



Full wwPDB EM Validation Report ⓘ

Oct 1, 2026 – 04:54 PM EDT

PDB ID : 38LP / pdb_000038lp
EMDB ID : EMD-78907
Title : Salmonella Flagellar Export Apparatus (FliPQR/FlhB/FlhA) in the context of the intact basal body with an asymmetric FlhA ring
Authors : Johnson, S.; Johnson, M.K.; Lea, S.M.
Deposited on : 2026-09-01
Resolution : 4.20 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:

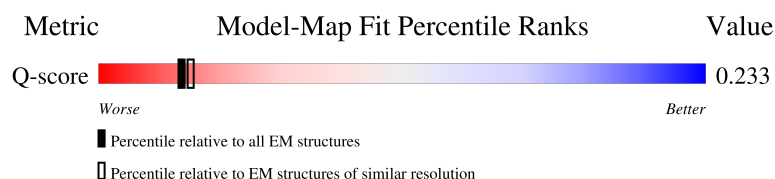
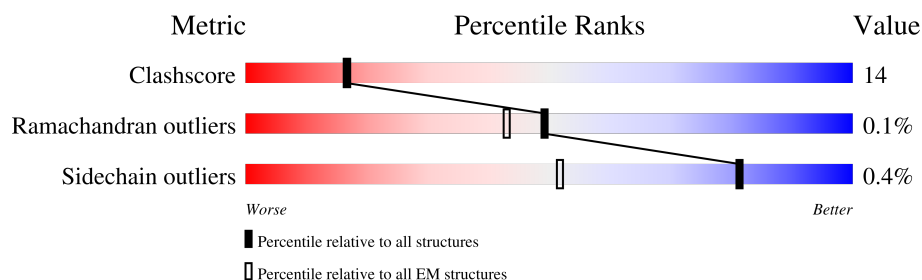
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.2
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

1 Overall quality at a glance

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

The reported resolution of this entry is 4.20 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	5410 (3.70 - 4.70)

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	A1	245	15% 58% 25% 15%
1	B1	245	14% 57% 28% 15%
1	C1	245	11% 61% 23% 15%
1	D1	245	10% 62% 22% 15%

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Mol	Chain	Length	Quality of chain
1	E1	245	
2	F1	264	
3	G1	89	
3	H1	89	
3	I1	89	
3	J1	89	
4	K1	383	
5	A2	692	
5	B2	692	
5	C2	692	
5	D2	692	
5	E2	692	
5	F2	692	
5	G2	692	
5	H2	692	
5	I2	692	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 35427 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 Flagellar biosynthetic protein FliP.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	209	Total	C	N	O	S	0	0
			1623	1084	251	276	12		
1	B1	209	Total	C	N	O	S	0	0
			1623	1084	251	276	12		
1	C1	209	Total	C	N	O	S	0	0
			1623	1084	251	276	12		
1	D1	209	Total	C	N	O	S	0	0
			1623	1084	251	276	12		
1	E1	209	Total	C	N	O	S	0	0
			1623	1084	251	276	12		

- Molecule 2 is a protein called Flagellar biosynthetic protein FliR.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F1	250	Total	C	N	O	S	0	0
			1925	1293	304	313	15		

- Molecule 3 is a protein called Flagellar biosynthetic protein FliQ.

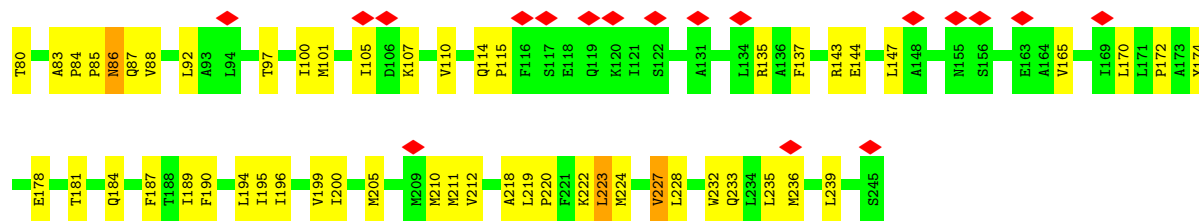
Mol	Chain	Residues	Atoms					AltConf	Trace
3	G1	89	Total	C	N	O	S	0	0
			670	449	100	114	7		
3	H1	89	Total	C	N	O	S	0	0
			670	449	100	114	7		
3	I1	89	Total	C	N	O	S	0	0
			670	449	100	114	7		
3	J1	89	Total	C	N	O	S	0	0
			670	449	100	114	7		

- Molecule 4 is a protein called Flagellar biosynthetic protein FlhB.

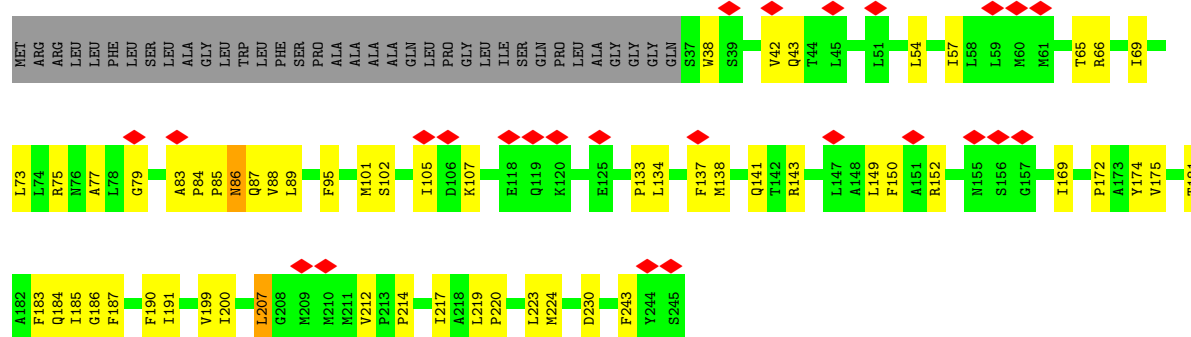
Mol	Chain	Residues	Atoms					AltConf	Trace
4	K1	249	Total	C	N	O	S	0	0
			1926	1245	333	331	17		

- Molecule 5 is a protein called Flagellar biosynthesis protein FlhA.

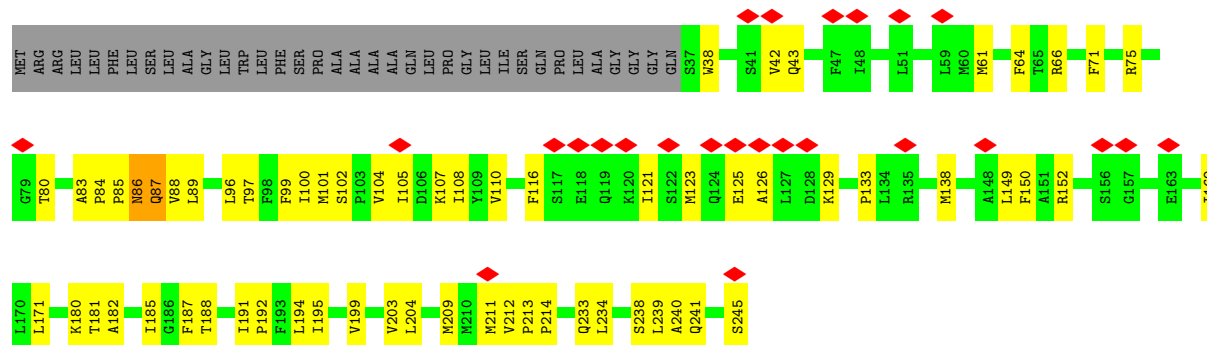
Mol	Chain	Residues	Atoms					AltConf	Trace
5	A2	311	Total	C	N	O	S	0	0
			2309	1516	377	401	15		
5	B2	311	Total	C	N	O	S	0	0
			2309	1516	377	401	15		
5	C2	311	Total	C	N	O	S	0	0
			2309	1516	377	401	15		
5	D2	311	Total	C	N	O	S	0	0
			2309	1516	377	401	15		
5	E2	311	Total	C	N	O	S	0	0
			2309	1516	377	401	15		
5	F2	311	Total	C	N	O	S	0	0
			2309	1516	377	401	15		
5	G2	311	Total	C	N	O	S	0	0
			2309	1516	377	401	15		
5	H2	311	Total	C	N	O	S	0	0
			2309	1516	377	401	15		
5	I2	311	Total	C	N	O	S	0	0
			2309	1516	377	401	15		



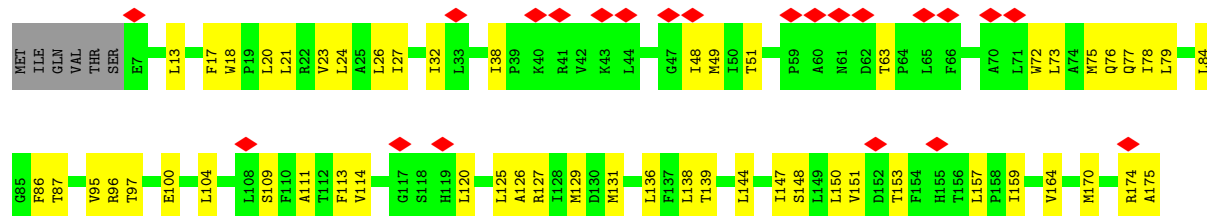
• Molecule 1: Flagellar biosynthetic protein Flp



• Molecule 1: Flagellar biosynthetic protein Flp

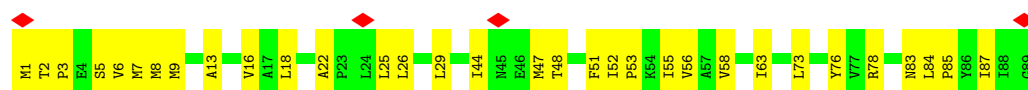


• Molecule 2: Flagellar biosynthetic protein Flr

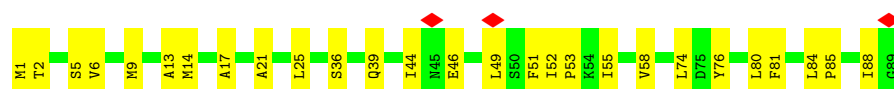




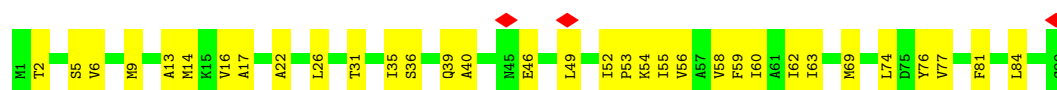
• Molecule 3: Flagellar biosynthetic protein FliQ



• Molecule 3: Flagellar biosynthetic protein FliQ



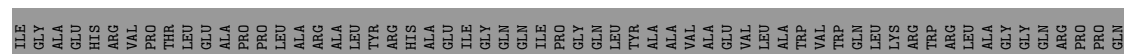
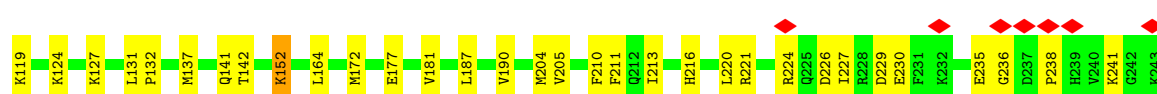
• Molecule 3: Flagellar biosynthetic protein FliQ



• Molecule 3: Flagellar biosynthetic protein FliQ



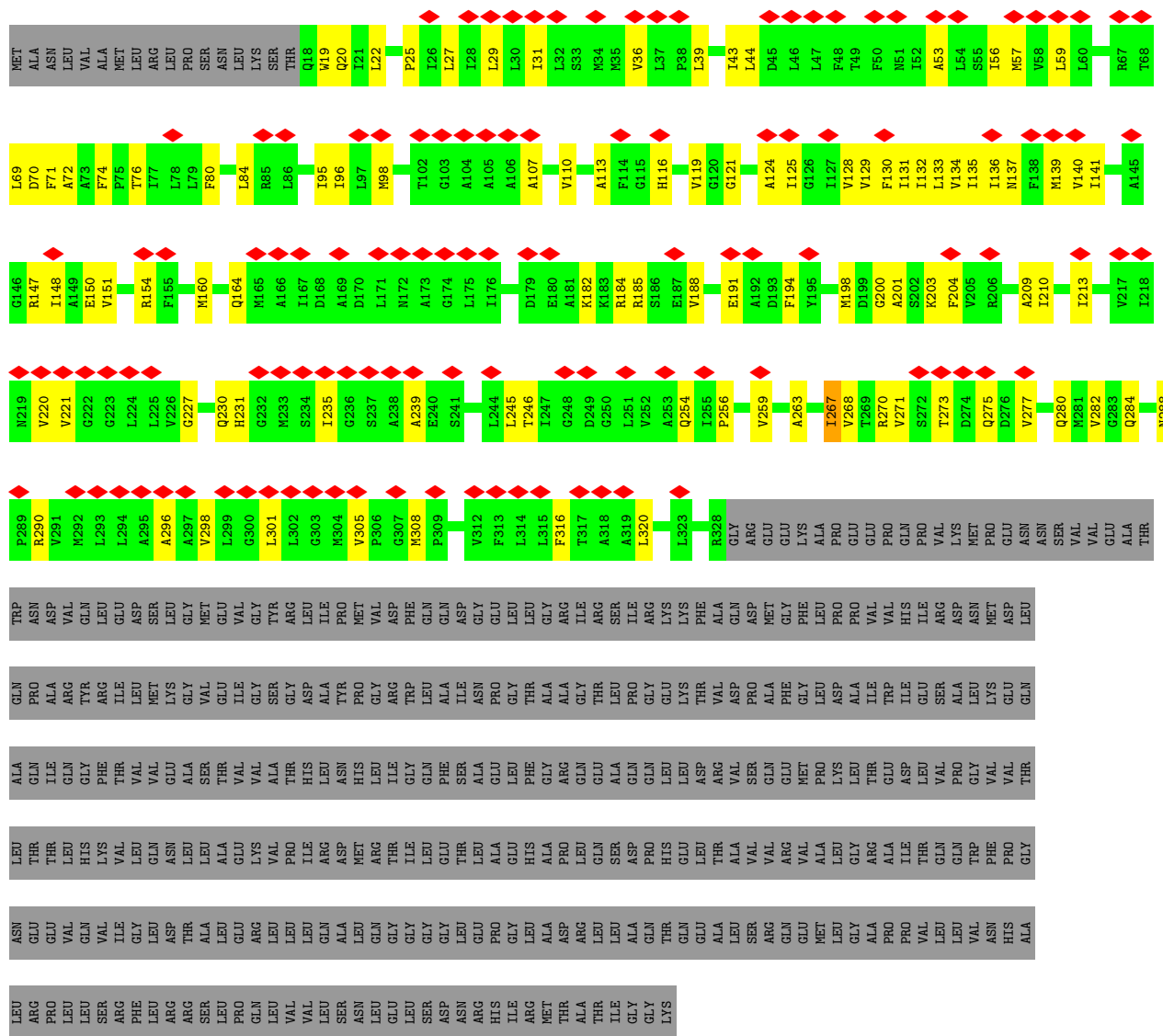
• Molecule 4: Flagellar biosynthetic protein FlhB



PRO GLU
ASN
LEU
PRO
VAL
MET
PRO
GLU
LEU
ASP
PHE
MET
ASN
GLU
LYS
ASN
THR
ASP
GLY

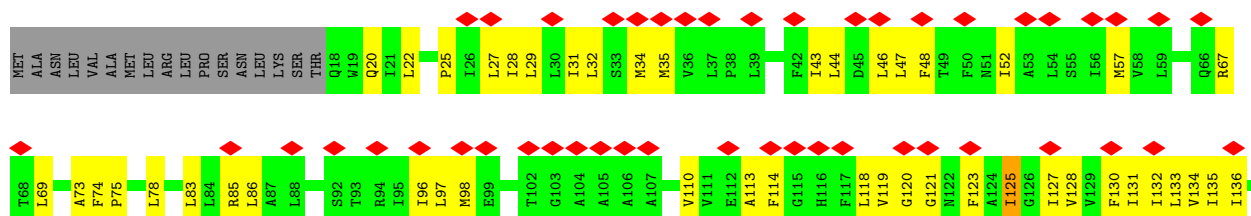
• Molecule 5: Flagellar biosynthesis protein FlhA

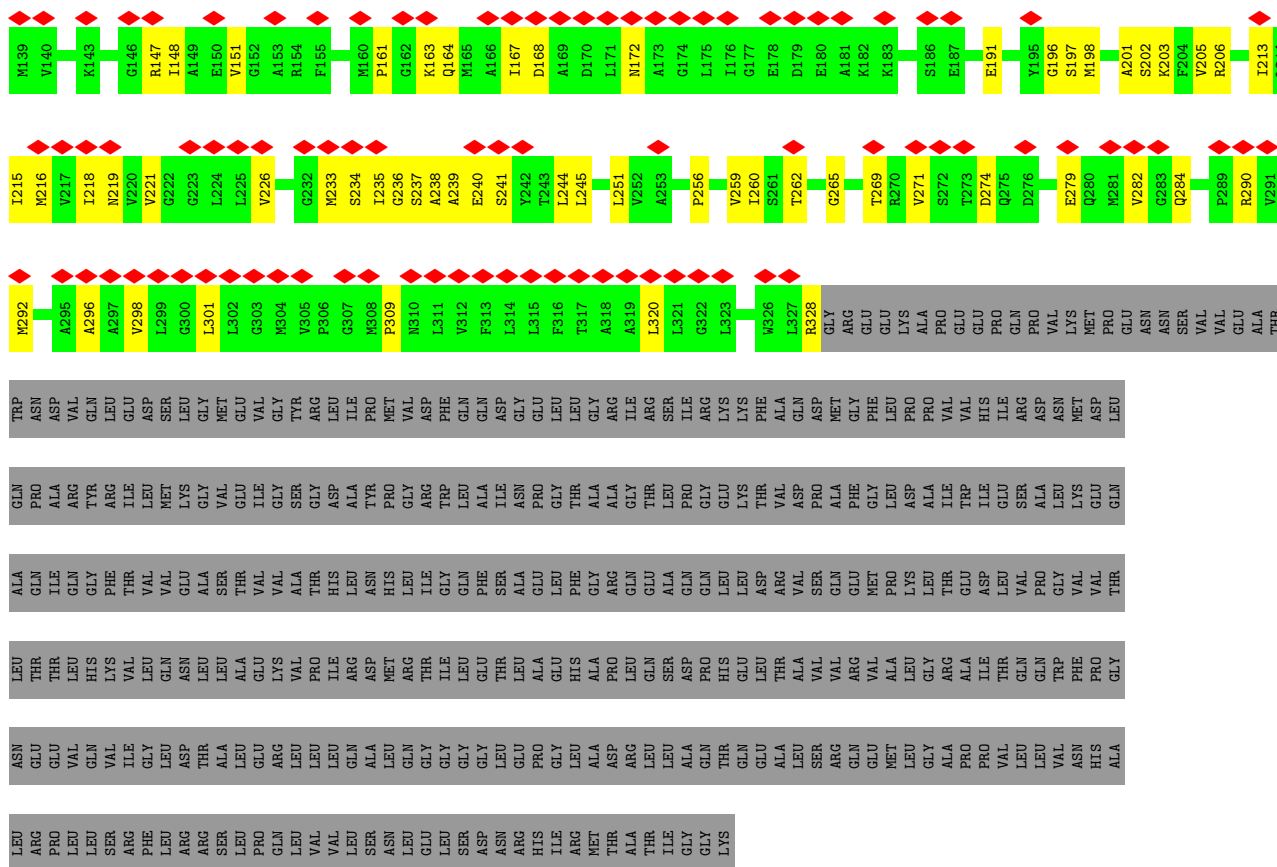
Chain A2: 18% 30% 14% 55%



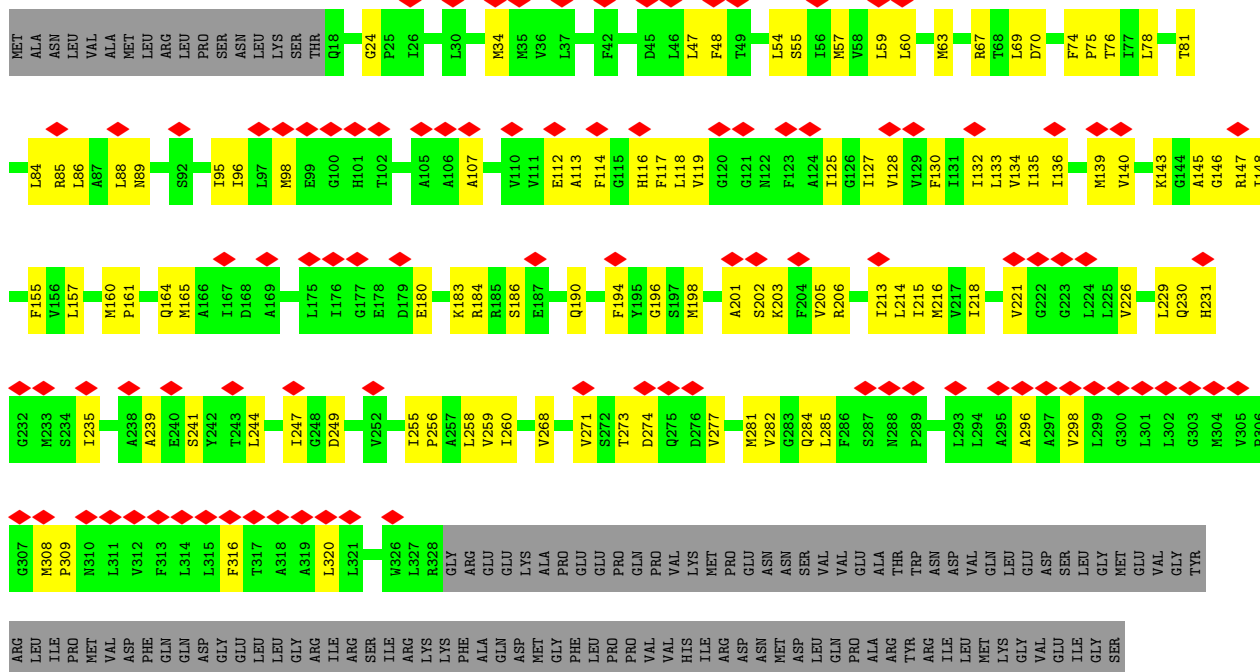
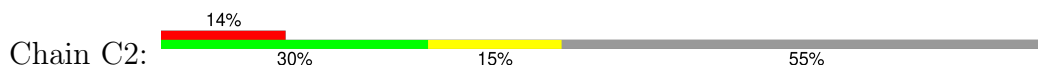
• Molecule 5: Flagellar biosynthesis protein FlhA

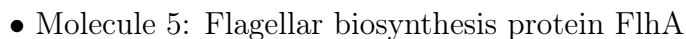
Chain B2: 20% 30% 15% 55%

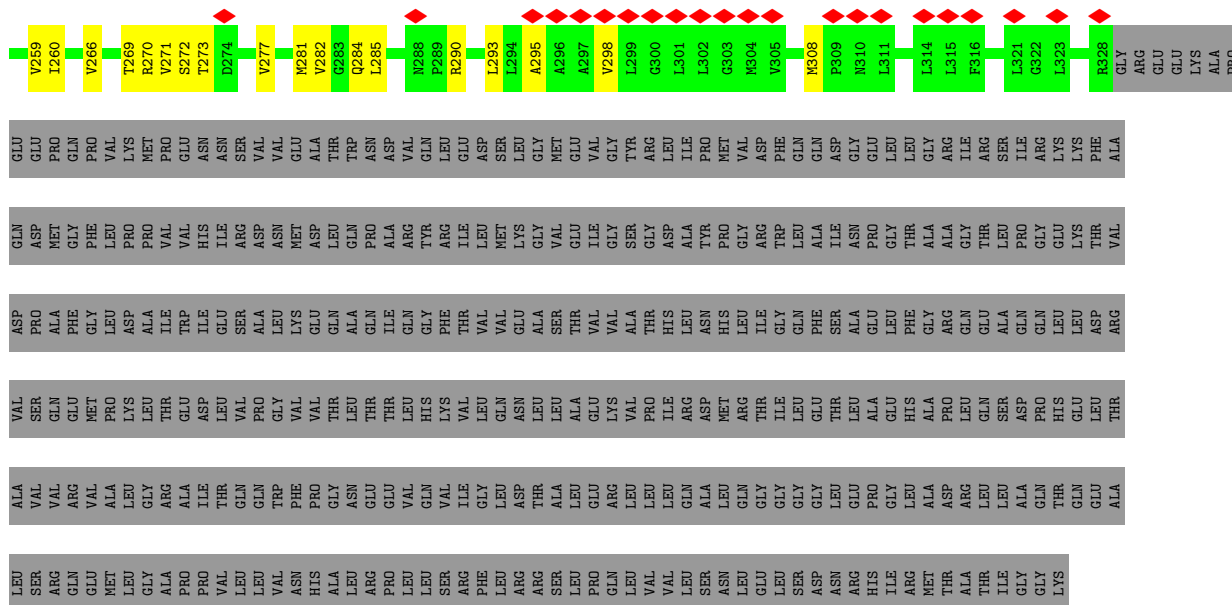




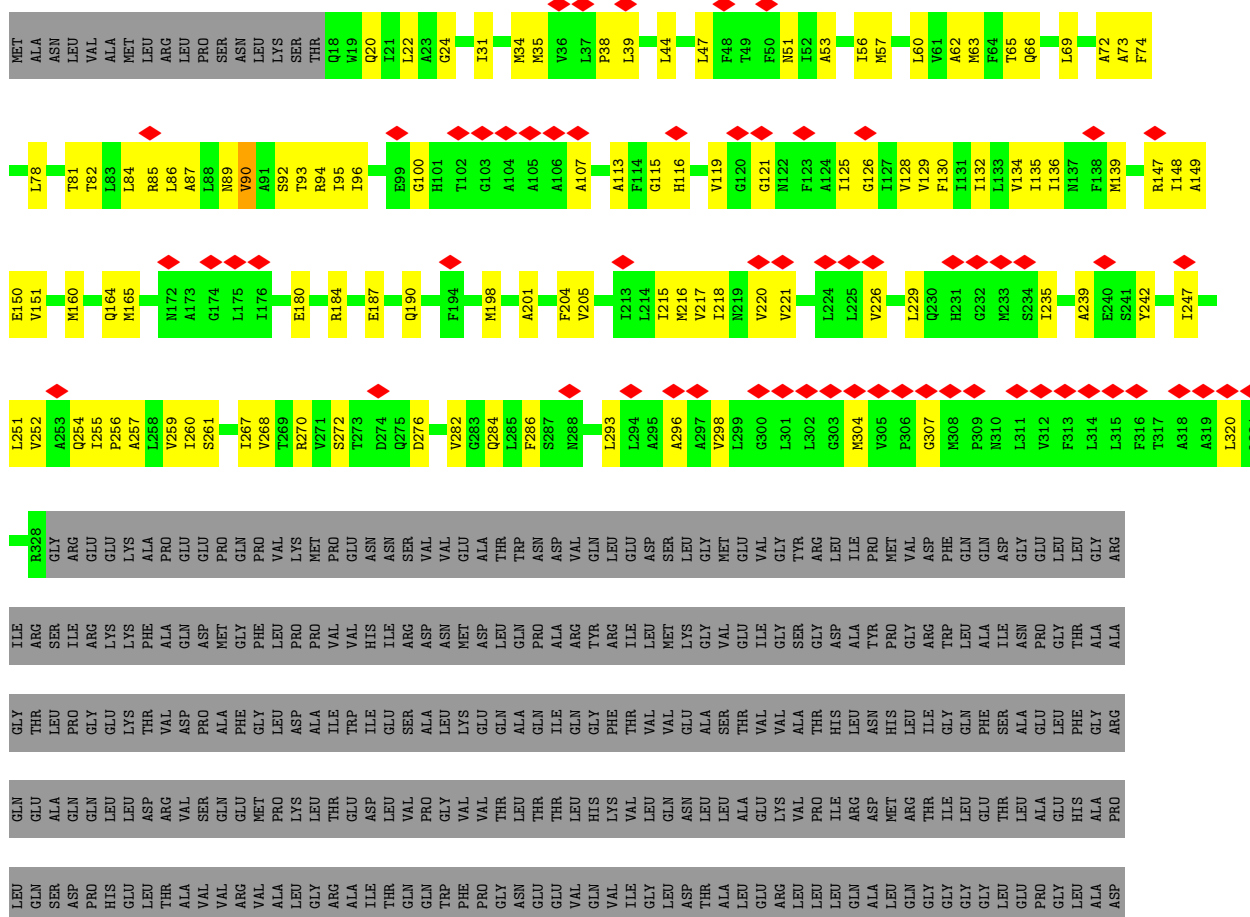
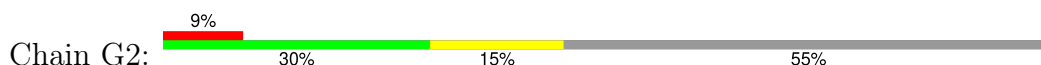
- Molecule 5: Flagellar biosynthesis protein FlhA

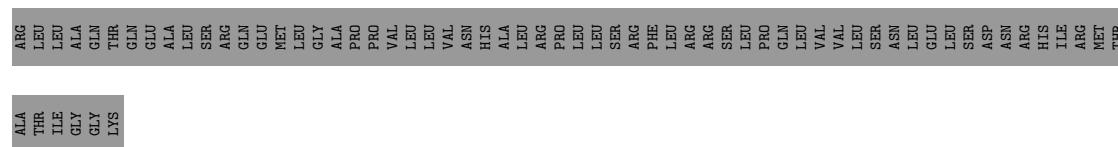




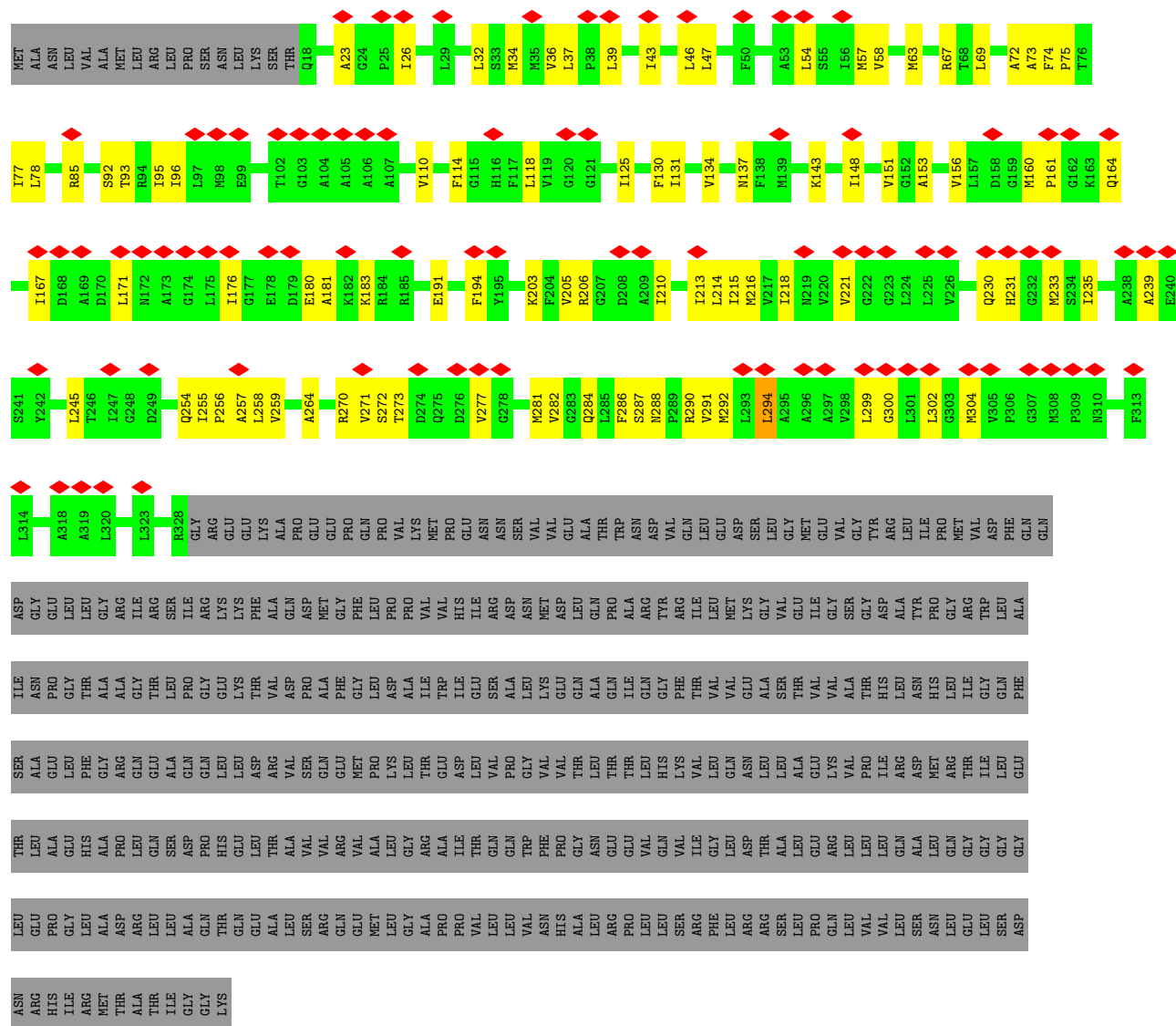
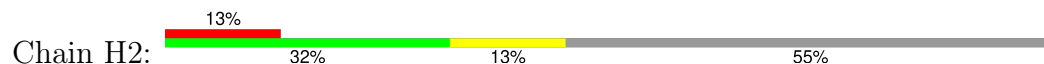


- Molecule 5: Flagellar biosynthesis protein FlhA

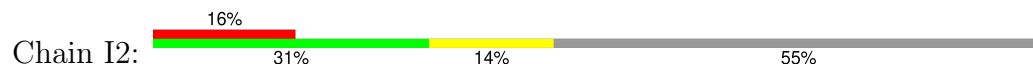


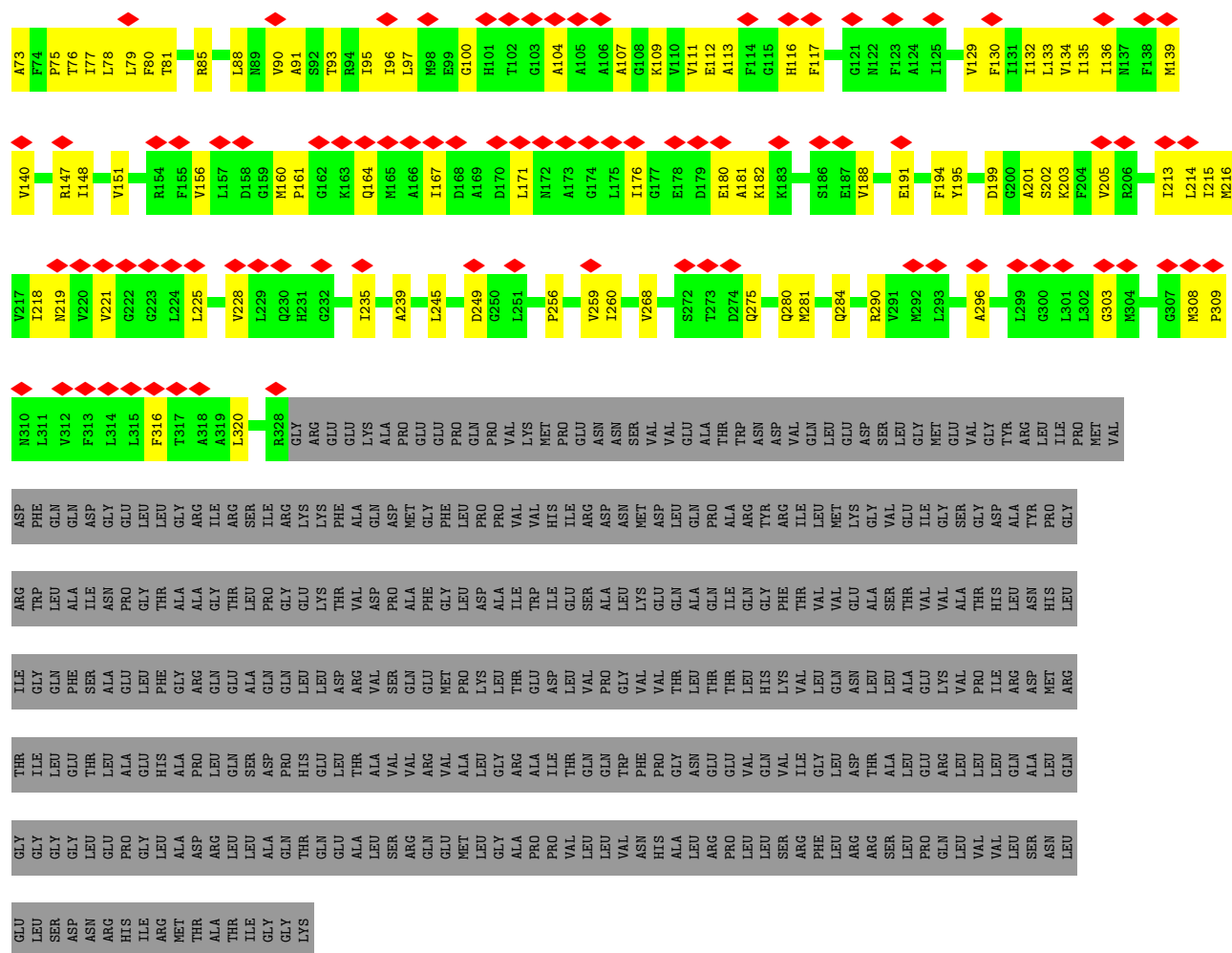


• Molecule 5: Flagellar biosynthesis protein FlhA



• Molecule 5: Flagellar biosynthesis protein FlhA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	51079	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58.5	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.397	Depositor
Minimum map value	-0.674	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	537.6, 537.6, 537.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A1	0.14	0/1662	0.40	1/2263 (0.0%)
1	B1	0.15	0/1662	0.39	0/2263
1	C1	0.14	0/1662	0.41	0/2263
1	D1	0.15	0/1662	0.37	0/2263
1	E1	0.14	0/1662	0.37	0/2263
2	F1	0.13	0/1974	0.30	0/2696
3	G1	0.13	0/681	0.34	0/930
3	H1	0.14	0/681	0.42	0/930
3	I1	0.14	0/681	0.36	0/930
3	J1	0.13	0/681	0.36	0/930
4	K1	0.14	0/1963	0.36	0/2647
5	A2	0.13	0/2346	0.33	0/3187
5	B2	0.13	0/2346	0.37	0/3187
5	C2	0.14	0/2346	0.38	0/3187
5	D2	0.15	0/2346	0.39	0/3187
5	E2	0.14	0/2346	0.37	0/3187
5	F2	0.14	0/2346	0.36	0/3187
5	G2	0.15	0/2346	0.39	0/3187
5	H2	0.13	0/2346	0.34	0/3187
5	I2	0.14	0/2346	0.38	0/3187
All	All	0.14	0/36085	0.37	1/49061 (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	A1	0	1
1	B1	0	1
1	C1	0	1
1	D1	0	1
1	E1	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	B2	0	1
5	E2	0	1
5	F2	0	1
5	H2	0	1
5	I2	0	1
All	All	0	10

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	223	LEU	CA-CB-CG	5.09	134.10	116.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A1	86	ASN	Peptide
1	B1	86	ASN	Peptide
5	B2	125	ILE	Peptide
1	C1	86	ASN	Peptide
1	D1	86	ASN	Peptide
1	E1	86	ASN	Peptide
5	E2	125	ILE	Peptide
5	F2	125	ILE	Peptide
5	H2	125	ILE	Peptide
5	I2	268	VAL	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	A1	1623	0	1715	55	0
1	B1	1623	0	1715	63	0
1	C1	1623	0	1715	49	0
1	D1	1623	0	1715	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E1	1623	0	1715	54	0
2	F1	1925	0	2042	71	0
3	G1	670	0	739	35	0
3	H1	670	0	739	27	0
3	I1	670	0	739	24	0
3	J1	670	0	739	20	0
4	K1	1926	0	2031	52	0
5	A2	2309	0	2450	86	0
5	B2	2309	0	2450	81	0
5	C2	2309	0	2450	82	0
5	D2	2309	0	2450	84	0
5	E2	2309	0	2450	71	0
5	F2	2309	0	2450	78	0
5	G2	2309	0	2450	86	0
5	H2	2309	0	2450	70	0
5	I2	2309	0	2450	73	0
All	All	35427	0	37654	1023	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 14.

All (1023) 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)
5:A2:147:ARG:HD3	5:I2:203:LYS:HD3	1.48	0.92
5:C2:89:ASN:HD21	5:C2:215:ILE:HG12	1.34	0.89
1:A1:87:GLN:HB3	1:B1:59:LEU:HD11	1.57	0.87
5:E2:137:ASN:HD21	5:E2:254:GLN:HE21	1.26	0.82
1:B1:118:GLU:HG3	1:B1:120:LYS:HG2	1.61	0.82
5:H2:137:ASN:HD22	5:H2:254:GLN:HE22	1.29	0.80
1:C1:223:LEU:HG	1:D1:187:PHE:HE1	1.46	0.79
3:H1:39:GLN:HE22	3:H1:46:GLU:HG3	1.48	0.78
1:E1:64:PHE:HA	1:E1:97:THR:HG21	1.66	0.78
5:D2:203:LYS:HD3	5:E2:147:ARG:HD3	1.65	0.78
1:A1:71:PHE:HB3	1:A1:89:LEU:HD23	1.63	0.78
5:A2:160:MET:O	5:A2:164:GLN:HB2	1.84	0.78
5:B2:28:ILE:HA	5:B2:31:ILE:HD12	1.66	0.77
1:A1:138:MET:HE2	1:A1:170:LEU:HG	1.69	0.74
5:F2:73:ALA:H	5:G2:284:GLN:HE22	1.35	0.74
5:G2:34:MET:HA	5:G2:39:LEU:HD11	1.68	0.74
5:H2:110:VAL:HA	5:I2:309:PRO:HG3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C2:146:GLY:HA3	5:C2:206:ARG:HH22	1.53	0.73
5:F2:25:PRO:HG3	5:G2:60:LEU:HD11	1.71	0.73
4:K1:74:ASP:HB3	4:K1:77:LEU:HD23	1.70	0.73
2:F1:207:MET:HG3	4:K1:152:LYS:HD3	1.71	0.73
2:F1:111:ALA:HB3	2:F1:120:LEU:HD11	1.71	0.72
1:E1:181:THR:HG21	4:K1:72:VAL:HG23	1.72	0.71
5:I2:69:LEU:HD22	5:I2:191:GLU:HG3	1.72	0.71
5:H2:134:VAL:HG21	5:H2:213:ILE:HB	1.73	0.70
5:A2:210:ILE:HA	5:A2:213:ILE:HD12	1.72	0.70
5:F2:33:SER:HA	5:F2:37:LEU:HD23	1.73	0.70
5:F2:85:ARG:HH22	5:F2:260:ILE:HD11	1.57	0.70
2:F1:215:VAL:HG13	2:F1:216:ILE:HG12	1.74	0.69
1:C1:223:LEU:HG	1:D1:187:PHE:CE1	2.27	0.69
2:F1:20:LEU:HD11	2:F1:48:ILE:HG22	1.75	0.69
5:D2:204:PHE:HE1	5:E2:141:ILE:HA	1.57	0.69
2:F1:227:MET:HE1	3:G1:18:LEU:HB2	1.75	0.69
2:F1:32:ILE:HG21	2:F1:138:LEU:HD21	1.75	0.69
5:G2:235:ILE:O	5:G2:239:ALA:CB	2.41	0.69
4:K1:235:GLU:HB2	4:K1:238:PRO:HG3	1.75	0.69
5:B2:86:LEU:HD13	5:C2:136:ILE:HD12	1.73	0.69
2:F1:193:LEU:HD22	2:F1:228:LEU:HD11	1.73	0.68
1:E1:192:PRO:HA	1:E1:195:ILE:HD12	1.75	0.68
5:A2:110:VAL:HG23	5:B2:309:PRO:HG3	1.74	0.68
5:B2:296:ALA:HB2	5:B2:320:LEU:HD22	1.75	0.68
4:K1:103:VAL:HA	4:K1:106:ILE:HG12	1.76	0.68
5:A2:56:ILE:HG23	5:A2:57:MET:HE2	1.75	0.68
3:G1:22:ALA:O	3:G1:26:LEU:HB2	1.93	0.67
5:A2:39:LEU:HA	5:A2:43:ILE:HD11	1.76	0.67
5:H2:143:LYS:HA	5:H2:206:ARG:HE	1.59	0.67
1:A1:192:PRO:HA	1:A1:195:ILE:HD12	1.75	0.67
5:B2:67:ARG:HH22	5:B2:274:ASP:HA	1.58	0.67
1:B1:185:ILE:HD11	3:H1:84:LEU:HG	1.77	0.67
5:F2:39:LEU:HB2	5:F2:94:ARG:HH22	1.60	0.67
5:E2:252:VAL:HA	5:E2:255:ILE:HD12	1.77	0.66
5:G2:100:GLY:HA3	5:G2:242:TYR:HE1	1.60	0.66
1:C1:219:LEU:HA	1:C1:222:LYS:HE2	1.75	0.66
5:B2:290:ARG:HH22	5:B2:328:ARG:HH12	1.42	0.66
5:A2:182:LYS:HA	5:A2:185:ARG:HE	1.59	0.66
5:E2:134:VAL:HG11	5:E2:213:ILE:HB	1.77	0.66
1:D1:184:GLN:HE21	3:J1:1:MET:HB2	1.60	0.66
2:F1:21:LEU:HD21	2:F1:78:ILE:HG12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G2:256:PRO:HA	5:G2:259:VAL:HG22	1.77	0.66
5:I2:35:MET:HG3	5:I2:36:VAL:HG13	1.76	0.66
1:D1:75:ARG:HH21	1:D1:89:LEU:HD23	1.60	0.66
5:D2:137:ASN:HD22	5:D2:141:ILE:HD11	1.61	0.65
1:D1:212:VAL:HG22	1:E1:214:PRO:HG2	1.77	0.65
5:A2:227:GLY:HA2	5:A2:230:GLN:HE21	1.61	0.65
5:A2:133:LEU:HD13	5:A2:254:GLN:HG3	1.79	0.65
1:E1:96:LEU:HD13	2:F1:170:MET:HE1	1.77	0.65
5:B2:134:VAL:HG21	5:B2:213:ILE:HB	1.79	0.65
5:F2:256:PRO:HA	5:F2:259:VAL:HG22	1.77	0.65
4:K1:226:ASP:HA	4:K1:229:ASP:HB2	1.77	0.65
1:A1:121:ILE:HG23	1:A1:123:MET:H	1.63	0.64
5:I2:85:ARG:HH22	5:I2:260:ILE:HD11	1.62	0.64
5:B2:110:VAL:HA	5:C2:309:PRO:HG3	1.78	0.64
5:G2:126:GLY:HA3	5:G2:247:ILE:HD12	1.78	0.64
5:B2:203:LYS:HG2	5:C2:147:ARG:HH11	1.62	0.64
5:C2:235:ILE:O	5:C2:239:ALA:CB	2.46	0.64
5:D2:235:ILE:O	5:D2:239:ALA:CB	2.46	0.64
5:F2:94:ARG:NH1	5:F2:95:ILE:HB	2.12	0.64
1:B1:223:LEU:HD11	1:C1:187:PHE:HB2	1.79	0.64
5:B2:78:LEU:HD12	5:B2:201:ALA:HB1	1.79	0.64
1:C1:220:PRO:HB3	1:D1:190:PHE:HD2	1.62	0.64
1:D1:73:LEU:HD23	1:D1:186:GLY:HA3	1.79	0.63
5:C2:81:THR:HA	5:C2:84:LEU:HD12	1.80	0.63
5:A2:74:PHE:HB3	5:A2:198:MET:HE1	1.80	0.63
5:E2:114:PHE:HA	5:F2:308:MET:HE1	1.78	0.63
5:E2:235:ILE:O	5:E2:239:ALA:CB	2.46	0.63
5:E2:20:GLN:HG3	5:F2:282:VAL:HG21	1.81	0.63
2:F1:178:LEU:HA	2:F1:181:LEU:HB3	1.79	0.63
3:I1:81:PHE:HA	3:I1:84:LEU:HG	1.79	0.63
1:B1:66:ARG:HB2	1:B1:182:ALA:HB2	1.80	0.63
1:C1:228:LEU:HD21	3:J1:3:PRO:HG3	1.81	0.63
5:E2:256:PRO:HA	5:E2:259:VAL:HG22	1.81	0.63
1:E1:80:THR:HG22	2:F1:104:LEU:HD12	1.79	0.62
5:B2:235:ILE:O	5:B2:239:ALA:CB	2.47	0.62
5:E2:97:LEU:HD12	5:F2:128:VAL:HG11	1.81	0.62
5:H2:156:VAL:HG22	5:H2:160:MET:HE3	1.81	0.62
5:E2:213:ILE:O	5:E2:216:MET:HG3	1.99	0.62
5:H2:203:LYS:HG2	5:I2:147:ARG:HD2	1.80	0.62
5:C2:34:MET:HE2	5:C2:47:LEU:HD13	1.82	0.62
1:B1:77:ALA:HB2	1:B1:190:PHE:HE1	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A2:20:GLN:HB2	5:B2:279:GLU:HA	1.80	0.62
5:D2:94:ARG:HH22	5:E2:118:LEU:HB3	1.64	0.62
1:B1:235:LEU:HB3	1:B1:236:MET:HE2	1.81	0.61
1:C1:233:GLN:HE21	1:D1:149:LEU:HD11	1.65	0.61
1:E1:121:ILE:HD11	1:E1:125:GLU:HG2	1.81	0.61
1:E1:150:PHE:HB3	1:E1:169:ILE:HD11	1.81	0.61
5:C2:24:GLY:HA3	5:D2:63:MET:HE3	1.80	0.61
1:B1:78:LEU:HA	1:B1:222:LYS:HD2	1.80	0.61
5:B2:96:ILE:HD11	5:B2:245:LEU:HD13	1.81	0.61
1:B1:228:LEU:HB3	3:H1:74:LEU:HD11	1.83	0.61
4:K1:24:GLU:HB2	4:K1:119:LYS:HD2	1.82	0.61
5:E2:226:VAL:O	5:E2:230:GLN:HB3	2.01	0.61
5:G2:128:VAL:O	5:G2:132:ILE:HG13	2.00	0.61
3:H1:39:GLN:NE2	3:H1:46:GLU:HG3	2.14	0.61
2:F1:190:VAL:HG22	2:F1:228:LEU:HB3	1.83	0.61
5:D2:271:VAL:HG13	5:D2:273:THR:H	1.66	0.61
2:F1:18:TRP:HH2	2:F1:63:THR:HB	1.66	0.61
5:C2:235:ILE:O	5:C2:239:ALA:HB3	2.00	0.61
5:A2:296:ALA:HB2	5:A2:320:LEU:HD22	1.83	0.61
5:G2:252:VAL:HA	5:G2:255:ILE:HD12	1.82	0.60
5:G2:73:ALA:H	5:H2:284:GLN:HE22	1.49	0.60
3:H1:2:THR:HG23	3:H1:5:SER:H	1.65	0.60
5:A2:151:VAL:HA	5:A2:154:ARG:HE	1.65	0.60
1:E1:83:ALA:HB3	1:E1:84:PRO:HD3	1.82	0.60
5:B2:29:LEU:HD13	5:B2:32:LEU:HD21	1.83	0.60
5:B2:215:ILE:HA	5:B2:218:ILE:HG12	1.81	0.60
5:A2:275:GLN:HB3	5:A2:280:GLN:HE21	1.66	0.60
5:E2:265:GLY:O	5:E2:269:THR:HB	2.02	0.60
1:B1:220:PRO:HB3	1:C1:190:PHE:HD2	1.67	0.60
5:D2:34:MET:HA	5:D2:39:LEU:HD11	1.84	0.60
2:F1:193:LEU:HD21	4:K1:164:LEU:HD13	1.84	0.59
5:A2:137:ASN:HA	5:A2:141:ILE:HG22	1.84	0.59
5:E2:73:ALA:H	5:F2:284:GLN:HE22	1.48	0.59
5:F2:98:MET:HE2	5:G2:125:ILE:HG21	1.84	0.59
5:D2:281:MET:O	5:D2:285:LEU:HB2	2.01	0.59
5:H2:34:MET:HE2	5:H2:47:LEU:HD13	1.83	0.59
5:I2:296:ALA:HB2	5:I2:320:LEU:HD22	1.84	0.59
5:C2:256:PRO:HA	5:C2:259:VAL:HG22	1.85	0.59
3:I1:39:GLN:NE2	3:I1:46:GLU:HG3	2.17	0.59
5:E2:74:PHE:HD2	5:E2:198:MET:HE1	1.67	0.59
1:E1:75:ARG:HD2	1:E1:84:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F1:213:ILE:HG13	2:F1:217:GLY:HA3	1.84	0.59
5:C2:76:THR:HG22	5:D2:269:THR:HG23	1.83	0.59
5:E2:126:GLY:H	5:E2:129:VAL:HG12	1.68	0.59
5:D2:256:PRO:HA	5:D2:259:VAL:HG12	1.83	0.59
4:K1:13:PRO:HG3	4:K1:220:LEU:HB3	1.85	0.59
4:K1:227:ILE:HA	4:K1:230:GLU:HG3	1.85	0.59
5:A2:39:LEU:HB3	5:A2:44:LEU:HD21	1.85	0.59
1:B1:63:SER:HB3	1:B1:101:MET:HE3	1.83	0.58
4:K1:124:LYS:HD3	4:K1:127:LYS:HE2	1.85	0.58
5:A2:69:LEU:HD22	5:A2:191:GLU:HG2	1.84	0.58
5:D2:33:SER:HA	5:D2:37:LEU:HD23	1.84	0.58
5:D2:75:PRO:HB3	5:D2:201:ALA:HB2	1.85	0.58
1:A1:211:MET:HB2	1:B1:214:PRO:HD3	1.85	0.58
1:A1:233:GLN:HA	1:A1:236:MET:HE2	1.86	0.58
5:B2:256:PRO:HA	5:B2:259:VAL:HG22	1.85	0.58
5:C2:214:LEU:HD11	5:D2:135:ILE:HG21	1.84	0.58
1:C1:233:GLN:HG3	1:D1:149:LEU:HD21	1.86	0.58
1:E1:126:ALA:HA	1:E1:129:LYS:HG2	1.85	0.58
4:K1:24:GLU:HG2	4:K1:26:GLN:OE1	2.04	0.58
5:E2:130:PHE:HE2	5:E2:216:MET:HG2	1.69	0.58
5:G2:74:PHE:HD2	5:G2:198:MET:HE1	1.68	0.58
5:I2:34:MET:HA	5:I2:39:LEU:HD11	1.86	0.58
2:F1:72:TRP:HA	2:F1:75:MET:HE3	1.85	0.58
5:F2:25:PRO:HG2	5:H2:294:LEU:HD11	1.86	0.57
5:D2:308:MET:HG2	5:D2:309:PRO:HD2	1.86	0.57
5:I2:235:ILE:O	5:I2:239:ALA:CB	2.53	0.57
4:K1:224:ARG:HA	4:K1:227:ILE:HG12	1.86	0.57
5:G2:81:THR:HA	5:G2:84:LEU:HD12	1.86	0.57
5:A2:98:MET:HE2	5:B2:125:ILE:HB	1.86	0.57
5:G2:235:ILE:O	5:G2:239:ALA:HB3	2.04	0.57
5:H2:255:ILE:HD13	5:H2:258:LEU:HD21	1.86	0.57
1:E1:239:LEU:HD22	4:K1:67:PHE:HZ	1.69	0.57
4:K1:41:VAL:HG11	4:K1:103:VAL:HG21	1.87	0.57
5:A2:119:VAL:HG12	5:A2:121:GLY:H	1.69	0.57
5:G2:93:THR:HA	5:G2:96:ILE:HG22	1.86	0.57
1:D1:199:VAL:HG23	3:J1:21:ALA:HB2	1.85	0.57
1:E1:121:ILE:HG12	1:E1:126:ALA:HB2	1.86	0.57
2:F1:175:ALA:O	2:F1:178:LEU:HG	2.04	0.57
5:A2:200:GLY:HA2	5:A2:203:LYS:HE2	1.87	0.57
5:A2:316:PHE:HE2	5:I2:50:PHE:HD1	1.51	0.57
5:F2:277:VAL:O	5:F2:281:MET:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F1:127:ARG:O	2:F1:131:MET:HG2	2.05	0.56
5:D2:86:LEU:HD13	5:E2:136:ILE:HD13	1.86	0.56
1:B1:77:ALA:HB2	1:B1:190:PHE:CE1	2.40	0.56
5:D2:148:ILE:HG22	5:D2:268:VAL:HG22	1.87	0.56
5:G2:69:LEU:HD21	5:G2:190:GLN:HB3	1.88	0.56
3:J1:53:PRO:HA	3:J1:56:VAL:HG12	1.88	0.56
5:H2:256:PRO:HA	5:H2:259:VAL:HG22	1.86	0.56
1:C1:143:ARG:HG3	1:C1:144:GLU:H	1.69	0.56
5:C2:113:ALA:O	5:C2:117:PHE:HB2	2.05	0.56
5:F2:290:ARG:HD3	5:F2:293:LEU:HD21	1.88	0.56
5:H2:277:VAL:O	5:H2:281:MET:HG2	2.05	0.56
5:I2:133:LEU:HD23	5:I2:136:ILE:HD11	1.87	0.56
2:F1:20:LEU:HB2	2:F1:51:THR:HG21	1.86	0.56
5:B2:57:MET:HE1	5:C2:285:LEU:HB3	1.88	0.56
5:G2:147:ARG:O	5:G2:150:GLU:HG3	2.06	0.55
5:G2:251:LEU:HA	5:G2:254:GLN:HE21	1.70	0.55
1:C1:83:ALA:HB3	1:C1:84:PRO:HD3	1.89	0.55
2:F1:104:LEU:HB3	2:F1:113:PHE:HZ	1.70	0.55
3:J1:81:PHE:HA	3:J1:84:LEU:HG	1.88	0.55
5:A2:267:ILE:HG22	5:A2:268:VAL:HG23	1.88	0.55
5:C2:69:LEU:HD21	5:C2:190:GLN:HB2	1.89	0.55
5:B2:235:ILE:O	5:B2:239:ALA:HB2	2.07	0.55
1:E1:116:PHE:HE2	1:E1:123:MET:HB3	1.72	0.55
5:C2:296:ALA:HB2	5:C2:320:LEU:HD22	1.88	0.55
5:G2:72:ALA:HB1	5:H2:271:VAL:HG21	1.87	0.55
1:B1:211:MET:HE3	2:F1:114:VAL:HG22	1.88	0.55
5:B2:234:SER:HB3	5:B2:237:SER:HB3	1.88	0.55
1:E1:188:THR:HA	1:E1:191:ILE:HD12	1.88	0.55
5:D2:235:ILE:O	5:D2:239:ALA:HB3	2.05	0.55
5:G2:235:ILE:O	5:G2:239:ALA:HB2	2.05	0.55
5:A2:160:MET:HE1	5:A2:188:VAL:HB	1.87	0.55
5:I2:256:PRO:HA	5:I2:259:VAL:HG22	1.89	0.55
1:A1:74:LEU:HD13	1:A1:235:LEU:HD21	1.88	0.55
2:F1:197:LEU:HD13	2:F1:224:VAL:HG21	1.87	0.55
5:B2:114:PHE:HA	5:C2:308:MET:HE1	1.87	0.55
5:E2:196:GLY:HA3	5:F2:155:PHE:HE2	1.72	0.55
1:B1:199:VAL:HG23	3:H1:21:ALA:HB2	1.88	0.55
1:D1:54:LEU:HD23	1:D1:57:ILE:HD11	1.89	0.55
1:E1:80:THR:HB	1:E1:83:ALA:HB2	1.89	0.55
3:H1:46:GLU:HG2	3:H1:49:LEU:HD12	1.89	0.55
5:E2:74:PHE:CD2	5:E2:198:MET:HE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E2:277:VAL:O	5:E2:281:MET:HG2	2.07	0.55
5:G2:218:ILE:HA	5:G2:221:VAL:HG22	1.88	0.55
5:H2:75:PRO:HD3	5:H2:194:PHE:HE1	1.71	0.55
1:B1:71:PHE:HB3	1:B1:89:LEU:HD23	1.89	0.55
1:E1:199:VAL:O	1:E1:203:VAL:HG12	2.07	0.55
5:A2:235:ILE:O	5:A2:239:ALA:CB	2.55	0.55
5:B2:265:GLY:O	5:B2:269:THR:HB	2.06	0.55
1:E1:66:ARG:HG2	1:E1:182:ALA:HB2	1.89	0.54
5:E2:215:ILE:HA	5:E2:218:ILE:HG22	1.88	0.54
5:F2:92:SER:HA	5:F2:95:ILE:HG22	1.88	0.54
2:F1:26:LEU:HD22	2:F1:150:LEU:HD13	1.89	0.54
5:C2:127:ILE:HD13	5:C2:247:ILE:HD13	1.89	0.54
5:C2:230:GLN:HE22	5:C2:231:HIS:CD2	2.25	0.54
1:A1:143:ARG:HE	1:A1:144:GLU:H	1.55	0.54
1:D1:184:GLN:NE2	3:J1:1:MET:HB2	2.22	0.54
1:D1:220:PRO:O	1:D1:224:MET:HG2	2.08	0.54
5:I2:76:THR:O	5:I2:79:LEU:HB3	2.07	0.54
3:G1:48:THR:HA	3:G1:51:PHE:HD2	1.72	0.54
3:I1:52:ILE:HD12	3:J1:29:LEU:HB2	1.88	0.54
4:K1:69:HIS:O	4:K1:72:VAL:HG12	2.07	0.54
5:C2:133:LEU:HD23	5:C2:136:ILE:HD11	1.88	0.54
1:A1:43:GLN:HG2	1:A1:123:MET:HE1	1.90	0.54
1:E1:100:ILE:HG22	1:E1:101:MET:HE2	1.90	0.54
2:F1:192:THR:O	2:F1:195:LEU:HB3	2.08	0.54
5:I2:130:PHE:CZ	5:I2:216:MET:HG3	2.41	0.54
5:E2:235:ILE:O	5:E2:239:ALA:HB3	2.06	0.54
5:H2:37:LEU:HB3	5:H2:39:LEU:HG	1.89	0.54
5:A2:135:ILE:HG21	5:I2:214:LEU:HD11	1.90	0.54
1:A1:226:PHE:O	1:A1:229:VAL:HG12	2.08	0.54
1:B1:181:THR:HB	3:H1:88:ILE:HD11	1.90	0.54
4:K1:45:ILE:HD11	4:K1:96:LEU:HD12	1.90	0.54
5:B2:74:PHE:HD2	5:B2:198:MET:HE1	1.73	0.54
5:F2:122:ASN:HD21	5:F2:124:ALA:HB3	1.73	0.54
1:D1:77:ALA:HB2	1:D1:190:PHE:CE1	2.43	0.54
4:K1:29:ARG:HD3	4:K1:111:LEU:HG	1.89	0.54
1:C1:92:LEU:HD11	1:C1:236:MET:HE1	1.90	0.53
5:E2:92:SER:HA	5:E2:95:ILE:HG22	1.89	0.53
5:G2:119:VAL:HG23	5:G2:121:GLY:H	1.74	0.53
1:B1:195:ILE:HD11	3:H1:13:ALA:HB1	1.90	0.53
5:F2:24:GLY:HA3	5:G2:63:MET:HE3	1.89	0.53
5:F2:86:LEU:HD13	5:G2:136:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B1:63:SER:HB2	1:B1:243:PHE:CE1	2.44	0.53
3:J1:39:GLN:HE21	3:J1:49:LEU:HD12	1.73	0.53
5:G2:51:ASN:HD21	5:G2:84:LEU:HB3	1.73	0.53
1:D1:38:TRP:HB3	1:D1:42:VAL:HB	1.90	0.53
1:D1:219:LEU:HB3	1:D1:220:PRO:HD3	1.91	0.53
1:D1:223:LEU:HD13	1:E1:187:PHE:CE1	2.43	0.53
1:E1:85:PRO:HD3	2:F1:96:ARG:HD2	1.91	0.53
5:A2:98:MET:HE3	5:B2:120:GLY:H	1.73	0.53
5:C2:86:LEU:HD13	5:D2:136:ILE:HD11	1.91	0.53
5:B2:233:MET:HE2	5:B2:238:ALA:HB3	1.91	0.53
5:I2:176:ILE:HD12	5:I2:180:GLU:HB3	1.91	0.53
1:E1:211:MET:H	2:F1:205:ASN:HD21	1.57	0.53
2:F1:196:THR:HG22	4:K1:190:VAL:HG23	1.91	0.53
3:G1:6:VAL:HG13	3:G1:7:MET:HE2	1.91	0.53
3:J1:48:THR:HA	3:J1:51:PHE:HB3	1.90	0.53
5:F2:235:ILE:O	5:F2:239:ALA:CB	2.57	0.53
1:E1:238:SER:HA	1:E1:241:GLN:HG3	1.91	0.53
5:E2:25:PRO:HD3	5:F2:63:MET:HE1	1.90	0.53
5:F2:39:LEU:HB2	5:F2:94:ARG:NH2	2.23	0.53
5:F2:73:ALA:H	5:G2:284:GLN:NE2	2.06	0.52
5:F2:235:ILE:O	5:F2:239:ALA:HB2	2.09	0.52
5:G2:85:ARG:HH22	5:G2:260:ILE:HG12	1.73	0.52
1:A1:200:ILE:HD13	1:A1:218:ALA:HA	1.90	0.52
5:A2:125:ILE:HG23	5:I2:97:LEU:HD11	1.90	0.52
5:D2:270:ARG:HE	5:D2:272:SER:HA	1.75	0.52
5:G2:270:ARG:HE	5:G2:272:SER:HA	1.73	0.52
1:B1:55:PRO:O	1:B1:59:LEU:HB2	2.09	0.52
2:F1:237:ALA:HB2	3:G1:7:MET:HE3	1.91	0.52
5:E2:33:SER:HA	5:E2:37:LEU:HD13	1.91	0.52
5:E2:133:LEU:HB3	5:E2:254:GLN:NE2	2.25	0.52
2:F1:207:MET:CG	4:K1:152:LYS:HD3	2.38	0.52
5:H2:130:PHE:CZ	5:H2:216:MET:HG3	2.45	0.52
5:A2:148:ILE:HA	5:A2:151:VAL:HG22	1.90	0.52
1:E1:83:ALA:HB1	2:F1:97:THR:HG23	1.91	0.52
1:E1:195:ILE:HD13	4:K1:85:LEU:HB3	1.91	0.52
5:C2:125:ILE:HA	5:C2:128:VAL:HG12	1.92	0.52
1:D1:187:PHE:O	1:D1:191:ILE:HG12	2.10	0.52
1:E1:241:GLN:HE22	4:K1:68:ASP:HA	1.74	0.52
3:I1:31:THR:HG23	3:I1:54:LYS:HG2	1.92	0.52
5:C2:218:ILE:HA	5:C2:221:VAL:HG12	1.91	0.52
5:D2:95:ILE:HG23	5:D2:107:ALA:HB1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B2:97:LEU:HB2	5:C2:125:ILE:HD12	1.91	0.51
5:I2:134:VAL:HG11	5:I2:213:ILE:HB	1.93	0.51
1:B1:75:ARG:HH12	1:B1:82:SER:HA	1.76	0.51
5:B2:69:LEU:HD13	5:B2:191:GLU:HA	1.91	0.51
5:B2:98:MET:HE1	5:C2:119:VAL:HA	1.92	0.51
1:C1:227:VAL:HG11	1:D1:187:PHE:HE2	1.75	0.51
5:H2:54:LEU:O	5:H2:57:MET:HG3	2.11	0.51
1:A1:57:ILE:HG13	1:A1:61:MET:HE2	1.93	0.51
5:D2:182:LYS:HA	5:D2:185:ARG:HG2	1.93	0.51
2:F1:97:THR:O	2:F1:100:GLU:HG3	2.10	0.51
3:G1:47:MET:HB3	3:G1:51:PHE:HE2	1.75	0.51
3:G1:2:THR:HG23	3:G1:5:SER:H	1.76	0.51
4:K1:13:PRO:HD3	4:K1:221:ARG:HG2	1.93	0.51
5:C2:164:GLN:HG3	5:C2:165:MET:HE2	1.92	0.51
5:D2:135:ILE:HG23	5:D2:139:MET:HE2	1.91	0.51
1:A1:209:MET:HE1	1:B1:202:SER:HA	1.92	0.51
1:B1:207:LEU:HG	1:B1:209:MET:HE2	1.93	0.51
2:F1:139:THR:HA	3:G1:1:MET:HE1	1.93	0.51
5:C2:255:ILE:O	5:C2:258:LEU:HG	2.11	0.51
5:G2:65:THR:HG23	5:G2:270:ARG:HH11	1.76	0.51
5:H2:85:ARG:CZ	5:H2:257:ALA:HB2	2.41	0.51
3:J1:85:PRO:HA	3:J1:88:ILE:HG12	1.92	0.51
5:B2:197:SER:HA	5:C2:148:ILE:HD11	1.91	0.51
5:I2:199:ASP:O	5:I2:203:LYS:HD2	2.11	0.51
2:F1:87:THR:HG21	2:F1:251:LEU:HD13	1.93	0.51
5:D2:209:ALA:O	5:D2:213:ILE:HG23	2.11	0.51
5:E2:22:LEU:HA	5:E2:25:PRO:HG2	1.92	0.51
1:B1:204:LEU:HD21	1:B1:212:VAL:HB	1.93	0.50
1:D1:79:GLY:HA3	1:D1:219:LEU:HD12	1.92	0.50
1:A1:196:ILE:HA	1:A1:199:VAL:HG12	1.93	0.50
4:K1:102:LEU:HG	4:K1:106:ILE:HD13	1.93	0.50
5:D2:129:VAL:HA	5:D2:132:ILE:HD12	1.93	0.50
5:F2:130:PHE:CD2	5:F2:216:MET:HG2	2.46	0.50
5:H2:235:ILE:O	5:H2:239:ALA:CB	2.58	0.50
4:K1:216:HIS:CE1	4:K1:220:LEU:HD11	2.46	0.50
5:D2:171:LEU:HD22	5:D2:181:ALA:HB2	1.94	0.50
5:F2:94:ARG:HH12	5:F2:95:ILE:HB	1.75	0.50
5:I2:32:LEU:O	5:I2:36:VAL:HG22	2.11	0.50
5:I2:96:ILE:HD11	5:I2:219:ASN:HD21	1.76	0.50
1:A1:45:LEU:HD12	1:A1:48:ILE:HD11	1.92	0.50
1:C1:232:TRP:HA	1:C1:235:LEU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D1:107:LYS:HD3	1:D1:133:PRO:HB3	1.93	0.50
5:A2:96:ILE:HG13	5:A2:245:LEU:HD23	1.93	0.50
1:E1:38:TRP:HB3	1:E1:42:VAL:HB	1.92	0.50
5:A2:131:ILE:HA	5:A2:134:VAL:HG12	1.93	0.50
5:E2:76:THR:HG22	5:F2:269:THR:HG23	1.94	0.50
5:F2:252:VAL:HA	5:F2:255:ILE:HD12	1.93	0.50
5:I2:78:LEU:HD12	5:I2:201:ALA:HB1	1.93	0.50
5:I2:215:ILE:HA	5:I2:218:ILE:HG22	1.93	0.50
5:F2:39:LEU:HA	5:F2:43:ILE:HD11	1.93	0.50
1:B1:235:LEU:HA	3:H1:81:PHE:CZ	2.47	0.50
1:E1:107:LYS:HA	1:E1:110:VAL:HG22	1.94	0.50
3:I1:2:THR:HG23	3:I1:5:SER:H	1.75	0.50
5:A2:20:GLN:HA	5:B2:282:VAL:HG21	1.94	0.50
1:B1:238:SER:OG	3:H1:85:PRO:HD3	2.12	0.50
1:C1:212:VAL:HG12	1:D1:214:PRO:HG2	1.94	0.50
1:C1:220:PRO:HB3	1:D1:190:PHE:CD2	2.46	0.50
5:D2:270:ARG:HH21	5:D2:272:SER:HA	1.76	0.50
5:E2:235:ILE:O	5:E2:239:ALA:HB2	2.12	0.50
5:H2:206:ARG:O	5:H2:210:ILE:HG12	2.11	0.50
5:B2:206:ARG:HH22	5:C2:143:LYS:HE2	1.76	0.49
5:C2:75:PRO:HD3	5:C2:194:PHE:HE1	1.77	0.49
5:D2:142:THR:HB	5:D2:206:ARG:HG2	1.94	0.49
5:G2:164:GLN:HG3	5:G2:165:MET:HE2	1.92	0.49
1:A1:220:PRO:HG3	1:B1:194:LEU:HD11	1.94	0.49
3:J1:42:THR:HA	4:K1:115:ILE:O	2.12	0.49
4:K1:28:PRO:HD3	4:K1:216:HIS:CE1	2.47	0.49
5:B2:29:LEU:HD21	5:D2:298:VAL:HG13	1.94	0.49
5:F2:281:MET:O	5:F2:285:LEU:HB2	2.12	0.49
1:B1:121:ILE:HD12	1:B1:126:ALA:HB2	1.93	0.49
5:H2:171:LEU:HD22	5:H2:181:ALA:HB2	1.94	0.49
5:F2:94:ARG:HH11	5:F2:94:ARG:HG2	1.78	0.49
5:A2:263:ALA:O	5:A2:267:ILE:HG12	2.12	0.49
5:B2:164:GLN:HA	5:B2:167:ILE:HG12	1.95	0.49
5:D2:210:ILE:O	5:D2:213:ILE:HG12	2.12	0.49
5:D2:265:GLY:O	5:D2:269:THR:HB	2.12	0.49
5:H2:67:ARG:C	5:H2:270:ARG:HH12	2.20	0.49
1:B1:138:MET:HE1	1:B1:171:LEU:HD22	1.94	0.49
1:C1:220:PRO:HA	1:C1:223:LEU:HD23	1.94	0.49
3:I1:22:ALA:O	3:I1:26:LEU:HB2	2.12	0.49
5:B2:216:MET:HE2	5:B2:219:ASN:HD22	1.76	0.49
5:C2:78:LEU:HD12	5:C2:201:ALA:HB1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E2:171:LEU:HD22	5:E2:181:ALA:HB2	1.95	0.49
5:F2:20:GLN:HE21	5:G2:282:VAL:HG11	1.78	0.49
5:I2:39:LEU:HD12	5:I2:91:ALA:HB1	1.94	0.49
1:B1:224:MET:HA	1:B1:227:VAL:HG12	1.95	0.49
1:C1:196:ILE:HA	1:C1:199:VAL:HG12	1.94	0.49
3:I1:59:PHE:O	3:I1:62:ILE:HG22	2.13	0.49
5:D2:126:GLY:C	5:D2:247:ILE:HG12	2.38	0.49
5:F2:248:GLY:O	5:F2:252:VAL:HG23	2.13	0.49
5:G2:184:ARG:O	5:G2:187:GLU:HG2	2.13	0.49
1:B1:184:GLN:HB2	3:H1:1:MET:HE1	1.95	0.49
1:D1:223:LEU:HB3	1:E1:187:PHE:CE2	2.48	0.49
3:G1:5:SER:O	3:G1:8:MET:HG2	2.13	0.49
3:G1:53:PRO:HA	3:G1:56:VAL:HG12	1.94	0.49
5:A2:201:ALA:HA	5:A2:204:PHE:CD2	2.47	0.49
5:B2:22:LEU:HA	5:B2:25:PRO:HG2	1.95	0.49
1:A1:185:ILE:HG23	3:G1:84:LEU:HD21	1.95	0.48
2:F1:95:VAL:HG22	2:F1:129:MET:HB3	1.93	0.48
2:F1:188:LEU:O	2:F1:192:THR:HG23	2.13	0.48
3:G1:44:ILE:HD11	3:H1:36:SER:C	2.37	0.48
5:I2:235:ILE:O	5:I2:239:ALA:HB2	2.13	0.48
1:A1:83:ALA:HB3	1:A1:84:PRO:HD3	1.96	0.48
1:E1:213:PRO:HD3	2:F1:213:ILE:HG21	1.94	0.48
2:F1:23:VAL:HG12	2:F1:150:LEU:HD21	1.94	0.48
1:A1:69:ILE:HD12	2:F1:38:ILE:HD13	1.95	0.48
5:D2:66:GLN:HG2	5:D2:276:ASP:OD1	2.13	0.48
5:G2:39:LEU:HB3	5:G2:44:LEU:HD21	1.96	0.48
5:G2:85:ARG:NH1	5:G2:257:ALA:HA	2.27	0.48
1:D1:38:TRP:HB2	1:D1:43:GLN:HB2	1.96	0.48
1:D1:75:ARG:HH22	1:D1:86:ASN:HA	1.78	0.48
1:E1:234:LEU:HD11	4:K1:65:LEU:HD13	1.94	0.48
5:E2:73:ALA:H	5:F2:284:GLN:NE2	2.12	0.48
5:B2:27:LEU:HD23	5:B2:31:ILE:HD11	1.95	0.48
5:D2:60:LEU:HD13	5:E2:295:ALA:HB2	1.95	0.48
5:G2:100:GLY:HA3	5:G2:242:TYR:CE1	2.44	0.48
1:A1:92:LEU:HD21	1:A1:236:MET:SD	2.53	0.48
5:C2:98:MET:HE2	5:D2:125:ILE:HD13	1.96	0.48
5:C2:135:ILE:O	5:C2:139:MET:HG3	2.13	0.48
5:F2:78:LEU:HD13	5:F2:201:ALA:HB1	1.94	0.48
5:F2:171:LEU:HD22	5:F2:181:ALA:HB2	1.94	0.48
5:I2:93:THR:HA	5:I2:96:ILE:HG12	1.96	0.48
3:I1:39:GLN:HE22	3:I1:46:GLU:HG3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E2:85:ARG:HD2	5:E2:253:ALA:O	2.14	0.48
3:G1:6:VAL:O	3:G1:9:MET:HG3	2.13	0.48
5:D2:235:ILE:O	5:D2:239:ALA:HB2	2.12	0.48
5:E2:157:LEU:HB2	5:F2:155:PHE:HE1	1.78	0.48
5:E2:164:GLN:HA	5:E2:167:ILE:HG12	1.95	0.48
5:G2:126:GLY:H	5:G2:129:VAL:HG22	1.79	0.48
1:B1:189:ILE:HD13	3:H1:81:PHE:HE1	1.78	0.48
1:C1:80:THR:HB	1:C1:83:ALA:HB2	1.96	0.48
5:A2:132:ILE:HG12	5:I2:90:VAL:HB	1.96	0.48
5:D2:86:LEU:O	5:D2:89:ASN:HB2	2.13	0.48
1:C1:63:SER:HB3	1:C1:97:THR:HG23	1.96	0.48
3:H1:44:ILE:HG13	3:I1:40:ALA:HB2	1.96	0.48
1:A1:223:LEU:HG	1:B1:187:PHE:CZ	2.49	0.47
1:D1:224:MET:HE1	4:K1:78:ILE:HD11	1.95	0.47
1:E1:88:VAL:HA	2:F1:86:PHE:CE1	2.49	0.47
3:I1:60:ILE:HA	3:I1:63:ILE:HD12	1.96	0.47
5:A2:27:LEU:O	5:A2:31:ILE:HG12	2.13	0.47
5:F2:27:LEU:O	5:F2:31:ILE:HG12	2.13	0.47
1:C1:205:MET:HE2	1:C1:205:MET:HB2	1.80	0.47
5:A2:71:PHE:CE2	5:A2:267:ILE:HD12	2.50	0.47
5:C2:48:PHE:HD1	5:C2:88:LEU:HD21	1.79	0.47
1:D1:224:MET:HE1	1:E1:191:ILE:HD11	1.96	0.47
5:B2:148:ILE:HA	5:B2:151:VAL:HG22	1.96	0.47
5:D2:83:LEU:HD12	5:D2:86:LEU:HD11	1.96	0.47
5:E2:230:GLN:HG3	5:E2:231:HIS:ND1	2.29	0.47
5:F2:148:ILE:HA	5:F2:151:VAL:HG22	1.95	0.47
5:F2:164:GLN:HG3	5:F2:165:MET:HE2	1.95	0.47
5:I2:171:LEU:HD22	5:I2:181:ALA:HB2	1.94	0.47
1:A1:195:ILE:HD11	3:G1:13:ALA:HB1	1.97	0.47
1:E1:61:MET:HE1	1:E1:138:MET:HE2	1.96	0.47
5:B2:125:ILE:HA	5:B2:128:VAL:HG12	1.95	0.47
5:D2:161:PRO:HA	5:D2:164:GLN:HE21	1.80	0.47
5:H2:255:ILE:O	5:H2:258:LEU:HG	2.13	0.47
1:D1:65:THR:O	1:D1:69:ILE:HG12	2.15	0.47
3:H1:76:TYR:OH	3:H1:80:LEU:HD12	2.13	0.47
5:B2:73:ALA:H	5:C2:284:GLN:HE22	1.63	0.47
5:H2:203:LYS:HE2	5:I2:147:ARG:CZ	2.44	0.47
5:I2:69:LEU:HD13	5:I2:191:GLU:HA	1.97	0.47
3:G1:63:ILE:HD11	3:H1:14:MET:HB2	1.95	0.47
3:I1:69:MET:HE2	3:I1:69:MET:HB2	1.73	0.47
5:B2:28:ILE:HG12	5:C2:59:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D2:136:ILE:HD12	5:D2:136:ILE:HA	1.78	0.47
1:E1:43:GLN:HE22	1:E1:123:MET:HG2	1.79	0.47
2:F1:23:VAL:O	2:F1:27:ILE:HG12	2.15	0.47
2:F1:73:LEU:HD21	2:F1:159:ILE:HG23	1.96	0.47
4:K1:15:PRO:HA	4:K1:18:LEU:HD12	1.97	0.47
5:A2:22:LEU:HA	5:A2:25:PRO:HG2	1.95	0.47
5:A2:36:VAL:HG22	5:B2:118:LEU:HD22	1.96	0.47
5:A2:70:ASP:O	5:B2:284:GLN:HG2	2.15	0.47
5:A2:235:ILE:O	5:A2:239:ALA:HB3	2.13	0.47
5:B2:27:LEU:O	5:B2:31:ILE:HG13	2.15	0.47
5:B2:218:ILE:HA	5:B2:221:VAL:HG12	1.96	0.47
5:B2:235:ILE:O	5:B2:239:ALA:HB3	2.14	0.47
5:C2:54:LEU:O	5:C2:57:MET:HG3	2.13	0.47
5:D2:266:VAL:HA	5:D2:269:THR:HG22	1.96	0.47
5:F2:91:ALA:HA	5:F2:94:ARG:CD	2.45	0.47
3:G1:52:ILE:HA	3:G1:55:ILE:HD12	1.97	0.47
3:I1:53:PRO:HA	3:I1:56:VAL:HG12	1.96	0.47
5:A2:284:GLN:NE2	5:I2:73:ALA:H	2.13	0.47
1:A1:223:LEU:HG	1:B1:187:PHE:CE1	2.49	0.47
1:B1:135:ARG:O	1:B1:138:MET:HG2	2.14	0.47
2:F1:224:VAL:O	2:F1:228:LEU:HG	2.15	0.47
5:B2:130:PHE:CZ	5:B2:216:MET:HG3	2.50	0.47
5:D2:30:LEU:O	5:D2:34:MET:HG2	2.15	0.47
5:D2:62:ALA:HB1	5:D2:267:ILE:HG13	1.95	0.47
5:D2:94:ARG:NH2	5:E2:118:LEU:HB3	2.30	0.47
5:G2:95:ILE:HG23	5:G2:107:ALA:HB1	1.96	0.47
5:H2:78:LEU:HD21	5:H2:205:VAL:HB	1.96	0.47
5:I2:160:MET:HE1	5:I2:188:VAL:HG22	1.97	0.47
1:E1:85:PRO:HB2	1:E1:87:GLN:HB2	1.96	0.47
1:E1:185:ILE:HG12	4:K1:71:MET:HG2	1.96	0.47
5:C2:134:VAL:HG11	5:C2:213:ILE:HD12	1.97	0.47
5:E2:255:ILE:O	5:E2:258:LEU:HG	2.15	0.47
1:C1:67:ILE:HD12	1:C1:239:LEU:HD23	1.97	0.46
1:C1:195:ILE:HD11	3:I1:13:ALA:HB1	1.97	0.46
1:C1:223:LEU:HD12	1:D1:183:PHE:CD2	2.51	0.46
4:K1:124:LYS:HG2	4:K1:127:LYS:HG2	1.97	0.46
5:A2:133:LEU:HD22	5:A2:254:GLN:CD	2.40	0.46
5:C2:67:ARG:HB2	5:C2:70:ASP:CG	2.40	0.46
5:E2:137:ASN:ND2	5:E2:254:GLN:HE21	2.03	0.46
5:A2:282:VAL:HG21	5:I2:20:GLN:HG3	1.97	0.46
5:G2:148:ILE:HA	5:G2:151:VAL:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B1:192:PRO:HA	1:B1:195:ILE:HD12	1.97	0.46
1:C1:224:MET:O	1:C1:227:VAL:HG12	2.15	0.46
3:J1:84:LEU:HB2	3:J1:85:PRO:HD3	1.96	0.46
5:A2:151:VAL:O	5:A2:154:ARG:HG2	2.15	0.46
5:A2:184:ARG:HA	5:A2:184:ARG:HD3	1.75	0.46
5:H2:164:GLN:HA	5:H2:167:ILE:HG12	1.98	0.46
1:A1:85:PRO:O	1:A1:88:VAL:HG22	2.15	0.46
1:B1:193:PHE:HA	1:B1:196:ILE:HG22	1.97	0.46
5:A2:31:ILE:HD11	5:A2:84:LEU:HG	1.97	0.46
5:I2:148:ILE:HA	5:I2:151:VAL:HG22	1.96	0.46
1:A1:224:MET:O	1:A1:227:VAL:HG12	2.16	0.46
1:C1:174:TYR:O	1:C1:178:GLU:HG2	2.15	0.46
4:K1:236:GLY:HA3	5:E2:154:ARG:HH22	1.80	0.46
5:D2:59:LEU:O	5:D2:63:MET:HG3	2.16	0.46
5:F2:37:LEU:HD21	5:H2:302:LEU:HD11	1.96	0.46
5:H2:58:VAL:HG21	5:H2:77:ILE:HG21	1.97	0.46
1:A1:228:LEU:HD21	3:H1:6:VAL:HG11	1.97	0.46
1:C1:143:ARG:HG3	1:C1:144:GLU:N	2.30	0.46
1:D1:85:PRO:O	1:D1:88:VAL:HG22	2.16	0.46
1:D1:181:THR:O	1:D1:185:ILE:HG13	2.15	0.46
5:A2:220:VAL:HA	5:A2:246:THR:HG21	1.97	0.46
5:B2:133:LEU:HD12	5:B2:136:ILE:HD11	1.97	0.46
5:B2:292:MET:HG2	5:B2:320:LEU:HD21	1.98	0.46
5:F2:119:VAL:HB	5:F2:125:ILE:HD12	1.97	0.46
5:F2:270:ARG:HG2	5:F2:272:SER:H	1.81	0.46
1:D1:184:GLN:HA	1:D1:187:PHE:CD2	2.51	0.46
2:F1:104:LEU:HD21	2:F1:109:SER:HB2	1.97	0.46
4:K1:75:PRO:O	4:K1:78:ILE:HG22	2.16	0.46
5:B2:218:ILE:HD11	5:C2:132:ILE:HG12	1.98	0.46
5:C2:75:PRO:HB3	5:C2:201:ALA:HB2	1.98	0.46
5:F2:63:MET:HE2	5:F2:63:MET:HB3	1.77	0.46
5:G2:66:GLN:HG2	5:G2:276:ASP:OD1	2.16	0.46
5:H2:156:VAL:O	5:H2:160:MET:HG2	2.16	0.46
5:H2:235:ILE:O	5:H2:239:ALA:HB2	2.16	0.46
2:F1:84:LEU:HD13	2:F1:251:LEU:HD11	1.98	0.46
5:A2:113:ALA:HA	5:A2:116:HIS:CE1	2.51	0.46
5:A2:130:PHE:HD1	5:A2:133:LEU:HD21	1.79	0.46
5:F2:215:ILE:HD11	5:G2:132:ILE:HG12	1.98	0.46
5:H2:39:LEU:HA	5:H2:43:ILE:HD11	1.98	0.46
5:I2:202:SER:O	5:I2:205:VAL:HG12	2.16	0.46
1:E1:204:LEU:O	1:E1:209:MET:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F1:49:MET:HE2	2:F1:49:MET:HB2	1.80	0.46
2:F1:192:THR:O	2:F1:196:THR:HG23	2.16	0.46
5:B2:114:PHE:HE1	5:B2:251:LEU:HD23	1.80	0.46
5:C2:277:VAL:O	5:C2:281:MET:HG2	2.16	0.46
5:F2:91:ALA:HA	5:F2:94:ARG:NE	2.31	0.46
5:G2:38:PRO:HA	5:G2:94:ARG:CZ	2.46	0.46
5:G2:78:LEU:HD13	5:G2:201:ALA:HB1	1.97	0.46
1:A1:57:ILE:HG13	1:A1:61:MET:HB2	1.97	0.45
1:E1:191:ILE:HD13	4:K1:82:ILE:HD11	1.97	0.45
5:C2:67:ARG:NH2	5:C2:274:ASP:HA	2.31	0.45
5:D2:202:SER:O	5:D2:205:VAL:HG12	2.16	0.45
5:H2:143:LYS:HA	5:H2:206:ARG:NE	2.29	0.45
5:H2:148:ILE:HA	5:H2:151:VAL:HG22	1.97	0.45
1:B1:196:ILE:HA	1:B1:199:VAL:HG12	1.98	0.45
3:G1:83:ASN:O	3:G1:87:ILE:HG12	2.16	0.45
3:J1:6:VAL:HA	3:J1:9:MET:HE3	1.97	0.45
5:A2:71:PHE:CE2	5:A2:194:PHE:HZ	2.34	0.45
5:B2:32:LEU:HA	5:B2:35:MET:HG2	1.98	0.45
5:D2:123:PHE:O	5:D2:127:ILE:HG22	2.15	0.45
5:F2:67:ARG:HA	5:F2:270:ARG:HH22	1.82	0.45
5:F2:149:ALA:HB1	5:F2:198:MET:HG3	1.99	0.45
5:G2:53:ALA:O	5:G2:57:MET:HG2	2.16	0.45
1:C1:210:MET:HG3	1:C1:211:MET:HG3	1.99	0.45
4:K1:27:ILE:HD12	4:K1:28:PRO:HD2	1.97	0.45
5:G2:129:VAL:HA	5:G2:132:ILE:HD12	1.98	0.45
1:A1:171:LEU:HG	2:F1:49:MET:HE3	1.99	0.45
2:F1:76:GLN:O	2:F1:79:LEU:HG	2.16	0.45
3:G1:16:VAL:HG21	3:G1:76:TYR:CE2	2.52	0.45
5:G2:89:ASN:O	5:G2:93:THR:HG23	2.16	0.45
5:G2:139:MET:HE3	5:G2:139:MET:HB3	1.88	0.45
5:H2:32:LEU:O	5:H2:36:VAL:HG22	2.16	0.45
3:H1:51:PHE:CE2	3:H1:55:ILE:HD11	2.52	0.45
5:E2:266:VAL:HA	5:E2:269:THR:HG22	1.99	0.45
5:G2:115:GLY:O	5:G2:119:VAL:HG22	2.17	0.45
5:H2:131:ILE:HA	5:H2:134:VAL:HG12	1.99	0.45
5:H2:300:GLY:O	5:H2:304:MET:HG2	2.16	0.45
1:C1:114:GLN:HB3	1:C1:115:PRO:HD3	1.99	0.45
2:F1:18:TRP:CH2	2:F1:63:THR:HB	2.48	0.45
2:F1:21:LEU:HD22	2:F1:77:GLN:HB2	1.98	0.45
5:C2:226:VAL:HA	5:C2:229:LEU:HG	1.97	0.45
5:D2:113:ALA:O	5:D2:117:PHE:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E2:186:SER:O	5:E2:190:GLN:HG2	2.17	0.45
5:I2:136:ILE:O	5:I2:140:VAL:HB	2.17	0.45
5:I2:303:GLY:HA2	5:I2:308:MET:HE1	1.99	0.45
1:A1:143:ARG:HE	1:A1:144:GLU:HG2	1.81	0.45
5:A2:256:PRO:HA	5:A2:259:VAL:HG22	1.98	0.45
5:C2:60:LEU:HD21	5:D2:295:ALA:HB2	1.98	0.45
5:D2:278:GLY:O	5:D2:281:MET:HG3	2.17	0.45
5:E2:201:ALA:HA	5:E2:204:PHE:HD2	1.82	0.45
5:F2:216:MET:HE1	5:F2:246:THR:HG23	1.99	0.45
5:G2:34:MET:HB3	5:G2:87:ALA:HB1	1.98	0.45
5:G2:87:ALA:O	5:G2:90:VAL:HG22	2.17	0.45
5:H2:215:ILE:HA	5:H2:218:ILE:HG12	1.98	0.45
1:B1:101:MET:HE1	1:B1:137:PHE:CZ	2.51	0.45
1:B1:174:TYR:O	1:B1:178:GLU:HG2	2.17	0.45
1:C1:74:LEU:HD12	1:C1:189:ILE:HG21	1.99	0.45
1:D1:181:THR:HA	1:D1:184:GLN:OE1	2.16	0.45
2:F1:13:LEU:O	2:F1:17:PHE:HB2	2.16	0.45
2:F1:157:LEU:HD21	2:F1:255:VAL:HG21	1.99	0.45
5:C2:186:SER:O	5:C2:190:GLN:HG2	2.17	0.45
5:E2:31:ILE:HD12	5:E2:83:LEU:HG	1.98	0.45
5:E2:71:PHE:CD1	5:F2:284:GLN:HB3	2.52	0.45
5:H2:43:ILE:O	5:H2:46:LEU:HG	2.16	0.45
5:H2:96:ILE:HD11	5:H2:245:LEU:HB3	1.99	0.45
1:A1:203:VAL:HA	3:G1:25:LEU:HD21	1.98	0.45
1:B1:115:PRO:HB2	1:B1:121:ILE:HD13	1.99	0.45
5:B2:83:LEU:HA	5:B2:86:LEU:HG	1.99	0.45
5:C2:180:GLU:HA	5:C2:183:LYS:HG2	1.99	0.45
5:C2:196:GLY:HA3	5:D2:155:PHE:HE2	1.82	0.45
5:D2:200:GLY:HA3	5:E2:148:ILE:CG2	2.47	0.45
5:I2:93:THR:HG22	5:I2:97:LEU:HD23	1.98	0.45
1:A1:167:MET:HB3	1:A1:167:MET:HE3	1.77	0.45
1:C1:85:PRO:O	1:C1:88:VAL:HG22	2.16	0.45
1:D1:141:GLN:NE2	1:D1:243:PHE:HA	2.32	0.45
2:F1:20:LEU:HA	2:F1:23:VAL:HG22	1.99	0.45
4:K1:141:GLN:HA	4:K1:211:PHE:CZ	2.52	0.45
5:A2:27:LEU:HB3	5:A2:80:PHE:CE1	2.52	0.45
5:A2:271:VAL:HG13	5:A2:273:THR:H	1.82	0.45
5:G2:130:PHE:O	5:G2:134:VAL:HG22	2.16	0.45
5:H2:230:GLN:HG3	5:H2:231:HIS:ND1	2.32	0.45
2:F1:20:LEU:HD23	2:F1:24:LEU:HD23	1.99	0.44
5:C2:202:SER:O	5:C2:205:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C2:203:LYS:HA	5:C2:206:ARG:HG2	1.98	0.44
5:D2:164:GLN:HA	5:D2:167:ILE:HG12	1.99	0.44
5:F2:161:PRO:O	5:F2:164:GLN:HG2	2.17	0.44
1:B1:83:ALA:HB3	1:B1:84:PRO:HD3	1.98	0.44
1:B1:86:ASN:O	1:B1:88:VAL:N	2.49	0.44
2:F1:220:LEU:HD12	3:G1:29:LEU:HD21	1.98	0.44
5:B2:168:ASP:O	5:B2:172:ASN:HB2	2.17	0.44
5:F2:78:LEU:HD21	5:F2:205:VAL:HG13	1.98	0.44
1:A1:207:LEU:HD11	3:G1:55:ILE:HA	1.99	0.44
1:C1:147:LEU:HD21	1:C1:170:LEU:HA	1.99	0.44
1:D1:138:MET:HE3	1:D1:174:TYR:HB2	2.00	0.44
1:D1:143:ARG:HD2	1:D1:143:ARG:HA	1.62	0.44
5:B2:196:GLY:HA3	5:C2:155:PHE:HE2	1.81	0.44
5:F2:92:SER:O	5:F2:96:ILE:HG12	2.17	0.44
5:G2:113:ALA:HA	5:G2:116:HIS:NE2	2.32	0.44
1:A1:138:MET:HG3	1:A1:174:TYR:CG	2.53	0.44
3:I1:14:MET:HE2	3:I1:14:MET:HB3	1.83	0.44
5:A2:284:GLN:HE22	5:I2:73:ALA:H	1.63	0.44
5:C2:215:ILE:HA	5:C2:218:ILE:HG12	1.99	0.44
5:D2:33:SER:O	5:D2:37:LEU:HB2	2.17	0.44
5:D2:43:ILE:O	5:D2:46:LEU:HG	2.17	0.44
5:F2:266:VAL:HA	5:F2:269:THR:HG22	1.99	0.44
1:A1:229:VAL:HG23	3:G1:78:ARG:HG3	1.99	0.44
1:D1:230:ASP:HB3	1:E1:180:LYS:HZ3	1.82	0.44
3:H1:6:VAL:O	3:H1:9:MET:HG2	2.17	0.44
5:A2:305:VAL:HG13	5:A2:308:MET:HB2	1.98	0.44
5:B2:97:LEU:HD22	5:B2:226:VAL:HG21	1.99	0.44
5:G2:34:MET:HE1	5:G2:47:LEU:HD22	1.99	0.44
5:G2:149:ALA:HA	5:G2:268:VAL:HG21	1.98	0.44
1:B1:172:PRO:HA	1:B1:175:VAL:HG22	1.99	0.44
1:B1:205:MET:HB2	1:B1:205:MET:HE3	1.68	0.44
1:C1:100:ILE:HG22	1:C1:101:MET:HE2	2.00	0.44
5:F2:91:ALA:HA	5:F2:94:ARG:HD3	2.00	0.44
1:A1:184:GLN:HE21	3:G1:1:MET:HG3	1.83	0.44
1:D1:149:LEU:HA	1:D1:152:ARG:HD2	2.00	0.44
4:K1:131:LEU:HB3	4:K1:132:PRO:HD3	2.00	0.44
5:C2:95:ILE:HG12	5:C2:107:ALA:HB2	1.99	0.44
5:D2:200:GLY:HA3	5:E2:148:ILE:HG22	2.00	0.44
5:H2:287:SER:H	5:H2:292:MET:HE1	1.82	0.44
5:I2:100:GLY:C	5:I2:104:ALA:HA	2.43	0.44
1:B1:226:PHE:O	1:B1:229:VAL:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E1:104:VAL:O	1:E1:108:ILE:HG12	2.17	0.44
3:G1:1:MET:HE3	3:G1:1:MET:HB3	1.86	0.44
3:G1:2:THR:HG22	3:G1:5:SER:HB3	2.00	0.44
5:E2:148:ILE:HA	5:E2:151:VAL:HG22	1.98	0.44
1:B1:99:PHE:HE2	1:C1:172:PRO:HG3	1.83	0.44
1:C1:63:SER:O	1:C1:67:ILE:HG12	2.17	0.44
1:C1:101:MET:HE1	1:C1:137:PHE:CE2	2.53	0.44
1:C1:228:LEU:HD22	3:I1:74:LEU:HG	1.99	0.44
2:F1:96:ARG:HG3	2:F1:126:ALA:HB1	1.99	0.44
3:I1:49:LEU:HD21	3:J1:32:GLY:HA3	1.99	0.44
3:I1:52:ILE:HA	3:I1:55:ILE:HG22	1.99	0.44
5:C2:85:ARG:HH22	5:C2:260:ILE:HG21	1.81	0.44
5:E2:180:GLU:HB3	5:E2:184:ARG:NH1	2.33	0.44
5:E2:203:LYS:HA	5:E2:206:ARG:HG2	2.00	0.44
5:F2:54:LEU:HA	5:F2:57:MET:HG2	2.00	0.44
5:G2:160:MET:HE3	5:G2:160:MET:HB3	1.90	0.44
5:G2:293:LEU:HD23	5:G2:293:LEU:HA	1.87	0.44
5:I2:112:GLU:HG2	5:I2:116:HIS:CE1	2.52	0.44
1:E1:245:SER:HB3	4:K1:69:HIS:CD2	2.53	0.43
3:J1:39:GLN:HG2	3:J1:44:ILE:HG23	2.00	0.43
5:C2:198:MET:HE2	5:C2:268:VAL:HG12	1.99	0.43
5:D2:87:ALA:O	5:D2:90:VAL:HG12	2.18	0.43
5:E2:74:PHE:CD2	5:E2:267:ILE:HG21	2.53	0.43
5:H2:288:ASN:O	5:H2:291:VAL:HG12	2.18	0.43
1:A1:207:LEU:HD13	3:G1:58:VAL:HG11	1.99	0.43
1:D1:101:MET:HE1	1:D1:137:PHE:CE2	2.53	0.43
1:D1:207:LEU:HD13	1:D1:207:LEU:HA	1.82	0.43
1:E1:107:LYS:HD2	1:E1:133:PRO:HB3	2.00	0.43
3:J1:35:ILE:HG21	3:J1:50:SER:HA	2.00	0.43
5:A2:76:THR:HB	5:B2:269:THR:HG21	2.01	0.43
5:B2:196:GLY:HA3	5:C2:155:PHE:CE2	2.53	0.43
5:C2:85:ARG:HH12	5:C2:260:ILE:CD1	2.31	0.43
5:C2:255:ILE:O	5:C2:259:VAL:HG13	2.18	0.43
5:D2:130:PHE:CZ	5:D2:216:MET:HG3	2.53	0.43
5:G2:92:SER:HA	5:G2:95:ILE:HG22	2.00	0.43
5:G2:255:ILE:O	5:G2:259:VAL:HG13	2.18	0.43
5:H2:46:LEU:HB2	5:I2:316:PHE:CE2	2.53	0.43
5:I2:290:ARG:HA	5:I2:290:ARG:HD3	1.81	0.43
5:D2:183:LYS:O	5:D2:187:GLU:HG2	2.18	0.43
5:F2:160:MET:HE3	5:F2:160:MET:HB3	1.91	0.43
5:G2:82:THR:O	5:G2:85:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H2:74:PHE:HE2	5:H2:264:ALA:HA	1.82	0.43
5:H2:282:VAL:HG13	5:H2:286:PHE:HD2	1.83	0.43
1:A1:209:MET:N	1:B1:205:MET:HE1	2.33	0.43
1:A1:238:SER:OG	3:G1:85:PRO:HD3	2.17	0.43
1:C1:223:LEU:HD12	1:D1:183:PHE:CE2	2.53	0.43
5:B2:113:ALA:HB3	5:C2:309:PRO:HD3	2.00	0.43
5:B2:163:LYS:HD3	5:B2:163:LYS:HA	1.79	0.43
5:F2:80:PHE:O	5:F2:83:LEU:HG	2.18	0.43
5:H2:210:ILE:HG13	5:I2:139:MET:HE1	2.01	0.43
1:A1:183:PHE:CZ	2:F1:38:ILE:HD11	2.53	0.43
1:A1:200:ILE:HD11	1:A1:217:ILE:HG22	2.01	0.43
1:B1:182:ALA:O	1:B1:185:ILE:HG22	2.18	0.43
2:F1:111:ALA:HA	2:F1:114:VAL:HG12	1.99	0.43
2:F1:148:SER:O	2:F1:151:VAL:HG12	2.18	0.43
5:B2:48:PHE:O	5:B2:52:ILE:HG12	2.18	0.43
5:F2:295:ALA:HA	5:F2:298:VAL:HG22	2.00	0.43
5:G2:282:VAL:HG13	5:G2:286:PHE:HD2	1.83	0.43
5:H2:75:PRO:HD3	5:H2:194:PHE:CE1	2.51	0.43
1:A1:65:THR:O	1:A1:69:ILE:HG12	2.18	0.43
1:A1:86:ASN:O	1:A1:88:VAL:N	2.51	0.43
1:B1:185:ILE:HD12	1:B1:185:ILE:HA	1.81	0.43
2:F1:170:MET:HE2	2:F1:170:MET:HA	1.99	0.43
5:A2:203:LYS:HE3	5:B2:147:ARG:HB3	1.99	0.43
5:B2:131:ILE:HA	5:B2:134:VAL:HG12	1.99	0.43
5:C2:130:PHE:CE2	5:C2:216:MET:HG2	2.53	0.43
5:D2:41:ALA:HA	5:D2:44:LEU:HG	2.01	0.43
5:G2:22:LEU:HD23	5:G2:22:LEU:H	1.83	0.43
5:G2:304:MET:HE3	5:G2:304:MET:HB3	1.81	0.43
5:H2:69:LEU:HD21	5:H2:191:GLU:HA	2.00	0.43
1:E1:100:ILE:HD11	1:E1:240:ALA:HA	1.99	0.43
5:B2:298:VAL:O	5:B2:301:LEU:HG	2.19	0.43
5:D2:160:MET:HE3	5:D2:160:MET:HB3	1.87	0.43
5:D2:292:MET:HG3	5:D2:324:ALA:HB2	1.99	0.43
5:F2:113:ALA:HA	5:F2:116:HIS:CE1	2.53	0.43
5:G2:63:MET:HE2	5:G2:63:MET:HB2	1.88	0.43
5:H2:46:LEU:HB2	5:I2:316:PHE:CZ	2.53	0.43
1:C1:227:VAL:HG11	1:D1:187:PHE:CE2	2.53	0.43
1:D1:150:PHE:HB3	1:D1:169:ILE:HG23	1.99	0.43
2:F1:153:THR:O	2:F1:157:LEU:HB2	2.18	0.43
3:G1:52:ILE:HG23	3:H1:25:LEU:HD12	2.01	0.43
3:H1:51:PHE:CD2	3:H1:55:ILE:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C2:136:ILE:O	5:C2:140:VAL:HB	2.18	0.43
5:D2:85:ARG:HH21	5:D2:208:ASP:CG	2.27	0.43
5:G2:78:LEU:HD21	5:G2:205:VAL:HG13	2.00	0.43
5:G2:86:LEU:O	5:G2:90:VAL:HG13	2.19	0.43
5:I2:44:LEU:HA	5:I2:47:LEU:HB2	2.00	0.43
5:I2:48:PHE:HD1	5:I2:88:LEU:HD21	1.83	0.43
3:I1:6:VAL:O	3:I1:9:MET:HG2	2.19	0.43
5:A2:128:VAL:HA	5:A2:131:ILE:HG12	1.99	0.43
5:B2:132:ILE:O	5:B2:135:ILE:HG22	2.19	0.43
5:I2:28:ILE:HD12	5:I2:28:ILE:HA	1.89	0.43
1:C1:195:ILE:HG23	3:I1:17:ALA:HB2	2.00	0.43
1:E1:99:PHE:CG	2:F1:170:MET:HE3	2.54	0.43
1:E1:102:SER:HA	1:E1:105:ILE:HG12	2.01	0.43
3:G1:63:ILE:HD13	3:G1:63:ILE:HA	1.85	0.43
5:A2:59:LEU:HB2	5:A2:263:ALA:HB2	2.01	0.43
5:B2:85:ARG:HH12	5:B2:260:ILE:HD11	1.83	0.43
5:C2:134:VAL:HG11	5:C2:213:ILE:HB	2.00	0.43
5:C2:157:LEU:HD22	5:D2:155:PHE:HE1	1.84	0.43
5:D2:188:VAL:O	5:D2:191:GLU:HG2	2.18	0.43
5:E2:130:PHE:HD2	5:E2:216:MET:HE3	1.84	0.43
5:E2:203:LYS:HD3	5:F2:147:ARG:HD2	2.01	0.43
5:H2:161:PRO:O	5:H2:164:GLN:HG2	2.19	0.43
5:I2:95:ILE:HG12	5:I2:107:ALA:HB2	2.01	0.43
5:I2:109:LYS:HE3	5:I2:109:LYS:HB3	1.86	0.43
1:B1:232:TRP:HA	1:B1:235:LEU:HB2	2.02	0.42
2:F1:136:LEU:HD21	3:G1:7:MET:HE3	2.01	0.42
4:K1:204:MET:HE3	4:K1:204:MET:HB3	1.81	0.42
5:A2:124:ALA:O	5:A2:128:VAL:HG22	2.18	0.42
5:B2:74:PHE:CD2	5:B2:198:MET:HE1	2.54	0.42
5:B2:235:ILE:HG13	5:B2:236:GLY:N	2.33	0.42
5:C2:143:LYS:HA	5:C2:206:ARG:HH21	1.84	0.42
5:D2:48:PHE:CZ	5:D2:252:VAL:HB	2.53	0.42
5:E2:292:MET:SD	5:E2:320:LEU:HD11	2.59	0.42
5:F2:212:GLY:O	5:F2:215:ILE:HG22	2.18	0.42
5:H2:214:LEU:O	5:H2:218:ILE:HG23	2.19	0.42
5:I2:32:LEU:HA	5:I2:35:MET:HG2	2.01	0.42
1:E1:233:GLN:OE1	2:F1:174:ARG:HA	2.19	0.42
5:A2:185:ARG:HA	5:A2:188:VAL:HG22	1.99	0.42
5:D2:43:ILE:O	5:D2:47:LEU:HG	2.19	0.42
5:D2:48:PHE:CE1	5:D2:252:VAL:HB	2.54	0.42
5:D2:75:PRO:O	5:D2:78:LEU:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D2:148:ILE:HA	5:D2:151:VAL:HG12	2.01	0.42
5:F2:281:MET:O	5:F2:285:LEU:CB	2.67	0.42
5:G2:20:GLN:HG3	5:H2:282:VAL:HG21	2.01	0.42
5:I2:78:LEU:O	5:I2:81:THR:HG22	2.19	0.42
1:C1:135:ARG:NH2	1:C1:165:VAL:H	2.18	0.42
4:K1:32:GLU:HG2	4:K1:205:VAL:HG23	2.00	0.42
5:A2:19:TRP:HA	5:A2:22:LEU:HG	2.00	0.42
5:A2:230:GLN:HG3	5:A2:231:HIS:ND1	2.34	0.42
5:F2:185:ARG:O	5:F2:188:VAL:HG12	2.20	0.42
5:H2:114:PHE:CE2	5:H2:118:LEU:HD12	2.55	0.42
5:I2:164:GLN:HA	5:I2:167:ILE:HG12	2.00	0.42
1:B1:220:PRO:HG3	1:C1:194:LEU:HD21	2.01	0.42
4:K1:28:PRO:HD3	4:K1:216:HIS:NE2	2.34	0.42
5:A2:194:PHE:CE1	5:A2:198:MET:HE3	2.55	0.42
5:A2:298:VAL:O	5:A2:301:LEU:HG	2.19	0.42
5:C2:85:ARG:HH22	5:C2:260:ILE:CG2	2.32	0.42
5:D2:190:GLN:HE22	5:E2:272:SER:C	2.27	0.42
5:D2:235:ILE:HG13	5:D2:236:GLY:N	2.34	0.42
5:E2:235:ILE:HG13	5:E2:236:GLY:N	2.34	0.42
5:F2:48:PHE:O	5:F2:52:ILE:HG12	2.19	0.42
5:G2:56:ILE:HG13	5:G2:57:MET:HE2	2.01	0.42
5:H2:92:SER:HA	5:H2:95:ILE:HG22	2.01	0.42
5:H2:270:ARG:HE	5:H2:272:SER:HA	1.84	0.42
5:I2:113:ALA:O	5:I2:117:PHE:HB2	2.19	0.42
5:I2:135:ILE:O	5:I2:139:MET:HG3	2.19	0.42
5:I2:235:ILE:O	5:I2:239:ALA:HB3	2.18	0.42
1:D1:134:LEU:O	1:D1:138:MET:HG3	2.18	0.42
3:G1:3:PRO:HA	3:G1:6:VAL:HG12	2.00	0.42
5:A2:150:GLU:HG3	5:A2:154:ARG:HH21	1.85	0.42
5:C2:55:SER:HB3	5:C2:85:ARG:HH21	1.85	0.42
5:C2:235:ILE:O	5:C2:239:ALA:HB2	2.19	0.42
5:E2:137:ASN:HD21	5:E2:254:GLN:NE2	2.06	0.42
5:F2:54:LEU:HD13	5:F2:81:THR:HG22	2.01	0.42
5:G2:24:GLY:HA3	5:H2:63:MET:HG3	2.01	0.42
5:G2:217:VAL:O	5:G2:220:VAL:HG12	2.20	0.42
5:H2:34:MET:HA	5:H2:39:LEU:HD11	2.01	0.42
1:C1:48:ILE:O	1:C1:51:LEU:HG	2.20	0.42
1:D1:172:PRO:HA	1:D1:175:VAL:HG22	2.00	0.42
3:I1:74:LEU:HA	3:I1:77:VAL:HG12	2.01	0.42
5:B2:20:GLN:HG3	5:C2:282:VAL:HG21	2.01	0.42
5:C2:145:ALA:O	5:C2:148:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D2:218:ILE:HA	5:D2:221:VAL:HG12	2.01	0.42
5:E2:99:GLU:CD	5:E2:106:ALA:HB3	2.43	0.42
5:F2:202:SER:HA	5:F2:205:VAL:HG22	2.02	0.42
1:A1:204:LEU:HD12	1:A1:212:VAL:HG21	2.01	0.42
1:D1:73:LEU:HD12	1:D1:73:LEU:HA	1.82	0.42
4:K1:137:MET:O	4:K1:142:THR:HG21	2.19	0.42
5:A2:71:PHE:HD2	5:A2:74:PHE:HB2	1.85	0.42
5:A2:72:ALA:HB1	5:B2:271:VAL:HG11	2.00	0.42
5:C2:112:GLU:HG2	5:C2:116:HIS:CD2	2.55	0.42
5:G2:190:GLN:HE22	5:H2:273:THR:HB	1.84	0.42
5:H2:74:PHE:CE2	5:H2:264:ALA:HA	2.55	0.42
5:H2:180:GLU:HA	5:H2:183:LYS:HG2	2.01	0.42
1:A1:100:ILE:HG22	1:A1:101:MET:HE2	2.02	0.42
1:B1:85:PRO:O	1:B1:88:VAL:HG22	2.18	0.42
3:J1:77:VAL:O	3:J1:80:LEU:HG	2.19	0.42
5:A2:69:LEU:HB2	5:A2:191:GLU:CD	2.44	0.42
5:B2:259:VAL:O	5:B2:262:THR:HG22	2.19	0.42
5:C2:114:PHE:CE2	5:C2:118:LEU:HD12	2.55	0.42
5:D2:161:PRO:HA	5:D2:164:GLN:HG2	2.01	0.42
5:F2:59:LEU:HD12	5:F2:259:VAL:O	2.19	0.42
5:G2:130:PHE:CD1	5:G2:216:MET:HE2	2.55	0.42
5:H2:73:ALA:HB1	5:I2:281:MET:HE1	2.01	0.42
5:H2:176:ILE:HD12	5:H2:180:GLU:HB3	2.02	0.42
5:I2:75:PRO:HD3	5:I2:194:PHE:HE1	1.85	0.42
1:E1:116:PHE:CE2	1:E1:123:MET:HB3	2.52	0.42
2:F1:227:MET:HE3	3:G1:18:LEU:HD13	2.02	0.42
3:I1:16:VAL:HG11	3:I1:76:TYR:CD2	2.55	0.42
5:A2:220:VAL:HG23	5:A2:221:VAL:HG13	2.02	0.42
5:C2:241:SER:O	5:C2:244:LEU:HG	2.20	0.42
5:D2:171:LEU:HD23	5:D2:176:ILE:HG13	2.02	0.42
5:E2:233:MET:HG2	5:E2:234:SER:O	2.20	0.42
5:F2:130:PHE:CE1	5:F2:251:LEU:HG	2.55	0.42
5:I2:67:ARG:NH1	5:I2:69:LEU:HB3	2.35	0.42
5:I2:182:LYS:HB3	5:I2:182:LYS:HE3	1.83	0.42
1:A1:193:PHE:HB3	1:A1:222:LYS:HE2	2.02	0.42
1:B1:195:ILE:HG23	3:H1:17:ALA:HB2	2.02	0.42
1:B1:207:LEU:HD13	3:H1:58:VAL:HG11	2.01	0.42
1:C1:105:ILE:HD12	1:C1:105:ILE:HA	1.88	0.42
1:C1:200:ILE:HG21	1:C1:218:ALA:HB2	2.02	0.42
5:A2:53:ALA:O	5:A2:57:MET:HG2	2.20	0.42
5:C2:160:MET:HB3	5:C2:160:MET:HE3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D2:292:MET:O	5:D2:295:ALA:HB3	2.19	0.42
5:E2:160:MET:N	5:E2:161:PRO:HD2	2.34	0.42
5:G2:31:ILE:O	5:G2:35:MET:HG2	2.20	0.42
5:H2:218:ILE:HA	5:H2:221:VAL:HG22	2.02	0.42
1:B1:107:LYS:HA	1:B1:110:VAL:HG12	2.01	0.41
1:B1:181:THR:O	1:B1:184:GLN:HG2	2.20	0.41
1:D1:141:GLN:HE22	1:D1:243:PHE:HA	1.84	0.41
5:A2:71:PHE:CZ	5:A2:267:ILE:HG23	2.55	0.41
5:B2:25:PRO:HA	5:B2:28:ILE:HG22	2.01	0.41
5:B2:46:LEU:HB2	5:C2:316:PHE:CZ	2.54	0.41
5:B2:202:SER:O	5:B2:205:VAL:HG12	2.20	0.41
5:B2:235:ILE:HG13	5:B2:236:GLY:H	1.85	0.41
5:C2:96:ILE:HD11	5:C2:249:ASP:OD2	2.20	0.41
5:G2:60:LEU:HD12	5:G2:60:LEU:HA	1.85	0.41
4:K1:187:LEU:HA	4:K1:190:VAL:HG12	2.02	0.41
5:A2:71:PHE:HZ	5:A2:267:ILE:HG23	1.85	0.41
5:A2:128:VAL:O	5:A2:132:ILE:HG22	2.21	0.41
5:E2:29:LEU:HD21	5:G2:298:VAL:HG13	2.02	0.41
5:F2:270:ARG:NE	5:F2:272:SER:HA	2.36	0.41
5:G2:56:ILE:HD11	5:H2:299:LEU:HG	2.03	0.41
5:I2:111:VAL:HG21	5:I2:249:ASP:OD1	2.20	0.41
5:I2:147:ARG:O	5:I2:151:VAL:HG13	2.20	0.41
1:A1:180:LYS:HG2	1:A1:184:GLN:OE1	2.20	0.41
5:A2:136:ILE:O	5:A2:140:VAL:HB	2.19	0.41
5:D2:215:ILE:HA	5:D2:218:ILE:HG22	2.02	0.41
5:E2:124:ALA:O	5:E2:128:VAL:HG12	2.20	0.41
5:I2:77:ILE:HA	5:I2:80:PHE:CE1	2.54	0.41
5:I2:156:VAL:HG21	5:I2:195:TYR:HD2	1.86	0.41
1:A1:143:ARG:HG3	1:A1:144:GLU:H	1.85	0.41
1:B1:184:GLN:HA	1:B1:187:PHE:CD2	2.56	0.41
2:F1:144:LEU:O	2:F1:147:ILE:HG22	2.21	0.41
5:A2:270:ARG:HB3	5:A2:277:VAL:HG22	2.02	0.41
5:C2:74:PHE:HB3	5:C2:75:PRO:HD3	2.03	0.41
5:F2:36:VAL:HG11	5:G2:255:ILE:HD11	2.02	0.41
5:G2:201:ALA:HA	5:G2:204:PHE:CD2	2.55	0.41
5:I2:225:LEU:O	5:I2:228:VAL:HG12	2.20	0.41
1:A1:47:PHE:HZ	1:A1:116:PHE:HZ	1.68	0.41
1:A1:104:VAL:O	1:A1:107:LYS:HG2	2.20	0.41
1:C1:107:LYS:HA	1:C1:110:VAL:HG12	2.00	0.41
1:D1:217:ILE:O	1:D1:220:PRO:HD2	2.20	0.41
1:E1:209:MET:HB3	1:E1:212:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F1:243:LEU:HD13	2:F1:243:LEU:HA	1.82	0.41
4:K1:177:GLU:HG3	4:K1:181:VAL:HG13	2.01	0.41
5:C2:184:ARG:HA	5:C2:184:ARG:HD2	1.85	0.41
5:D2:133:LEU:O	5:D2:136:ILE:HG22	2.21	0.41
5:F2:215:ILE:CD1	5:G2:132:ILE:HG12	2.50	0.41
2:F1:104:LEU:HD23	2:F1:104:LEU:HA	1.81	0.41
5:C2:63:MET:HE3	5:C2:63:MET:HB3	1.96	0.41
5:C2:161:PRO:HA	5:C2:164:GLN:HG2	2.03	0.41
5:G2:260:ILE:HG13	5:G2:261:SER:N	2.35	0.41
5:I2:35:MET:HE3	5:I2:35:MET:HB2	1.89	0.41
1:A1:208:GLY:C	1:B1:205:MET:HE1	2.46	0.41
1:A1:219:LEU:O	1:A1:222:LYS:HG2	2.21	0.41
1:C1:181:THR:O	1:C1:184:GLN:HG2	2.21	0.41
5:A2:95:ILE:HD13	5:A2:107:ALA:HA	2.02	0.41
5:A2:130:PHE:O	5:A2:133:LEU:HG	2.20	0.41
5:B2:74:PHE:N	5:B2:75:PRO:HD2	2.35	0.41
5:E2:270:ARG:HH21	5:E2:272:SER:HA	1.85	0.41
2:F1:125:LEU:HD22	2:F1:229:MET:HE2	2.03	0.41
3:G1:63:ILE:HD11	3:H1:14:MET:CB	2.51	0.41
3:I1:35:ILE:HD13	3:I1:53:PRO:HG2	2.02	0.41
4:K1:13:PRO:HG2	4:K1:18:LEU:HD21	2.02	0.41
4:K1:241:LYS:HA	4:K1:244:ILE:HG22	2.03	0.41
5:B2:241:SER:O	5:B2:244:LEU:HG	2.21	0.41
5:D2:185:ARG:HA	5:D2:188:VAL:HG12	2.02	0.41
5:D2:295:ALA:O	5:D2:298:VAL:HB	2.21	0.41
5:G2:62:ALA:HB1	5:G2:267:ILE:HG13	2.02	0.41
5:G2:215:ILE:HA	5:G2:218:ILE:HG12	2.02	0.41
5:G2:296:ALA:HB2	5:G2:320:LEU:HD22	2.03	0.41
1:A1:143:ARG:O	1:A1:147:LEU:HD23	2.21	0.41
1:A1:193:PHE:O	1:A1:196:ILE:HG22	2.20	0.41
1:C1:73:LEU:HD12	1:C1:190:PHE:CZ	2.55	0.41
1:D1:102:SER:HA	1:D1:105:ILE:HG22	2.03	0.41
3:I1:55:ILE:O	3:I1:58:VAL:HG12	2.21	0.41
3:J1:9:MET:O	3:J1:12:GLU:HG2	2.21	0.41
5:A2:129:VAL:HA	5:A2:132:ILE:HG22	2.03	0.41
5:A2:288:ASN:ND2	5:A2:290:ARG:HG2	2.36	0.41
5:B2:123:PHE:O	5:B2:127:ILE:HG22	2.20	0.41
5:B2:161:PRO:O	5:B2:164:GLN:HG3	2.21	0.41
5:C2:271:VAL:HG13	5:C2:273:THR:H	1.85	0.41
5:D2:79:LEU:O	5:D2:80:PHE:C	2.64	0.41
5:E2:218:ILE:HA	5:E2:221:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F2:271:VAL:HG13	5:F2:273:THR:H	1.86	0.41
5:H2:23:ALA:O	5:H2:26:ILE:HG22	2.21	0.41
5:H2:93:THR:HA	5:H2:96:ILE:HG22	2.02	0.41
5:H2:233:MET:HE2	5:H2:233:MET:HB3	1.91	0.41
5:I2:78:LEU:O	5:I2:79:LEU:C	2.64	0.41
5:I2:161:PRO:O	5:I2:164:GLN:HG2	2.21	0.41
1:A1:225:LEU:HD22	3:G1:73:LEU:HD21	2.03	0.41
1:B1:86:ASN:C	1:B1:88:VAL:H	2.28	0.41
1:B1:189:ILE:HD12	1:B1:189:ILE:HA	1.89	0.41
1:D1:86:ASN:O	1:D1:88:VAL:N	2.51	0.41
1:D1:95:PHE:HE2	1:E1:171:LEU:HD23	1.86	0.41
2:F1:21:LEU:O	2:F1:24:LEU:HG	2.21	0.41
4:K1:16:HIS:O	4:K1:19:GLU:HG2	2.21	0.41
4:K1:210:PHE:O	4:K1:213:ILE:HG22	2.21	0.41
5:G2:135:ILE:HD13	5:G2:135:ILE:HA	1.89	0.41
1:D1:66:ARG:HD3	1:D1:243:PHE:CZ	2.56	0.40
2:F1:227:MET:CE	3:G1:18:LEU:HD13	2.51	0.40
4:K1:82:ILE:HA	4:K1:85:LEU:HD12	2.02	0.40
5:A2:209:ALA:O	5:A2:213:ILE:HG13	2.21	0.40
5:B2:34:MET:HE1	5:B2:44:LEU:HD22	2.02	0.40
5:B2:119:VAL:HG12	5:B2:121:GLY:H	1.85	0.40
5:E2:31:ILE:HD13	5:E2:34:MET:HE3	2.02	0.40
5:E2:33:SER:O	5:E2:37:LEU:HB2	2.21	0.40
5:F2:117:PHE:CZ	5:G2:307:GLY:HA3	2.56	0.40
5:G2:226:VAL:HA	5:G2:229:LEU:HG	2.03	0.40
5:H2:288:ASN:HD21	5:H2:290:ARG:HG2	1.86	0.40
5:I2:130:PHE:CE2	5:I2:216:MET:HG3	2.56	0.40
5:I2:218:ILE:HA	5:I2:221:VAL:HG22	2.02	0.40
1:D1:217:ILE:HA	1:E1:194:LEU:HD21	2.03	0.40
1:E1:86:ASN:O	1:E1:88:VAL:N	2.52	0.40
3:H1:44:ILE:HD11	3:I1:36:SER:C	2.46	0.40
5:A2:130:PHE:O	5:A2:134:VAL:HG12	2.21	0.40
5:A2:139:MET:HE2	5:A2:139:MET:HB3	1.97	0.40
5:H2:153:ALA:O	5:H2:156:VAL:HG12	2.21	0.40
1:B1:104:VAL:HA	1:B1:107:LYS:HE3	2.03	0.40
1:D1:200:ILE:HD12	1:D1:200:ILE:HA	1.95	0.40
1:E1:71:PHE:CG	1:E1:89:LEU:HD12	2.56	0.40
3:J1:74:LEU:HB3	3:J1:78:ARG:HH22	1.86	0.40
4:K1:172:MET:HA	4:K1:172:MET:HE2	2.04	0.40
4:K1:244:ILE:HA	4:K1:247:MET:HG2	2.03	0.40
5:A2:25:PRO:O	5:A2:29:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B2:43:ILE:HG22	5:B2:47:LEU:HD13	2.02	0.40
5:E2:65:THR:HG23	5:E2:270:ARG:HH11	1.86	0.40
5:F2:270:ARG:HE	5:F2:272:SER:HA	1.86	0.40
1:D1:86:ASN:C	1:D1:88:VAL:H	2.29	0.40
3:H1:52:ILE:N	3:H1:53:PRO:HD2	2.36	0.40
3:J1:46:GLU:HB3	3:J1:49:LEU:HG	2.03	0.40
5:D2:165:MET:HE3	5:D2:165:MET:HB3	1.83	0.40
5:E2:325:TRP:NE1	5:E2:328:ARG:HH22	2.19	0.40
5:G2:180:GLU:O	5:G2:184:ARG:HG2	2.21	0.40
5:I2:129:VAL:HA	5:I2:132:ILE:HG22	2.03	0.40
5:I2:275:GLN:HB2	5:I2:280:GLN:HE21	1.86	0.40
1:B1:69:ILE:HD13	1:B1:69:ILE:HA	1.94	0.40
1:C1:86:ASN:O	1:C1:88:VAL:N	2.52	0.40
1:D1:83:ALA:HB3	1:D1:84:PRO:HD3	2.04	0.40
1:E1:149:LEU:HA	1:E1:152:ARG:HD3	2.03	0.40
5:A2:29:LEU:HD11	5:C2:298:VAL:HG22	2.03	0.40
5:A2:182:LYS:O	5:A2:185:ARG:HG2	2.22	0.40
5:D2:67:ARG:HB3	5:D2:69:LEU:HD23	2.03	0.40
5:D2:126:GLY:H	5:D2:129:VAL:HG12	1.85	0.40
5:E2:185:ARG:O	5:E2:188:VAL:HG12	2.22	0.40
5:F2:20:GLN:HG3	5:G2:282:VAL:HG21	2.02	0.40
5:H2:72:ALA:HB3	5:I2:284:GLN:HE22	1.86	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	A1	207/245 (84%)	197 (95%)	9 (4%)	1 (0%)	24	62
1	B1	207/245 (84%)	192 (93%)	14 (7%)	1 (0%)	24	62
1	C1	207/245 (84%)	195 (94%)	11 (5%)	1 (0%)	24	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D1	207/245 (84%)	196 (95%)	10 (5%)	1 (0%)	24	62
1	E1	207/245 (84%)	194 (94%)	12 (6%)	1 (0%)	24	62
2	F1	248/264 (94%)	237 (96%)	10 (4%)	1 (0%)	30	66
3	G1	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
3	H1	87/89 (98%)	83 (95%)	4 (5%)	0	100	100
3	I1	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
3	J1	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
4	K1	247/383 (64%)	235 (95%)	12 (5%)	0	100	100
5	A2	309/692 (45%)	289 (94%)	20 (6%)	0	100	100
5	B2	309/692 (45%)	287 (93%)	22 (7%)	0	100	100
5	C2	309/692 (45%)	291 (94%)	18 (6%)	0	100	100
5	D2	309/692 (45%)	288 (93%)	21 (7%)	0	100	100
5	E2	309/692 (45%)	290 (94%)	19 (6%)	0	100	100
5	F2	309/692 (45%)	291 (94%)	18 (6%)	0	100	100
5	G2	309/692 (45%)	291 (94%)	18 (6%)	0	100	100
5	H2	309/692 (45%)	294 (95%)	15 (5%)	0	100	100
5	I2	309/692 (45%)	286 (93%)	23 (7%)	0	100	100
All	All	4659/8456 (55%)	4391 (94%)	262 (6%)	6 (0%)	49	82

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A1	87	GLN
1	B1	87	GLN
1	C1	87	GLN
1	D1	87	GLN
1	E1	87	GLN
2	F1	164	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	A1	179/204 (88%)	177 (99%)	2 (1%)	65	73
1	B1	179/204 (88%)	179 (100%)	0	100	100
1	C1	179/204 (88%)	177 (99%)	2 (1%)	65	73
1	D1	179/204 (88%)	178 (99%)	1 (1%)	78	80
1	E1	179/204 (88%)	179 (100%)	0	100	100
2	F1	207/221 (94%)	207 (100%)	0	100	100
3	G1	74/74 (100%)	74 (100%)	0	100	100
3	H1	74/74 (100%)	74 (100%)	0	100	100
3	I1	74/74 (100%)	74 (100%)	0	100	100
3	J1	74/74 (100%)	74 (100%)	0	100	100
4	K1	210/316 (66%)	209 (100%)	1 (0%)	81	81
5	A2	241/561 (43%)	240 (100%)	1 (0%)	84	82
5	B2	241/561 (43%)	240 (100%)	1 (0%)	84	82
5	C2	241/561 (43%)	241 (100%)	0	100	100
5	D2	241/561 (43%)	241 (100%)	0	100	100
5	E2	241/561 (43%)	240 (100%)	1 (0%)	84	82
5	F2	241/561 (43%)	238 (99%)	3 (1%)	63	73
5	G2	241/561 (43%)	240 (100%)	1 (0%)	84	82
5	H2	241/561 (43%)	240 (100%)	1 (0%)	84	82
5	I2	241/561 (43%)	240 (100%)	1 (0%)	84	82
All	All	3777/6902 (55%)	3762 (100%)	15 (0%)	81	82

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	138	MET
1	A1	235	LEU
1	C1	223	LEU
1	C1	227	VAL
1	D1	207	LEU
4	K1	152	LYS
5	A2	267	ILE
5	B2	240	GLU
5	E2	291	VAL

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Mol	Chain	Res	Type
5	F2	47	LEU
5	F2	94	ARG
5	F2	249	ASP
5	G2	90	VAL
5	H2	294	LEU
5	I2	245	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	87	GLN
1	A1	119	GLN
1	A1	124	GLN
1	A1	184	GLN
1	A1	241	GLN
1	B1	76	ASN
1	B1	233	GLN
1	C1	43	GLN
1	C1	76	ASN
1	C1	141	GLN
1	C1	233	GLN
1	D1	43	GLN
1	D1	141	GLN
1	E1	76	ASN
2	F1	162	ASN
2	F1	205	ASN
3	G1	43	GLN
3	G1	45	ASN
3	G1	83	ASN
3	H1	39	GLN
3	H1	45	ASN
3	H1	71	ASN
3	I1	71	ASN
3	J1	39	GLN
4	K1	66	HIS
4	K1	129	ASN
4	K1	216	HIS
4	K1	239	HIS
4	K1	246	GLN
4	K1	248	GLN
5	A2	116	HIS
5	A2	137	ASN

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Mol	Chain	Res	Type
5	A2	230	GLN
5	A2	280	GLN
5	B2	122	ASN
5	B2	172	ASN
5	B2	190	GLN
5	B2	254	GLN
5	C2	89	ASN
5	C2	116	HIS
5	C2	219	ASN
5	C2	230	GLN
5	C2	231	HIS
5	D2	51	ASN
5	D2	101	HIS
5	D2	116	HIS
5	D2	137	ASN
5	D2	164	GLN
5	D2	190	GLN
5	D2	254	GLN
5	E2	254	GLN
5	F2	164	GLN
5	F2	219	ASN
5	G2	51	ASN
5	G2	164	GLN
5	G2	190	GLN
5	G2	254	GLN
5	G2	284	GLN
5	H2	51	ASN
5	H2	137	ASN
5	H2	284	GLN
5	I2	137	ASN
5	I2	219	ASN
5	I2	230	GLN
5	I2	288	ASN

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.

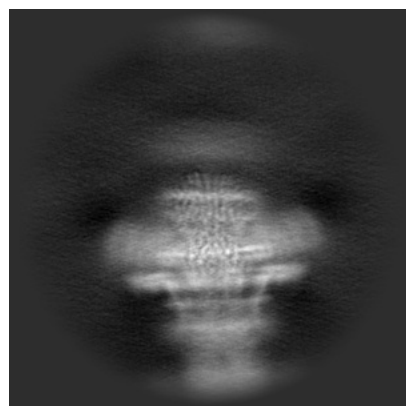
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-78907. These allow visual inspection of the internal detail of the map and identification of artifacts.

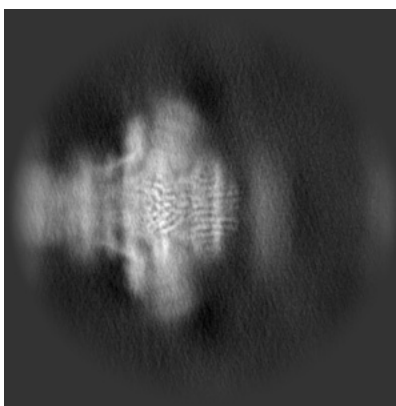
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

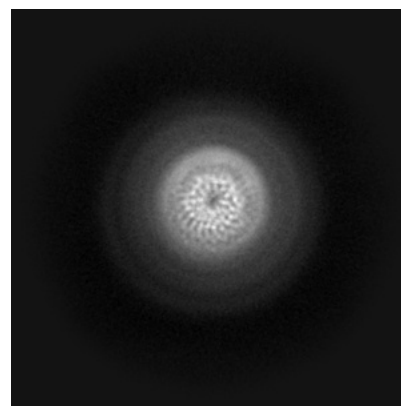
6.1.1 Primary map



X

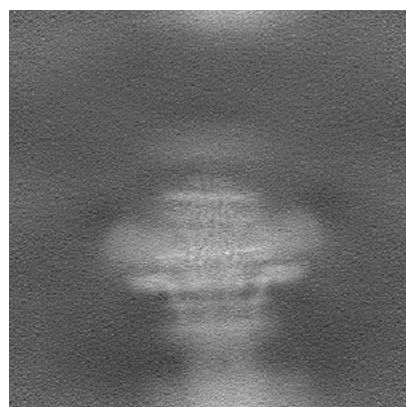


Y

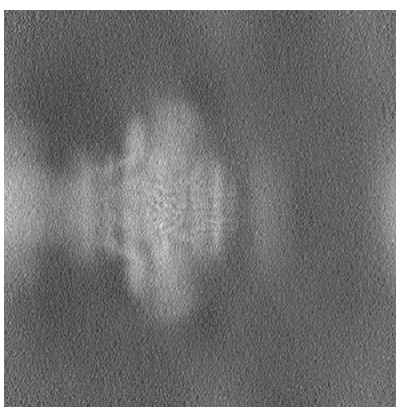


Z

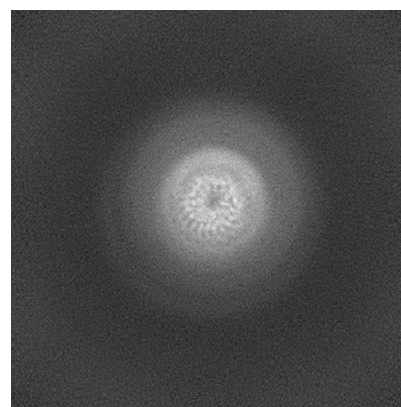
6.1.2 Raw map



X



Y

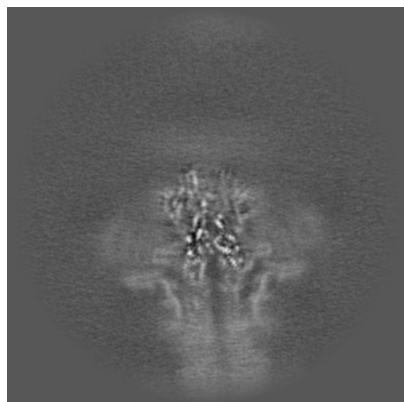


Z

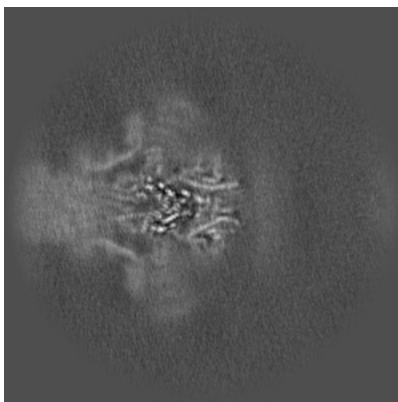
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

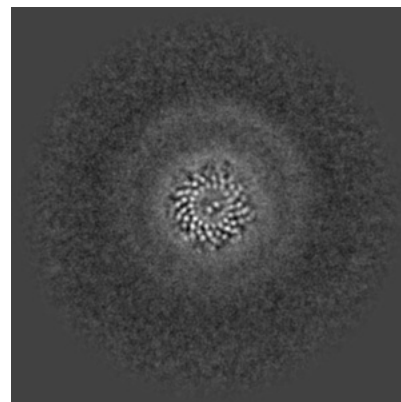
6.2.1 Primary map



X Index: 256

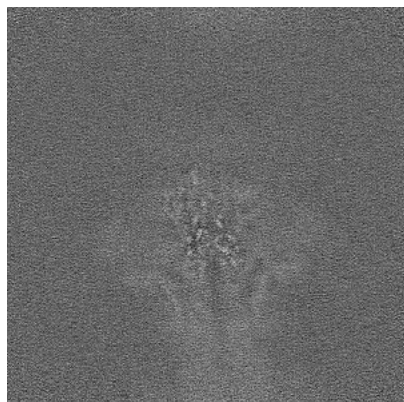


Y Index: 256

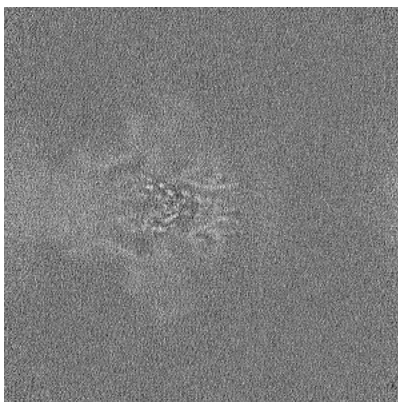


Z Index: 256

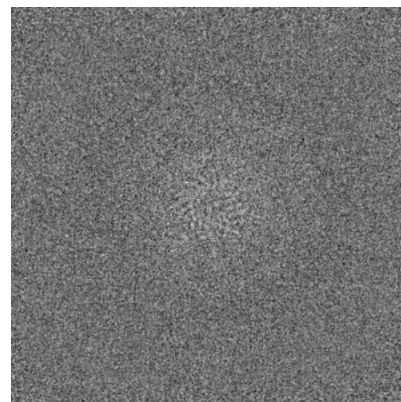
6.2.2 Raw map



X Index: 256



Y Index: 256

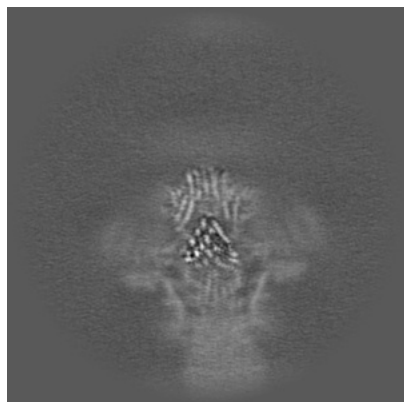


Z Index: 256

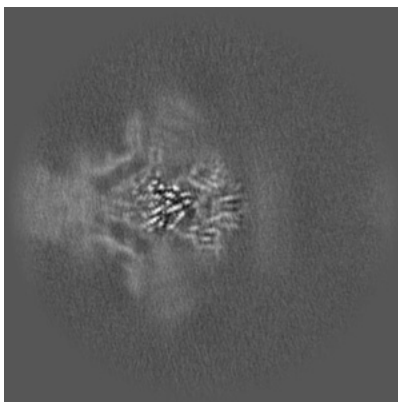
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

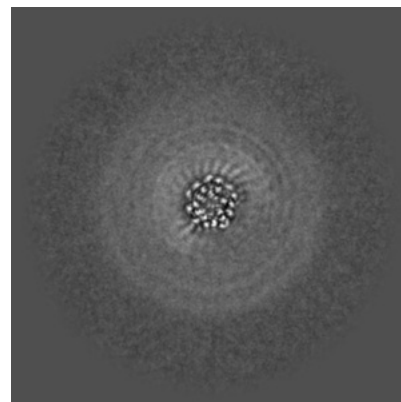
6.3.1 Primary map



X Index: 242

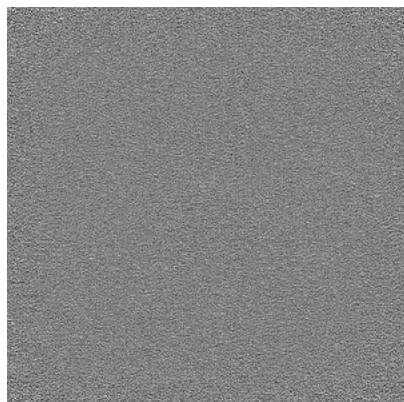


Y Index: 245

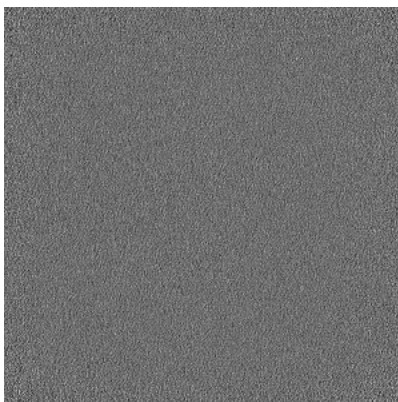


Z Index: 204

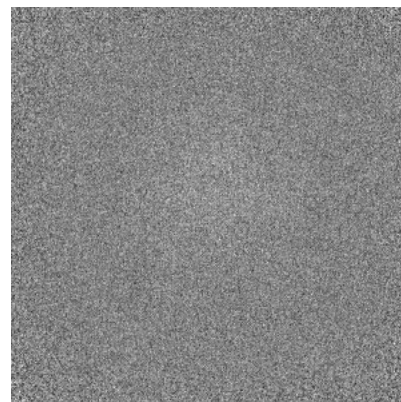
6.3.2 Raw map



X Index: 0



Y Index: 0

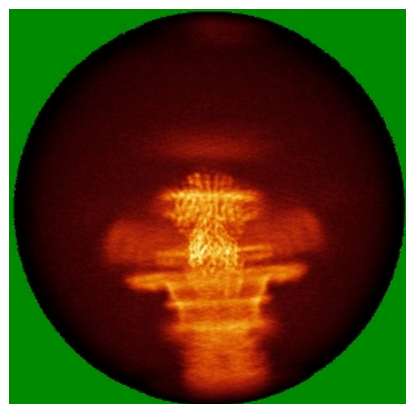


Z Index: 0

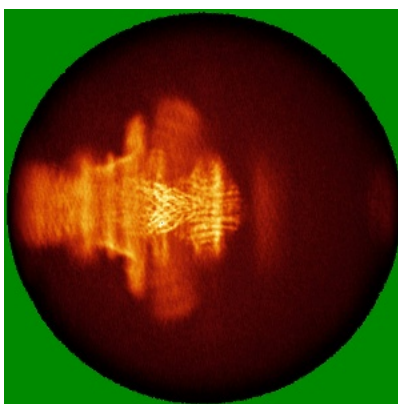
The images above show the largest variance slices of the map in three orthogonal directions.

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

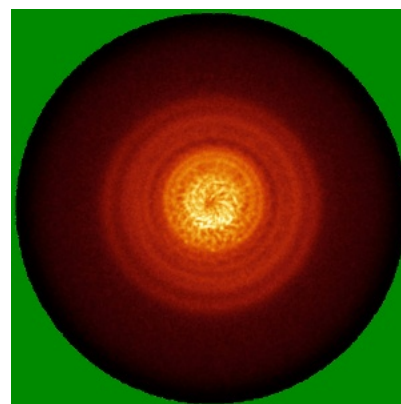
6.4.1 Primary map



X

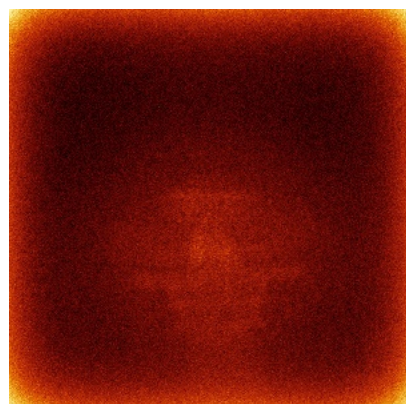


Y

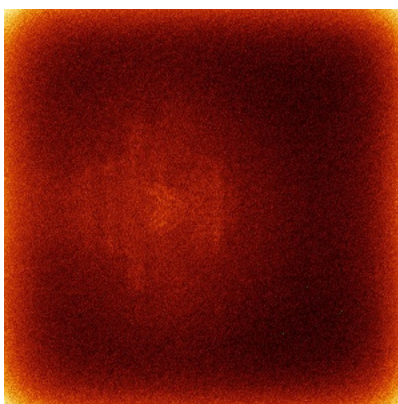


Z

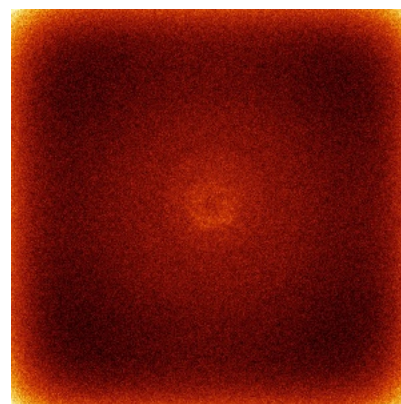
6.4.2 Raw map



X



Y

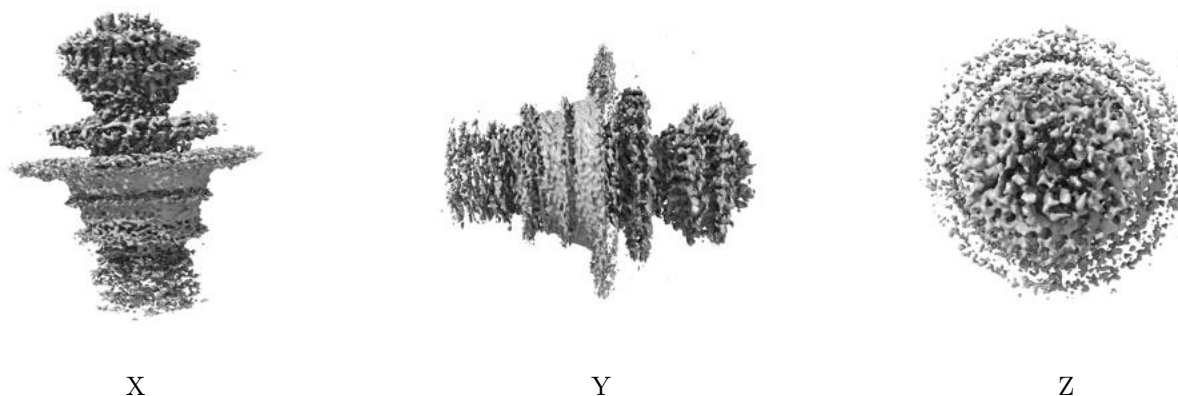


Z

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.

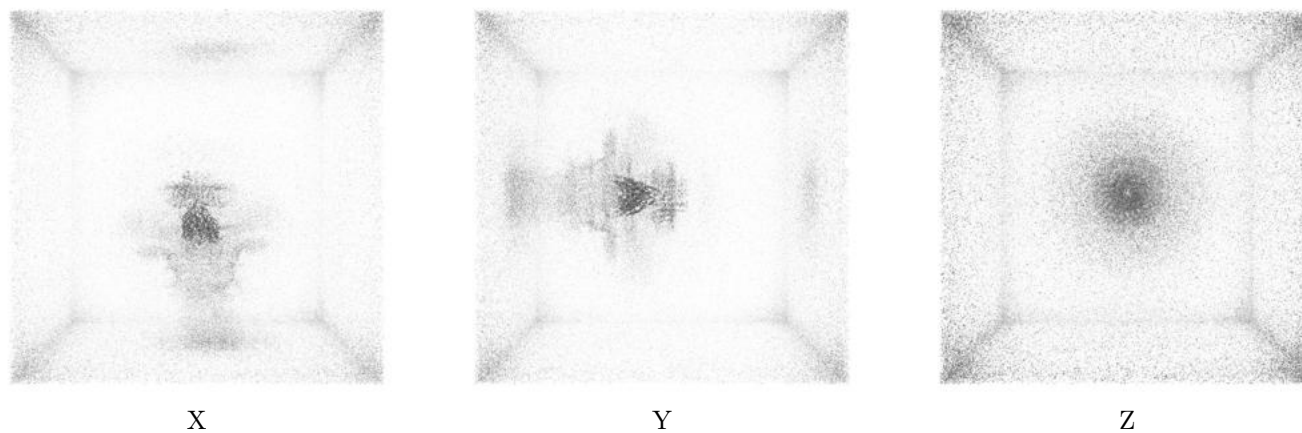
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

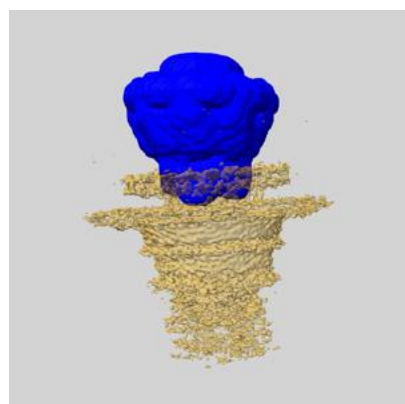
6.6 Mask visualisation [i](#)

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

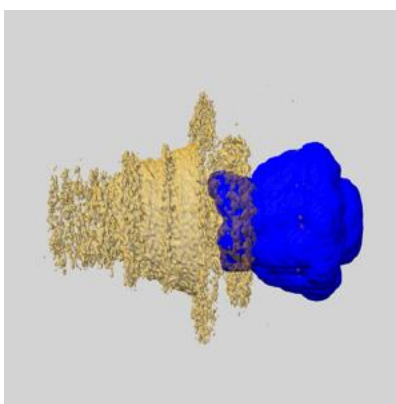
A mask typically either:

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

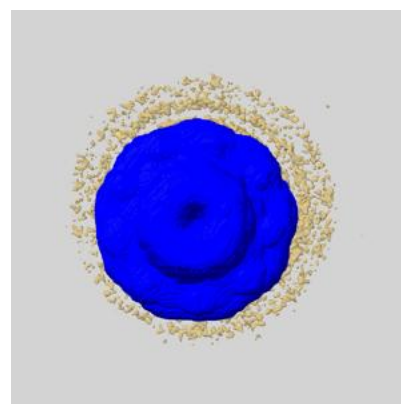
6.6.1 emd_78907_msk_1.map [i](#)



X



Y

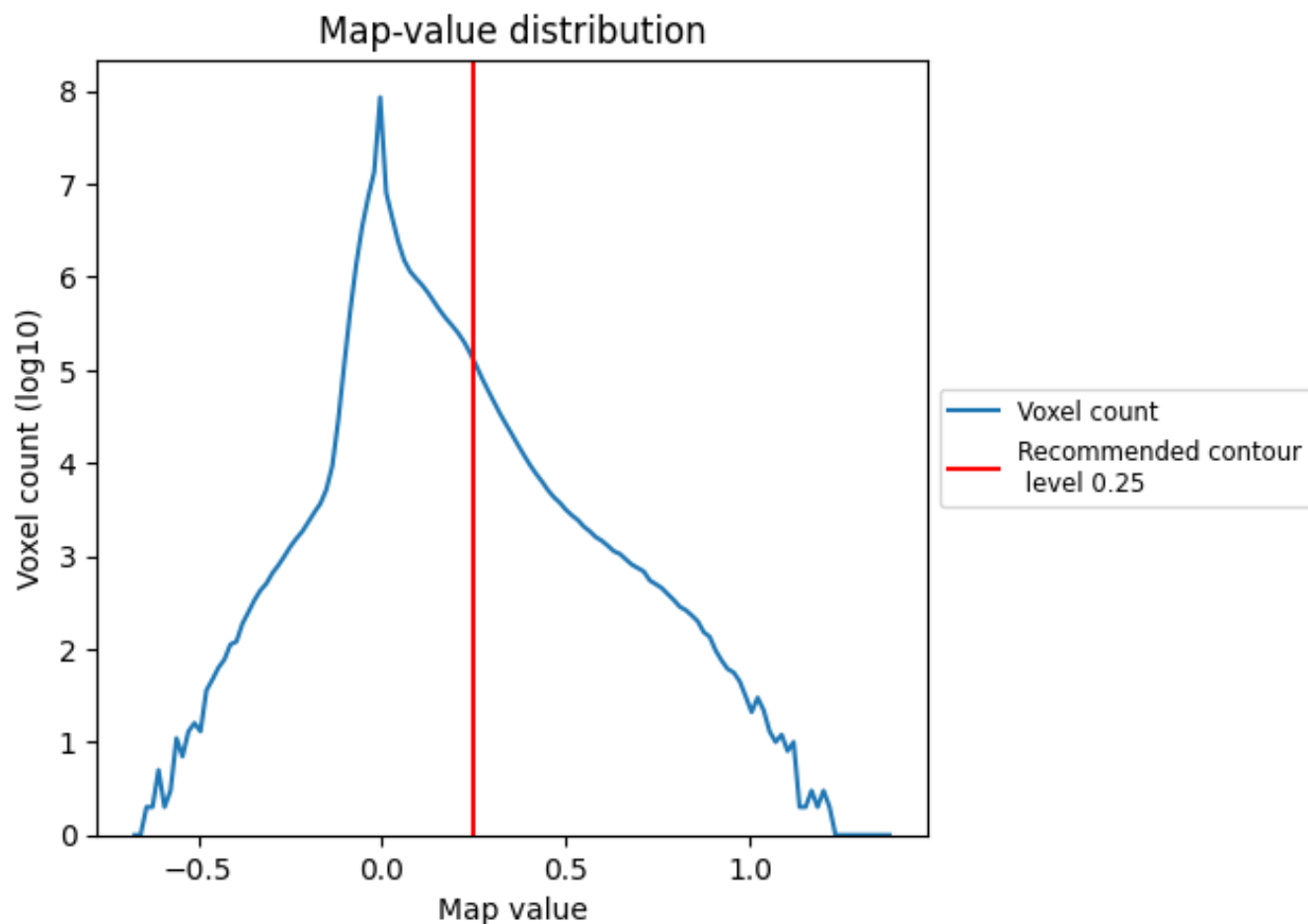


Z

7 Map analysis [i](#)

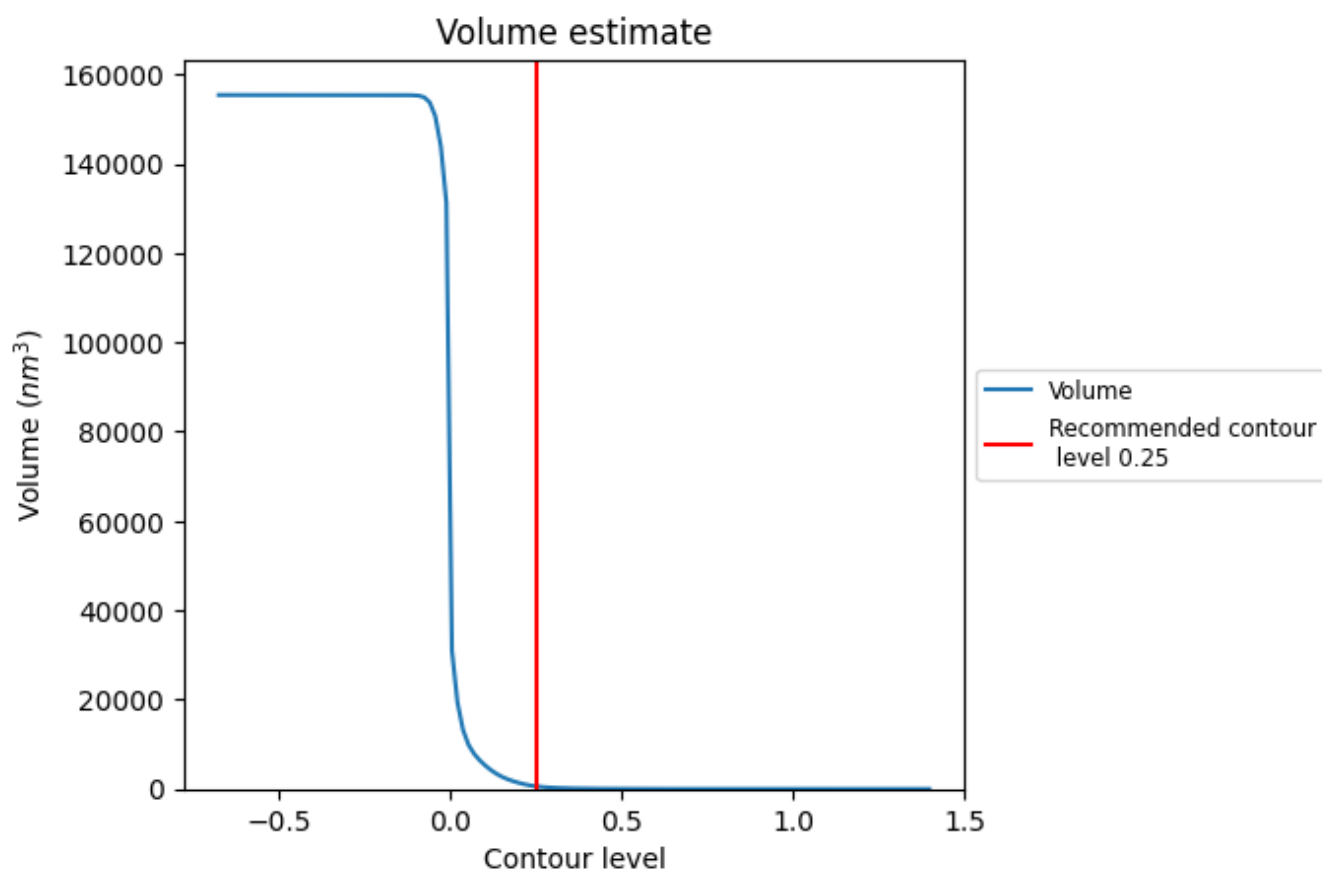
This section contains the results of statistical analysis of the map.

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.

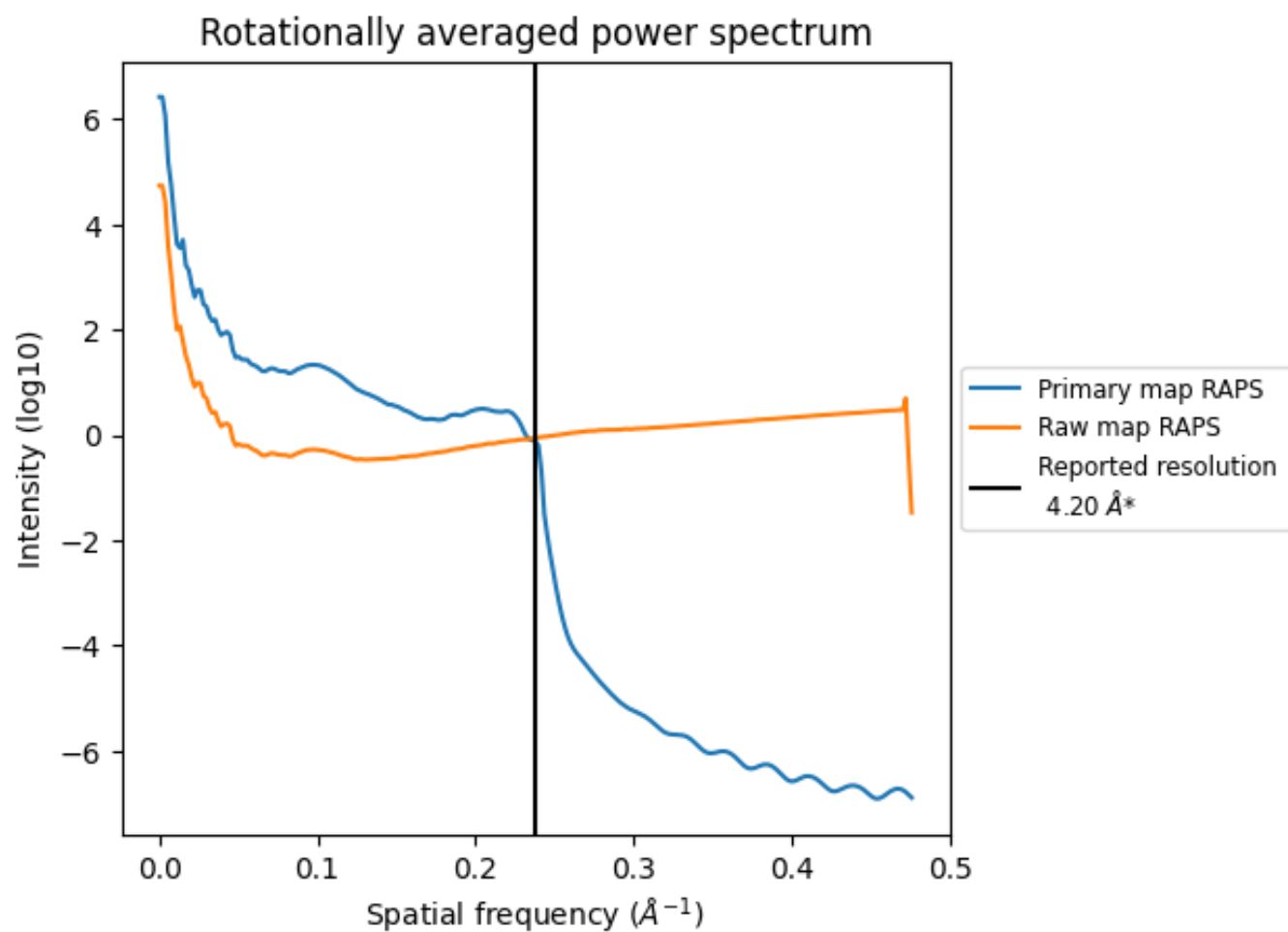
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 602 nm³; this corresponds to an approximate mass of 544 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 ⓘ

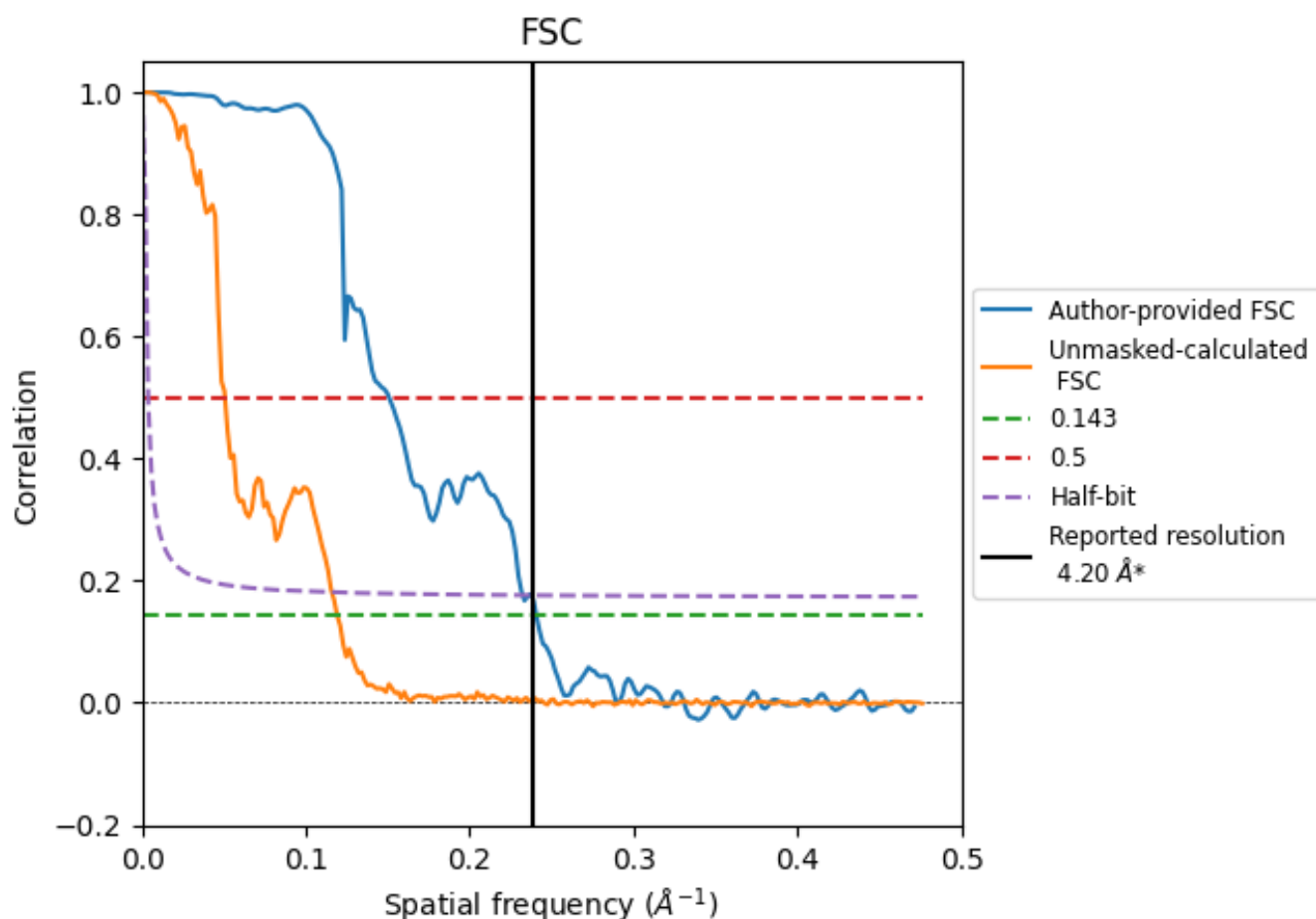


*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.238 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

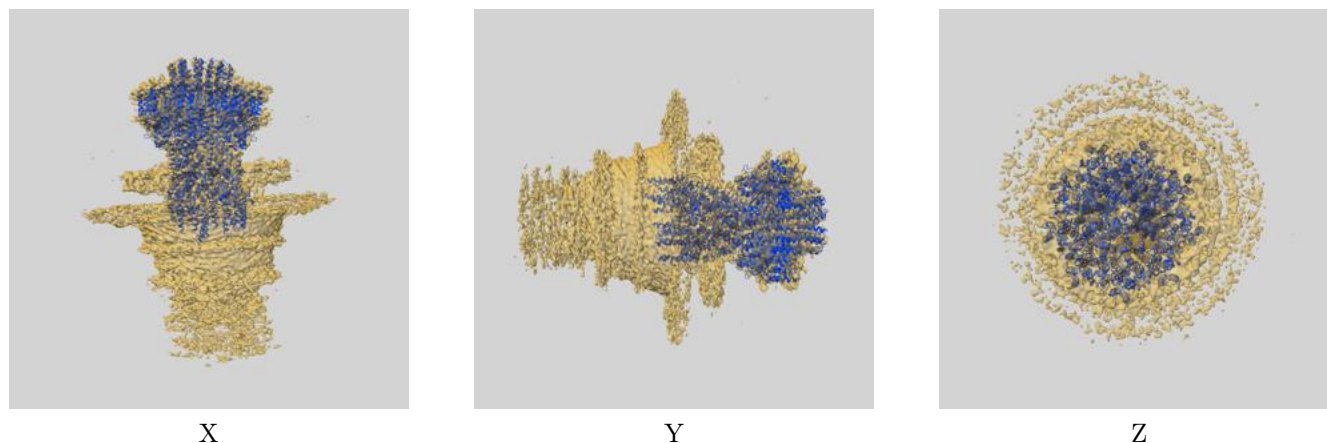
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.16	6.63	4.30
Unmasked-calculated*	8.40	19.80	8.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.40 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

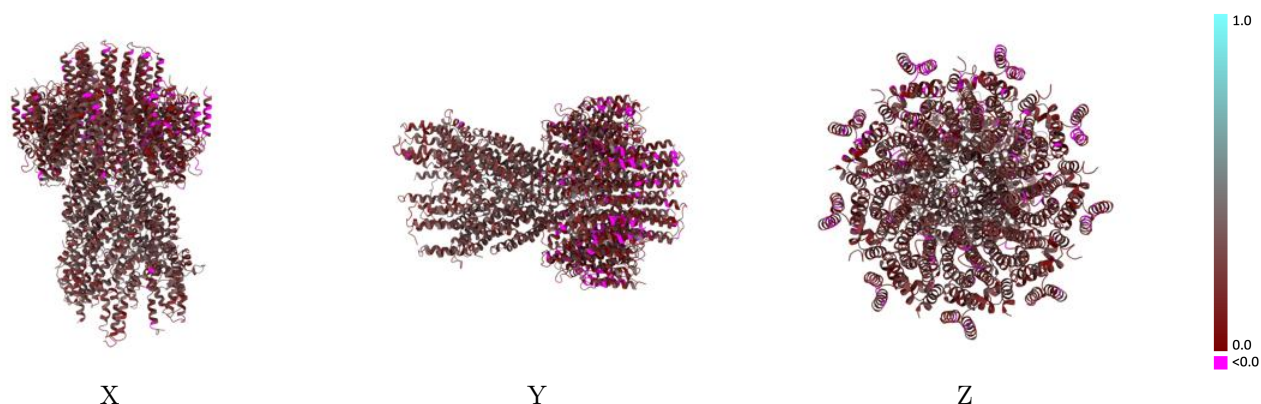
This section contains information regarding the fit between EMDB map EMD-78907 and PDB model 38LP. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



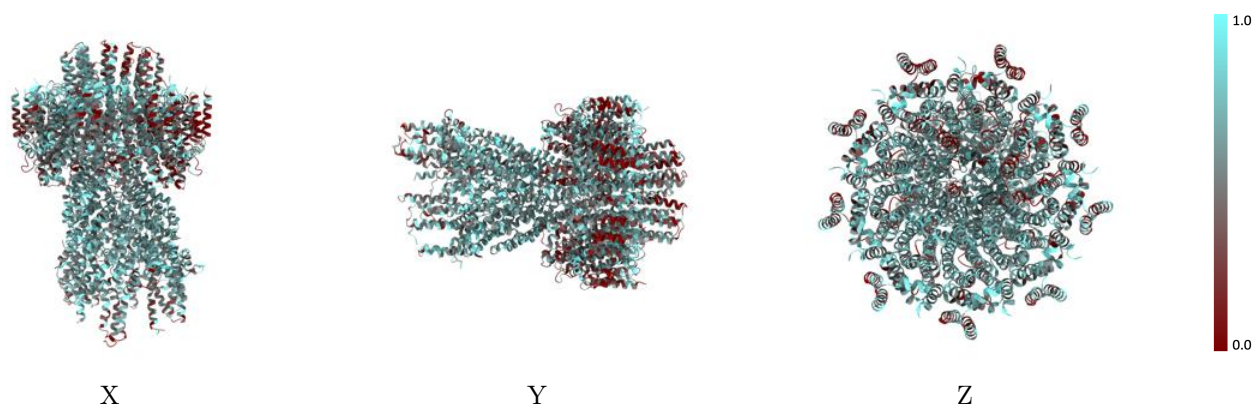
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



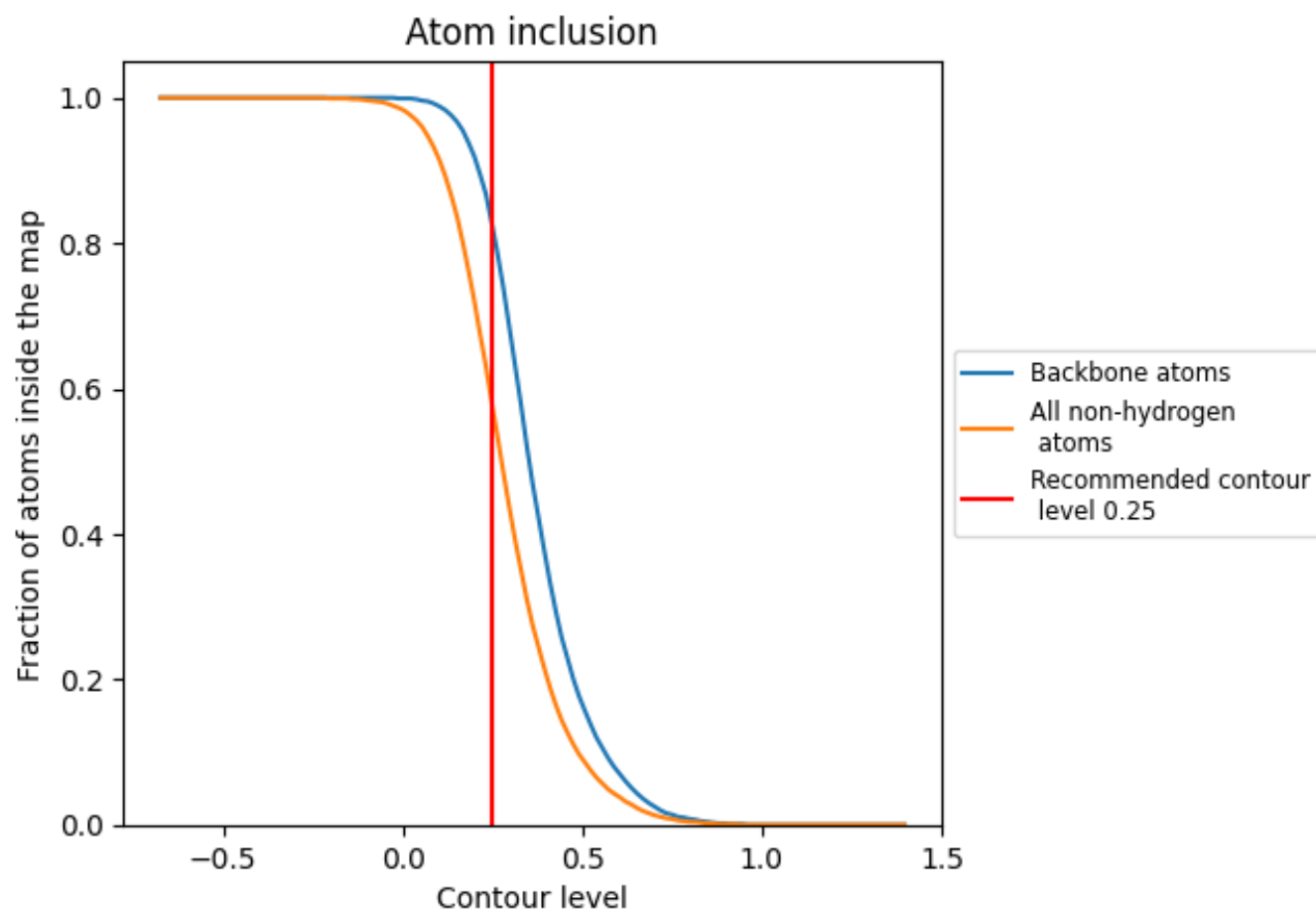
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 57% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5750	 0.2330
A1	 0.5740	 0.2890
A2	 0.5010	 0.1730
B1	 0.6100	 0.2860
B2	 0.4520	 0.1590
C1	 0.6380	 0.2930
C2	 0.5180	 0.1670
D1	 0.6480	 0.3110
D2	 0.5450	 0.1960
E1	 0.6360	 0.2960
E2	 0.5900	 0.2150
F1	 0.6130	 0.3090
F2	 0.5930	 0.2180
G1	 0.6260	 0.2890
G2	 0.5900	 0.2190
H1	 0.6450	 0.2760
H2	 0.5360	 0.2000
I1	 0.6380	 0.2750
I2	 0.5120	 0.1840
J1	 0.6500	 0.2800
K1	 0.6660	 0.2650

