



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:38 AM UTC

PDB ID : 6LAR / pdb_00006lar
EMDB ID : EMD-0862
Title : Structure of ESX-3 complex
Authors : Wang, S.H.; Zhou, K.X.; Li, J.; Rao, Z.H.
Deposited on : 2019-11-13
Resolution : 3.70 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:

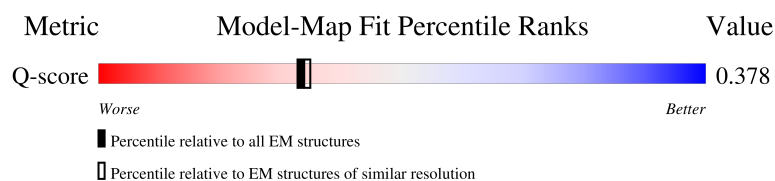
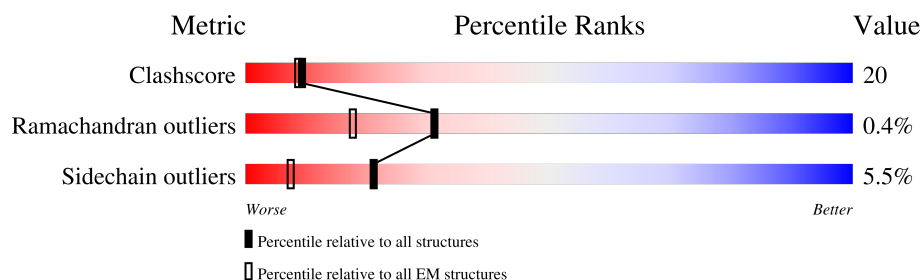
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.70 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.



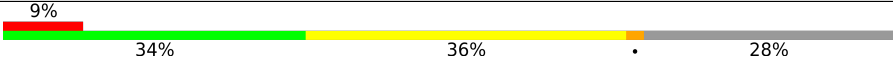
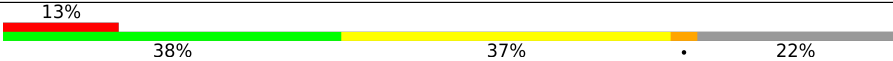
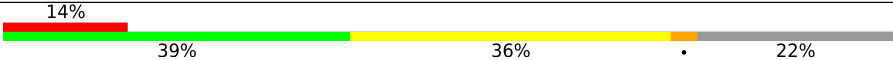
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	518	 8% 5% 84%
1	I	518	 8% 89%
2	B	475	 11% 61% 28% 10%
2	C	475	 23% 69% 24% 7%

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Mol	Chain	Length	Quality of chain
2	E	475	
2	H	475	
3	F	449	
3	J	449	
4	D	309	
4	G	309	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22448 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 ESX-3 secretion system ATPase EccB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	81	Total	C	N	O	S	0	0
			642	402	127	110	3		
1	I	59	Total	C	N	O	S	0	0
			461	297	87	74	3		

- Molecule 2 is a protein called ESX-3 secretion system protein EccD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	427	Total	C	N	O	S	0	0
			3055	1986	527	534	8		
2	C	442	Total	C	N	O	S	0	0
			3168	2063	548	549	8		
2	E	427	Total	C	N	O	S	0	0
			3055	1986	527	534	8		
2	H	442	Total	C	N	O	S	0	0
			3168	2063	548	549	8		

- Molecule 3 is a protein called ESX-3 secretion system protein EccC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	336	Total	C	N	O	S	0	0
			2667	1671	501	491	4		
3	J	324	Total	C	N	O	S	0	0
			2574	1608	483	479	4		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	432	HIS	-	expression tag	UNP A0QQ40
F	433	LEU	-	expression tag	UNP A0QQ40
F	434	GLY	-	expression tag	UNP A0QQ40
F	435	GLY	-	expression tag	UNP A0QQ40
F	436	ILE	-	expression tag	UNP A0QQ40

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Chain	Residue	Modelled	Actual	Comment	Reference
F	437	LYS	-	expression tag	UNP A0QQ40
F	438	ALA	-	expression tag	UNP A0QQ40
F	439	PHE	-	expression tag	UNP A0QQ40
F	440	HIS	-	expression tag	UNP A0QQ40
F	441	HIS	-	expression tag	UNP A0QQ40
F	442	HIS	-	expression tag	UNP A0QQ40
F	443	HIS	-	expression tag	UNP A0QQ40
F	444	HIS	-	expression tag	UNP A0QQ40
F	445	HIS	-	expression tag	UNP A0QQ40
F	446	HIS	-	expression tag	UNP A0QQ40
F	447	HIS	-	expression tag	UNP A0QQ40
F	448	HIS	-	expression tag	UNP A0QQ40
F	449	HIS	-	expression tag	UNP A0QQ40
J	432	HIS	-	expression tag	UNP A0QQ40
J	433	LEU	-	expression tag	UNP A0QQ40
J	434	GLY	-	expression tag	UNP A0QQ40
J	435	GLY	-	expression tag	UNP A0QQ40
J	436	ILE	-	expression tag	UNP A0QQ40
J	437	LYS	-	expression tag	UNP A0QQ40
J	438	ALA	-	expression tag	UNP A0QQ40
J	439	PHE	-	expression tag	UNP A0QQ40
J	440	HIS	-	expression tag	UNP A0QQ40
J	441	HIS	-	expression tag	UNP A0QQ40
J	442	HIS	-	expression tag	UNP A0QQ40
J	443	HIS	-	expression tag	UNP A0QQ40
J	444	HIS	-	expression tag	UNP A0QQ40
J	445	HIS	-	expression tag	UNP A0QQ40
J	446	HIS	-	expression tag	UNP A0QQ40
J	447	HIS	-	expression tag	UNP A0QQ40
J	448	HIS	-	expression tag	UNP A0QQ40
J	449	HIS	-	expression tag	UNP A0QQ40

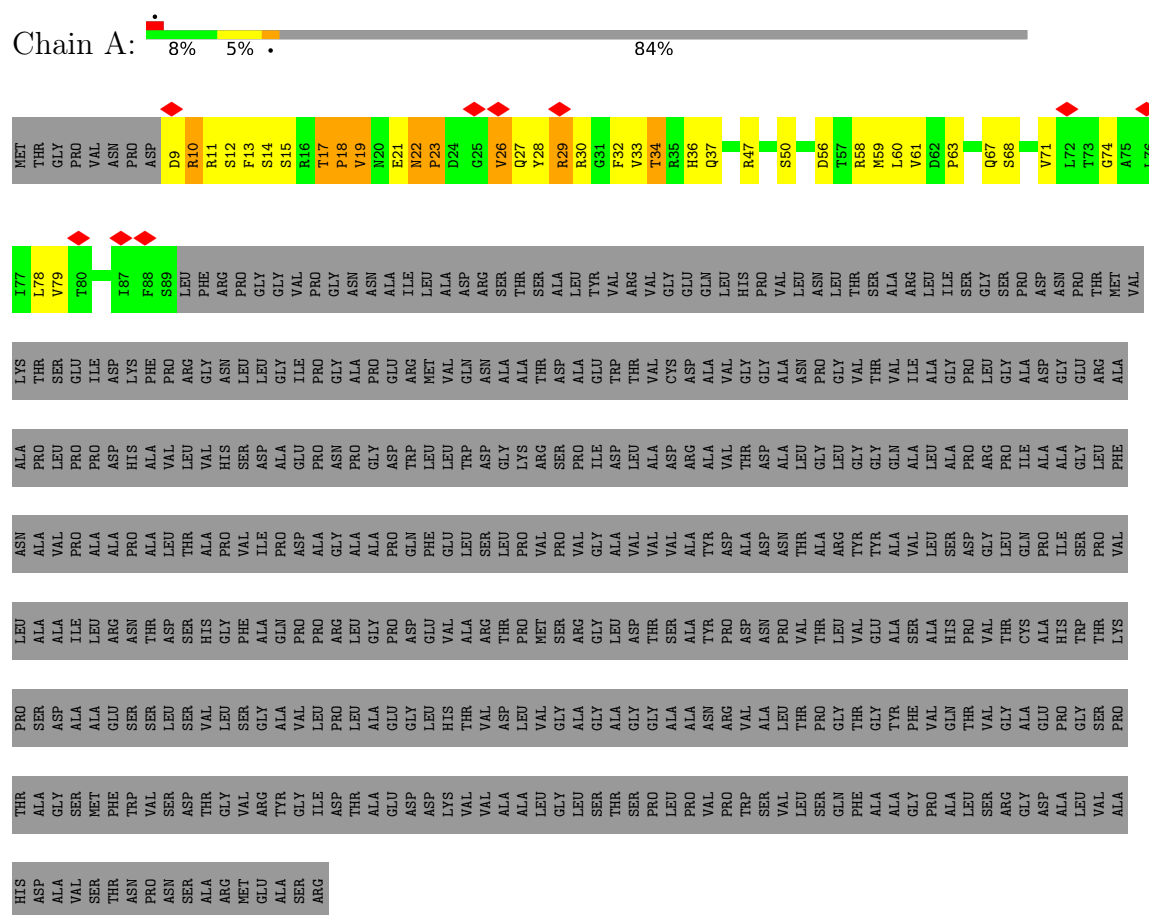
- Molecule 4 is a protein called ESX-3 secretion system protein EccE3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	241	Total	C	N	O	S	0	0
			1829	1160	336	328	5		
4	D	241	Total	C	N	O	S	0	0
			1829	1160	336	328	5		

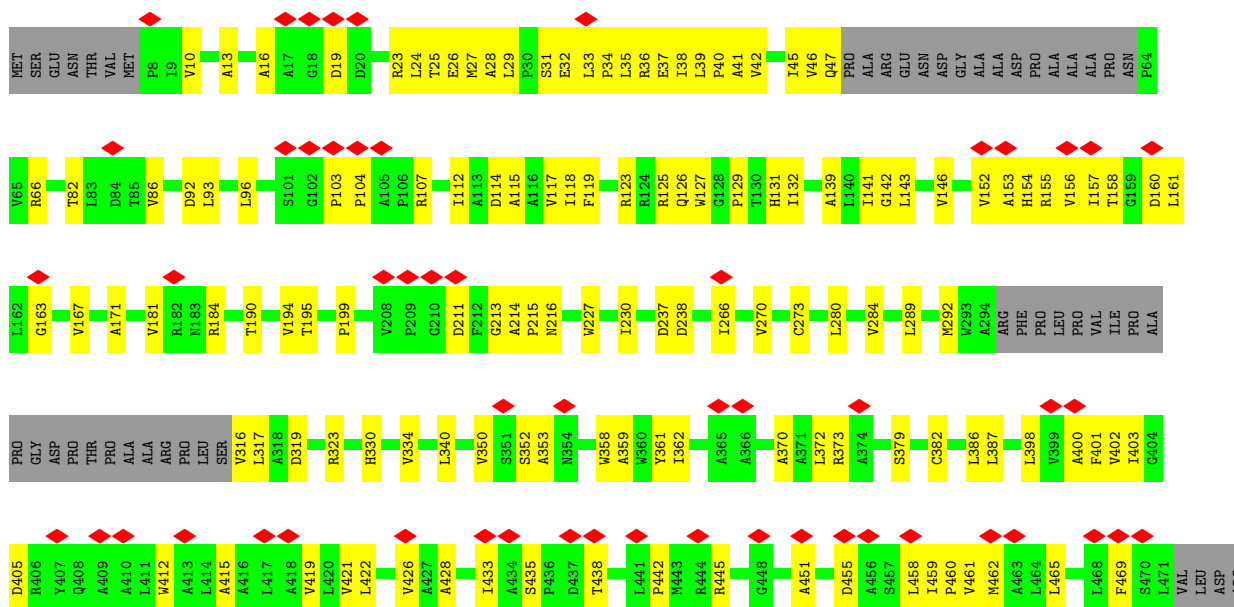
3 Residue-property plots

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: ESX-3 secretion system ATPase EccB3

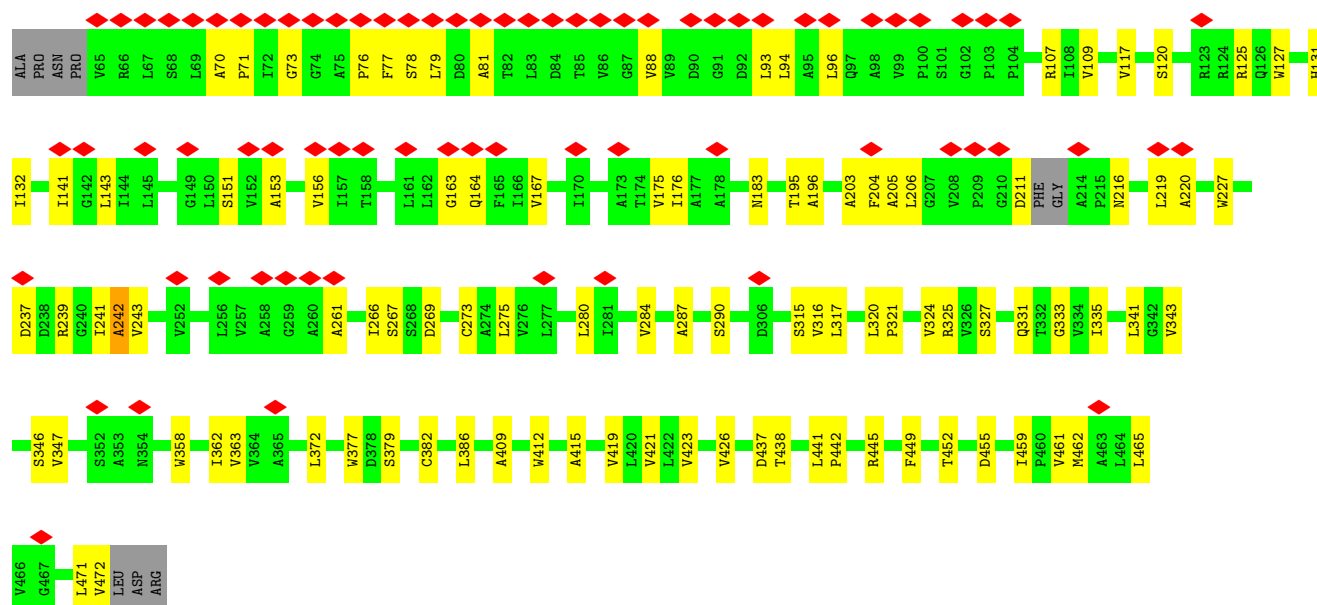


- Molecule 2: ESX-3 secretion system protein EccD3

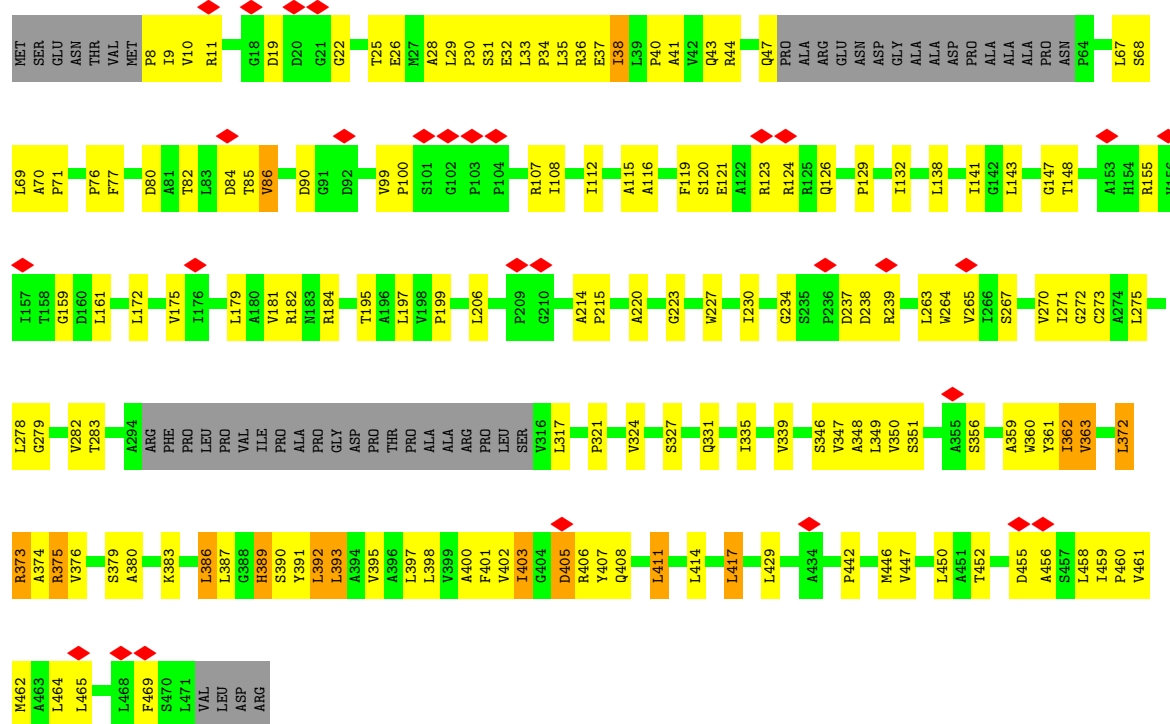


- Molecule 2: ESX-3 secretion system protein EccD3



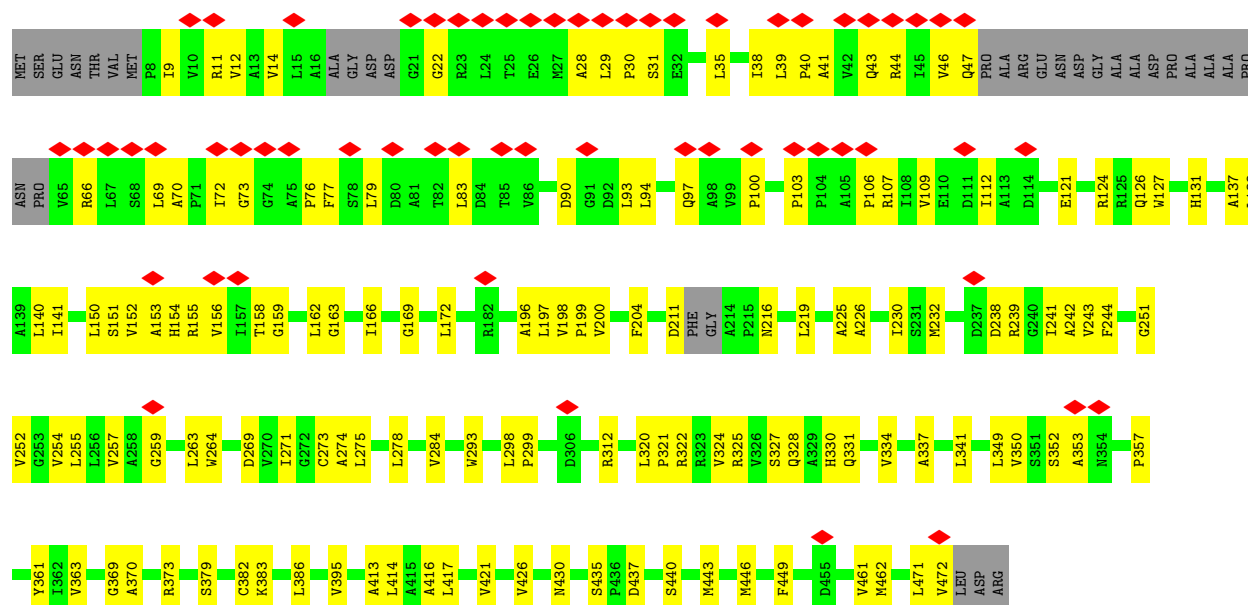


• Molecule 2: ESX-3 secretion system protein EccD3

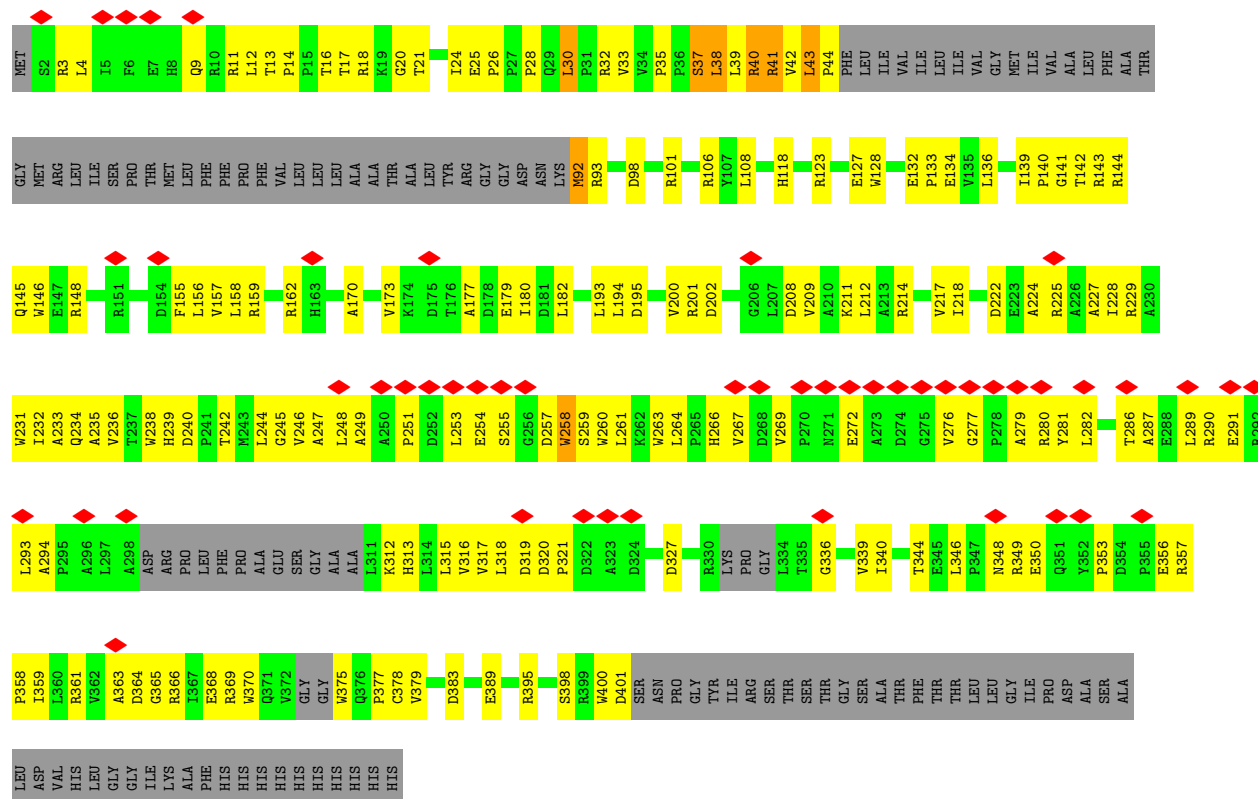


• Molecule 2: ESX-3 secretion system protein EccD3



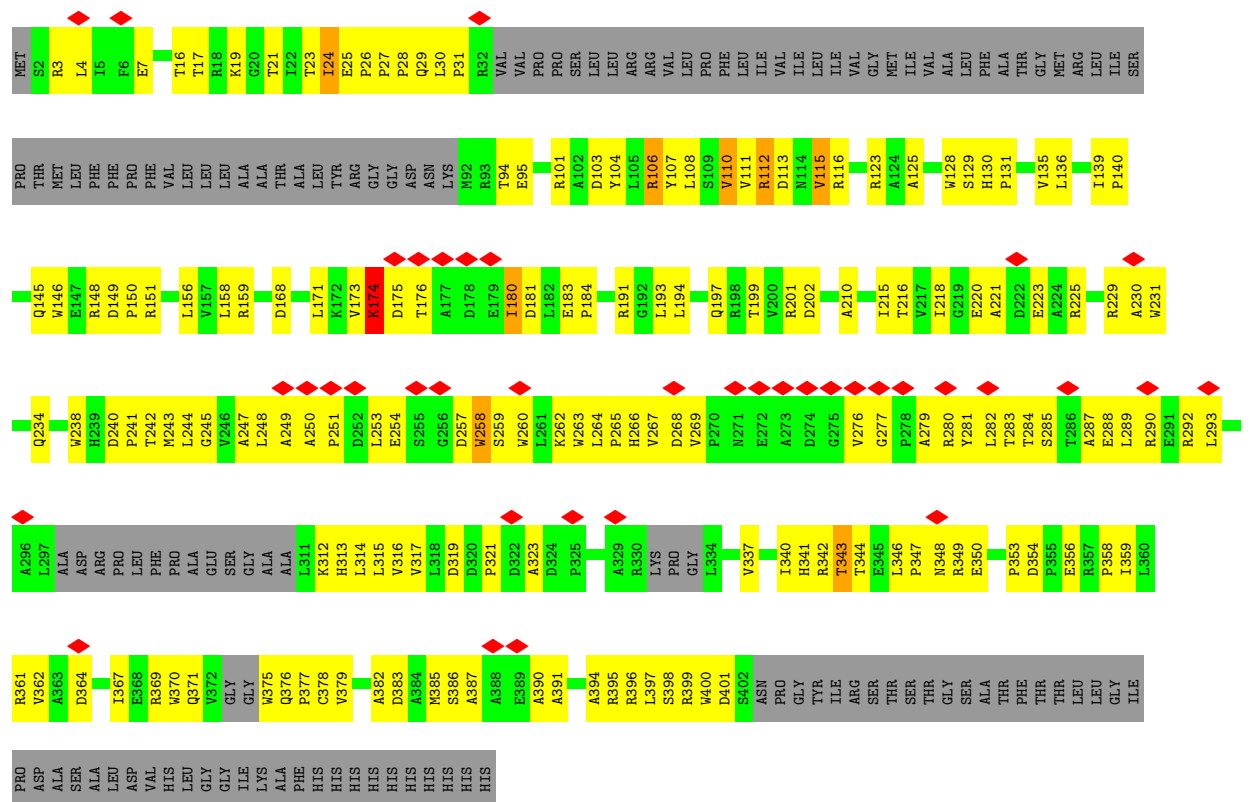


• Molecule 3: ESX-3 secretion system protein EccC3

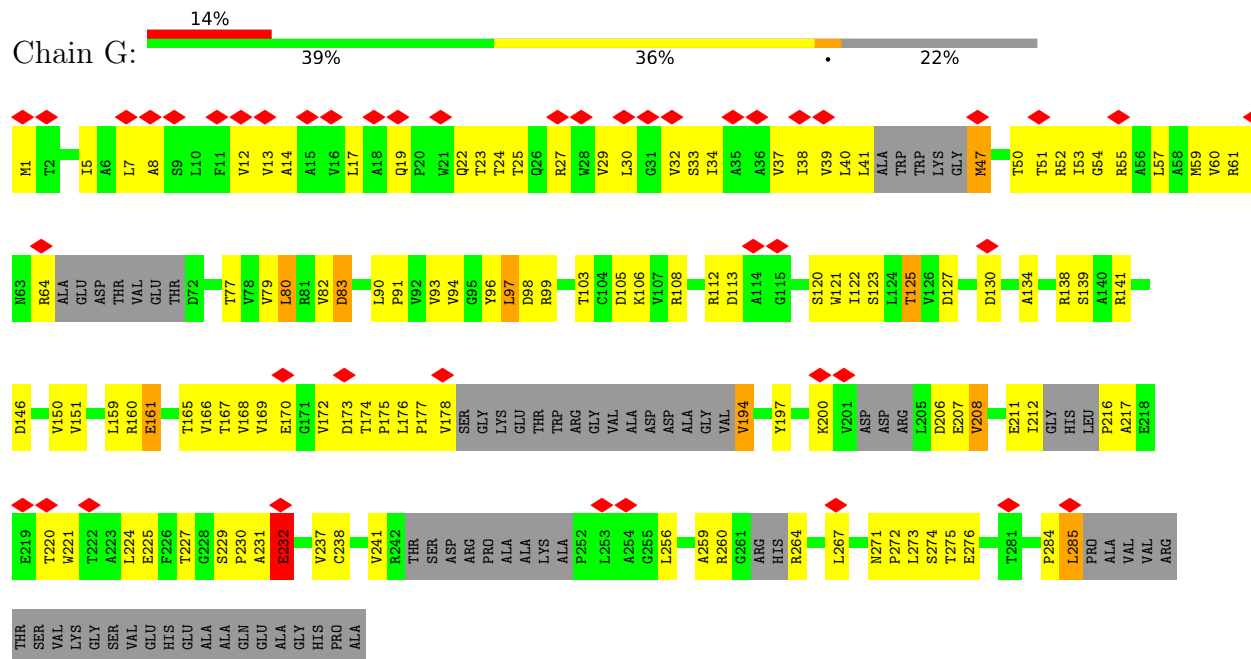


• Molecule 3: ESX-3 secretion system protein EccC3





• Molecule 4: ESX-3 secretion system protein EccE3



• Molecule 4: ESX-3 secretion system protein EccE3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	215839	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.113	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	360.8, 360.8, 360.8	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	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	0.63	0/654	0.77	0/883
1	I	0.43	0/469	0.55	0/634
2	B	0.31	0/3111	0.55	0/4271
2	C	0.33	0/3229	0.54	0/4438
2	E	0.46	0/3111	0.67	1/4271 (0.0%)
2	H	0.38	0/3229	0.57	0/4438
3	F	0.38	0/2727	0.61	0/3727
3	J	0.43	0/2631	0.69	0/3593
4	D	0.30	0/1855	0.58	2/2531 (0.1%)
4	G	0.30	0/1855	0.58	2/2531 (0.1%)
All	All	0.38	0/22871	0.61	5/31317 (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
3	J	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	232	GLU	CA-CB-CG	7.45	129.01	114.10
4	D	232	GLU	CA-CB-CG	7.42	128.94	114.10
2	E	86	VAL	N-CA-C	-6.95	105.95	112.83
4	D	232	GLU	CB-CG-CD	5.56	122.05	112.60
4	G	232	GLU	CB-CG-CD	5.54	122.02	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	323	ALA	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	642	0	653	56	0
1	I	461	0	487	17	0
2	B	3055	0	3235	98	0
2	C	3168	0	3367	81	0
2	E	3055	0	3235	156	0
2	H	3168	0	3367	105	0
3	F	2667	0	2661	147	0
3	J	2574	0	2549	198	0
4	D	1829	0	1907	84	0
4	G	1829	0	1907	75	0
All	All	22448	0	23368	930	0

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

All (930) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:PHE:CE2	3:J:104:TYR:HD1	1.39	1.39
2:E:346:SER:OG	2:E:363:VAL:HG12	1.20	1.33
2:E:346:SER:OG	2:E:363:VAL:CG1	1.86	1.24
1:A:13:PHE:CE2	3:J:104:TYR:CD1	2.30	1.18
2:E:107:ARG:NE	3:J:116:ARG:HH21	1.39	1.17
3:J:26:PRO:HG3	3:J:175:ASP:HB3	1.16	1.13
1:A:22:ASN:HB2	1:A:23:PRO:CD	1.79	1.11
2:E:107:ARG:HE	3:J:116:ARG:NH2	1.47	1.10
1:A:18:PRO:HD2	3:J:110:VAL:HG11	1.31	1.07
1:A:13:PHE:CD2	3:J:104:TYR:HD1	1.73	1.06
2:E:107:ARG:NE	3:J:116:ARG:NH2	2.01	1.04
2:E:414:LEU:HD12	2:H:150:LEU:CD2	1.87	1.03
1:A:18:PRO:HG2	3:J:110:VAL:CG1	1.91	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:PHE:HE2	3:J:104:TYR:HA	1.26	0.99
1:A:18:PRO:CD	3:J:110:VAL:HG11	1.93	0.99
3:J:26:PRO:HG3	3:J:175:ASP:CB	1.94	0.98
2:E:414:LEU:HD12	2:H:150:LEU:HD23	1.46	0.96
1:A:22:ASN:HB2	1:A:23:PRO:HD2	1.46	0.95
1:A:29:ARG:HG2	1:A:29:ARG:HH11	1.29	0.94
2:E:350:VAL:HG11	2:E:360:TRP:CZ3	2.03	0.94
2:E:107:ARG:CD	3:J:116:ARG:NH2	2.32	0.93
1:A:13:PHE:CD2	3:J:104:TYR:CD1	2.53	0.93
3:J:371:GLN:HB3	3:J:376:GLN:HE21	1.32	0.92
2:E:346:SER:HG	2:E:363:VAL:HG12	0.92	0.92
1:A:18:PRO:CG	3:J:110:VAL:CG1	2.48	0.91
3:J:264:LEU:HB2	3:J:267:VAL:HG23	1.53	0.91
3:F:35:PRO:HG2	3:J:95:GLU:CB	2.02	0.89
3:F:248:LEU:HD11	3:F:258:TRP:HB3	1.54	0.89
2:E:107:ARG:HD3	3:J:116:ARG:NH2	1.89	0.88
3:F:35:PRO:HG2	3:J:95:GLU:HB2	1.56	0.87
3:J:26:PRO:CG	3:J:175:ASP:HB3	2.04	0.87
3:J:341:HIS:NE2	3:J:343:THR:OG1	2.08	0.87
2:E:107:ARG:CD	3:J:116:ARG:HH21	1.89	0.85
3:F:127:GLU:OE1	3:F:162:ARG:NH1	2.10	0.85
3:F:38:LEU:HA	3:F:41:ARG:HG2	1.59	0.84
2:E:414:LEU:CD1	2:H:150:LEU:HD23	2.08	0.84
2:E:414:LEU:O	2:E:414:LEU:HD23	1.79	0.83
1:A:22:ASN:HB2	1:A:23:PRO:HD3	1.61	0.83
3:F:43:LEU:H	3:F:44:PRO:HD2	1.44	0.82
2:H:298:LEU:O	2:H:312:ARG:NH1	2.12	0.82
1:A:18:PRO:CG	3:J:110:VAL:HG11	2.09	0.82
1:A:13:PHE:CE2	3:J:104:TYR:HA	2.14	0.82
4:D:108:ARG:HB3	4:D:123:SER:HB2	1.62	0.82
3:J:264:LEU:HD21	3:J:394:ALA:HA	1.62	0.82
2:E:107:ARG:HE	3:J:116:ARG:HH21	0.84	0.81
4:G:108:ARG:HB3	4:G:123:SER:HB2	1.62	0.81
2:E:82:THR:HG23	2:E:84:ASP:H	1.47	0.80
3:J:251:PRO:HA	3:J:284:THR:HG23	1.64	0.79
4:G:194:VAL:N	4:G:241:VAL:O	2.16	0.79
3:J:3:ARG:NH2	3:J:263:TRP:O	2.15	0.79
2:E:143:LEU:HD22	2:H:421:VAL:HG11	1.64	0.79
3:J:262:LYS:HD2	3:J:280:ARG:HG2	1.65	0.79
4:D:194:VAL:N	4:D:241:VAL:O	2.16	0.78
3:J:229:ARG:HH21	3:J:386:SER:HA	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:PHE:HE2	3:J:104:TYR:HD1	1.29	0.78
2:E:392:LEU:HD12	2:E:392:LEU:O	1.84	0.78
3:J:26:PRO:CG	3:J:175:ASP:CB	2.61	0.78
1:A:22:ASN:CB	1:A:23:PRO:CD	2.60	0.78
2:E:11:ARG:N	2:E:90:ASP:OD1	2.16	0.77
2:E:335:ILE:HG21	2:E:386:LEU:CD2	2.14	0.77
2:C:379:SER:HG	2:C:382:CYS:HG	1.28	0.77
3:F:254:GLU:HA	3:F:259:SER:HB3	1.65	0.77
2:H:379:SER:OG	2:H:382:CYS:SG	2.43	0.77
2:C:331:GLN:NE2	2:C:382:CYS:SG	2.58	0.77
2:E:414:LEU:HD12	2:H:150:LEU:HD22	1.66	0.77
2:E:335:ILE:HG21	2:E:386:LEU:HD23	1.67	0.76
2:B:153:ALA:HA	2:B:156:VAL:HG22	1.68	0.76
3:F:43:LEU:N	3:F:44:PRO:HD2	2.00	0.75
4:G:17:LEU:HD12	4:G:19:GLN:HE22	1.51	0.75
3:J:229:ARG:NE	3:J:385:MET:O	2.20	0.74
1:A:58:ARG:O	3:F:106:ARG:NH1	2.19	0.74
2:E:335:ILE:CG2	2:E:386:LEU:HD23	2.16	0.74
3:J:314:LEU:HB2	3:J:337:VAL:HG22	1.69	0.74
3:J:243:MET:SD	3:J:312:LYS:NZ	2.59	0.74
4:D:17:LEU:HD12	4:D:19:GLN:HE22	1.51	0.74
2:B:154:HIS:CE1	2:B:160:ASP:HB3	2.23	0.74
1:A:13:PHE:HE2	3:J:104:TYR:CD1	2.03	0.73
3:J:94:THR:OG1	3:J:95:GLU:OE2	2.04	0.73
3:F:313:HIS:NE2	3:F:336:GLY:O	2.22	0.73
2:E:155:ARG:O	2:E:155:ARG:NH1	2.20	0.72
2:E:346:SER:OG	2:E:363:VAL:HG11	1.89	0.72
2:B:107:ARG:HH22	2:B:118:ILE:HG21	1.54	0.72
3:J:369:ARG:NE	3:J:378:CYS:SG	2.62	0.72
2:C:358:TRP:HB2	2:C:465:LEU:HD13	1.71	0.72
2:B:36:ARG:NE	3:F:389:GLU:OE1	2.23	0.71
2:E:26:GLU:OE1	4:D:154:ARG:NH1	2.22	0.71
2:E:350:VAL:CG1	2:E:360:TRP:CH2	2.73	0.71
3:J:112:ARG:HG3	3:J:112:ARG:HH11	1.53	0.71
2:B:273:CYS:HB3	2:B:462:MET:HE3	1.72	0.71
2:C:379:SER:OG	2:C:382:CYS:SG	2.46	0.71
1:A:29:ARG:HG2	1:A:29:ARG:NH1	1.97	0.70
3:J:248:LEU:HD21	3:J:258:TRP:HB3	1.74	0.70
2:C:11:ARG:HD3	3:F:276:VAL:HB	1.73	0.70
3:J:341:HIS:HE2	3:J:343:THR:HG1	1.28	0.70
4:D:59:MET:SD	4:D:62:ARG:NH1	2.59	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:59:MET:SD	4:G:62:ARG:NH1	2.59	0.70
2:E:99:VAL:HG22	2:E:100:PRO:HD2	1.72	0.70
2:H:211:ASP:OD1	2:H:216:ASN:ND2	2.25	0.70
3:F:98:ASP:OD1	3:F:101:ARG:NH1	2.24	0.70
3:J:371:GLN:HB3	3:J:376:GLN:NE2	2.06	0.70
2:B:157:ILE:HG23	2:B:158:THR:HG23	1.73	0.70
2:B:155:ARG:NH1	2:B:160:ASP:O	2.24	0.70
2:E:29:LEU:HD13	2:E:38:ILE:HD12	1.72	0.69
2:E:393:LEU:O	2:E:393:LEU:HD12	1.92	0.69
3:F:264:LEU:HD11	3:F:266:HIS:HB2	1.74	0.69
3:J:254:GLU:HA	3:J:259:SER:HB2	1.73	0.69
3:F:370:TRP:HA	3:F:375:TRP:HE1	1.56	0.69
1:A:18:PRO:HG2	3:J:110:VAL:HG11	1.71	0.69
3:J:24:ILE:HD13	3:J:24:ILE:N	2.06	0.69
3:F:43:LEU:H	3:F:44:PRO:CD	2.05	0.69
2:E:182:ARG:NH1	2:E:234:GLY:O	2.25	0.69
2:C:273:CYS:HA	2:C:462:MET:HE2	1.75	0.68
3:J:253:LEU:HG	3:J:254:GLU:HG3	1.74	0.68
3:F:225:ARG:HA	3:F:228:ILE:HD12	1.75	0.68
1:A:22:ASN:ND2	3:J:113:ASP:O	2.26	0.68
2:C:205:ALA:HB2	2:C:220:ALA:HB2	1.75	0.68
2:B:372:LEU:HD23	2:B:451:ALA:HB2	1.76	0.68
3:F:158:LEU:HD23	3:F:231:TRP:HB2	1.76	0.68
3:F:41:ARG:O	3:F:41:ARG:HG3	1.94	0.67
3:F:363:ALA:HB3	3:F:366:ARG:HB2	1.74	0.67
1:A:18:PRO:HG2	3:J:110:VAL:HG13	1.76	0.67
2:H:241:ILE:HG13	2:H:243:VAL:HG12	1.75	0.67
2:B:421:VAL:HG21	2:C:143:LEU:HD13	1.77	0.67
2:C:71:PRO:HD3	2:C:77:PHE:CZ	2.30	0.67
2:E:392:LEU:HD12	2:E:392:LEU:C	2.20	0.67
3:F:9:GLN:HG2	3:F:143:ARG:HE	1.61	0.66
2:E:414:LEU:CD1	2:H:150:LEU:CD2	2.67	0.66
2:H:35:LEU:HB2	2:H:79:LEU:HD12	1.77	0.65
3:F:43:LEU:N	3:F:44:PRO:CD	2.59	0.65
3:F:212:LEU:HD12	3:F:358:PRO:HD3	1.77	0.65
4:D:60:VAL:O	4:D:64:ARG:NH2	2.29	0.65
3:F:225:ARG:NH1	3:F:257:ASP:OD2	2.30	0.65
4:G:60:VAL:O	4:G:64:ARG:NH2	2.29	0.65
2:E:350:VAL:HG11	2:E:360:TRP:CH2	2.32	0.65
2:H:121:GLU:OE1	2:H:124:ARG:NH2	2.28	0.65
3:F:253:LEU:HG	3:F:254:GLU:HG2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:PRO:CD	3:J:110:VAL:CG1	2.73	0.64
3:F:353:PRO:HG3	3:F:370:TRP:CD1	2.31	0.64
2:E:22:GLY:N	2:H:112:ILE:O	2.29	0.64
3:F:11:ARG:NH1	3:F:12:LEU:O	2.30	0.64
3:F:142:THR:HG22	3:F:143:ARG:H	1.62	0.64
2:H:155:ARG:HA	2:H:158:THR:O	1.98	0.64
3:J:243:MET:HA	3:J:312:LYS:HD2	1.77	0.64
2:B:92:ASP:OD1	2:B:93:LEU:N	2.31	0.64
2:B:160:ASP:OD1	2:B:161:LEU:N	2.29	0.64
2:B:123:ARG:HG3	2:B:125:ARG:HB3	1.80	0.64
2:C:141:ILE:HD12	2:C:195:THR:HG21	1.80	0.64
4:G:161:GLU:OE1	4:G:161:GLU:HA	1.98	0.63
4:G:54:GLY:HA2	4:G:57:LEU:HD12	1.80	0.63
4:D:174:THR:OG1	4:D:176:LEU:O	2.16	0.63
4:D:220:THR:HA	4:D:241:VAL:HG12	1.80	0.63
2:B:379:SER:OG	2:B:382:CYS:SG	2.52	0.63
3:F:258:TRP:NE1	3:F:319:ASP:OD2	2.31	0.63
3:F:350:GLU:HB3	3:F:370:TRP:HE1	1.63	0.63
3:J:248:LEU:HD23	3:J:282:LEU:HG	1.80	0.63
2:C:409:ALA:HA	2:C:412:TRP:HD1	1.61	0.63
3:F:261:LEU:HD22	3:F:264:LEU:HD22	1.81	0.63
3:J:115:VAL:HG21	3:J:171:LEU:HD11	1.81	0.62
3:J:230:ALA:HA	3:J:385:MET:HB2	1.81	0.62
4:D:54:GLY:HA2	4:D:57:LEU:HD12	1.80	0.62
2:E:141:ILE:HD12	2:E:195:THR:HG21	1.81	0.62
2:B:114:ASP:HA	2:B:117:VAL:HG12	1.81	0.62
4:G:174:THR:OG1	4:G:176:LEU:O	2.16	0.62
4:G:220:THR:HA	4:G:241:VAL:HG12	1.81	0.62
3:J:341:HIS:CD2	3:J:343:THR:HG1	2.16	0.62
2:C:73:GLY:O	2:C:107:ARG:NH1	2.32	0.62
3:F:247:ALA:HB3	3:F:316:VAL:HG12	1.82	0.62
3:J:112:ARG:HH11	3:J:112:ARG:CG	2.13	0.62
3:J:159:ARG:N	3:J:234:GLN:OE1	2.30	0.62
3:F:370:TRP:HA	3:F:375:TRP:NE1	2.13	0.62
2:E:324:VAL:O	2:E:327:SER:OG	2.16	0.62
2:E:275:LEU:O	2:E:279:GLY:N	2.28	0.62
2:E:373:ARG:O	2:E:376:VAL:HG12	1.99	0.62
3:J:343:THR:HG22	3:J:344:THR:H	1.65	0.61
4:D:161:GLU:HA	4:D:161:GLU:OE1	1.99	0.61
3:J:262:LYS:HD3	3:J:282:LEU:HD13	1.81	0.61
1:A:22:ASN:CB	1:A:23:PRO:HD2	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:70:ALA:HB2	2:E:76:PRO:HA	1.83	0.61
1:I:62:ASP:OD1	1:I:62:ASP:N	2.32	0.61
3:F:35:PRO:HG2	3:J:95:GLU:HB3	1.81	0.61
4:G:47:MET:O	4:G:47:MET:HG3	2.00	0.61
3:J:260:TRP:CE3	3:J:391:ALA:HA	2.35	0.61
2:B:37:GLU:HB2	2:C:93:LEU:HD21	1.82	0.61
2:H:275:LEU:O	2:H:278:LEU:N	2.34	0.60
3:F:42:VAL:HG13	3:F:42:VAL:O	2.01	0.60
3:J:317:VAL:HG12	3:J:340:ILE:HD13	1.82	0.60
1:A:26:VAL:HG22	1:A:26:VAL:O	2.01	0.60
3:F:290:ARG:O	3:F:294:ALA:N	2.35	0.60
2:B:139:ALA:HB1	2:C:421:VAL:HG12	1.83	0.60
2:B:361:TYR:HE2	2:B:461:VAL:HG11	1.67	0.60
2:H:73:GLY:O	2:H:107:ARG:NH2	2.34	0.60
3:F:92:MET:O	3:F:92:MET:HE3	2.01	0.60
2:E:398:LEU:C	2:E:398:LEU:HD23	2.27	0.60
2:H:263:LEU:HB2	2:H:264:TRP:CE3	2.36	0.60
2:H:46:VAL:HG13	2:H:47:GLN:HG2	1.84	0.60
1:I:34:THR:HG23	1:I:37:GLN:H	1.66	0.60
4:D:47:MET:HG3	4:D:47:MET:O	2.00	0.60
3:J:353:PRO:HG3	3:J:370:TRP:HD1	1.67	0.59
2:H:9:ILE:HD11	2:H:28:ALA:HB1	1.83	0.59
3:F:359:ILE:HB	3:F:370:TRP:HB3	1.82	0.59
2:E:126:GLN:CD	2:E:126:GLN:H	2.09	0.59
2:E:350:VAL:HG11	2:E:360:TRP:CE3	2.37	0.59
3:J:257:ASP:O	3:J:259:SER:N	2.35	0.59
2:B:66:ARG:NH2	3:F:389:GLU:OE2	2.25	0.59
2:H:440:SER:HG	2:H:443:MET:H	1.47	0.59
3:J:399:ARG:HB2	3:J:400:TRP:CE3	2.37	0.59
2:B:155:ARG:NH1	2:B:160:ASP:H	2.00	0.59
3:J:276:VAL:HG13	3:J:280:ARG:HD2	1.84	0.59
3:J:387:ALA:HA	3:J:390:ALA:HB3	1.83	0.59
4:D:82:VAL:O	4:D:120:SER:OG	2.20	0.59
2:H:169:GLY:HA2	2:H:172:LEU:HD12	1.85	0.59
2:H:395:VAL:HG22	2:H:417:LEU:HD21	1.85	0.59
3:J:218:ILE:HG21	3:J:346:LEU:HG	1.85	0.59
2:C:167:VAL:HG12	2:C:203:ALA:HB2	1.83	0.59
4:G:208:VAL:O	4:G:212:ILE:HD12	2.03	0.59
4:D:208:VAL:O	4:D:212:ILE:HD12	2.03	0.59
1:A:32:PHE:CE1	1:I:63:PRO:HG3	2.38	0.58
3:F:11:ARG:HH12	3:F:13:THR:HA	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:41:ALA:HA	2:E:44:ARG:HE	1.68	0.58
1:A:58:ARG:HB3	3:F:106:ARG:HH11	1.69	0.58
3:J:260:TRP:CE2	3:J:390:ALA:HB1	2.38	0.58
4:G:82:VAL:O	4:G:120:SER:OG	2.20	0.58
2:E:350:VAL:HG21	2:E:363:VAL:HG21	1.84	0.58
4:D:91:PRO:HA	4:D:94:VAL:HG12	1.86	0.58
2:E:11:ARG:HG2	2:E:28:ALA:HB2	1.86	0.58
3:J:3:ARG:HH21	3:J:398:SER:HA	1.69	0.58
2:C:211:ASP:O	2:C:216:ASN:ND2	2.36	0.58
2:C:287:ALA:O	2:C:290:SER:OG	2.18	0.58
2:C:335:ILE:HD11	2:C:377:TRP:CE2	2.39	0.58
2:C:196:ALA:HB3	2:C:227:TRP:HE1	1.69	0.58
1:A:18:PRO:CG	3:J:110:VAL:HG12	2.34	0.58
2:H:322:ARG:HA	2:H:325:ARG:HH11	1.69	0.57
3:J:215:ILE:HB	3:J:340:ILE:HG13	1.85	0.57
2:E:238:ASP:OD1	2:E:239:ARG:N	2.32	0.57
4:G:79:VAL:HG23	4:G:169:VAL:HG23	1.87	0.57
4:D:22:GLN:O	4:D:23:THR:OG1	2.20	0.57
2:B:29:LEU:HD13	2:B:38:ILE:HG21	1.84	0.57
3:J:247:ALA:HB3	3:J:316:VAL:HA	1.87	0.57
4:D:79:VAL:HG23	4:D:169:VAL:HG23	1.86	0.57
3:F:14:PRO:HG3	3:F:128:TRP:CD1	2.40	0.57
4:G:91:PRO:HA	4:G:94:VAL:HG12	1.86	0.57
3:J:145:GLN:HG3	3:J:146:TRP:H	1.69	0.57
4:G:259:ALA:O	4:G:264:ARG:NH2	2.38	0.57
3:F:208:ASP:OD2	3:F:211:LYS:NZ	2.37	0.57
2:H:151:SER:OG	2:H:163:GLY:O	2.23	0.57
2:E:10:VAL:O	2:E:29:LEU:N	2.34	0.56
2:H:40:PRO:HA	2:H:43:GLN:HB2	1.87	0.56
2:C:241:ILE:HG13	2:C:243:VAL:HG12	1.86	0.56
2:E:11:ARG:HA	2:E:28:ALA:HA	1.86	0.56
3:J:244:LEU:HD11	3:J:315:LEU:HD23	1.87	0.56
3:F:218:ILE:HD13	3:F:359:ILE:HG23	1.87	0.56
3:F:257:ASP:O	3:F:259:SER:N	2.38	0.56
4:G:105:ASP:OD2	4:G:127:ASP:N	2.39	0.56
2:E:401:PHE:HB3	2:E:406:ARG:HB3	1.86	0.56
2:H:331:GLN:NE2	2:H:382:CYS:SG	2.78	0.56
3:J:283:THR:OG1	3:J:284:THR:N	2.39	0.56
3:J:361:ARG:HH21	3:J:375:TRP:HZ3	1.53	0.56
4:D:259:ALA:O	4:D:264:ARG:NH2	2.38	0.56
1:A:50:SER:O	1:A:50:SER:OG	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:229:ARG:HG2	3:F:260:TRP:CZ2	2.40	0.56
4:G:97:LEU:HD11	4:G:227:THR:HA	1.88	0.56
1:A:13:PHE:CZ	3:J:107:TYR:CD2	2.94	0.56
2:H:232:MET:HE2	2:H:293:TRP:HZ3	1.70	0.56
2:C:442:PRO:HA	2:C:445:ARG:HD3	1.88	0.56
2:E:347:VAL:O	2:E:351:SER:HB3	2.05	0.56
2:E:37:GLU:OE2	3:J:395:ARG:NH1	2.39	0.56
2:E:350:VAL:CG1	2:E:360:TRP:CZ3	2.84	0.56
2:H:327:SER:OG	2:H:328:GLN:N	2.38	0.56
3:J:26:PRO:CG	3:J:175:ASP:HB2	2.35	0.56
4:D:105:ASP:OD2	4:D:127:ASP:N	2.39	0.56
3:F:263:TRP:HB3	3:F:398:SER:HB3	1.86	0.56
4:G:50:THR:HA	4:G:53:ILE:HD12	1.88	0.56
2:E:335:ILE:CG2	2:E:386:LEU:CD2	2.81	0.56
4:D:50:THR:HA	4:D:53:ILE:HD12	1.88	0.56
4:D:83:ASP:N	4:D:83:ASP:OD1	2.37	0.56
3:F:224:ALA:O	3:F:228:ILE:HG13	2.06	0.56
2:H:39:LEU:HG	2:H:40:PRO:HD3	1.88	0.56
2:B:35:LEU:O	2:B:39:LEU:HD23	2.06	0.56
3:J:27:PRO:CB	3:J:28:PRO:HD2	2.36	0.55
2:H:151:SER:O	2:H:154:HIS:HB3	2.06	0.55
3:J:220:GLU:O	3:J:342:ARG:NH2	2.39	0.55
2:C:321:PRO:HB2	2:C:325:ARG:HH12	1.71	0.55
3:F:370:TRP:HE3	3:F:375:TRP:NE1	2.03	0.55
1:A:33:VAL:HG23	1:A:33:VAL:O	2.06	0.55
2:E:82:THR:O	2:E:86:VAL:HG12	2.06	0.55
2:H:440:SER:OG	2:H:443:MET:N	2.21	0.55
2:B:23:ARG:HH11	2:C:109:VAL:HG11	1.72	0.55
4:G:146:ASP:O	4:G:150:VAL:HG23	2.07	0.55
3:J:130:HIS:O	3:J:159:ARG:NE	2.39	0.55
3:J:131:PRO:HB2	3:J:135:VAL:HB	1.88	0.55
3:J:258:TRP:HE1	3:J:319:ASP:HB2	1.71	0.55
2:B:227:TRP:HA	2:B:230:ILE:HD12	1.87	0.55
3:J:158:LEU:HD23	3:J:231:TRP:CD1	2.42	0.55
2:B:155:ARG:HH11	2:B:160:ASP:H	1.55	0.55
4:G:83:ASP:OD1	4:G:83:ASP:N	2.37	0.55
2:E:356:SER:HB3	2:E:359:ALA:HB2	1.88	0.55
3:F:146:TRP:CH2	3:F:266:HIS:HE1	2.25	0.55
3:J:245:GLY:O	3:J:314:LEU:HA	2.07	0.55
2:B:330:HIS:O	2:B:334:VAL:HG23	2.07	0.54
2:H:471:LEU:HD23	2:H:472:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:129:SER:O	3:J:130:HIS:ND1	2.39	0.54
3:J:158:LEU:HD23	3:J:231:TRP:HD1	1.72	0.54
2:B:19:ASP:OD1	2:B:19:ASP:N	2.36	0.54
2:C:153:ALA:HA	2:C:156:VAL:HG12	1.89	0.54
4:G:113:ASP:HB3	4:G:220:THR:HB	1.89	0.54
4:D:113:ASP:HB3	4:D:220:THR:HB	1.89	0.54
4:D:146:ASP:O	4:D:150:VAL:HG23	2.07	0.54
2:B:352:SER:OG	2:B:353:ALA:N	2.39	0.54
3:F:3:ARG:HD2	3:F:401:ASP:HB2	1.90	0.54
4:D:97:LEU:HD11	4:D:227:THR:HA	1.88	0.54
4:D:106:LYS:HE3	4:D:125:THR:HG21	1.90	0.54
2:B:125:ARG:NH1	2:B:126:GLN:OE1	2.39	0.54
2:B:350:VAL:HG22	2:B:359:ALA:HB1	1.89	0.54
3:F:247:ALA:HB2	3:F:293:LEU:HD21	1.88	0.54
2:E:227:TRP:HA	2:E:230:ILE:HD12	1.90	0.54
3:J:174:LYS:HD2	3:J:174:LYS:O	2.08	0.54
2:C:261:ALA:HA	2:C:266:ILE:HG13	1.90	0.54
4:G:108:ARG:HA	4:G:225:GLU:HA	1.89	0.54
2:E:35:LEU:HD11	2:E:69:LEU:HD12	1.87	0.54
2:E:270:VAL:HA	2:E:273:CYS:SG	2.48	0.54
3:J:247:ALA:HB1	3:J:289:LEU:HD11	1.89	0.54
4:D:172:VAL:HG13	4:D:173:ASP:H	1.73	0.54
2:C:164:GLN:NE2	2:C:206:LEU:O	2.41	0.54
3:F:139:ILE:HD11	3:F:144:ARG:HB2	1.88	0.54
3:F:370:TRP:HE3	3:F:375:TRP:HE1	1.54	0.54
2:E:349:LEU:HD23	2:E:362:ILE:HG21	1.89	0.54
2:E:414:LEU:HD23	2:E:414:LEU:C	2.32	0.54
3:J:221:ALA:HA	3:J:342:ARG:HH22	1.73	0.54
1:A:29:ARG:O	1:A:29:ARG:HD3	2.07	0.53
2:B:35:LEU:HD12	2:B:35:LEU:H	1.74	0.53
2:B:459:ILE:HD12	2:B:459:ILE:H	1.72	0.53
3:F:229:ARG:HG2	3:F:260:TRP:HZ2	1.73	0.53
4:G:106:LYS:HE3	4:G:125:THR:HG21	1.90	0.53
4:G:172:VAL:HG13	4:G:173:ASP:H	1.73	0.53
2:E:271:ILE:HD12	2:E:271:ILE:H	1.73	0.53
3:J:104:TYR:O	3:J:107:TYR:N	2.33	0.53
2:B:33:LEU:N	2:B:82:THR:OG1	2.42	0.53
2:B:154:HIS:HE1	2:B:160:ASP:HB3	1.70	0.53
3:F:133:PRO:HA	3:F:136:LEU:HD22	1.90	0.53
2:E:442:PRO:O	2:E:446:MET:N	2.26	0.53
3:F:240:ASP:HB3	3:F:242:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:156:LEU:HB2	3:J:210:ALA:HB2	1.90	0.53
4:D:108:ARG:HA	4:D:225:GLU:HA	1.89	0.53
4:D:224:LEU:HD12	4:D:225:GLU:H	1.74	0.53
3:F:159:ARG:NE	3:F:383:ASP:OD2	2.35	0.53
3:F:227:ALA:HB1	3:F:231:TRP:CZ3	2.42	0.53
4:G:224:LEU:HD12	4:G:225:GLU:H	1.74	0.53
3:J:149:ASP:HB2	3:J:150:PRO:HD2	1.91	0.53
2:B:266:ILE:H	2:B:266:ILE:HD12	1.73	0.53
2:E:458:LEU:O	2:E:462:MET:N	2.36	0.53
3:F:214:ARG:HB3	3:F:357:ARG:HG2	1.90	0.53
2:B:171:ALA:HB2	2:B:199:PRO:HB2	1.91	0.53
3:F:108:LEU:HD11	3:F:193:LEU:HD13	1.91	0.53
2:H:155:ARG:HH11	2:H:159:GLY:HA3	1.74	0.53
3:J:348:ASN:OD1	3:J:349:ARG:N	2.40	0.53
3:F:368:GLU:HG2	3:F:377:PRO:HA	1.91	0.53
3:J:3:ARG:HB3	3:J:401:ASP:HB2	1.91	0.53
3:J:264:LEU:HD22	3:J:397:LEU:HD23	1.90	0.53
2:B:317:LEU:H	2:B:317:LEU:HD23	1.74	0.52
2:H:11:ARG:HA	2:H:28:ALA:HA	1.89	0.52
2:H:70:ALA:HB2	2:H:76:PRO:HA	1.91	0.52
2:C:362:ILE:HD11	2:C:461:VAL:HG23	1.90	0.52
2:E:359:ALA:N	2:E:465:LEU:HD11	2.25	0.52
2:E:374:ALA:HB2	2:E:386:LEU:HD12	1.92	0.52
2:H:273:CYS:HB3	2:H:462:MET:SD	2.49	0.52
1:I:57:THR:O	1:I:57:THR:OG1	2.28	0.52
2:B:163:GLY:O	2:B:167:VAL:HG23	2.09	0.52
2:C:415:ALA:O	2:C:419:VAL:HG23	2.09	0.52
2:B:181:VAL:HA	2:B:184:ARG:HD2	1.91	0.52
1:A:11:ARG:HD2	3:J:29:GLN:HG3	1.92	0.52
2:C:70:ALA:HB2	2:C:76:PRO:HA	1.91	0.52
3:F:361:ARG:HH12	3:F:363:ALA:HB2	1.74	0.52
3:F:136:LEU:O	3:F:139:ILE:HG22	2.10	0.52
2:E:82:THR:HG23	2:E:85:THR:H	1.75	0.52
2:H:153:ALA:O	2:H:156:VAL:HG12	2.10	0.52
1:A:13:PHE:CD1	1:A:13:PHE:C	2.87	0.52
2:C:237:ASP:N	2:C:237:ASP:OD1	2.41	0.52
2:H:239:ARG:C	2:H:241:ILE:H	2.18	0.52
4:G:61:ARG:HA	4:G:64:ARG:NH1	2.25	0.51
2:B:211:ASP:C	2:B:213:GLY:H	2.19	0.51
2:C:13:ALA:HB2	3:F:395:ARG:HD3	1.91	0.51
3:F:244:LEU:N	3:F:312:LYS:HZ3	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:77:THR:OG1	4:G:275:THR:HG22	2.10	0.51
2:E:391:TYR:CE1	2:E:417:LEU:CD2	2.94	0.51
4:D:77:THR:OG1	4:D:275:THR:HG22	2.10	0.51
2:E:30:PRO:HG3	2:H:72:ILE:HD12	1.91	0.51
3:J:123:ARG:NH1	3:J:202:ASP:O	2.44	0.51
1:A:63:PRO:O	1:A:67:GLN:HG2	2.11	0.51
2:B:190:THR:O	2:B:194:VAL:HG23	2.11	0.51
3:F:177:ALA:HB1	3:F:180:ILE:HG13	1.91	0.51
3:F:234:GLN:O	3:F:238:TRP:HD1	1.94	0.51
2:E:348:ALA:O	2:E:351:SER:OG	2.29	0.51
1:A:10:ARG:HE	3:J:31:PRO:HB3	1.75	0.51
3:J:260:TRP:CZ3	3:J:394:ALA:HB2	2.46	0.51
1:I:39:SER:O	3:J:101:ARG:NH1	2.38	0.51
3:J:199:THR:OG1	3:J:201:ARG:NH2	2.44	0.51
4:G:22:GLN:O	4:G:23:THR:OG1	2.19	0.50
2:E:361:TYR:CD1	2:E:361:TYR:C	2.89	0.50
2:H:198:VAL:HG13	2:H:199:PRO:HD3	1.92	0.50
4:D:61:ARG:HA	4:D:64:ARG:NH1	2.25	0.50
3:F:11:ARG:HH22	3:F:14:PRO:HD2	1.76	0.50
3:F:251:PRO:HD3	3:F:320:ASP:OD1	2.12	0.50
3:J:248:LEU:C	3:J:289:LEU:HD22	2.37	0.50
3:J:361:ARG:NH2	3:J:375:TRP:HZ3	2.08	0.50
2:B:46:VAL:HG23	2:B:47:GLN:HG2	1.93	0.50
2:E:82:THR:CG2	2:E:85:THR:H	2.24	0.50
2:C:41:ALA:HA	2:C:44:ARG:NH2	2.27	0.50
2:E:350:VAL:CG1	2:E:360:TRP:CZ2	2.93	0.50
2:E:43:GLN:HE21	2:E:67:LEU:HD12	1.76	0.50
3:J:173:VAL:HG12	3:J:173:VAL:O	2.11	0.50
3:J:359:ILE:HB	3:J:370:TRP:HB3	1.93	0.50
2:B:152:VAL:O	2:B:156:VAL:HG13	2.10	0.50
3:J:241:PRO:HA	3:J:266:HIS:CE1	2.47	0.50
4:D:34:ILE:O	4:D:38:ILE:HG12	2.12	0.50
3:F:139:ILE:N	3:F:140:PRO:HD2	2.27	0.50
2:E:237:ASP:N	2:E:237:ASP:OD1	2.44	0.50
3:J:264:LEU:HB2	3:J:267:VAL:CG2	2.35	0.50
2:B:13:ALA:HB1	2:B:24:LEU:HD11	1.94	0.50
2:B:455:ASP:N	2:B:455:ASP:OD1	2.45	0.50
3:F:30:LEU:HD22	3:F:30:LEU:O	2.12	0.50
3:F:248:LEU:HD23	3:F:249:ALA:N	2.27	0.50
2:B:34:PRO:O	2:B:37:GLU:HG2	2.12	0.49
3:F:317:VAL:HG12	3:F:340:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:TRP:O	2:B:131:HIS:HD2	1.95	0.49
2:E:452:THR:HA	2:E:455:ASP:OD2	2.12	0.49
2:H:273:CYS:HB3	2:H:462:MET:HE3	1.94	0.49
2:C:471:LEU:HD23	2:C:472:VAL:HG23	1.95	0.49
3:F:377:PRO:C	3:F:379:VAL:H	2.19	0.49
3:J:21:THR:O	3:J:21:THR:OG1	2.26	0.49
3:J:146:TRP:CE3	3:J:241:PRO:HD2	2.46	0.49
3:J:370:TRP:HA	3:J:375:TRP:HE1	1.76	0.49
2:C:242:ALA:HB1	2:C:333:GLY:HA2	1.93	0.49
3:J:193:LEU:HD12	3:J:197:GLN:HG3	1.94	0.49
2:B:400:ALA:HA	2:B:403:ILE:HG22	1.94	0.49
4:G:97:LEU:HB3	4:G:230:PRO:HD3	1.94	0.49
2:E:107:ARG:HD3	3:J:116:ARG:CZ	2.42	0.49
3:J:148:ARG:HD2	3:J:238:TRP:HB3	1.93	0.49
4:D:206:ASP:OD1	4:D:206:ASP:N	2.46	0.49
2:H:383:LYS:O	2:H:386:LEU:N	2.40	0.49
3:J:288:GLU:HG3	3:J:292:ARG:HH21	1.77	0.49
4:D:19:GLN:CD	4:D:19:GLN:H	2.20	0.49
1:A:32:PHE:CZ	1:I:63:PRO:HG2	2.48	0.49
4:G:34:ILE:O	4:G:38:ILE:HG12	2.12	0.49
2:E:327:SER:O	2:E:331:GLN:HG3	2.13	0.49
1:I:39:SER:C	3:J:101:ARG:HH12	2.18	0.49
3:J:230:ALA:HA	3:J:385:MET:CB	2.42	0.49
2:B:433:ILE:HD12	2:B:433:ILE:H	1.77	0.49
3:F:369:ARG:NH2	3:F:378:CYS:SG	2.86	0.49
4:G:19:GLN:H	4:G:19:GLN:CD	2.20	0.49
2:E:265:VAL:HG22	2:E:267:SER:N	2.28	0.49
3:F:277:GLY:HA3	3:F:280:ARG:HG3	1.95	0.49
2:E:34:PRO:HB2	2:E:36:ARG:HG2	1.94	0.49
3:F:25:GLU:CD	3:F:26:PRO:HD2	2.38	0.48
3:F:132:GLU:OE2	3:F:134:GLU:HG2	2.13	0.48
3:J:220:GLU:C	3:J:342:ARG:HH22	2.20	0.48
3:F:247:ALA:HB1	3:F:289:LEU:HD21	1.93	0.48
2:B:25:THR:OG1	2:C:109:VAL:HG12	2.13	0.48
2:E:32:GLU:CD	2:H:22:GLY:H	2.22	0.48
1:I:58:ARG:HA	3:J:106:ARG:HG3	1.94	0.48
3:J:27:PRO:CB	3:J:28:PRO:CD	2.92	0.48
3:J:249:ALA:HB2	3:J:289:LEU:HB3	1.95	0.48
3:F:257:ASP:O	3:F:259:SER:OG	2.29	0.48
2:H:162:LEU:O	2:H:166:ILE:HG12	2.13	0.48
3:J:267:VAL:O	3:J:279:ALA:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:195:ASP:OD1	3:F:195:ASP:N	2.47	0.48
3:F:248:LEU:HD12	3:F:261:LEU:HD12	1.96	0.48
4:D:208:VAL:O	4:D:211:GLU:N	2.46	0.48
2:B:398:LEU:O	2:B:402:VAL:HG23	2.13	0.48
3:F:21:THR:HA	3:F:170:ALA:HB3	1.94	0.48
3:F:255:SER:O	3:F:255:SER:OG	2.25	0.48
4:D:97:LEU:HB3	4:D:230:PRO:HD3	1.94	0.48
2:B:428:ALA:HB2	2:C:132:ILE:HG22	1.95	0.48
2:B:435:SER:HB2	2:B:438:THR:HG22	1.96	0.48
2:E:464:LEU:HD23	2:E:469:PHE:HE1	1.77	0.48
1:I:76:LEU:HA	1:I:79:VAL:HG22	1.96	0.48
3:J:112:ARG:CG	3:J:112:ARG:NH1	2.73	0.48
2:B:280:LEU:O	2:B:284:VAL:HG22	2.13	0.48
2:E:25:THR:HG22	2:H:109:VAL:HB	1.95	0.48
3:J:314:LEU:HD13	3:J:337:VAL:HG22	1.95	0.48
4:G:79:VAL:HA	4:G:122:ILE:O	2.13	0.48
2:H:138:LEU:HA	2:H:141:ILE:HD12	1.96	0.48
2:C:320:LEU:N	2:C:321:PRO:HD2	2.28	0.47
4:G:284:PRO:O	4:G:285:LEU:HD23	2.14	0.47
3:J:276:VAL:HG13	3:J:277:GLY:H	1.79	0.47
2:H:126:GLN:HG3	2:H:127:TRP:H	1.79	0.47
2:B:213:GLY:HA3	2:B:216:ASN:ND2	2.29	0.47
2:C:423:VAL:HA	2:C:426:VAL:HG12	1.95	0.47
2:E:393:LEU:HD12	2:E:393:LEU:C	2.39	0.47
3:F:16:THR:OG1	3:F:17:THR:N	2.48	0.47
2:E:459:ILE:N	2:E:460:PRO:HD2	2.29	0.47
2:H:76:PRO:HG2	2:H:100:PRO:HD3	1.97	0.47
3:J:250:ALA:O	3:J:284:THR:HA	2.14	0.47
3:J:260:TRP:CZ2	3:J:390:ALA:HB1	2.49	0.47
2:E:9:ILE:HG13	2:E:29:LEU:C	2.39	0.47
3:J:145:GLN:HG3	3:J:146:TRP:N	2.29	0.47
2:B:33:LEU:HB3	2:B:37:GLU:OE2	2.14	0.47
3:F:316:VAL:HG23	3:F:339:VAL:HG23	1.95	0.47
3:F:366:ARG:HB3	3:F:368:GLU:HG3	1.96	0.47
2:H:426:VAL:O	2:H:430:ASN:HB3	2.15	0.47
3:J:225:ARG:HB3	3:J:258:TRP:CZ2	2.49	0.47
2:B:359:ALA:HA	2:B:362:ILE:HG22	1.97	0.47
2:C:117:VAL:O	2:C:120:SER:OG	2.27	0.47
2:H:70:ALA:O	2:H:94:LEU:HA	2.15	0.47
2:H:320:LEU:N	2:H:321:PRO:HD2	2.30	0.47
3:J:146:TRP:HB3	3:J:240:ASP:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:240:ASP:HB2	3:J:242:THR:HG22	1.97	0.47
3:J:262:LYS:HZ2	3:J:280:ARG:NE	2.13	0.47
4:D:17:LEU:HA	4:D:19:GLN:HE22	1.79	0.47
4:D:79:VAL:HA	4:D:122:ILE:O	2.13	0.47
1:A:60:LEU:HD23	1:A:60:LEU:HA	1.75	0.47
2:C:125:ARG:H	2:C:125:ARG:HD3	1.80	0.47
4:G:197:TYR:CD1	4:G:256:LEU:HB3	2.50	0.47
4:G:208:VAL:O	4:G:211:GLU:N	2.46	0.47
2:B:280:LEU:HD11	2:B:373:ARG:HH22	1.80	0.47
2:H:369:GLY:O	2:H:373:ARG:NE	2.48	0.47
3:J:353:PRO:HG3	3:J:370:TRP:CD1	2.49	0.47
4:D:216:PRO:HB2	4:D:217:ALA:H	1.57	0.47
4:D:284:PRO:O	4:D:285:LEU:HD23	2.14	0.47
2:B:16:ALA:HB2	2:B:96:LEU:HD22	1.96	0.47
2:C:127:TRP:O	2:C:131:HIS:HD2	1.98	0.47
2:E:147:GLY:HA2	2:H:414:LEU:HD11	1.97	0.47
2:E:317:LEU:HD23	2:E:317:LEU:H	1.80	0.47
4:D:197:TYR:CD1	4:D:256:LEU:HB3	2.50	0.47
2:C:11:ARG:NH2	3:F:277:GLY:HA2	2.30	0.46
3:F:18:ARG:O	3:F:20:GLY:N	2.48	0.46
3:F:212:LEU:HD13	3:F:356:GLU:HA	1.96	0.46
3:J:136:LEU:HD11	3:J:385:MET:HE1	1.96	0.46
2:B:141:ILE:HD12	2:B:195:THR:HG21	1.95	0.46
2:B:415:ALA:O	2:B:419:VAL:HG23	2.15	0.46
2:C:36:ARG:HH21	2:C:79:LEU:HB3	1.80	0.46
2:C:38:ILE:HA	2:C:41:ALA:HB3	1.96	0.46
2:C:455:ASP:OD1	2:C:455:ASP:N	2.47	0.46
4:G:22:GLN:OE1	4:G:23:THR:HG23	2.14	0.46
4:G:206:ASP:OD1	4:G:206:ASP:N	2.46	0.46
2:E:155:ARG:NH1	2:E:159:GLY:HA2	2.30	0.46
2:E:181:VAL:HG13	2:E:184:ARG:HB2	1.95	0.46
1:I:86:PHE:O	1:I:90:LEU:HG	2.15	0.46
4:G:108:ARG:O	4:G:123:SER:N	2.48	0.46
1:I:36:HIS:CG	3:J:30:LEU:HD11	2.51	0.46
1:A:56:ASP:OD2	1:A:58:ARG:NH2	2.49	0.46
2:B:37:GLU:O	2:B:40:PRO:HD2	2.16	0.46
2:B:289:LEU:HD11	2:B:292:MET:HE3	1.98	0.46
3:F:28:PRO:O	3:F:182:LEU:HD12	2.15	0.46
2:H:126:GLN:CG	2:H:127:TRP:H	2.29	0.46
3:J:216:THR:OG1	3:J:358:PRO:O	2.33	0.46
4:D:96:TYR:HD1	4:D:99:ARG:HD3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:145:GLN:O	3:F:238:TRP:HA	2.16	0.46
3:F:321:PRO:CB	3:F:344:THR:HG23	2.45	0.46
3:F:378:CYS:O	3:F:379:VAL:HG23	2.16	0.46
2:E:389:HIS:ND1	2:E:389:HIS:C	2.73	0.46
3:J:399:ARG:HB2	3:J:400:TRP:CZ3	2.50	0.46
4:D:22:GLN:OE1	4:D:23:THR:HG23	2.14	0.46
2:B:82:THR:O	2:B:86:VAL:HG12	2.15	0.46
2:C:40:PRO:HB2	2:C:44:ARG:NH1	2.31	0.46
1:A:68:SER:O	1:A:71:VAL:HG12	2.16	0.46
2:C:409:ALA:HA	2:C:412:TRP:CD1	2.48	0.46
3:F:157:VAL:HA	3:F:208:ASP:HA	1.97	0.46
3:F:287:ALA:O	3:F:291:GLU:HG2	2.15	0.46
4:G:17:LEU:HA	4:G:19:GLN:HE22	1.79	0.46
2:E:339:VAL:HG21	2:E:386:LEU:HA	1.98	0.46
3:J:16:THR:OG1	3:J:17:THR:N	2.49	0.46
3:J:125:ALA:O	3:J:128:TRP:N	2.47	0.46
4:D:112:ARG:HG3	4:D:221:TRP:CE2	2.51	0.46
1:A:60:LEU:HG	3:F:106:ARG:HH12	1.80	0.46
2:B:143:LEU:HD22	2:C:421:VAL:HG21	1.96	0.46
3:F:123:ARG:NH1	3:F:202:ASP:O	2.44	0.46
2:H:100:PRO:HB3	4:D:161:GLU:OE1	2.15	0.46
2:C:78:SER:HB3	2:C:81:ALA:HB2	1.97	0.46
4:G:52:ARG:HA	4:G:55:ARG:HB2	1.98	0.46
4:G:96:TYR:HD1	4:G:99:ARG:HD3	1.80	0.46
4:G:97:LEU:HD22	4:G:230:PRO:HD3	1.98	0.46
2:E:68:SER:OG	2:E:69:LEU:N	2.46	0.46
3:J:148:ARG:HB2	3:J:238:TRP:O	2.16	0.46
3:J:281:TYR:CE1	3:J:292:ARG:HB3	2.51	0.46
3:J:314:LEU:O	3:J:337:VAL:HA	2.15	0.46
2:B:280:LEU:HD11	2:B:373:ARG:NH2	2.31	0.46
3:F:141:GLY:HA2	3:F:400:TRP:CH2	2.51	0.46
2:E:391:TYR:CE1	2:E:417:LEU:HD21	2.50	0.46
2:H:137:ALA:O	2:H:140:LEU:N	2.49	0.46
3:J:146:TRP:HZ2	3:J:397:LEU:HD11	1.81	0.46
4:G:112:ARG:HG3	4:G:221:TRP:CE2	2.51	0.45
2:E:8:PRO:HD2	2:H:97:GLN:HE22	1.81	0.45
3:J:107:TYR:CD1	3:J:107:TYR:C	2.94	0.45
4:D:77:THR:HG23	4:D:125:THR:HG22	1.98	0.45
1:A:74:GLY:HA3	2:C:459:ILE:HD12	1.98	0.45
4:G:77:THR:HG23	4:G:125:THR:HG22	1.98	0.45
1:A:36:HIS:CE1	3:F:30:LEU:HD21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:112:ILE:HD12	2:E:112:ILE:H	1.82	0.45
2:E:121:GLU:O	2:E:123:ARG:N	2.47	0.45
2:E:206:LEU:HD23	2:E:206:LEU:HA	1.77	0.45
3:J:104:TYR:O	3:J:107:TYR:HB3	2.16	0.45
4:G:8:ALA:HB2	4:G:40:LEU:HD22	1.98	0.45
2:E:405:ASP:N	2:E:405:ASP:OD1	2.49	0.45
1:I:85:CYS:HA	1:I:88:PHE:HB3	1.98	0.45
3:J:174:LYS:HB3	3:J:174:LYS:HE2	1.46	0.45
3:J:346:LEU:HD21	3:J:361:ARG:HG3	1.98	0.45
2:B:319:ASP:O	2:B:323:ARG:HG3	2.17	0.45
2:H:238:ASP:CG	2:H:239:ARG:H	2.25	0.45
2:H:269:ASP:HA	2:H:349:LEU:HD22	1.98	0.45
3:J:263:TRP:HB2	3:J:394:ALA:HB1	1.97	0.45
2:C:449:PHE:O	2:C:452:THR:OG1	2.32	0.45
2:E:82:THR:HG23	2:E:84:ASP:N	2.24	0.45
3:J:378:CYS:O	3:J:379:VAL:HG23	2.17	0.45
2:C:275:LEU:HD23	2:C:275:LEU:HA	1.77	0.45
3:F:24:ILE:O	3:F:173:VAL:HG23	2.17	0.45
4:G:175:PRO:HB3	4:G:221:TRP:CD2	2.52	0.45
2:E:36:ARG:HH22	2:E:80:ASP:HA	1.81	0.45
2:E:374:ALA:O	2:E:376:VAL:N	2.49	0.45
2:H:254:VAL:HA	2:H:257:VAL:HG12	1.98	0.45
2:H:417:LEU:O	2:H:421:VAL:HG12	2.17	0.45
4:D:175:PRO:HB3	4:D:221:TRP:CD2	2.52	0.45
4:G:197:TYR:CG	4:G:256:LEU:HD23	2.52	0.45
2:E:429:LEU:HD23	2:E:429:LEU:HA	1.77	0.45
2:H:204:PHE:HB3	2:H:219:LEU:HG	1.99	0.45
4:D:197:TYR:CG	4:D:256:LEU:HD23	2.52	0.45
1:A:13:PHE:HZ	3:J:107:TYR:CD2	2.35	0.45
1:A:34:THR:HG23	1:A:37:GLN:HG3	1.99	0.45
2:B:280:LEU:HD12	2:B:280:LEU:HA	1.74	0.45
3:F:232:ILE:HD11	3:F:246:VAL:HG21	1.98	0.45
3:F:246:VAL:O	3:F:267:VAL:HG23	2.17	0.45
2:E:398:LEU:C	2:E:398:LEU:CD2	2.90	0.45
4:D:52:ARG:HA	4:D:55:ARG:HB2	1.98	0.45
2:E:361:TYR:CD1	2:E:361:TYR:O	2.70	0.45
2:E:361:TYR:O	2:E:361:TYR:CG	2.70	0.45
3:J:183:GLU:CD	3:J:184:PRO:HD2	2.42	0.45
3:J:264:LEU:CD2	3:J:397:LEU:HB3	2.47	0.45
2:C:343:VAL:O	2:C:347:VAL:HG12	2.17	0.44
3:F:267:VAL:O	3:F:279:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:71:PRO:HD3	2:E:77:PHE:CZ	2.52	0.44
2:E:372:LEU:HD12	2:E:372:LEU:HA	1.77	0.44
2:H:29:LEU:HD11	2:H:38:ILE:HD12	1.98	0.44
3:J:276:VAL:HG13	3:J:277:GLY:N	2.33	0.44
3:J:285:SER:HB2	3:J:288:GLU:HB2	1.99	0.44
3:F:229:ARG:HA	3:F:232:ILE:HG22	1.99	0.44
3:F:264:LEU:HD23	3:F:267:VAL:HB	1.99	0.44
4:G:229:SER:O	4:G:231:ALA:N	2.50	0.44
2:E:238:ASP:CG	2:E:239:ARG:H	2.22	0.44
2:E:374:ALA:C	2:E:376:VAL:H	2.25	0.44
2:B:370:ALA:HA	2:B:373:ARG:NH1	2.32	0.44
3:F:37:SER:HB3	3:F:40:ARG:HE	1.81	0.44
3:F:261:LEU:HD23	3:F:261:LEU:HA	1.73	0.44
2:E:411:LEU:H	2:E:411:LEU:HG	1.57	0.44
2:H:14:VAL:HA	2:H:94:LEU:O	2.17	0.44
3:J:3:ARG:NH2	3:J:265:PRO:HD3	2.32	0.44
3:J:139:ILE:N	3:J:140:PRO:HD2	2.32	0.44
4:D:172:VAL:HG13	4:D:173:ASP:N	2.32	0.44
3:F:286:THR:OG1	3:F:287:ALA:N	2.50	0.44
2:E:33:LEU:HD22	2:E:34:PRO:HD2	1.99	0.44
2:E:124:ARG:NH2	2:E:126:GLN:HB2	2.32	0.44
4:D:50:THR:O	4:D:53:ILE:HB	2.18	0.44
4:D:229:SER:O	4:D:231:ALA:N	2.50	0.44
2:E:36:ARG:HH12	2:E:80:ASP:HB2	1.82	0.44
3:J:223:GLU:OE1	3:J:362:VAL:HG12	2.17	0.44
4:D:8:ALA:HB2	4:D:40:LEU:HD22	1.98	0.44
4:D:97:LEU:HD22	4:D:230:PRO:HD3	1.98	0.44
2:B:442:PRO:HA	2:B:445:ARG:HD3	1.99	0.44
2:B:458:LEU:HA	2:B:461:VAL:HG12	1.98	0.44
2:C:267:SER:C	2:C:269:ASP:H	2.25	0.44
3:F:327:ASP:OD1	3:F:327:ASP:N	2.47	0.44
4:G:134:ALA:HB1	4:G:138:ARG:HH12	1.83	0.44
4:G:175:PRO:HB3	4:G:221:TRP:CG	2.53	0.44
2:E:391:TYR:CD1	2:E:417:LEU:HD21	2.52	0.44
2:H:12:VAL:HG21	2:H:94:LEU:HD12	1.98	0.44
2:H:29:LEU:HD11	2:H:38:ILE:HG23	2.00	0.44
2:H:252:VAL:O	2:H:255:LEU:HB3	2.17	0.44
2:C:14:VAL:HA	2:C:94:LEU:O	2.17	0.44
3:F:233:ALA:HA	3:F:236:VAL:HG22	1.99	0.44
2:E:116:ALA:O	2:E:120:SER:OG	2.31	0.44
2:E:278:LEU:O	2:E:282:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:106:PRO:C	2:H:107:ARG:HG2	2.43	0.44
2:H:259:GLY:O	2:H:263:LEU:HG	2.18	0.44
3:J:107:TYR:CD1	3:J:107:TYR:O	2.70	0.44
2:C:315:SER:OG	2:C:316:VAL:N	2.51	0.44
4:G:172:VAL:HG22	4:G:173:ASP:CG	2.43	0.44
4:G:260:ARG:HD2	4:G:260:ARG:HA	1.79	0.44
1:I:79:VAL:O	1:I:82:LEU:HB3	2.18	0.44
4:D:108:ARG:O	4:D:123:SER:N	2.48	0.44
1:A:13:PHE:CZ	3:J:107:TYR:HD2	2.36	0.44
2:B:422:LEU:O	2:B:426:VAL:HG22	2.17	0.44
2:C:341:LEU:HD23	2:C:341:LEU:HA	1.76	0.44
3:F:12:LEU:HD12	3:F:12:LEU:H	1.82	0.44
3:F:202:ASP:OD1	3:F:202:ASP:N	2.51	0.44
4:G:172:VAL:HG13	4:G:173:ASP:N	2.33	0.44
2:H:196:ALA:O	2:H:200:VAL:HG23	2.18	0.44
1:I:60:LEU:HD23	1:I:60:LEU:HA	1.89	0.44
3:J:112:ARG:O	3:J:112:ARG:HG2	2.16	0.44
4:D:123:SER:OG	4:D:272:PRO:HB3	2.18	0.44
1:A:30:ARG:HD2	1:A:30:ARG:HA	1.66	0.43
3:F:280:ARG:NH2	3:F:282:LEU:HD11	2.33	0.43
3:J:354:ASP:HB3	3:J:356:GLU:O	2.18	0.43
4:D:172:VAL:HG22	4:D:173:ASP:CG	2.43	0.43
3:F:30:LEU:C	3:F:30:LEU:CD2	2.91	0.43
3:F:200:VAL:HG12	3:F:201:ARG:O	2.18	0.43
3:F:245:GLY:O	3:F:315:LEU:N	2.51	0.43
3:J:7:GLU:N	3:J:7:GLU:OE1	2.52	0.43
1:A:10:ARG:NH2	3:J:31:PRO:HG3	2.32	0.43
1:A:15:SER:OG	3:F:32:ARG:NH2	2.50	0.43
2:C:40:PRO:HB2	2:C:44:ARG:HH11	1.83	0.43
2:C:441:LEU:N	2:C:442:PRO:HD2	2.33	0.43
2:E:375:ARG:HA	2:E:375:ARG:HD3	1.65	0.43
2:E:379:SER:OG	2:E:380:ALA:N	2.51	0.43
2:E:447:VAL:HA	2:E:450:LEU:HB3	2.01	0.43
3:J:4:LEU:O	3:J:401:ASP:N	2.50	0.43
4:D:175:PRO:HB3	4:D:221:TRP:CG	2.53	0.43
2:C:445:ARG:HB3	2:C:449:PHE:CZ	2.52	0.43
3:F:247:ALA:O	3:F:317:VAL:HG22	2.18	0.43
3:F:281:TYR:CD2	3:F:293:LEU:HD11	2.54	0.43
2:E:119:PHE:CE2	2:H:321:PRO:HD3	2.54	0.43
3:J:240:ASP:N	3:J:240:ASP:OD1	2.49	0.43
2:B:238:ASP:OD1	2:B:238:ASP:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:324:VAL:O	2:C:327:SER:OG	2.28	0.43
2:E:155:ARG:HD2	2:E:155:ARG:HA	1.63	0.43
2:E:179:LEU:HD23	2:E:182:ARG:HH21	1.84	0.43
2:E:374:ALA:C	2:E:376:VAL:N	2.76	0.43
2:H:103:PRO:HD3	4:D:160:ARG:HB3	2.00	0.43
3:J:149:ASP:OD2	3:J:151:ARG:NH1	2.52	0.43
3:J:281:TYR:OH	3:J:293:LEU:HG	2.18	0.43
3:J:321:PRO:HA	3:J:342:ARG:O	2.18	0.43
2:C:88:VAL:HG11	2:C:94:LEU:HD11	2.00	0.43
4:G:50:THR:O	4:G:53:ILE:HB	2.18	0.43
2:E:273:CYS:HB3	2:E:462:MET:SD	2.59	0.43
2:H:9:ILE:HA	2:H:30:PRO:HA	2.01	0.43
2:H:446:MET:O	2:H:449:PHE:N	2.51	0.43
3:J:260:TRP:CE3	3:J:394:ALA:HB2	2.53	0.43
2:E:99:VAL:CG2	2:E:100:PRO:HD2	2.44	0.43
2:H:196:ALA:C	2:H:199:PRO:HD2	2.44	0.43
4:D:90:LEU:O	4:D:93:VAL:HG12	2.18	0.43
2:C:346:SER:OG	2:C:363:VAL:HG23	2.19	0.43
4:G:80:LEU:O	4:G:121:TRP:HA	2.19	0.43
2:E:115:ALA:O	2:H:324:VAL:HG21	2.19	0.43
2:H:197:LEU:HA	2:H:200:VAL:HB	2.01	0.43
2:H:435:SER:O	2:H:435:SER:OG	2.36	0.43
3:J:173:VAL:HG21	3:J:194:LEU:HD11	2.01	0.43
4:D:103:THR:HG23	4:D:103:THR:O	2.18	0.43
2:B:39:LEU:HA	2:B:42:VAL:HG22	2.00	0.43
2:B:129:PRO:HA	2:B:132:ILE:HD12	2.00	0.43
2:C:183:ASN:OD1	2:C:183:ASN:N	2.47	0.43
3:F:222:ASP:OD1	3:F:222:ASP:N	2.52	0.43
3:F:269:VAL:CG2	3:F:272:GLU:HB3	2.48	0.43
2:E:43:GLN:O	2:E:47:GLN:HB2	2.18	0.43
2:H:330:HIS:O	2:H:334:VAL:HG23	2.19	0.43
3:J:4:LEU:N	3:J:399:ARG:O	2.51	0.43
2:B:31:SER:OG	2:B:32:GLU:N	2.51	0.43
4:G:90:LEU:O	4:G:93:VAL:HG12	2.17	0.43
4:G:103:THR:HG23	4:G:103:THR:O	2.18	0.43
4:G:232:GLU:OE2	4:G:232:GLU:C	2.62	0.43
2:E:392:LEU:C	2:E:392:LEU:CD1	2.92	0.43
2:H:35:LEU:HD12	2:H:79:LEU:HA	2.01	0.43
2:H:93:LEU:HD21	3:J:395:ARG:HH11	1.84	0.43
2:H:352:SER:OG	2:H:353:ALA:N	2.52	0.43
3:J:191:ARG:HD3	3:J:191:ARG:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:80:LEU:O	4:D:121:TRP:HA	2.19	0.43
2:C:151:SER:HB3	2:C:163:GLY:O	2.19	0.42
2:H:320:LEU:HD12	2:H:320:LEU:HA	1.83	0.42
2:H:370:ALA:HA	2:H:373:ARG:HG2	2.00	0.42
2:C:317:LEU:HD23	2:C:317:LEU:HA	1.74	0.42
3:F:349:ARG:HD3	3:F:349:ARG:HA	1.72	0.42
4:G:27:ARG:O	4:G:30:LEU:HB3	2.20	0.42
3:J:3:ARG:HH21	3:J:398:SER:CA	2.32	0.42
3:J:347:PRO:HB2	3:J:350:GLU:HB2	2.01	0.42
4:D:134:ALA:HB1	4:D:138:ARG:HH12	1.83	0.42
2:C:386:LEU:HD23	2:C:386:LEU:HA	1.77	0.42
3:F:155:PHE:CD2	3:F:156:LEU:HG	2.55	0.42
3:F:208:ASP:OD1	3:F:209:VAL:N	2.52	0.42
4:G:123:SER:OG	4:G:272:PRO:HB3	2.18	0.42
4:G:224:LEU:HD12	4:G:225:GLU:N	2.35	0.42
2:E:361:TYR:HE1	2:E:461:VAL:HG21	1.85	0.42
4:D:139:SER:OG	4:D:141:ARG:HG3	2.20	0.42
4:D:232:GLU:C	4:D:232:GLU:OE2	2.62	0.42
1:A:15:SER:OG	3:J:103:ASP:OD2	2.28	0.42
1:A:78:LEU:HD23	1:A:79:VAL:HG23	2.01	0.42
2:B:118:ILE:HD13	2:B:118:ILE:HA	1.86	0.42
3:F:214:ARG:O	3:F:357:ARG:HA	2.20	0.42
3:F:348:ASN:O	3:F:349:ARG:NH1	2.44	0.42
2:E:172:LEU:O	2:E:175:VAL:HB	2.19	0.42
2:E:220:ALA:O	2:E:223:GLY:N	2.51	0.42
2:E:403:ILE:HD12	2:E:403:ILE:HA	1.77	0.42
3:J:287:ALA:HB2	3:J:290:ARG:HH21	1.83	0.42
3:J:377:PRO:C	3:J:379:VAL:H	2.28	0.42
4:D:40:LEU:HD23	4:D:41:LEU:HD22	2.02	0.42
2:B:161:LEU:HD23	2:B:161:LEU:HA	1.81	0.42
2:C:11:ARG:HA	2:C:28:ALA:HA	2.00	0.42
2:C:280:LEU:O	2:C:284:VAL:HG22	2.18	0.42
2:C:372:LEU:HD13	2:C:372:LEU:HA	1.90	0.42
3:F:194:LEU:HD23	3:F:194:LEU:HA	1.87	0.42
3:F:264:LEU:O	3:F:267:VAL:HG12	2.20	0.42
2:E:129:PRO:HA	2:E:132:ILE:HD12	2.00	0.42
2:H:31:SER:OG	2:H:83:LEU:HB2	2.19	0.42
2:B:10:VAL:O	2:B:28:ALA:HA	2.20	0.42
2:B:340:LEU:HA	2:B:340:LEU:HD23	1.75	0.42
2:H:284:VAL:HG23	1:I:67:GLN:HB3	2.02	0.42
3:J:364:ASP:OD1	3:J:364:ASP:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:175:PRO:HA	4:D:221:TRP:CD1	2.54	0.42
2:E:321:PRO:HA	2:E:324:VAL:HG12	2.01	0.42
3:J:281:TYR:HE1	3:J:292:ARG:HB3	1.84	0.42
3:J:281:TYR:CZ	3:J:293:LEU:HG	2.55	0.42
1:A:47:ARG:HD2	1:A:59:MET:HG3	2.01	0.42
2:B:103:PRO:HA	2:B:104:PRO:HD3	1.85	0.42
2:B:401:PHE:O	2:B:405:ASP:N	2.53	0.42
2:E:456:ALA:HB1	4:D:6:ALA:HB2	2.02	0.42
2:H:41:ALA:O	2:H:44:ARG:HB3	2.20	0.42
1:I:45:MET:HE3	1:I:45:MET:HB3	1.92	0.42
3:J:112:ARG:NH1	3:J:112:ARG:HB2	2.35	0.42
2:B:41:ALA:O	2:B:45:ILE:HG12	2.18	0.42
3:F:158:LEU:HD11	3:F:235:ALA:HB2	2.01	0.42
2:H:350:VAL:HG23	2:H:363:VAL:HG11	2.01	0.42
2:C:204:PHE:HB3	2:C:219:LEU:HG	2.02	0.42
2:C:239:ARG:C	2:C:241:ILE:H	2.27	0.42
3:F:158:LEU:HB3	3:F:231:TRP:HB2	2.02	0.42
4:G:40:LEU:HD23	4:G:41:LEU:HD22	2.01	0.42
4:G:175:PRO:HD2	4:G:271:ASN:HB3	2.02	0.42
4:G:176:LEU:HG	4:G:177:PRO:HD2	2.01	0.42
2:E:31:SER:HB2	2:E:84:ASP:OD1	2.20	0.42
2:E:40:PRO:HB3	3:J:396:ARG:NH1	2.35	0.42
2:H:69:LEU:HB2	2:H:77:PHE:HD2	1.84	0.42
2:B:214:ALA:HB3	2:B:215:PRO:HD3	2.02	0.41
2:C:24:LEU:HD11	3:F:395:ARG:NH2	2.34	0.41
3:F:245:GLY:N	3:F:313:HIS:O	2.38	0.41
3:F:246:VAL:HA	3:F:315:LEU:O	2.20	0.41
2:E:19:ASP:OD1	2:E:19:ASP:N	2.43	0.41
2:E:272:GLY:HA2	2:E:275:LEU:HB2	2.01	0.41
2:H:11:ARG:N	2:H:90:ASP:OD1	2.53	0.41
2:H:66:ARG:HA	2:H:66:ARG:NE	2.35	0.41
2:H:127:TRP:O	2:H:131:HIS:HD2	2.02	0.41
2:B:412:TRP:N	2:B:412:TRP:CD1	2.88	0.41
4:G:139:SER:OG	4:G:141:ARG:HG3	2.20	0.41
2:E:459:ILE:HG23	2:E:460:PRO:HD3	2.02	0.41
2:H:225:ALA:HB2	2:H:251:GLY:HA3	2.02	0.41
2:H:299:PRO:HG2	1:I:41:TRP:CZ3	2.55	0.41
3:J:244:LEU:HD12	3:J:313:HIS:O	2.20	0.41
4:D:160:ARG:HG3	4:D:166:VAL:HG22	2.02	0.41
2:B:142:GLY:O	2:B:146:VAL:HG12	2.20	0.41
3:F:346:LEU:HD23	3:F:346:LEU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:160:ARG:HG3	4:G:166:VAL:HG22	2.02	0.41
2:E:138:LEU:HD23	2:E:138:LEU:HA	1.81	0.41
2:E:386:LEU:H	2:E:386:LEU:HG	1.45	0.41
2:H:152:VAL:O	2:H:156:VAL:N	2.52	0.41
3:J:19:LYS:HD2	3:J:168:ASP:OD2	2.21	0.41
4:D:27:ARG:O	4:D:30:LEU:HB3	2.19	0.41
2:C:204:PHE:O	2:C:219:LEU:HD23	2.20	0.41
4:G:175:PRO:HA	4:G:221:TRP:CD1	2.55	0.41
4:G:216:PRO:HB2	4:G:217:ALA:H	1.57	0.41
2:H:357:PRO:O	2:H:361:TYR:N	2.53	0.41
3:J:148:ARG:CD	3:J:238:TRP:HB3	2.50	0.41
3:J:149:ASP:OD2	3:J:151:ARG:NH2	2.53	0.41
3:J:264:LEU:HD23	3:J:264:LEU:HA	1.68	0.41
2:B:112:ILE:HA	2:B:115:ALA:HB3	2.02	0.41
2:B:316:VAL:HG22	2:B:317:LEU:H	1.86	0.41
2:C:175:VAL:HG12	2:C:176:ILE:HD13	2.03	0.41
2:E:161:LEU:HD13	2:E:161:LEU:HA	1.92	0.41
2:E:214:ALA:HB3	2:E:215:PRO:HD3	2.02	0.41
2:E:263:LEU:HD12	2:E:264:TRP:N	2.35	0.41
2:H:435:SER:OG	2:H:437:ASP:OD1	2.29	0.41
4:D:49:LEU:O	4:D:53:ILE:HG13	2.20	0.41
4:D:97:LEU:CD2	4:D:230:PRO:HD3	2.51	0.41
4:D:176:LEU:HG	4:D:177:PRO:HD2	2.01	0.41
2:B:123:ARG:CG	2:B:125:ARG:HB3	2.49	0.41
3:F:253:LEU:O	3:F:259:SER:N	2.47	0.41
2:E:283:THR:HG21	2:E:373:ARG:HH11	1.85	0.41
2:H:361:TYR:HD2	2:H:461:VAL:HG11	1.84	0.41
3:J:262:LYS:HE2	3:J:282:LEU:HB2	2.02	0.41
2:B:26:GLU:H	2:B:26:GLU:HG3	1.73	0.41
2:C:239:ARG:C	2:C:241:ILE:N	2.79	0.41
2:C:437:ASP:OD1	2:C:438:THR:N	2.54	0.41
4:G:159:LEU:HD23	4:G:166:VAL:HG11	2.03	0.41
2:H:226:ALA:O	2:H:230:ILE:HG13	2.20	0.41
4:D:108:ARG:HG3	4:D:225:GLU:HB2	2.02	0.41
2:B:469:PHE:CE1	4:G:14:ALA:HA	2.56	0.41
2:C:16:ALA:HB3	2:C:21:GLY:O	2.21	0.41
2:C:96:LEU:HD23	2:C:96:LEU:HA	1.80	0.41
2:H:413:ALA:O	2:H:416:ALA:N	2.54	0.41
3:J:269:VAL:HG13	3:J:279:ALA:CB	2.51	0.41
4:D:175:PRO:HD2	4:D:271:ASN:HB3	2.02	0.41
2:B:237:ASP:OD1	2:B:238:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:ILE:HG22	2:B:270:VAL:HG11	2.02	0.41
2:B:373:ARG:HB2	2:B:386:LEU:HD13	2.03	0.41
2:C:79:LEU:HD12	2:C:79:LEU:HA	1.97	0.41
3:F:93:ARG:H	3:F:93:ARG:HD3	1.86	0.41
3:F:364:ASP:OD1	3:F:365:GLY:N	2.52	0.41
4:G:173:ASP:HB2	4:G:221:TRP:HH2	1.86	0.41
4:G:207:GLU:N	4:G:207:GLU:OE1	2.54	0.41
2:E:35:LEU:HD23	2:E:35:LEU:O	2.21	0.41
2:E:181:VAL:HG12	2:E:181:VAL:O	2.20	0.41
2:E:350:VAL:HG12	2:E:360:TRP:CH2	2.54	0.41
2:H:242:ALA:O	2:H:244:PHE:N	2.53	0.41
2:H:337:ALA:O	2:H:341:LEU:HG	2.20	0.41
3:J:367:ILE:HG13	3:J:382:ALA:HB2	2.02	0.41
4:D:159:LEU:HD23	4:D:166:VAL:HG11	2.02	0.41
4:D:170:GLU:OE1	4:D:170:GLU:N	2.54	0.41
4:D:175:PRO:HA	4:D:221:TRP:NE1	2.36	0.41
4:D:270:LEU:HD12	4:D:270:LEU:HA	1.96	0.41
1:A:9:ASP:HB3	1:A:10:ARG:H	1.64	0.41
1:A:61:VAL:O	1:A:63:PRO:HD3	2.21	0.41
3:F:18:ARG:HH21	3:F:118:HIS:CD2	2.39	0.41
2:E:36:ARG:NH2	2:E:80:ASP:HA	2.36	0.41
2:H:211:ASP:C	2:H:216:ASN:HD22	2.29	0.41
3:J:146:TRP:CD2	3:J:241:PRO:HD2	2.56	0.41
3:J:268:ASP:OD1	3:J:268:ASP:N	2.47	0.41
3:F:132:GLU:HA	3:F:159:ARG:CZ	2.52	0.40
4:G:170:GLU:N	4:G:170:GLU:OE1	2.54	0.40
2:E:148:THR:OG1	2:E:199:PRO:HB3	2.20	0.40
2:H:241:ILE:O	2:H:242:ALA:C	2.64	0.40
4:D:121:TRP:CE3	4:D:172:VAL:HG23	2.56	0.40
2:E:107:ARG:HG2	2:E:108:ILE:H	1.85	0.40
2:E:197:LEU:HB3	2:E:227:TRP:HD1	1.86	0.40
4:D:224:LEU:HD12	4:D:225:GLU:N	2.35	0.40
2:B:27:MET:HE2	2:B:27:MET:HB3	1.85	0.40
2:B:119:PHE:HE2	2:C:321:PRO:HD3	1.87	0.40
3:F:92:MET:O	3:F:92:MET:SD	2.79	0.40
3:F:148:ARG:HD2	3:F:239:HIS:NE2	2.36	0.40
3:F:217:VAL:C	3:F:218:ILE:HD12	2.45	0.40
4:G:97:LEU:CD2	4:G:230:PRO:HD3	2.51	0.40
2:E:356:SER:HB3	2:E:359:ALA:CB	2.51	0.40
2:E:397:LEU:O	2:E:400:ALA:HB3	2.21	0.40
4:D:259:ALA:HB3	4:D:264:ARG:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:260:ARG:HD2	4:D:260:ARG:HA	1.79	0.40
3:F:317:VAL:C	3:F:318:LEU:HD12	2.47	0.40
2:H:271:ILE:O	2:H:274:ALA:HB3	2.22	0.40
3:J:383:ASP:OD1	3:J:383:ASP:N	2.55	0.40
1:A:17:THR:O	3:F:179:GLU:HB3	2.21	0.40
2:B:358:TRP:HB2	2:B:465:LEU:HD13	2.03	0.40
2:B:387:LEU:HD23	2:B:387:LEU:HA	1.86	0.40
2:B:459:ILE:N	2:B:460:PRO:HD2	2.36	0.40
3:F:4:LEU:HD12	3:F:400:TRP:CD1	2.56	0.40
4:G:108:ARG:HG3	4:G:225:GLU:HB2	2.03	0.40
3:J:180:ILE:HA	3:J:180:ILE:HD12	1.69	0.40
3:J:262:LYS:NZ	3:J:282:LEU:HB2	2.36	0.40
4:D:173:ASP:HB2	4:D:221:TRP:HH2	1.86	0.40
4:D:232:GLU:OE1	4:D:284:PRO:HB3	2.22	0.40
4:D:234:LEU:HB3	4:D:282:ALA:HB1	2.04	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	79/518 (15%)	68 (86%)	6 (8%)	5 (6%)	1	14
1	I	57/518 (11%)	55 (96%)	2 (4%)	0	100	100
2	B	421/475 (89%)	384 (91%)	37 (9%)	0	100	100
2	C	434/475 (91%)	386 (89%)	47 (11%)	1 (0%)	43	72
2	E	421/475 (89%)	362 (86%)	58 (14%)	1 (0%)	43	72
2	H	434/475 (91%)	371 (86%)	63 (14%)	0	100	100
3	F	326/449 (73%)	263 (81%)	62 (19%)	1 (0%)	36	65
3	J	314/449 (70%)	256 (82%)	55 (18%)	3 (1%)	12	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	225/309 (73%)	196 (87%)	29 (13%)	0	100	100
4	G	225/309 (73%)	196 (87%)	29 (13%)	0	100	100
All	All	2936/4452 (66%)	2537 (86%)	388 (13%)	11 (0%)	31	60

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	18	PRO
1	A	26	VAL
3	F	258	TRP
2	C	242	ALA
2	E	375	ARG
3	J	258	TRP
3	J	181	ASP
3	J	174	LYS
1	A	23	PRO
1	A	19	VAL

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	70/398 (18%)	60 (86%)	10 (14%)	3	18
1	I	50/398 (13%)	50 (100%)	0	100	100
2	B	305/342 (89%)	305 (100%)	0	100	100
2	C	319/342 (93%)	319 (100%)	0	100	100
2	E	305/342 (89%)	285 (93%)	20 (7%)	15	42
2	H	319/342 (93%)	319 (100%)	0	100	100
3	F	281/369 (76%)	272 (97%)	9 (3%)	34	56
3	J	270/369 (73%)	257 (95%)	13 (5%)	23	48
4	D	192/241 (80%)	155 (81%)	37 (19%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	G	192/241 (80%)	155 (81%)	37 (19%)	1	9
All	All	2303/3384 (68%)	2177 (94%)	126 (6%)	21	46

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	12	SER
1	A	14	SER
1	A	17	THR
1	A	19	VAL
1	A	21	GLU
1	A	27	GLN
1	A	28	TYR
1	A	29	ARG
1	A	34	THR
3	F	30	LEU
3	F	33	VAL
3	F	37	SER
3	F	38	LEU
3	F	39	LEU
3	F	40	ARG
3	F	41	ARG
3	F	43	LEU
3	F	92	MET
4	G	1	MET
4	G	5	ILE
4	G	7	LEU
4	G	12	VAL
4	G	13	VAL
4	G	24	THR
4	G	25	THR
4	G	29	VAL
4	G	32	VAL
4	G	33	SER
4	G	37	VAL
4	G	39	VAL
4	G	47	MET
4	G	51	THR
4	G	80	LEU
4	G	83	ASP
4	G	97	LEU

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Mol	Chain	Res	Type
4	G	98	ASP
4	G	125	THR
4	G	130	ASP
4	G	151	VAL
4	G	161	GLU
4	G	165	THR
4	G	167	THR
4	G	168	VAL
4	G	178	VAL
4	G	194	VAL
4	G	200	LYS
4	G	208	VAL
4	G	232	GLU
4	G	237	VAL
4	G	238	CYS
4	G	267	LEU
4	G	273	LEU
4	G	274	SER
4	G	276	GLU
4	G	285	LEU
2	E	38	ILE
2	E	362	ILE
2	E	363	VAL
2	E	372	LEU
2	E	373	ARG
2	E	383	LYS
2	E	386	LEU
2	E	387	LEU
2	E	389	HIS
2	E	390	SER
2	E	392	LEU
2	E	393	LEU
2	E	395	VAL
2	E	402	VAL
2	E	403	ILE
2	E	405	ASP
2	E	407	TYR
2	E	408	GLN
2	E	411	LEU
2	E	417	LEU
3	J	23	THR
3	J	24	ILE

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Mol	Chain	Res	Type
3	J	25	GLU
3	J	106	ARG
3	J	108	LEU
3	J	110	VAL
3	J	111	VAL
3	J	112	ARG
3	J	115	VAL
3	J	174	LYS
3	J	176	THR
3	J	180	ILE
3	J	343	THR
4	D	1	MET
4	D	5	ILE
4	D	7	LEU
4	D	12	VAL
4	D	13	VAL
4	D	24	THR
4	D	25	THR
4	D	29	VAL
4	D	32	VAL
4	D	33	SER
4	D	37	VAL
4	D	39	VAL
4	D	47	MET
4	D	51	THR
4	D	80	LEU
4	D	83	ASP
4	D	97	LEU
4	D	98	ASP
4	D	125	THR
4	D	130	ASP
4	D	151	VAL
4	D	161	GLU
4	D	165	THR
4	D	167	THR
4	D	168	VAL
4	D	178	VAL
4	D	194	VAL
4	D	200	LYS
4	D	208	VAL
4	D	232	GLU
4	D	237	VAL

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Mol	Chain	Res	Type
4	D	238	CYS
4	D	267	LEU
4	D	273	LEU
4	D	274	SER
4	D	276	GLU
4	D	285	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
2	B	131	HIS
2	B	154	HIS
2	B	288	GLN
2	C	126	GLN
2	C	131	HIS
2	C	164	GLN
3	F	9	GLN
3	F	122	GLN
3	F	234	GLN
3	F	376	GLN
3	F	392	HIS
4	G	19	GLN
4	G	145	GLN
2	E	43	GLN
2	E	97	GLN
2	E	131	HIS
2	E	216	ASN
2	E	330	HIS
2	H	97	GLN
2	H	131	HIS
2	H	216	ASN
3	J	187	HIS
3	J	271	ASN
3	J	371	GLN
3	J	376	GLN
4	D	19	GLN
4	D	145	GLN
4	D	158	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

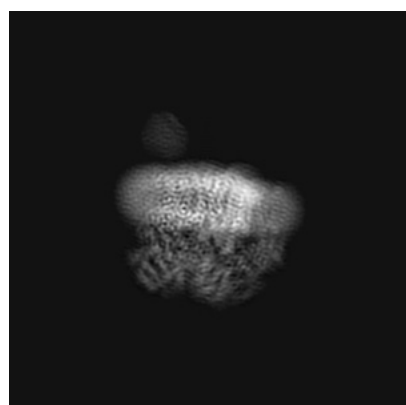
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0862. These allow visual inspection of the internal detail of the map and identification of artifacts.

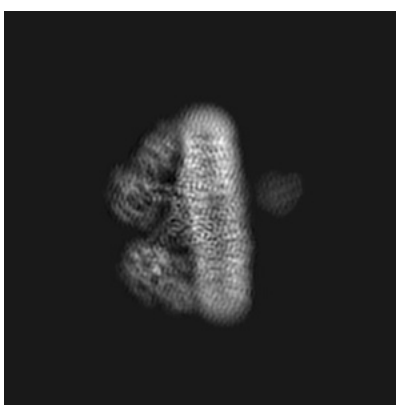
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

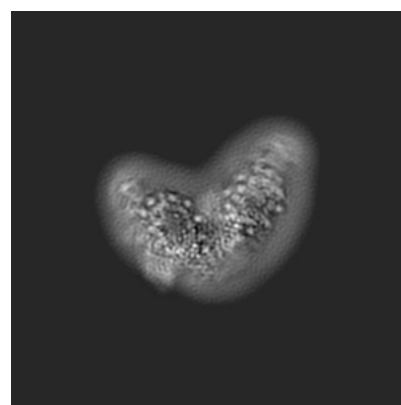
6.1.1 Primary map



X



Y

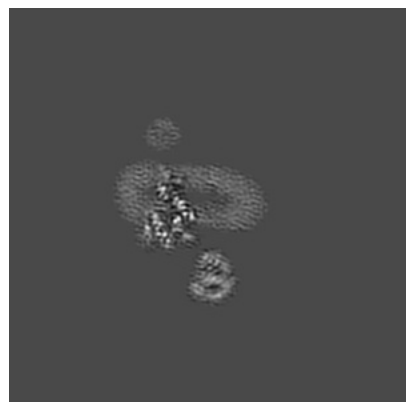


Z

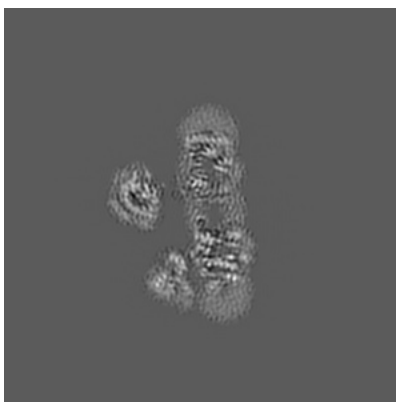
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

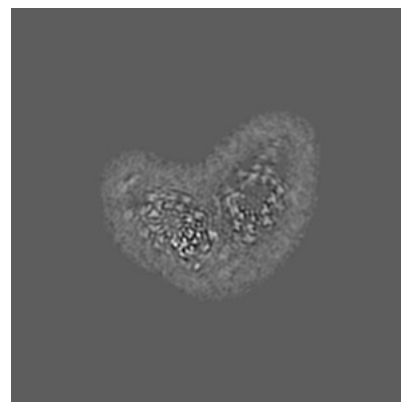
6.2.1 Primary map



X Index: 220



Y Index: 220

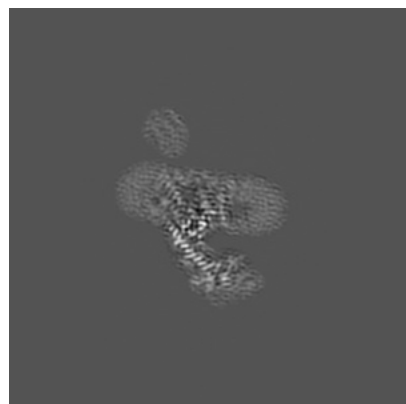


Z Index: 220

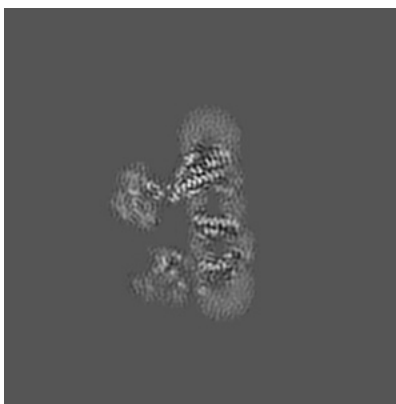
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

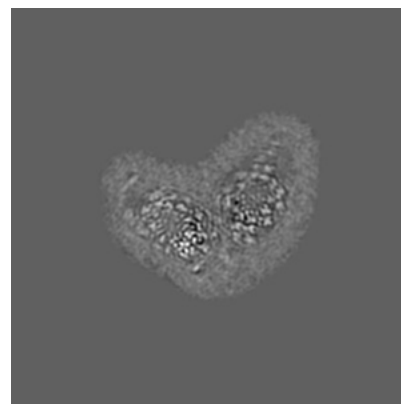
6.3.1 Primary map



X Index: 244



Y Index: 211

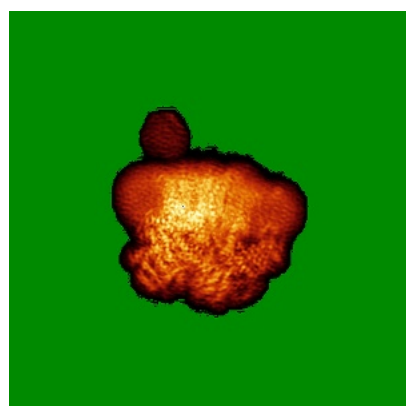


Z Index: 218

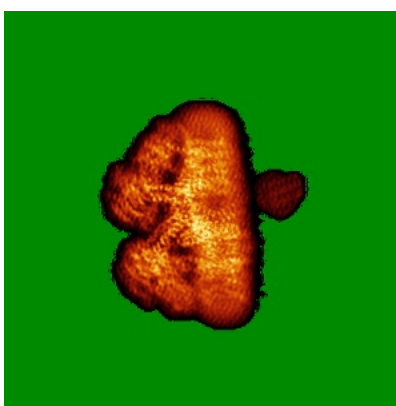
The images above show the largest variance slices of the map in three orthogonal directions.

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

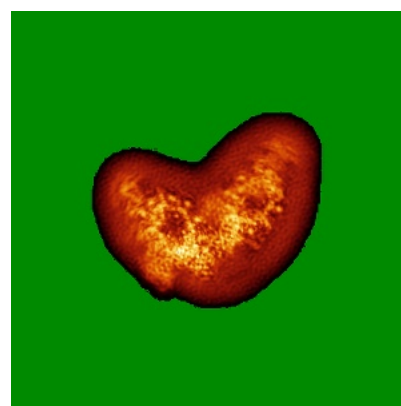
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

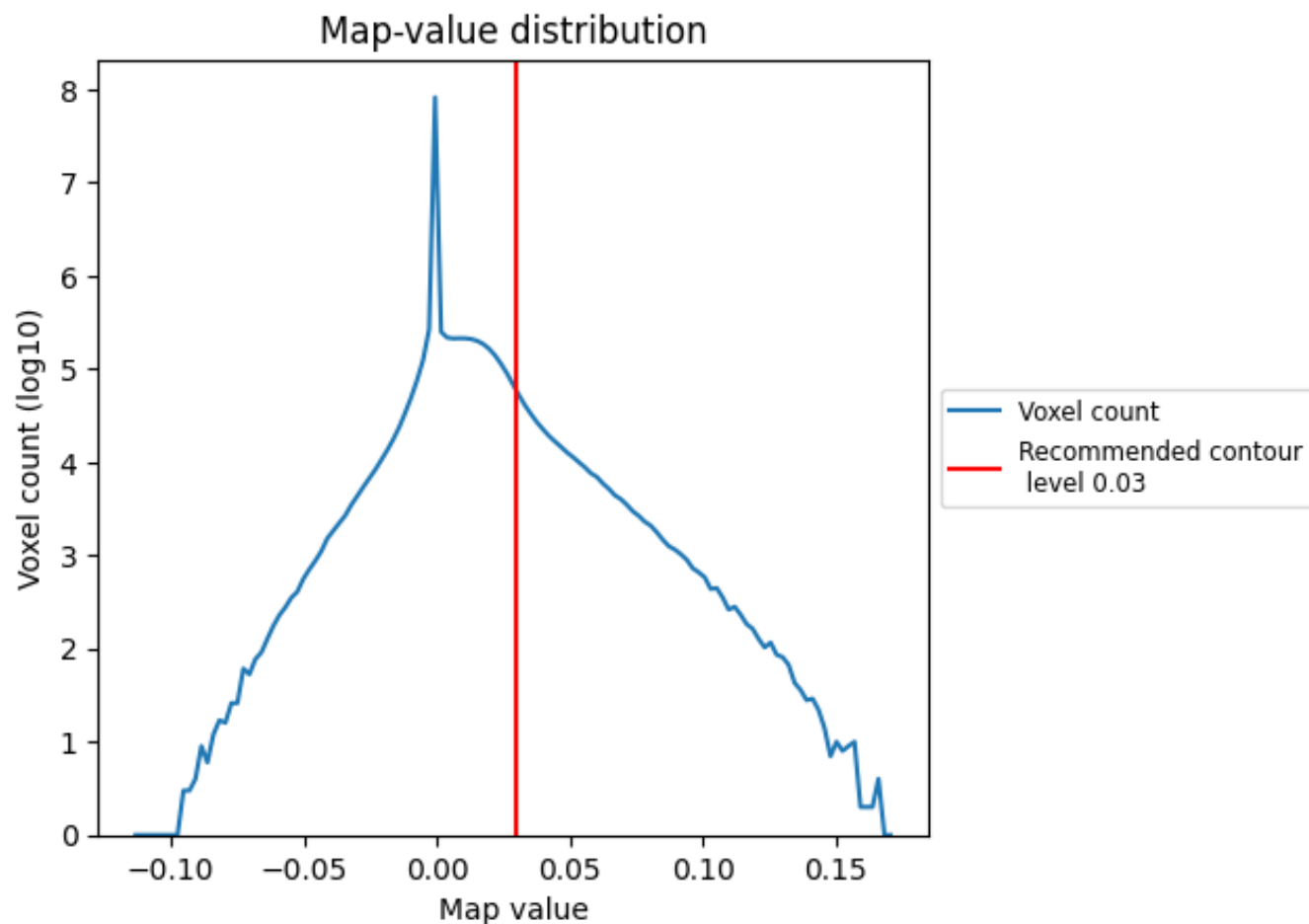
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

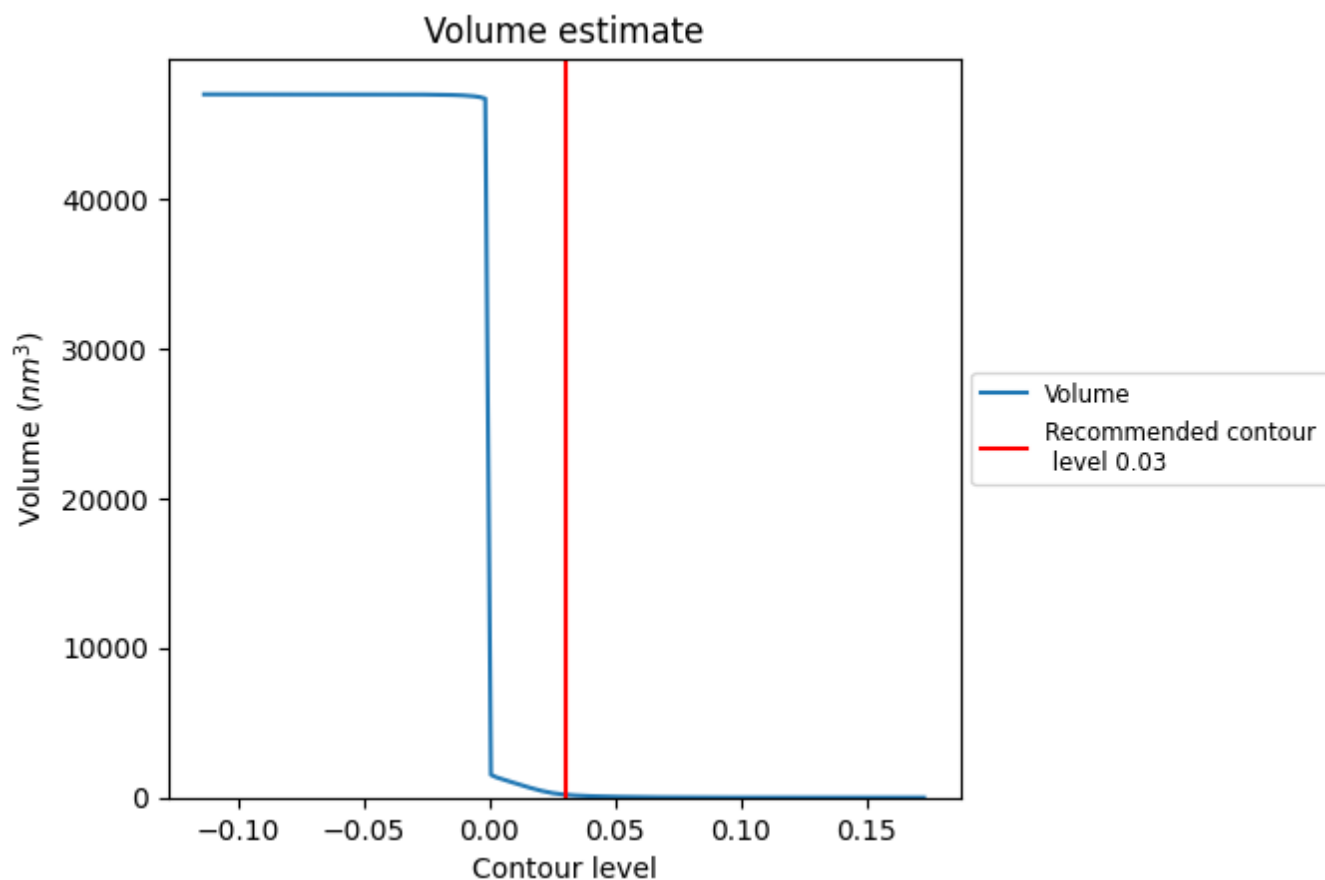
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

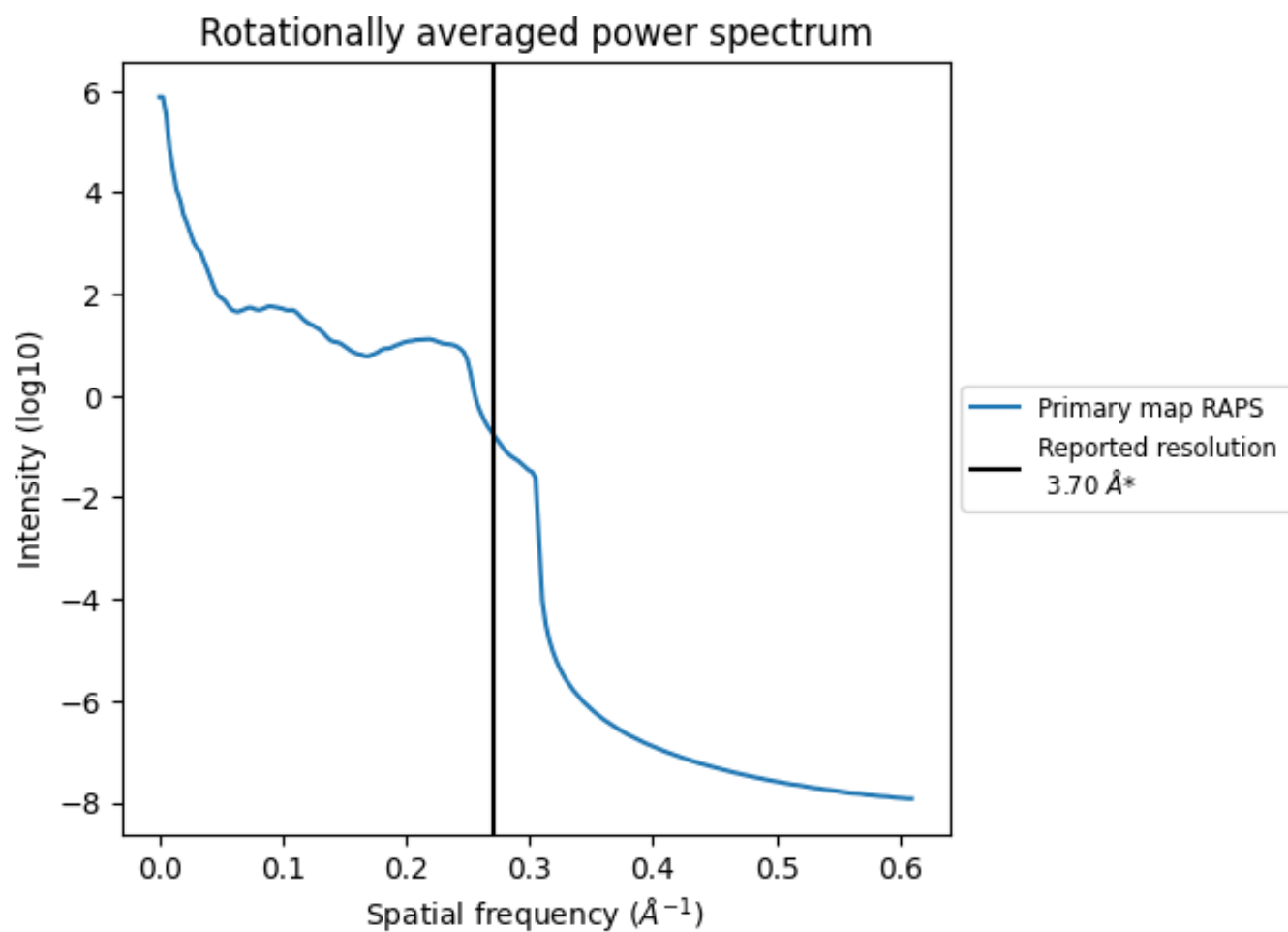
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 194 nm³; this corresponds to an approximate mass of 175 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 0.270 Å⁻¹

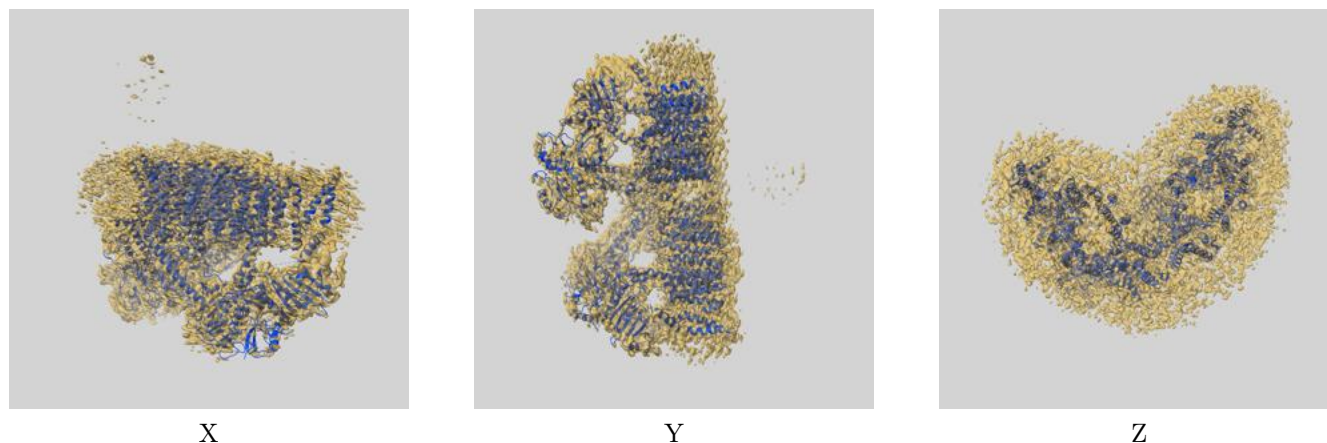
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

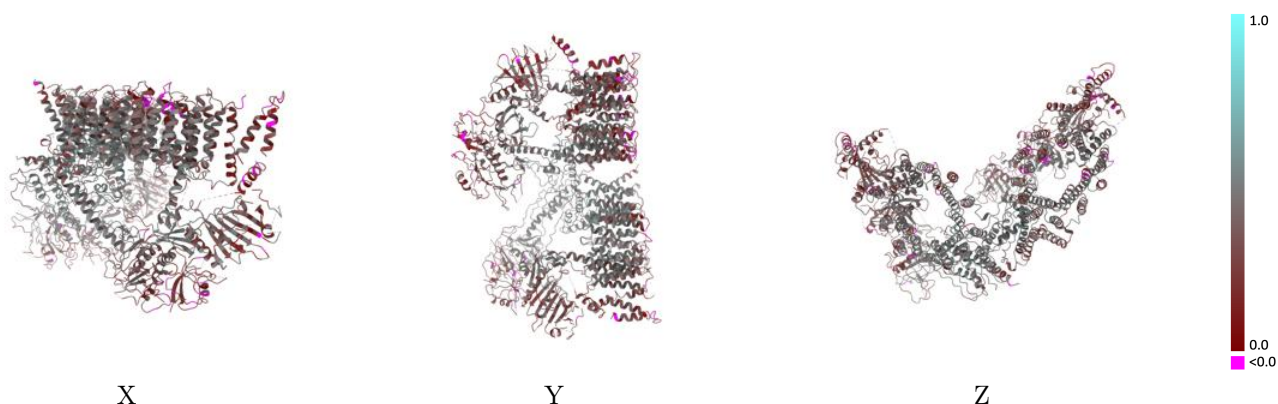
This section contains information regarding the fit between EMDB map EMD-0862 and PDB model 6LAR. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

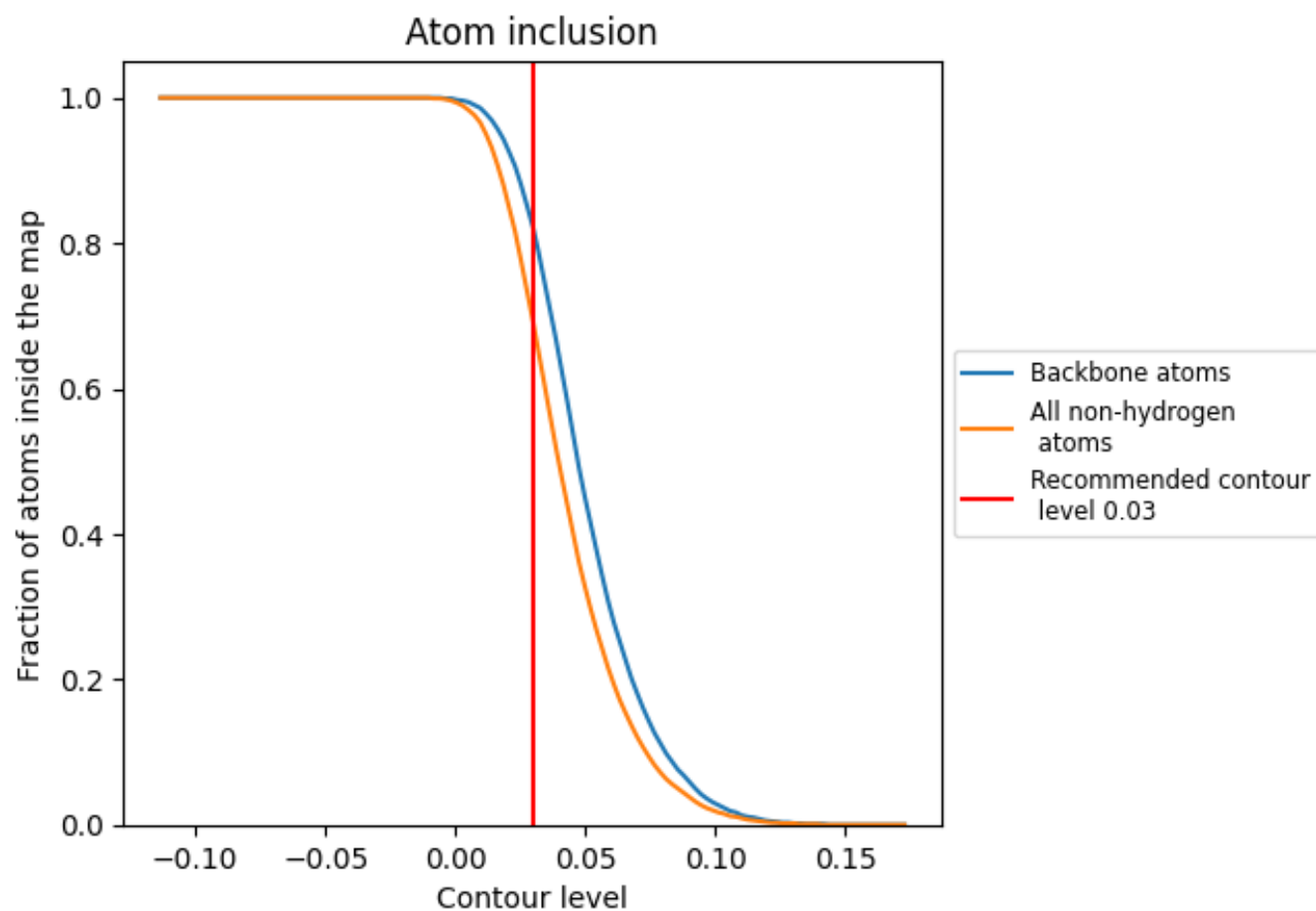


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 69% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6900	0.3780
A	0.7760	0.4450
B	0.6820	0.3860
C	0.6040	0.3620
D	0.6540	0.3160
E	0.7410	0.4070
F	0.6870	0.3640
G	0.6310	0.3110
H	0.7220	0.4260
I	0.7890	0.4410
J	0.7360	0.3740

1.0

0.0

<0.0