
1:A:243:GLN:OE1	1:W:246:CYS:N	2.46	0.48
1:L:257:MET:O	1:L:261:GLN:HG2	2.14	0.48
1:L:446:ASP:HB3	1:L:449:VAL:HG23	1.96	0.48
1:U:369:THR:C	1:U:391:GLN:HG2	2.35	0.48
1:V:246:CYS:HA	1:V:426:ARG:NH1	2.28	0.48
1:Y:299:VAL:HG13	1:Y:395:LEU:HD12	1.95	0.48
1:M:355:ALA:HA	1:M:360:LEU:HD23	1.96	0.47
1:O:401:PHE:O	1:O:416:MET:N	2.47	0.47
1:B:264:ARG:HE	1:B:280:GLY:HA2	1.80	0.47
1:C:271:PHE:CE1	1:C:277:LEU:HB2	2.48	0.47
1:G:249:LEU:HD11	1:P:386:ILE:HB	1.96	0.47
1:K:318:ILE:CD1	1:K:336:VAL:HG11	2.44	0.47
1:G:264:ARG:O	1:G:268:LYS:HB2	2.14	0.47
1:W:264:ARG:O	1:W:268:LYS:HG3	2.15	0.47
1:A:264:ARG:NH1	1:A:279:LEU:O	2.47	0.47
1:G:274:LYS:NZ	1:K:295:GLU:OE1	2.43	0.47
1:U:324:THR:OG1	1:U:327:GLY:O	2.25	0.47
1:Y:398:HIS:HD2	1:Y:422:THR:CG2	2.27	0.47
1:C:450:LEU:HB2	1:P:451:LEU:HD11	1.95	0.47
1:H:371:THR:N	1:H:391:GLN:OE1	2.47	0.47
1:O:263:MET:HB3	1:S:448:ARG:HE	1.79	0.47
1:O:318:ILE:HD13	1:O:370:PHE:HB3	1.96	0.47
1:F:357:LYS:HB2	1:F:359:GLU:HG3	1.95	0.47
1:F:264:ARG:O	1:F:268:LYS:HB3	2.15	0.47
1:F:273:LYS:HB3	1:F:273:LYS:HE3	1.58	0.47
1:H:449:VAL:HG13	1:H:454:LEU:HB2	1.97	0.47
1:S:337:GLU:HG2	1:S:338:THR:HG23	1.96	0.47
1:W:388:ASN:C	1:W:391:GLN:HE21	2.18	0.47
1:H:268:LYS:HG3	1:H:279:LEU:HD13	1.95	0.47
1:G:331:PRO:CB	1:G:351:LEU:HD13	2.44	0.47
1:G:356:ARG:HE	1:G:357:LYS:NZ	2.13	0.47
1:E:304:ASP:HB3	1:E:309:GLU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:427:LEU:HG	1:I:428:ILE:HG13	1.96	0.47
1:O:334:ARG:HH21	1:O:364:ASP:HA	1.81	0.47
1:S:318:ILE:HD13	1:S:370:PHE:HB3	1.96	0.47
1:T:264:ARG:HA	1:T:279:LEU:HD23	1.96	0.47
1:U:317:ASP:OD1	1:U:334:ARG:HA	2.13	0.47
1:E:412:GLU:OE1	1:E:412:GLU:N	2.49	0.46
1:K:343:ASP:HA	1:K:346:ARG:HG2	1.96	0.46
1:M:255:VAL:HG22	1:M:417:MET:HB3	1.97	0.46
1:Y:338:THR:O	1:Y:346:ARG:NH2	2.48	0.46
1:C:240:LYS:N	1:C:244:ASN:OD1	2.48	0.46
1:C:278:LYS:HD3	1:C:278:LYS:HA	1.74	0.46
1:M:257:MET:O	1:M:261:GLN:HG2	2.15	0.46
1:U:296:GLN:NE2	1:U:432:GLU:OE1	2.49	0.46
1:V:333:ILE:HG23	1:V:347:THR:HG21	1.96	0.46
1:C:294:GLN:HE21	1:C:337:GLU:HB2	1.80	0.46
1:C:357:LYS:HB2	1:C:357:LYS:HE3	1.64	0.46
1:E:264:ARG:NH1	1:E:279:LEU:O	2.47	0.46
1:L:275:HIS:NE2	1:T:453:ASP:O	2.36	0.46
1:T:294:GLN:HG3	1:T:337:GLU:OE1	2.15	0.46
1:W:318:ILE:HG12	1:W:336:VAL:HG21	1.98	0.46
1:Y:356:ARG:HH12	1:Y:362:ILE:HG23	1.80	0.46
1:B:248:MET:HA	1:B:248:MET:CE	2.45	0.46
1:C:250:THR:HA	1:C:422:THR:HA	1.97	0.46
1:J:373:SER:HB3	1:J:394:ILE:HD11	1.97	0.46
1:R:277:LEU:HD13	1:R:345:GLU:HB3	1.97	0.46
1:E:242:ALA:O	1:E:244:ASN:N	2.49	0.46
1:F:371:THR:HG23	1:F:394:ILE:HD12	1.97	0.46
1:I:249:LEU:HA	1:I:249:LEU:HD12	1.80	0.46
1:R:257:MET:HG3	1:R:400:ILE:HG12	1.98	0.46
1:X:446:ASP:O	1:X:449:VAL:HG22	2.15	0.46
1:Y:247:ALA:O	1:Y:426:ARG:HA	2.15	0.46
1:C:419:VAL:HG12	1:C:437:LEU:HD11	1.98	0.46
1:Y:334:ARG:NE	1:Y:370:PHE:HB2	2.30	0.46
1:Y:409:GLY:N	1:Y:412:GLU:O	2.49	0.46
1:P:318:ILE:HA	1:P:370:PHE:O	2.16	0.46
1:V:246:CYS:HA	1:V:426:ARG:HH12	1.80	0.46
1:X:285:PHE:HB3	1:X:372:ILE:HD11	1.97	0.46
1:Y:328:LEU:O	1:Y:329:VAL:HB	2.16	0.46
1:C:241:GLU:HB2	1:T:246:CYS:H	1.80	0.46
1:C:264:ARG:HG2	1:C:279:LEU:HB3	1.98	0.46
1:E:387:ILE:HG22	1:E:394:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:287:LYS:HG2	1:F:450:LEU:HD22	1.98	0.46
1:H:303:ILE:HD11	1:H:427:LEU:HB2	1.97	0.46
1:J:353:GLU:HA	1:J:356:ARG:NH1	2.31	0.46
1:M:259:ASN:O	1:M:262:GLU:HG2	2.15	0.46
1:S:354:LYS:HB3	1:S:354:LYS:HE3	1.68	0.46
1:V:429:ASP:OD1	1:V:429:ASP:N	2.39	0.46
1:Y:302:VAL:O	1:Y:313:ARG:HG2	2.16	0.46
1:I:378:PHE:CE1	1:S:431:ARG:HD2	2.50	0.45
1:K:319:SER:OG	1:K:332:VAL:HG22	2.15	0.45
1:W:318:ILE:HG22	1:W:320:VAL:HG23	1.97	0.45
1:Y:441:LYS:HA	1:Y:444:VAL:HB	1.97	0.45
1:C:324:THR:HG22	1:C:327:GLY:O	2.16	0.45
1:F:411:VAL:HG22	1:R:404:PRO:HB3	1.98	0.45
1:G:446:ASP:OD1	1:G:448:ARG:HB2	2.16	0.45
1:H:387:ILE:HD11	1:H:422:THR:HG22	1.99	0.45
1:J:282:MET:O	1:J:286:VAL:HG23	2.15	0.45
1:K:424:ASP:OD1	1:K:424:ASP:N	2.47	0.45
1:O:275:HIS:HE1	1:S:454:LEU:HD12	1.78	0.45
1:R:314:ASP:OD1	1:R:314:ASP:N	2.39	0.45
1:V:299:VAL:HG22	1:V:428:ILE:HD12	1.97	0.45
1:F:441:LYS:O	1:F:445:GLU:HB2	2.16	0.45
1:J:302:VAL:HB	1:J:313:ARG:NH2	2.30	0.45
1:G:303:ILE:HG12	1:G:427:LEU:HG	1.98	0.45
1:H:436:PHE:CE2	1:H:440:ILE:HD11	2.51	0.45
1:I:354:LYS:HG3	1:I:359:GLU:HG3	1.97	0.45
1:N:257:MET:O	1:N:261:GLN:HG3	2.16	0.45
1:T:412:GLU:N	1:T:412:GLU:OE2	2.49	0.45
1:C:250:THR:HG21	1:C:384:THR:HB	1.97	0.45
1:G:351:LEU:HD23	1:G:351:LEU:HA	1.78	0.45
1:N:313:ARG:HH21	1:N:369:THR:HA	1.82	0.45
1:V:321:ALA:HA	1:V:330:VAL:HG22	1.97	0.45
1:Y:400:ILE:HG22	1:Y:401:PHE:N	2.32	0.45
1:E:260:ILE:O	1:E:264:ARG:HG3	2.17	0.45
1:X:303:ILE:HD11	1:X:426:ARG:HE	1.82	0.45
1:Y:385:PRO:HG2	1:Y:398:HIS:CG	2.51	0.45
1:D:344:ILE:HG22	1:D:348:ILE:HD12	1.99	0.45
1:E:295:GLU:OE1	1:E:295:GLU:HA	2.17	0.45
1:G:392:SER:O	1:G:392:SER:OG	2.33	0.45
1:D:438:ARG:HG3	1:D:438:ARG:HH11	1.82	0.45
1:D:447:PRO:O	1:D:450:LEU:HB2	2.17	0.45
1:G:248:MET:HB3	1:G:422:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:314:ASP:OD1	1:L:314:ASP:N	2.48	0.45
1:R:273:LYS:HB3	1:R:273:LYS:HE3	1.67	0.45
1:S:330:VAL:O	1:S:330:VAL:HG13	2.17	0.45
1:Y:299:VAL:CG1	1:Y:395:LEU:HD12	2.47	0.45
1:G:318:ILE:HD12	1:G:372:ILE:HD11	1.98	0.45
1:R:318:ILE:HD13	1:R:370:PHE:HB3	1.98	0.45
1:Y:271:PHE:CE1	1:Y:344:ILE:HD11	2.52	0.45
1:Y:333:ILE:HG22	1:Y:334:ARG:H	1.81	0.45
1:D:448:ARG:HE	1:D:448:ARG:HB2	1.62	0.45
1:E:268:LYS:NZ	1:E:279:LEU:O	2.50	0.45
1:H:330:VAL:O	1:H:330:VAL:HG12	2.17	0.45
1:H:373:SER:HB3	1:H:394:ILE:HD11	1.99	0.45
1:B:255:VAL:HG23	1:B:445:GLU:HG3	1.99	0.44
1:E:256:ASP:HA	1:E:416:MET:SD	2.57	0.44
1:E:448:ARG:HH21	1:M:266:ARG:HH21	1.64	0.44
1:G:263:MET:SD	1:K:448:ARG:HD2	2.57	0.44
1:G:438:ARG:HG3	1:G:438:ARG:HH11	1.82	0.44
1:X:331:PRO:HB3	1:X:351:LEU:HD22	1.99	0.44
1:L:321:ALA:HB1	1:L:328:LEU:HD11	1.98	0.44
1:R:341:TYR:HB2	1:V:452:LEU:HA	1.99	0.44
1:Y:405:VAL:HG12	1:Y:407:VAL:HG13	1.97	0.44
1:A:452:LEU:HD13	1:A:454:LEU:HD11	1.99	0.44
1:D:287:LYS:HG2	1:D:450:LEU:HD11	1.99	0.44
1:H:320:VAL:O	1:H:331:PRO:HD2	2.16	0.44
1:I:449:VAL:HG13	1:I:454:LEU:HB3	1.99	0.44
1:O:374:ASN:HA	1:O:397:MET:HG3	1.99	0.44
1:U:264:ARG:O	1:U:268:LYS:HG3	2.17	0.44
1:U:328:LEU:HD23	1:U:328:LEU:HA	1.82	0.44
1:Y:388:ASN:O	1:Y:389:PRO:C	2.55	0.44
1:J:289:SER:O	1:J:293:LEU:HD13	2.17	0.44
1:J:443:ALA:HB1	1:J:450:LEU:HD21	2.00	0.44
1:L:277:LEU:HD13	1:L:345:GLU:OE1	2.18	0.44
1:M:330:VAL:HG23	1:M:330:VAL:O	2.16	0.44
1:Y:356:ARG:NH2	1:Y:363:GLU:H	2.15	0.44
1:Y:395:LEU:HA	1:Y:395:LEU:HD23	1.59	0.44
1:Y:398:HIS:CD2	1:Y:422:THR:OG1	2.71	0.44
1:S:257:MET:O	1:S:261:GLN:HG2	2.18	0.44
1:V:271:PHE:CD2	1:V:279:LEU:HB2	2.53	0.44
1:W:302:VAL:HG21	1:W:391:GLN:HA	1.98	0.44
1:Y:448:ARG:O	1:Y:451:LEU:HD12	2.18	0.44
1:E:448:ARG:CZ	1:M:263:MET:HB2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:264:ARG:HH11	1:G:281:PHE:HE1	1.62	0.44
1:G:437:LEU:HD23	1:G:437:LEU:HA	1.80	0.44
1:H:386:ILE:HD12	1:H:386:ILE:HA	1.85	0.44
1:O:337:GLU:OE2	1:O:337:GLU:N	2.33	0.44
1:P:337:GLU:OE1	1:P:337:GLU:N	2.38	0.44
1:T:264:ARG:NH2	1:T:279:LEU:O	2.35	0.44
1:Y:277:LEU:HB2	1:Y:351:LEU:HD13	1.99	0.44
1:Y:397:MET:HE1	1:Y:421:LEU:HD13	2.00	0.44
1:Y:400:ILE:CG2	1:Y:401:PHE:H	2.30	0.44
1:A:302:VAL:HG21	1:A:313:ARG:HH21	1.83	0.44
1:C:341:TYR:HB2	1:P:452:LEU:HA	2.00	0.44
1:D:279:LEU:HD12	1:D:279:LEU:HA	1.81	0.44
1:I:346:ARG:O	1:I:350:GLU:HG2	2.18	0.44
1:I:373:SER:HB3	1:I:394:ILE:HD11	2.00	0.44
1:J:305:ASP:O	1:J:308:LYS:NZ	2.37	0.44
1:L:321:ALA:HB3	1:L:373:SER:HA	2.00	0.44
1:N:443:ALA:HB1	1:N:450:LEU:HD21	1.99	0.44
1:P:441:LYS:O	1:P:445:GLU:HG3	2.17	0.44
1:X:313:ARG:HD2	1:X:369:THR:HG22	2.00	0.44
1:Y:381:LEU:CD2	1:Y:403:ARG:HH12	2.31	0.44
1:A:437:LEU:HD12	1:A:437:LEU:HA	1.80	0.43
1:D:393:ALA:HB1	1:D:421:LEU:HD11	2.00	0.43
1:G:425:HIS:ND1	1:P:239:LEU:HD21	2.32	0.43
1:N:405:VAL:HG11	1:N:416:MET:SD	2.57	0.43
1:V:303:ILE:HD12	1:V:426:ARG:HH21	1.83	0.43
1:C:295:GLU:OE1	1:P:274:LYS:NZ	2.51	0.43
1:D:303:ILE:HD11	1:D:308:LYS:HG3	2.01	0.43
1:G:452:LEU:HD11	1:K:279:LEU:HD21	1.99	0.43
1:V:304:ASP:N	1:V:309:GLU:O	2.42	0.43
1:C:378:PHE:CE1	1:T:431:ARG:HG3	2.53	0.43
1:D:437:LEU:HD12	1:D:437:LEU:HA	1.82	0.43
1:I:424:ASP:OD1	1:I:426:ARG:N	2.44	0.43
1:M:340:ASN:OD1	1:M:340:ASN:N	2.51	0.43
1:N:385:PRO:HB2	1:N:394:ILE:HD13	2.00	0.43
1:P:303:ILE:HD13	1:P:310:VAL:HG12	1.99	0.43
1:U:255:VAL:HG22	1:U:441:LYS:HB2	2.00	0.43
1:W:356:ARG:HG3	1:W:357:LYS:HD3	2.00	0.43
1:Y:400:ILE:HG22	1:Y:401:PHE:H	1.82	0.43
1:B:243:GLN:N	1:B:243:GLN:OE1	2.51	0.43
1:C:255:VAL:HG13	1:C:417:MET:HB3	2.00	0.43
1:C:414:ARG:HG3	1:C:415:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:287:LYS:HA	1:O:287:LYS:HD2	1.81	0.43
1:R:319:SER:HA	1:R:332:VAL:HA	2.00	0.43
1:D:262:GLU:O	1:D:266:ARG:HG2	2.19	0.43
1:E:293:LEU:HD11	1:E:370:PHE:CG	2.54	0.43
1:E:334:ARG:HE	1:E:334:ARG:HB2	1.66	0.43
1:P:268:LYS:HE2	1:P:268:LYS:HB3	1.74	0.43
1:U:268:LYS:HB2	1:U:268:LYS:HE3	1.90	0.43
1:U:368:GLY:HA3	1:U:391:GLN:HE21	1.83	0.43
1:A:242:ALA:O	1:A:244:ASN:N	2.51	0.43
1:J:360:LEU:HD23	1:J:365:MET:CE	2.48	0.43
1:T:320:VAL:O	1:T:331:PRO:HD2	2.18	0.43
1:T:429:ASP:HB3	1:T:432:GLU:HG3	2.00	0.43
1:V:355:ALA:HB2	1:V:360:LEU:HD11	2.01	0.43
1:Y:267:HIS:O	1:Y:271:PHE:HD2	2.01	0.43
1:Y:275:HIS:ND1	1:Y:344:ILE:HD13	2.34	0.43
1:Y:353:GLU:HA	1:Y:356:ARG:HB3	2.01	0.43
1:F:386:ILE:HB	1:H:249:LEU:HD21	2.00	0.43
1:J:431:ARG:HG3	1:X:378:PHE:CE1	2.54	0.43
1:B:334:ARG:NH2	1:B:364:ASP:HA	2.33	0.43
1:C:431:ARG:HG3	1:O:378:PHE:CE2	2.53	0.43
1:G:267:HIS:NE2	1:K:446:ASP:OD2	2.35	0.43
1:L:259:ASN:OD1	1:T:448:ARG:NH1	2.52	0.43
1:N:277:LEU:HD21	1:N:345:GLU:HB3	2.01	0.43
1:P:261:GLN:HE21	1:P:281:PHE:HZ	1.65	0.43
1:B:287:LYS:HA	1:B:287:LYS:HD2	1.86	0.43
1:E:406:ALA:HA	1:E:410:LYS:O	2.19	0.43
1:R:264:ARG:HE	1:R:280:GLY:HA2	1.84	0.43
1:G:387:ILE:HG13	1:G:422:THR:HG22	2.00	0.42
1:O:427:LEU:H	1:O:427:LEU:HD23	1.84	0.42
1:X:345:GLU:HA	1:X:348:ILE:HG12	2.00	0.42
1:K:269:ASP:OD1	1:K:270:ALA:N	2.52	0.42
1:L:333:ILE:HG12	1:L:351:LEU:HD11	2.01	0.42
1:N:373:SER:HB3	1:N:394:ILE:HD11	2.00	0.42
1:V:340:ASN:N	1:V:340:ASN:OD1	2.52	0.42
1:K:333:ILE:HD13	1:K:351:LEU:HD22	2.00	0.42
1:O:249:LEU:HD11	1:T:386:ILE:HB	2.01	0.42
1:T:410:LYS:HE2	1:T:410:LYS:HB2	1.86	0.42
1:Y:295:GLU:O	1:Y:297:PRO:HD3	2.18	0.42
1:A:249:LEU:HD13	1:A:425:HIS:HB2	2.00	0.42
1:B:329:VAL:HG23	1:B:331:PRO:HD3	2.01	0.42
1:D:244:ASN:C	1:G:243:GLN:HE22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:295:GLU:HG3	1:I:439:LYS:NZ	2.35	0.42
1:K:357:LYS:HB2	1:K:359:GLU:OE1	2.19	0.42
1:M:243:GLN:HE21	1:M:246:CYS:HB2	1.84	0.42
1:N:305:ASP:OD1	1:N:305:ASP:N	2.52	0.42
1:O:423:TYR:HB2	1:O:428:ILE:HD12	2.01	0.42
1:W:318:ILE:CD1	1:W:370:PHE:HB3	2.49	0.42
1:B:352:GLY:O	1:B:356:ARG:HG2	2.18	0.42
1:U:334:ARG:NH2	1:U:366:ASP:OD1	2.52	0.42
1:Y:387:ILE:HG12	1:Y:398:HIS:CE1	2.55	0.42
1:A:272:LEU:HD12	1:A:276:ASN:HA	2.01	0.42
1:C:250:THR:HG22	1:C:422:THR:HB	2.02	0.42
1:I:287:LYS:HG2	1:I:344:ILE:HD12	2.02	0.42
1:J:381:LEU:HD22	1:Y:254:GLU:HG3	2.00	0.42
1:L:429:ASP:OD1	1:L:429:ASP:N	2.41	0.42
1:X:337:GLU:HG2	1:X:338:THR:HG23	2.01	0.42
1:A:261:GLN:OE1	1:A:261:GLN:HA	2.20	0.42
1:A:454:LEU:HD21	1:D:271:PHE:HD1	1.85	0.42
1:B:279:LEU:HD12	1:B:279:LEU:HA	1.78	0.42
1:D:330:VAL:HG23	1:D:330:VAL:O	2.19	0.42
1:F:424:ASP:OD1	1:F:424:ASP:N	2.40	0.42
1:M:302:VAL:HA	1:M:427:LEU:HD21	2.00	0.42
1:R:303:ILE:HD13	1:R:426:ARG:NH1	2.35	0.42
1:X:276:ASN:O	1:X:277:LEU:HD23	2.19	0.42
1:E:331:PRO:HB3	1:E:351:LEU:HD22	2.01	0.42
1:L:424:ASP:OD1	1:L:424:ASP:N	2.53	0.42
1:X:426:ARG:H	1:X:426:ARG:HG2	1.63	0.42
1:Y:400:ILE:HD13	1:Y:420:ALA:HB3	2.01	0.42
1:A:360:LEU:HD23	1:A:360:LEU:HA	1.95	0.42
1:B:287:LYS:HG3	1:B:450:LEU:HD22	2.02	0.42
1:B:350:GLU:OE2	1:B:354:LYS:HE3	2.20	0.42
1:C:264:ARG:NH1	1:C:279:LEU:O	2.52	0.42
1:C:382:PHE:HA	1:C:398:HIS:CD2	2.55	0.42
1:K:439:LYS:HZ3	1:K:439:LYS:HG3	1.65	0.42
1:S:318:ILE:HB	1:S:336:VAL:HG21	2.00	0.42
1:V:308:LYS:HD3	1:V:308:LYS:HA	1.81	0.42
1:V:372:ILE:HG23	1:V:372:ILE:HD12	1.72	0.42
1:Y:243:GLN:HA	1:Y:248:MET:HE2	2.02	0.42
1:Y:333:ILE:HG12	1:Y:357:LYS:HD2	2.02	0.42
1:Y:377:VAL:HB	1:Y:399:GLY:O	2.19	0.42
1:A:263:MET:HB2	1:D:448:ARG:CZ	2.50	0.42
1:C:373:SER:HB3	1:C:394:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:LYS:NZ	1:C:454:LEU:OXT	2.52	0.42
1:L:276:ASN:O	1:L:277:LEU:HD23	2.20	0.42
1:L:290:ALA:O	1:L:294:GLN:HG3	2.20	0.42
1:S:439:LYS:HA	1:S:439:LYS:HD3	1.76	0.42
1:T:339:MET:HB3	1:T:343:ASP:HB2	2.02	0.42
1:U:260:ILE:HD12	1:U:263:MET:CE	2.50	0.42
1:X:291:PHE:O	1:X:295:GLU:HG2	2.20	0.42
1:A:316:ILE:HD12	1:A:316:ILE:N	2.35	0.41
1:D:264:ARG:O	1:D:268:LYS:HB2	2.19	0.41
1:E:359:GLU:OE1	1:E:359:GLU:N	2.49	0.41
1:H:359:GLU:N	1:H:359:GLU:OE1	2.52	0.41
1:I:263:MET:HG3	1:N:448:ARG:HE	1.85	0.41
1:I:388:ASN:OD1	1:I:391:GLN:NE2	2.53	0.41
1:I:448:ARG:NH2	1:N:262:GLU:OE1	2.52	0.41
1:O:448:ARG:HB3	1:S:263:MET:HE2	2.01	0.41
1:X:271:PHE:CE2	1:X:277:LEU:HB2	2.55	0.41
1:Y:313:ARG:NH2	1:Y:315:TYR:OH	2.47	0.41
1:Y:400:ILE:HG21	1:Y:420:ALA:HB3	2.02	0.41
1:Y:444:VAL:O	1:Y:447:PRO:HD2	2.19	0.41
1:F:407:VAL:HB	1:F:412:GLU:OE2	2.20	0.41
1:K:452:LEU:HB3	1:K:454:LEU:HD23	2.01	0.41
1:R:353:GLU:OE2	1:R:353:GLU:HA	2.20	0.41
1:W:350:GLU:O	1:W:353:GLU:HG3	2.19	0.41
1:D:318:ILE:N	1:D:318:ILE:HD12	2.36	0.41
1:E:282:MET:HE2	1:E:374:ASN:HD22	1.85	0.41
1:F:333:ILE:HG22	1:F:336:VAL:HG22	2.02	0.41
1:H:260:ILE:HD13	1:H:260:ILE:HA	1.88	0.41
1:H:350:GLU:O	1:H:353:GLU:HG2	2.21	0.41
1:N:318:ILE:O	1:N:333:ILE:HG12	2.20	0.41
1:Y:356:ARG:NH1	1:Y:362:ILE:HG23	2.35	0.41
1:H:318:ILE:HD13	1:H:370:PHE:HB3	2.03	0.41
1:H:451:LEU:HD13	1:Y:287:LYS:HZ2	1.85	0.41
1:V:291:PHE:HE2	1:V:439:LYS:HZ1	1.66	0.41
1:A:277:LEU:HD21	1:A:346:ARG:HG2	2.02	0.41
1:I:287:LYS:HA	1:I:287:LYS:HD2	1.79	0.41
1:J:386:ILE:HG21	1:Y:427:LEU:HD11	2.02	0.41
1:O:361:ALA:N	1:O:364:ASP:OD2	2.49	0.41
1:P:382:PHE:HA	1:P:398:HIS:CE1	2.56	0.41
1:R:372:ILE:HD13	1:R:395:LEU:HB3	2.02	0.41
1:R:439:LYS:HD2	1:R:439:LYS:HA	1.91	0.41
1:V:373:SER:OG	1:V:394:ILE:HD11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:346:ARG:O	1:X:350:GLU:HG2	2.21	0.41
1:E:243:GLN:O	1:U:248:MET:HG2	2.21	0.41
1:G:283:SER:OG	1:G:345:GLU:OE2	2.38	0.41
1:M:449:VAL:HG13	1:M:454:LEU:HB2	2.02	0.41
1:R:287:LYS:HA	1:R:287:LYS:HD2	1.87	0.41
1:T:357:LYS:HB2	1:T:359:GLU:OE2	2.21	0.41
1:T:440:ILE:O	1:T:444:VAL:HG23	2.21	0.41
1:U:248:MET:HB2	1:U:422:THR:CG2	2.50	0.41
1:U:373:SER:HB3	1:U:394:ILE:HD11	2.03	0.41
1:W:439:LYS:HB3	1:W:439:LYS:HE3	1.77	0.41
1:C:341:TYR:HB2	1:P:451:LEU:O	2.21	0.41
1:C:411:VAL:HG22	1:O:404:PRO:HB3	2.01	0.41
1:D:398:HIS:H	1:D:417:MET:HE3	1.86	0.41
1:E:333:ILE:HD11	1:E:348:ILE:HG13	2.03	0.41
1:H:317:ASP:H	1:H:369:THR:HG22	1.85	0.41
1:J:317:ASP:H	1:J:369:THR:CG2	2.33	0.41
1:O:452:LEU:HD23	1:O:452:LEU:HA	1.84	0.41
1:T:387:ILE:HG12	1:T:394:ILE:HG22	2.02	0.41
1:V:287:LYS:HA	1:V:287:LYS:HD2	1.78	0.41
1:V:382:PHE:HA	1:V:398:HIS:CG	2.56	0.41
1:Y:323:ALA:HB3	1:Y:376:GLY:H	1.86	0.41
1:Y:400:ILE:HB	1:Y:420:ALA:O	2.20	0.41
1:E:451:LEU:O	1:M:340:ASN:HB2	2.21	0.41
1:K:319:SER:HA	1:K:332:VAL:HA	2.03	0.41
1:M:439:LYS:HB2	1:M:439:LYS:HE2	1.84	0.41
1:P:287:LYS:HG3	1:P:450:LEU:HD13	2.02	0.41
1:U:258:SER:O	1:U:262:GLU:HG3	2.21	0.41
1:W:317:ASP:HB2	1:W:332:VAL:HG13	2.02	0.41
1:Y:334:ARG:NH2	1:Y:370:PHE:O	2.54	0.41
1:A:257:MET:HB3	1:A:261:GLN:HG2	2.02	0.41
1:B:338:THR:O	1:B:338:THR:OG1	2.38	0.41
1:B:452:LEU:HB3	1:J:271:PHE:CE1	2.55	0.41
1:C:324:THR:HG23	1:C:326:ARG:H	1.86	0.41
1:E:354:LYS:HB3	1:E:354:LYS:HE2	1.90	0.41
1:F:291:PHE:CZ	1:F:453:ASP:HA	2.56	0.41
1:F:323:ALA:HA	1:F:329:VAL:H	1.85	0.41
1:M:287:LYS:HB3	1:M:341:TYR:HE1	1.85	0.41
1:W:337:GLU:HG2	1:W:338:THR:HG23	2.02	0.41
1:W:357:LYS:HB2	1:W:359:GLU:OE1	2.21	0.41
1:Y:313:ARG:HG3	1:Y:313:ARG:O	2.20	0.41
1:Y:426:ARG:CZ	1:Y:428:ILE:HD12	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:340:ASN:HB2	1:K:451:LEU:O	2.20	0.41
1:J:287:LYS:HA	1:J:287:LYS:HD3	1.97	0.41
1:J:293:LEU:HD23	1:J:316:ILE:HG12	2.03	0.41
1:J:293:LEU:HD12	1:J:436:PHE:CE1	2.56	0.41
1:K:404:PRO:HD3	1:N:406:ALA:H	1.86	0.41
1:O:277:LEU:HD11	1:O:346:ARG:HA	2.03	0.41
1:U:291:PHE:HA	1:U:294:GLN:OE1	2.21	0.41
1:V:278:LYS:HA	1:V:278:LYS:HD3	1.69	0.41
1:V:371:THR:HG22	1:V:373:SER:H	1.85	0.41
1:Y:324:THR:HA	1:Y:325:PRO:HD3	1.95	0.41
1:B:397:MET:HB2	1:B:417:MET:SD	2.61	0.40
1:C:255:VAL:HG23	1:C:445:GLU:HG3	2.02	0.40
1:G:243:GLN:HA	1:G:248:MET:SD	2.61	0.40
1:J:453:ASP:O	1:J:453:ASP:OD1	2.39	0.40
1:L:402:ASP:N	1:L:402:ASP:OD1	2.54	0.40
1:O:260:ILE:O	1:O:263:MET:HG3	2.21	0.40
1:U:429:ASP:OD1	1:U:430:GLY:N	2.51	0.40
1:W:340:ASN:OD1	1:W:340:ASN:N	2.53	0.40
1:B:308:LYS:O	1:B:308:LYS:HG2	2.20	0.40
1:B:319:SER:HA	1:B:332:VAL:HA	2.03	0.40
1:B:325:PRO:HD2	1:B:356:ARG:NH1	2.32	0.40
1:C:324:THR:OG1	1:C:325:PRO:HD2	2.20	0.40
1:C:340:ASN:O	1:C:341:TYR:HD1	2.03	0.40
1:J:260:ILE:O	1:J:264:ARG:HG3	2.20	0.40
1:P:329:VAL:HG23	1:P:331:PRO:HD3	2.02	0.40
1:V:334:ARG:HA	1:V:334:ARG:HD3	1.85	0.40
1:X:323:ALA:HA	1:X:329:VAL:HG22	2.04	0.40
1:B:317:ASP:OD1	1:B:334:ARG:HD3	2.21	0.40
1:C:397:MET:HB3	1:C:417:MET:HE2	2.03	0.40
1:H:264:ARG:O	1:H:268:LYS:HB2	2.21	0.40
1:J:268:LYS:HG3	1:J:269:ASP:N	2.37	0.40
1:Y:385:PRO:HB2	1:Y:398:HIS:CE1	2.56	0.40
1:E:360:LEU:HD23	1:E:360:LEU:HA	1.96	0.40
1:F:454:LEU:HA	1:U:274:LYS:HD3	2.03	0.40
1:G:405:VAL:HG21	1:G:414:ARG:HD2	2.03	0.40
1:K:360:LEU:HD13	1:K:365:MET:HE2	2.04	0.40
1:S:285:PHE:CZ	1:S:444:VAL:HG11	2.57	0.40
1:U:423:TYR:HB2	1:U:428:ILE:HD13	2.04	0.40
1:Y:387:ILE:H	1:Y:387:ILE:HG13	1.80	0.40
1:G:294:GLN:HE22	1:G:337:GLU:HG2	1.87	0.40
1:G:324:THR:OG1	1:G:327:GLY:O	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:382:PHE:HA	1:H:398:HIS:CG	2.57	0.40
1:J:313:ARG:HG2	1:J:315:TYR:CZ	2.57	0.40
1:M:324:THR:HG22	1:M:326:ARG:H	1.86	0.40
1:P:293:LEU:HD12	1:P:316:ILE:HG23	2.03	0.40
1:R:324:THR:OG1	1:R:327:GLY:O	2.33	0.40
1:U:454:LEU:HD12	1:U:454:LEU:HA	1.90	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	211/216 (98%)	194 (92%)	16 (8%)	1 (0%)	25	58
1	B	210/216 (97%)	196 (93%)	14 (7%)	0	100	100
1	C	213/216 (99%)	207 (97%)	6 (3%)	0	100	100
1	D	209/216 (97%)	202 (97%)	7 (3%)	0	100	100
1	E	211/216 (98%)	202 (96%)	8 (4%)	1 (0%)	25	58
1	F	208/216 (96%)	191 (92%)	17 (8%)	0	100	100
1	G	214/216 (99%)	205 (96%)	9 (4%)	0	100	100
1	H	208/216 (96%)	197 (95%)	11 (5%)	0	100	100
1	I	212/216 (98%)	210 (99%)	2 (1%)	0	100	100
1	J	206/216 (95%)	201 (98%)	5 (2%)	0	100	100
1	K	209/216 (97%)	198 (95%)	11 (5%)	0	100	100
1	L	207/216 (96%)	201 (97%)	6 (3%)	0	100	100
1	M	210/216 (97%)	206 (98%)	4 (2%)	0	100	100
1	N	213/216 (99%)	204 (96%)	9 (4%)	0	100	100
1	O	206/216 (95%)	199 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	214/216 (99%)	207 (97%)	7 (3%)	0	100	100
1	R	210/216 (97%)	203 (97%)	6 (3%)	1 (0%)	25	58
1	S	210/216 (97%)	203 (97%)	6 (3%)	1 (0%)	25	58
1	T	208/216 (96%)	200 (96%)	8 (4%)	0	100	100
1	U	209/216 (97%)	202 (97%)	7 (3%)	0	100	100
1	V	211/216 (98%)	203 (96%)	8 (4%)	0	100	100
1	W	207/216 (96%)	199 (96%)	8 (4%)	0	100	100
1	X	207/216 (96%)	199 (96%)	8 (4%)	0	100	100
1	Y	210/216 (97%)	177 (84%)	26 (12%)	7 (3%)	3	17
All	All	5033/5184 (97%)	4806 (96%)	216 (4%)	11 (0%)	45	74

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	243	GLN
1	A	243	GLN
1	Y	305	ASP
1	Y	329	VAL
1	Y	393	ALA
1	Y	389	PRO
1	Y	390	PRO
1	S	329	VAL
1	Y	245	THR
1	Y	411	VAL
1	R	390	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	178/181 (98%)	172 (97%)	6 (3%)	32	62
1	B	178/181 (98%)	172 (97%)	6 (3%)	32	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	180/181 (99%)	176 (98%)	4 (2%)	47	71
1	D	177/181 (98%)	173 (98%)	4 (2%)	45	70
1	E	178/181 (98%)	173 (97%)	5 (3%)	38	66
1	F	176/181 (97%)	171 (97%)	5 (3%)	38	66
1	G	181/181 (100%)	173 (96%)	8 (4%)	24	54
1	H	176/181 (97%)	172 (98%)	4 (2%)	45	70
1	I	179/181 (99%)	175 (98%)	4 (2%)	47	71
1	J	174/181 (96%)	171 (98%)	3 (2%)	56	78
1	K	177/181 (98%)	174 (98%)	3 (2%)	56	78
1	L	175/181 (97%)	171 (98%)	4 (2%)	45	70
1	M	178/181 (98%)	178 (100%)	0	100	100
1	N	180/181 (99%)	173 (96%)	7 (4%)	27	58
1	O	174/181 (96%)	173 (99%)	1 (1%)	84	91
1	P	181/181 (100%)	176 (97%)	5 (3%)	38	66
1	R	178/181 (98%)	176 (99%)	2 (1%)	70	84
1	S	178/181 (98%)	175 (98%)	3 (2%)	56	78
1	T	176/181 (97%)	169 (96%)	7 (4%)	27	58
1	U	177/181 (98%)	171 (97%)	6 (3%)	32	62
1	V	178/181 (98%)	174 (98%)	4 (2%)	47	71
1	W	175/181 (97%)	171 (98%)	4 (2%)	45	70
1	X	175/181 (97%)	171 (98%)	4 (2%)	45	70
1	Y	178/181 (98%)	172 (97%)	6 (3%)	32	62
All	All	4257/4344 (98%)	4152 (98%)	105 (2%)	43	69

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	ASP
1	A	313	ARG
1	A	363	GLU
1	A	378	PHE
1	A	415	PRO
1	A	439	LYS
1	B	248	MET

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Mol	Chain	Res	Type
1	B	319	SER
1	B	339	MET
1	B	378	PHE
1	B	392	SER
1	B	402	ASP
1	C	269	ASP
1	C	359	GLU
1	C	402	ASP
1	C	414	ARG
1	D	253	ASN
1	D	258	SER
1	D	296	GLN
1	D	334	ARG
1	E	273	LYS
1	E	283	SER
1	E	313	ARG
1	E	356	ARG
1	E	373	SER
1	F	291	PHE
1	F	305	ASP
1	F	326	ARG
1	F	392	SER
1	F	416	MET
1	G	243	GLN
1	G	258	SER
1	G	263	MET
1	G	269	ASP
1	G	305	ASP
1	G	317	ASP
1	G	349	ASN
1	G	392	SER
1	H	281	PHE
1	H	294	GLN
1	H	346	ARG
1	H	366	ASP
1	I	258	SER
1	I	373	SER
1	I	397	MET
1	I	402	ASP
1	J	295	GLU
1	J	421	LEU
1	J	425	HIS

Continued on next page...

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Mol	Chain	Res	Type
1	K	276	ASN
1	K	370	PHE
1	K	378	PHE
1	L	263	MET
1	L	397	MET
1	L	402	ASP
1	L	424	ASP
1	N	253	ASN
1	N	271	PHE
1	N	313	ARG
1	N	314	ASP
1	N	343	ASP
1	N	364	ASP
1	N	378	PHE
1	O	397	MET
1	P	244	ASN
1	P	340	ASN
1	P	373	SER
1	P	380	SER
1	P	426	ARG
1	R	259	ASN
1	R	378	PHE
1	S	248	MET
1	S	281	PHE
1	S	304	ASP
1	T	271	PHE
1	T	378	PHE
1	T	402	ASP
1	T	416	MET
1	T	421	LEU
1	T	431	ARG
1	T	446	ASP
1	U	253	ASN
1	U	266	ARG
1	U	350	GLU
1	U	366	ASP
1	U	426	ARG
1	U	446	ASP
1	V	294	GLN
1	V	346	ARG
1	V	392	SER
1	V	452	LEU

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Mol	Chain	Res	Type
1	W	317	ASP
1	W	343	ASP
1	W	365	MET
1	W	392	SER
1	X	269	ASP
1	X	300	ASN
1	X	364	ASP
1	X	439	LYS
1	Y	339	MET
1	Y	382	PHE
1	Y	387	ILE
1	Y	388	ASN
1	Y	418	TYR
1	Y	423	TYR

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	267	HIS
1	B	243	GLN
1	C	244	ASN
1	C	294	GLN
1	F	398	HIS
1	I	391	GLN
1	K	425	HIS
1	N	243	GLN
1	N	275	HIS
1	W	391	GLN
1	Y	243	GLN
1	Y	261	GLN
1	Y	398	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

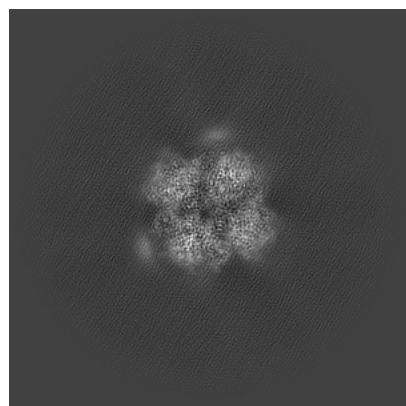
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38452. These allow visual inspection of the internal detail of the map and identification of artifacts.

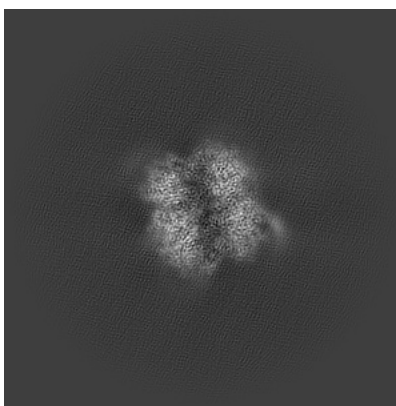
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

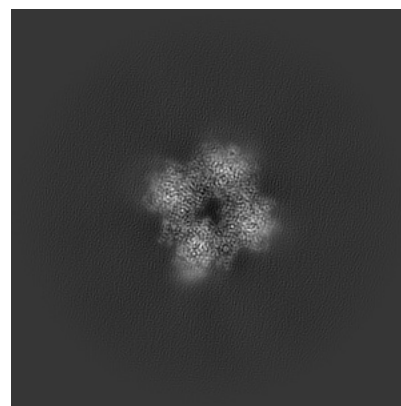
6.1.1 Primary map



X

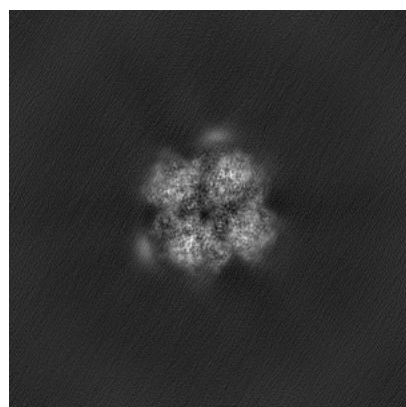


Y

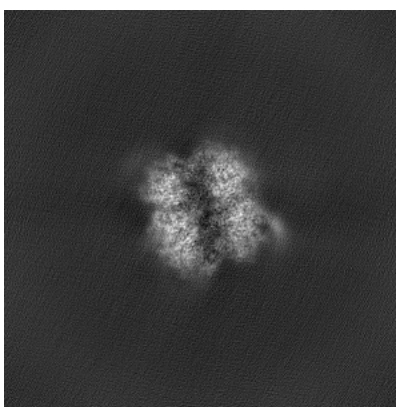


Z

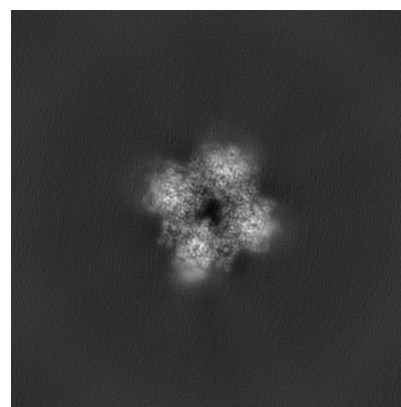
6.1.2 Raw map



X



Y



Z

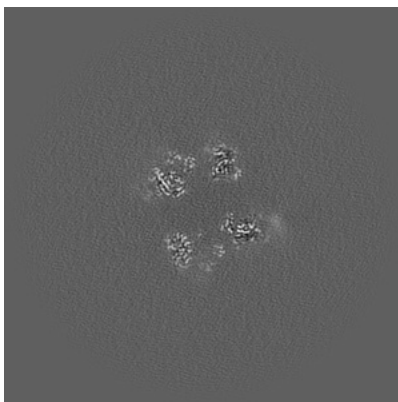
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 215

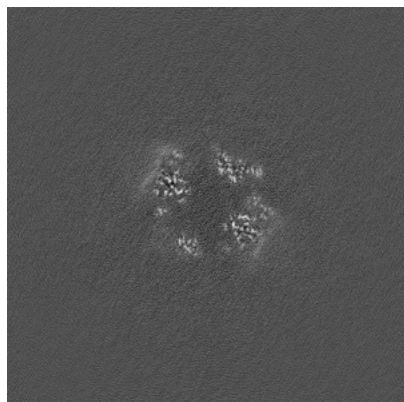


Y Index: 215

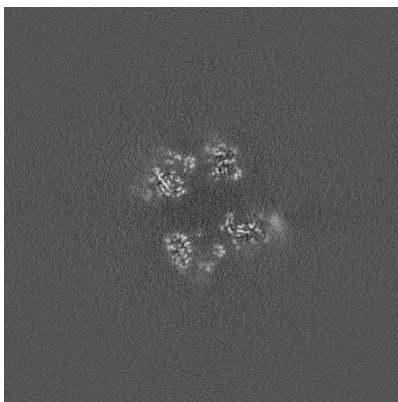


Z Index: 215

6.2.2 Raw map



X Index: 215



Y Index: 215

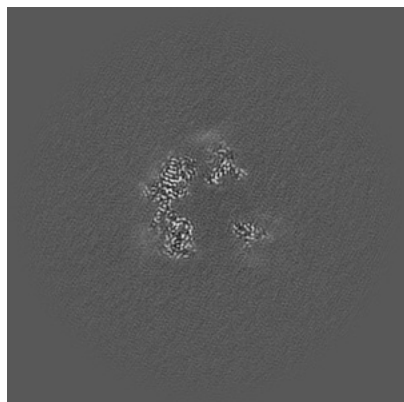


Z Index: 215

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

6.3 Largest variance slices [i](#)

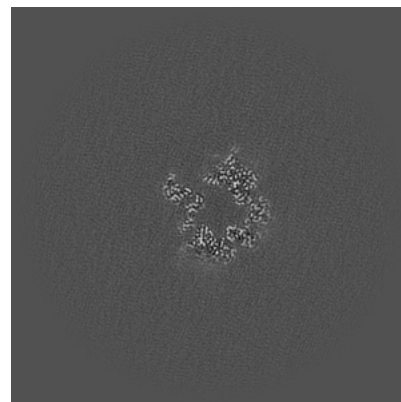
6.3.1 Primary map



X Index: 204

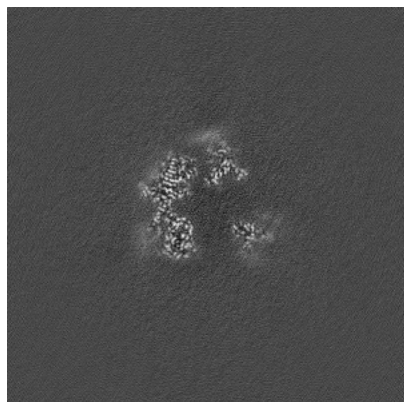


Y Index: 195

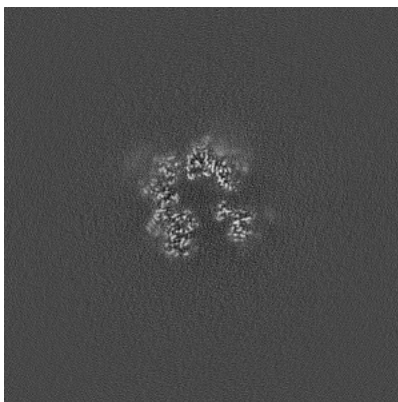


Z Index: 243

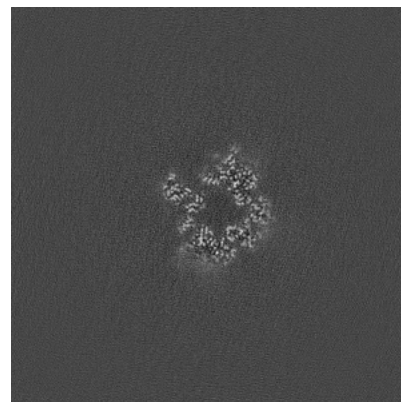
6.3.2 Raw map



X Index: 204



Y Index: 193

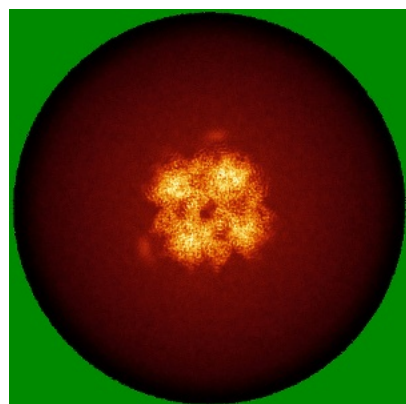


Z Index: 243

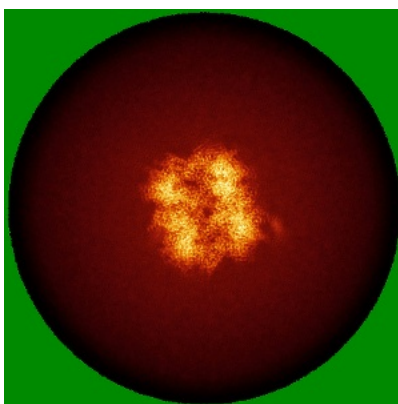
The images above show the largest variance slices of the map in three orthogonal directions.

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

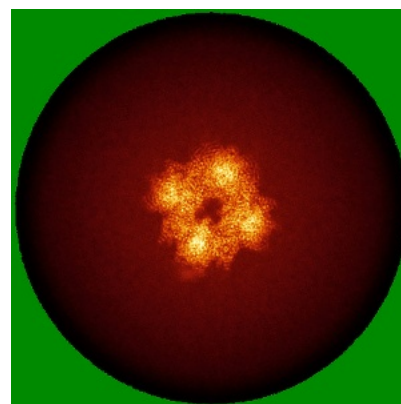
6.4.1 Primary map



X

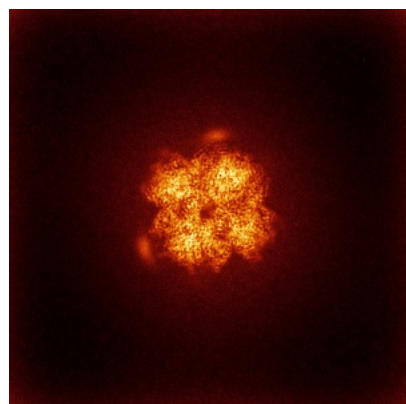


Y

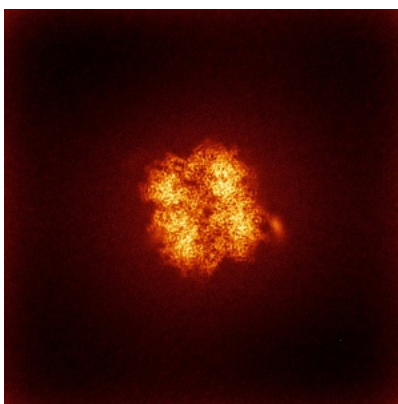


Z

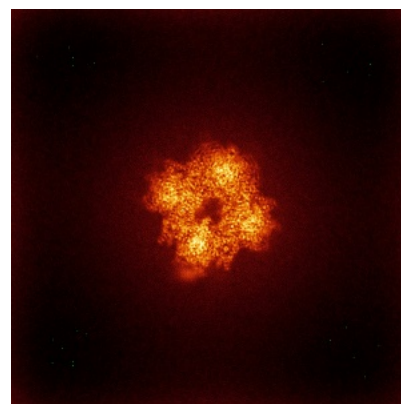
6.4.2 Raw map



X



Y

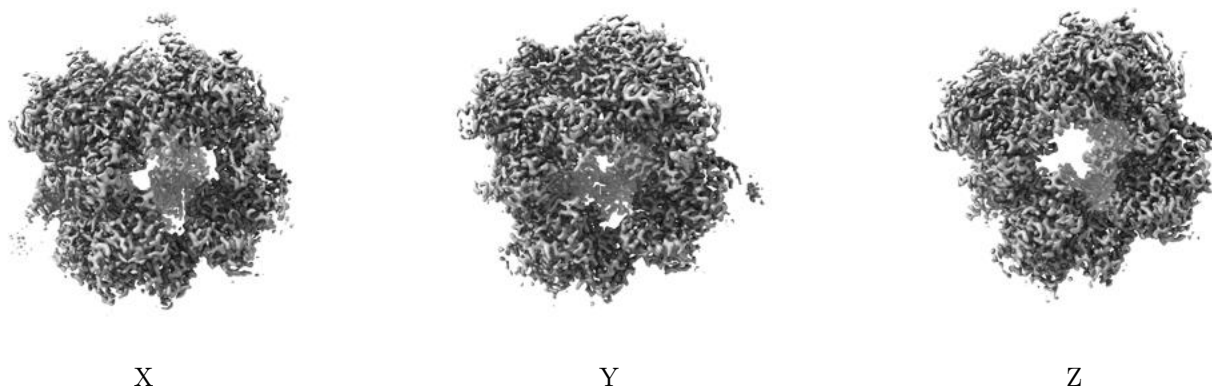


Z

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.

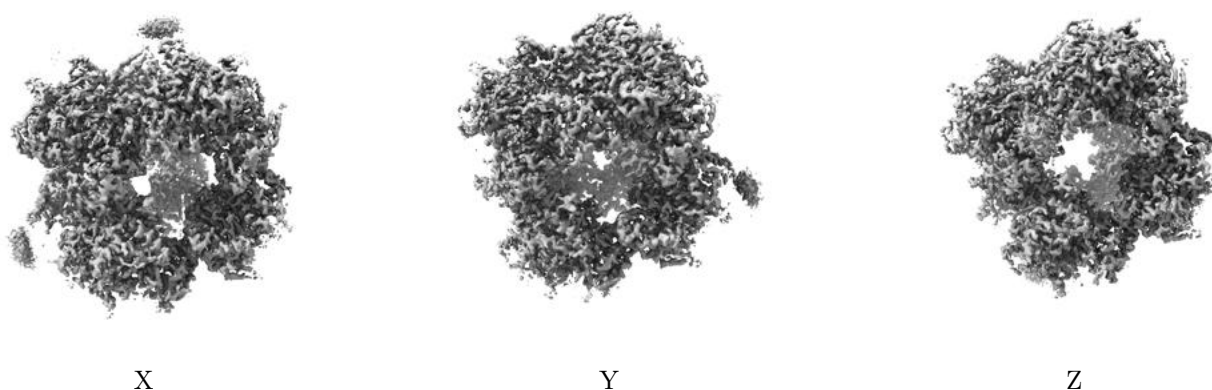
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.288. 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.

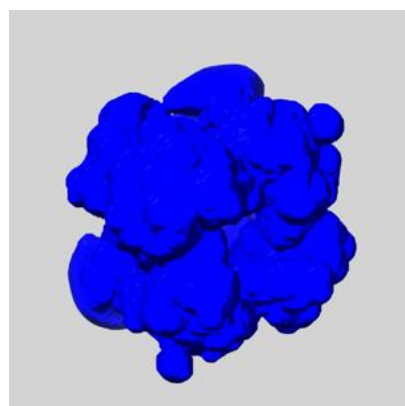
6.6 Mask visualisation [i](#)

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

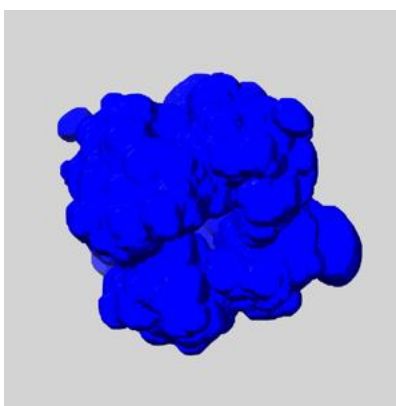
A mask typically either:

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

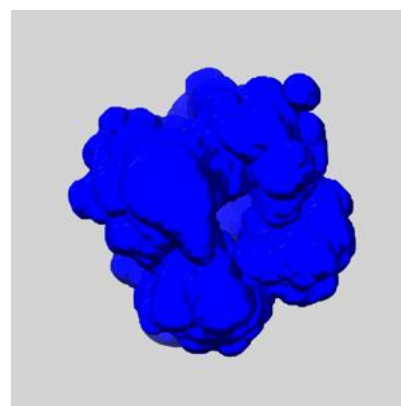
6.6.1 emd_38452_msk_1.map [i](#)



X



Y

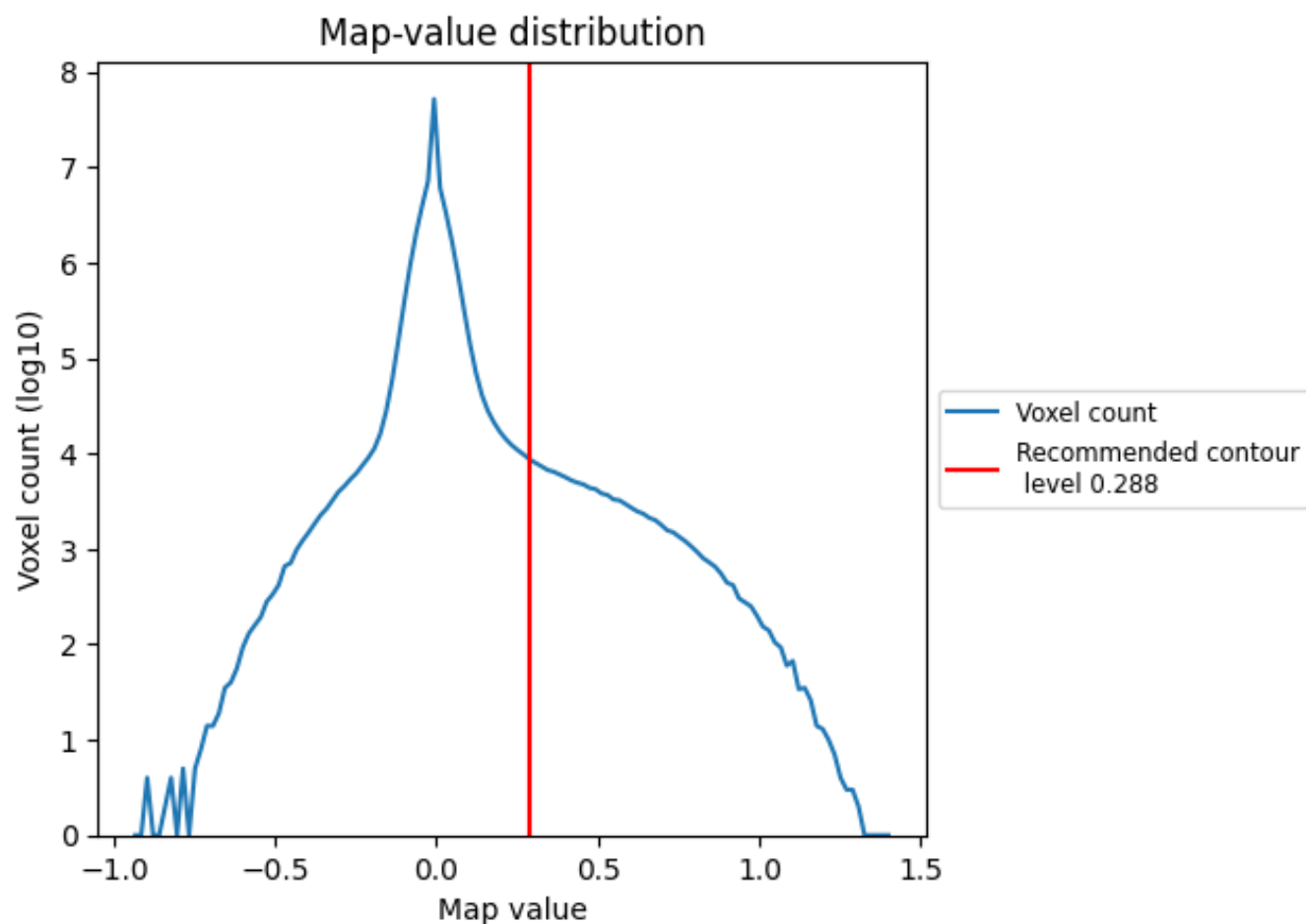


Z

7 Map analysis [i](#)

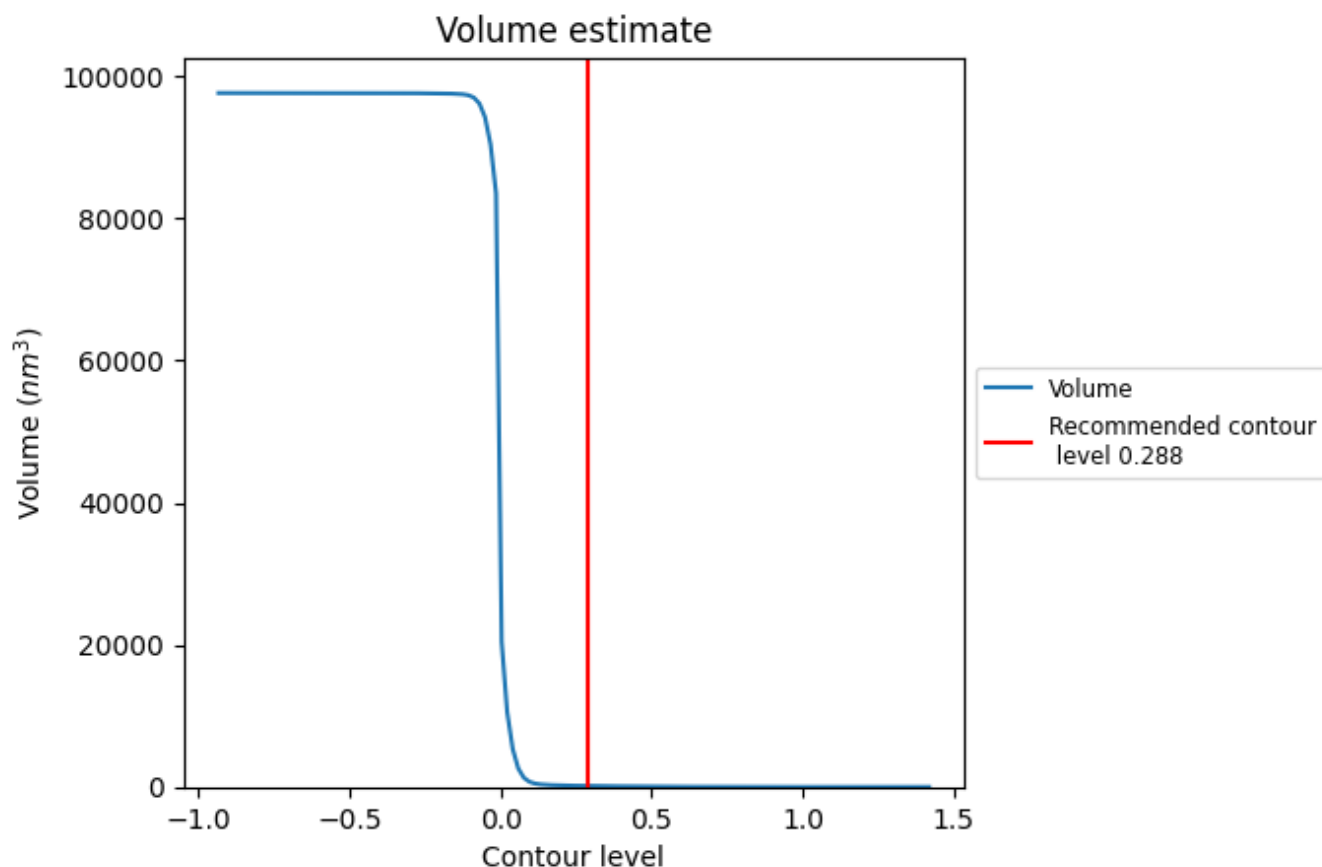
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

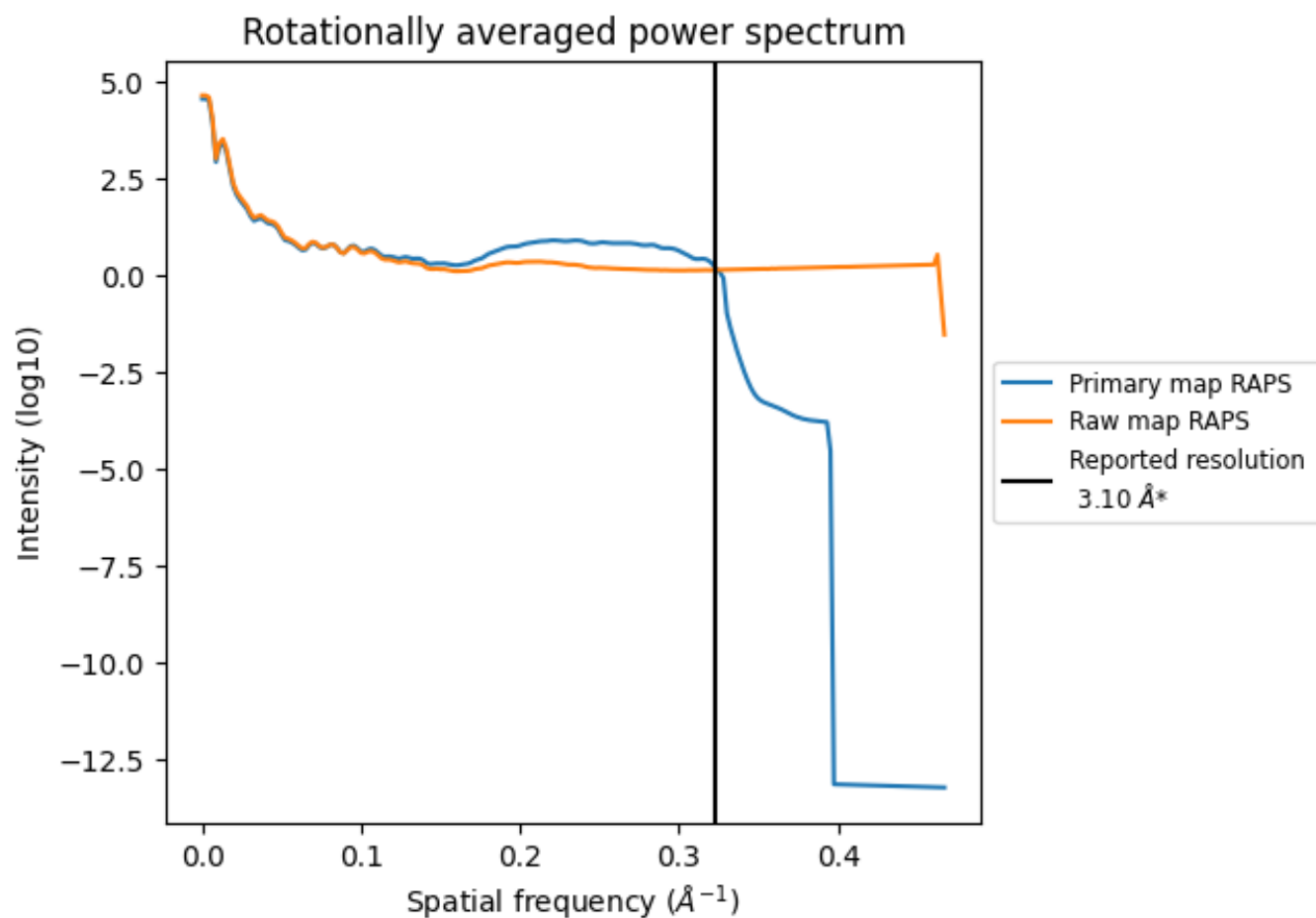
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 143 nm³; this corresponds to an approximate mass of 129 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 ⓘ

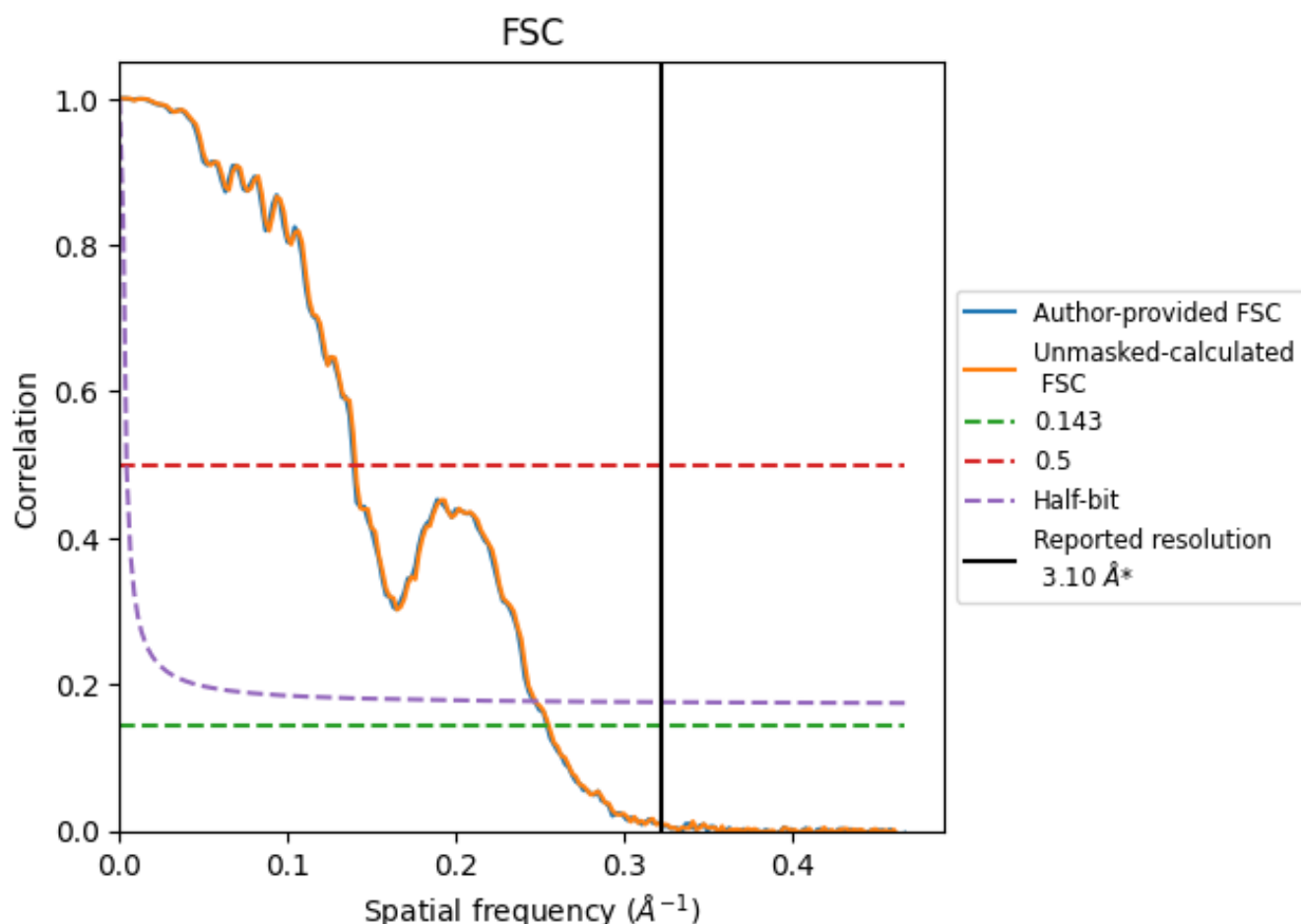


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.94	7.18	4.06
Unmasked-calculated*	3.92	7.13	4.05

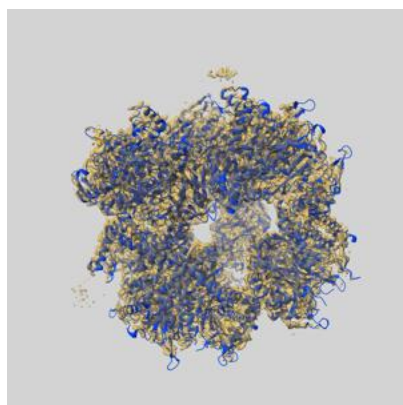
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.94 differs from the reported value 3.1 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.92 differs from the reported value 3.1 by more than 10 %

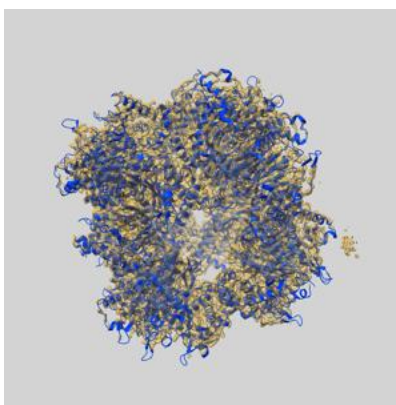
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38452 and PDB model 8XLL. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

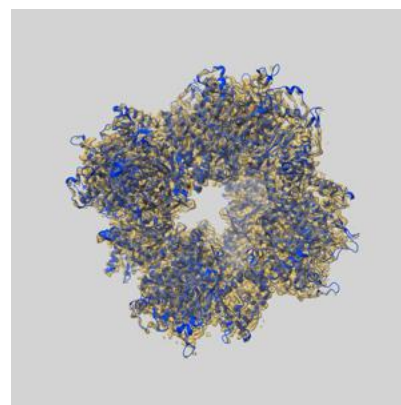
9.1 Map-model overlay [i](#)



X



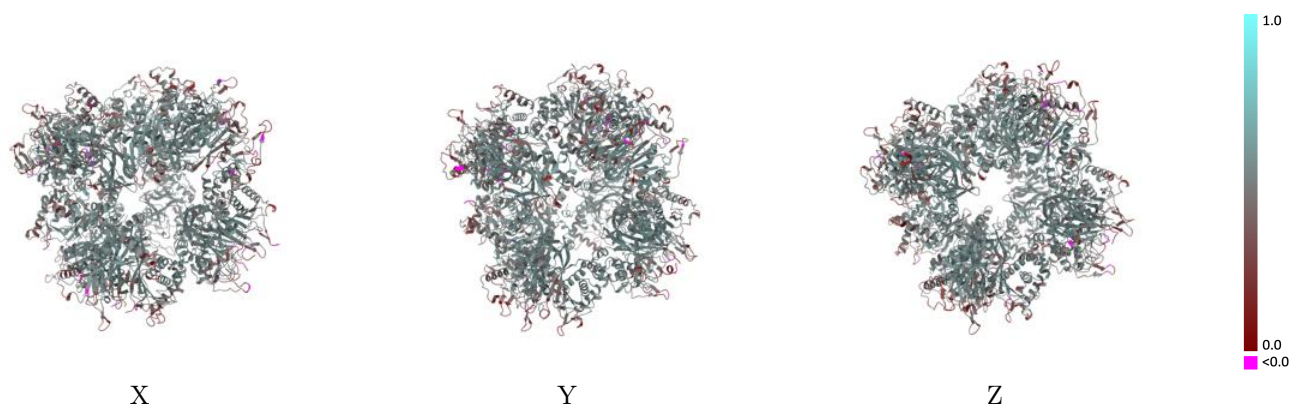
Y



Z

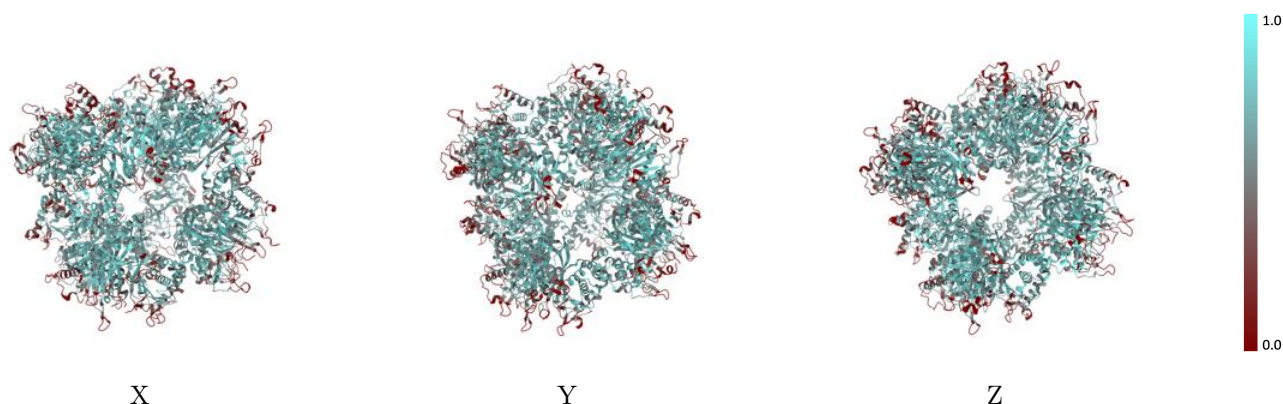
The images above show the 3D surface view of the map at the recommended contour level 0.288 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



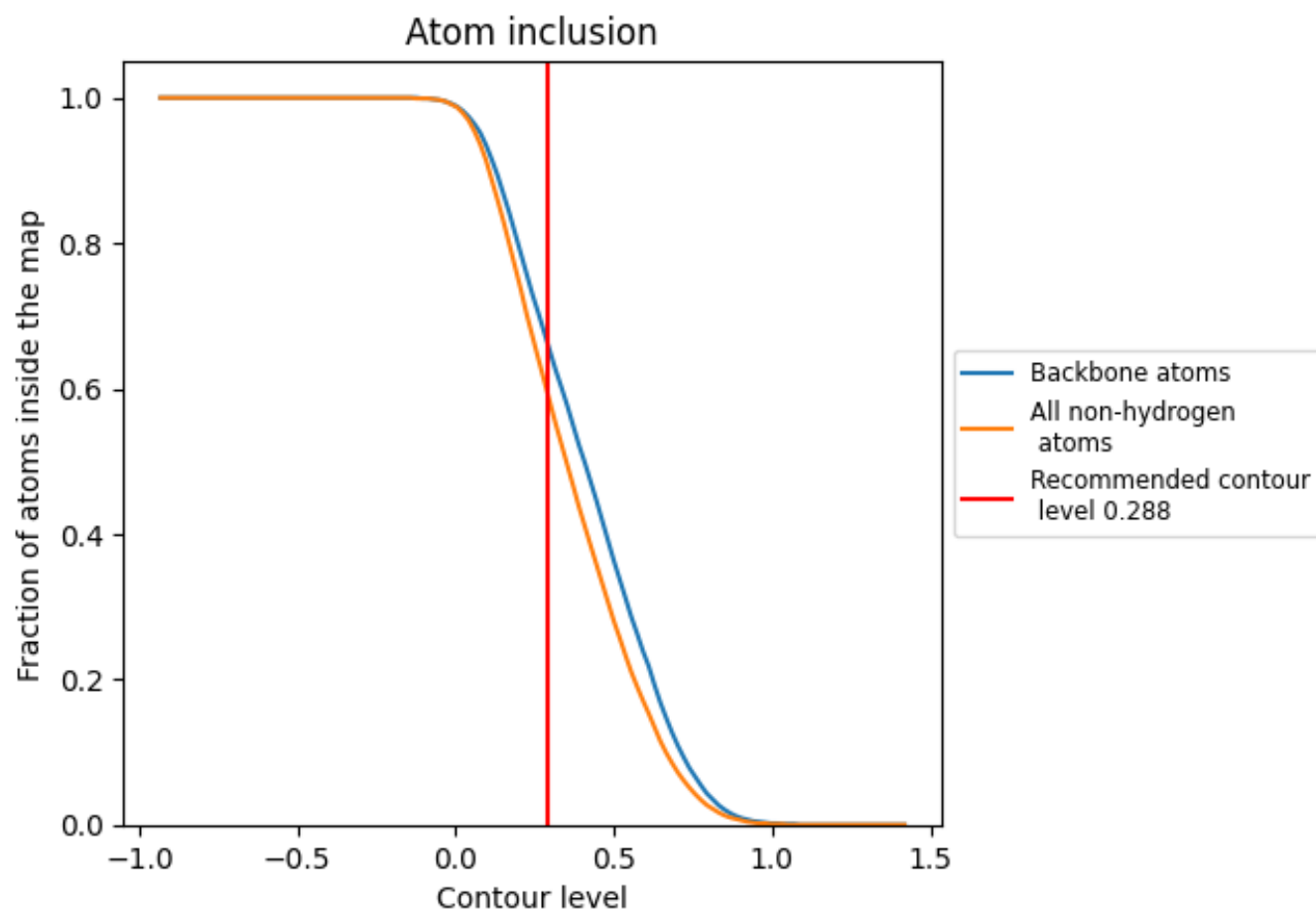
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.288).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 60% 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 (0.288) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5960	 0.4920
A	 0.6160	 0.4790
B	 0.6130	 0.5060
C	 0.5980	 0.4990
D	 0.6250	 0.4920
E	 0.6040	 0.4930
F	 0.5850	 0.4870
G	 0.6000	 0.4920
H	 0.5990	 0.5000
I	 0.5940	 0.5120
J	 0.6310	 0.5120
K	 0.6160	 0.4990
L	 0.5950	 0.4910
M	 0.6020	 0.4980
N	 0.5980	 0.4990
O	 0.5960	 0.4950
P	 0.5950	 0.5000
R	 0.5730	 0.4990
S	 0.5770	 0.4960
T	 0.5820	 0.4850
U	 0.5790	 0.4840
V	 0.5700	 0.4940
W	 0.6190	 0.5030
X	 0.6250	 0.5060
Y	 0.5160	 0.3990

