



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 06:15 AM UTC

PDB ID : 9ZE4 / pdb_00009ze4
EMDB ID : EMD-74091
Title : Asymmetric Tail Gating Complex of Pseudomonas Phage DEV
Authors : Bellis, N.F.; Cingolani, G.
Deposited on : 2025-11-27
Resolution : 8.50 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

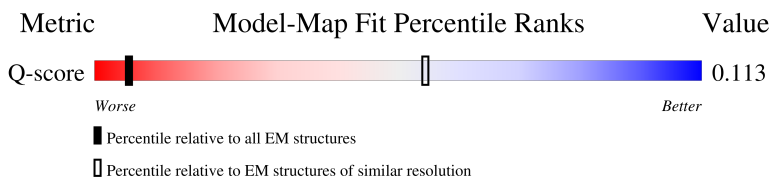
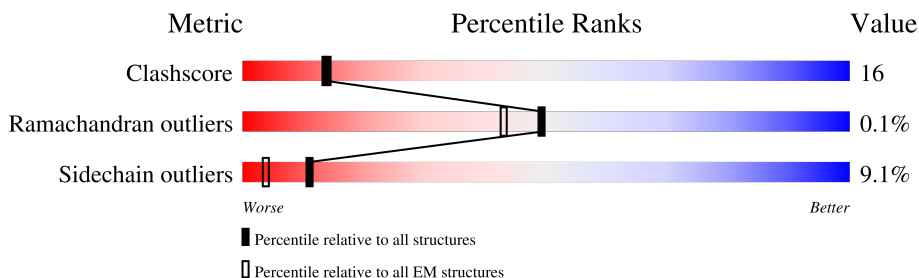
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.50 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.



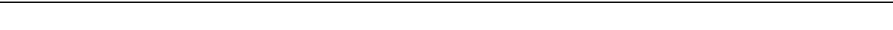
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	328 (8.00 - 9.00)

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	321	 69% 27% .
1	B	321	 72% 24% .
1	C	321	 71% 26% .
1	D	321	 69% 27% .

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Mol	Chain	Length	Quality of chain
1	E	321	 69% 29% .
1	F	321	 67% 29% .
1	G	321	 70% 26% .
1	H	321	 74% 21% .
1	I	321	 71% 26% .
1	J	321	 69% 29% .
1	K	321	 70% 27% .
1	L	321	 65% 32% .
2	M	740	 37% 30% . 32%
3	N	429	 29% 17% . 53%
3	O	429	 29% 16% . 53%
3	P	429	 30% 16% . 53%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 35853 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 gp75 tail tube.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	320	Total	C	N	O	S	0	0
			2336	1445	420	465	6		
1	B	320	Total	C	N	O	S	0	0
			2336	1445	420	465	6		
1	C	320	Total	C	N	O	S	0	0
			2336	1445	420	465	6		
1	D	320	Total	C	N	O	S	0	0
			2336	1445	420	465	6		
1	E	320	Total	C	N	O	S	0	0
			2336	1445	420	465	6		
1	F	320	Total	C	N	O	S	0	0
			2336	1445	420	465	6		
1	G	320	Total	C	N	O	S	0	0
			2336	1445	420	465	6		
1	H	320	Total	C	N	O	S	0	0
			2336	1445	420	465	6		
1	I	320	Total	C	N	O	S	0	0
			2336	1445	420	465	6		
1	J	320	Total	C	N	O	S	0	0
			2336	1445	420	465	6		
1	K	320	Total	C	N	O	S	0	0
			2336	1445	420	465	6		
1	L	320	Total	C	N	O	S	0	0
			2336	1445	420	465	6		

- Molecule 2 is a protein called N4 gp53-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	502	Total	C	N	O	S	0	0
			3990	2544	671	758	17		

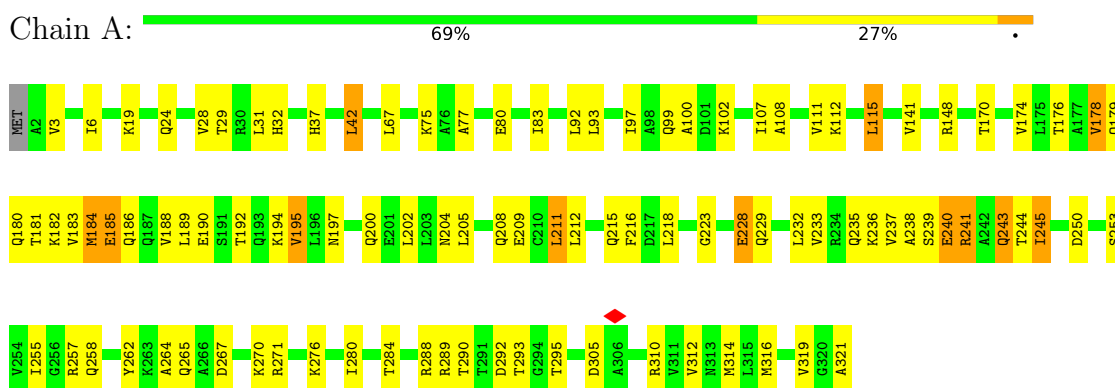
- Molecule 3 is a protein called Tip attachment protein J central straight fiber domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	203	Total 1277	C 793	N 232	O 251	S 1	0	0
3	O	203	Total 1277	C 793	N 232	O 251	S 1	0	0
3	P	203	Total 1277	C 793	N 232	O 251	S 1	0	0

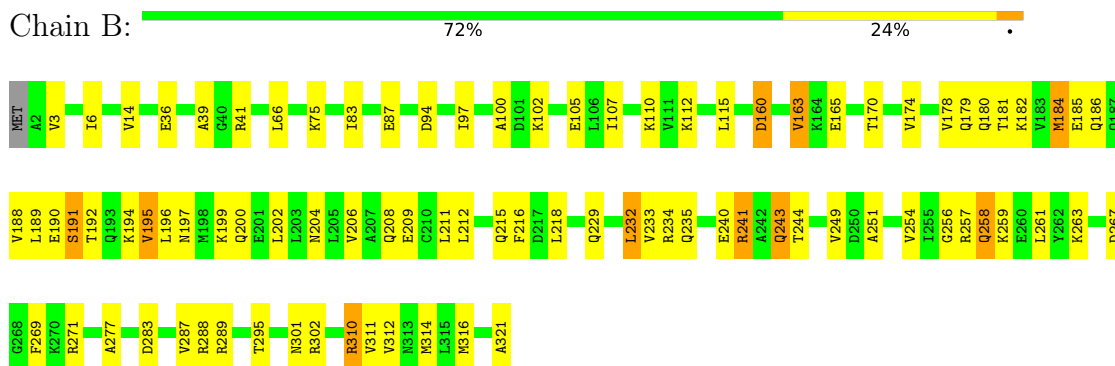
3 Residue-property plots

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.

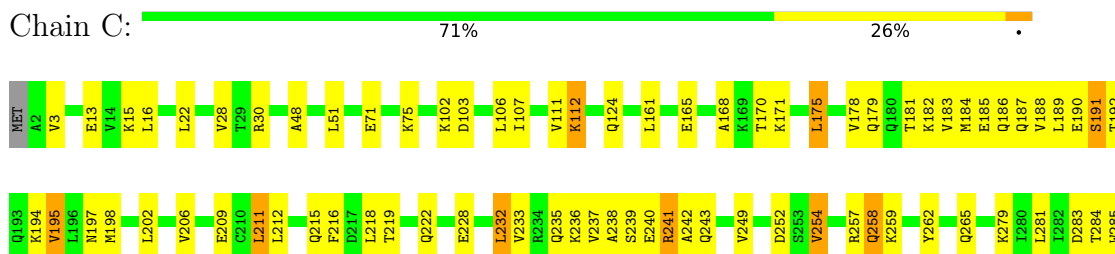
- Molecule 1: gp75 tail tube



- Molecule 1: gp75 tail tube



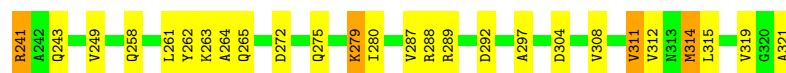
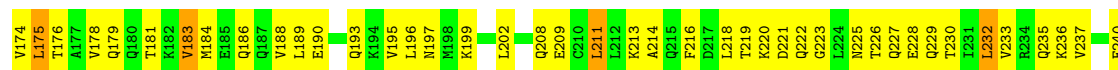
- Molecule 1: gp75 tail tube





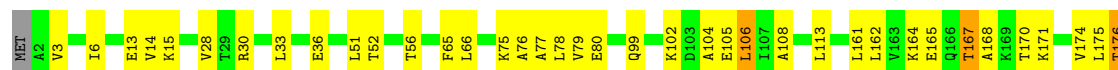
- Molecule 1: gp75 tail tube

Chain D: 69% 27% .



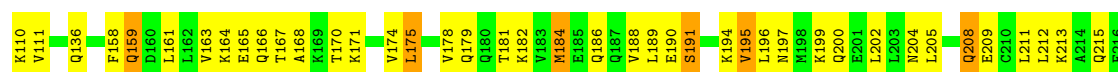
- Molecule 1: gp75 tail tube

Chain E: 69% 29% .



- Molecule 1: gp75 tail tube

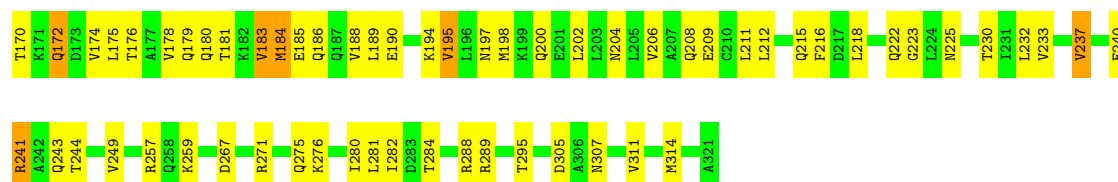
Chain F: 67% 29% .



- Molecule 1: gp75 tail tube

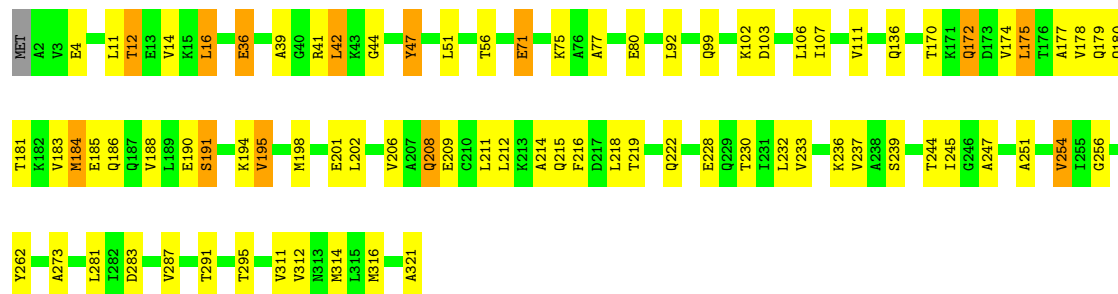
Chain G: 70% 26% .





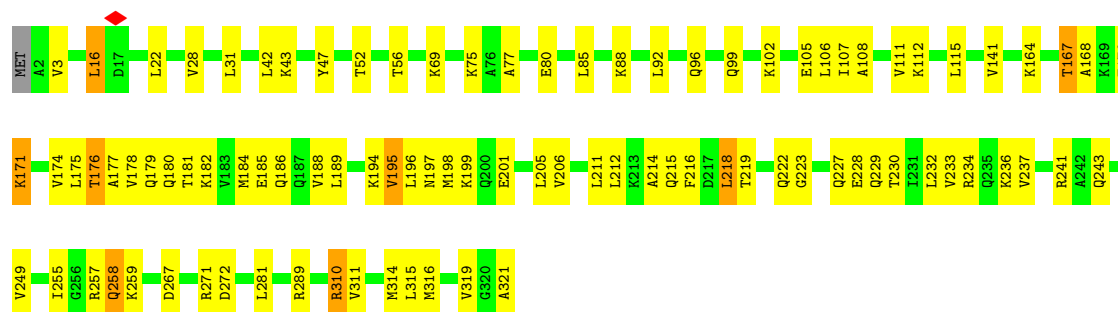
- Molecule 1: gp75 tail tube

Chain H: 74% 21% .



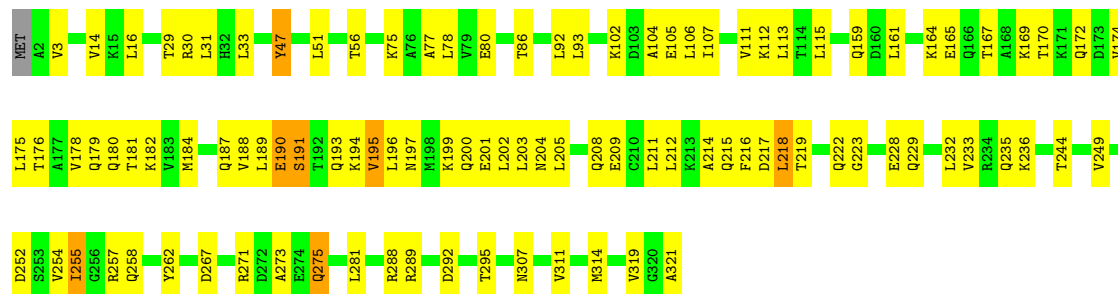
- Molecule 1: gp75 tail tube

Chain I: 71% 26% .



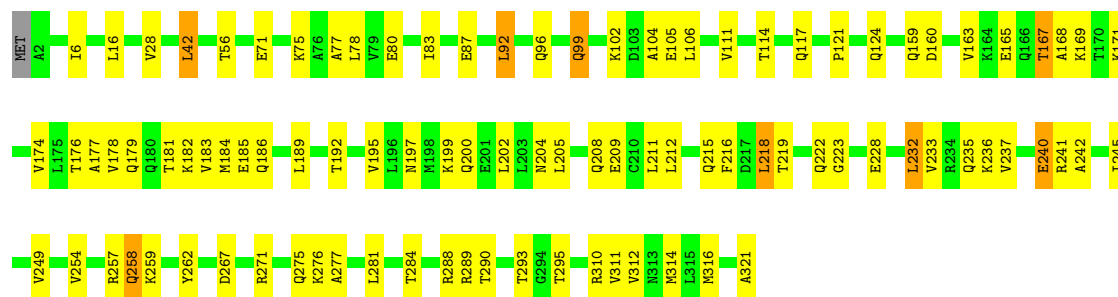
- Molecule 1: gp75 tail tube

Chain J: 69% 29% .



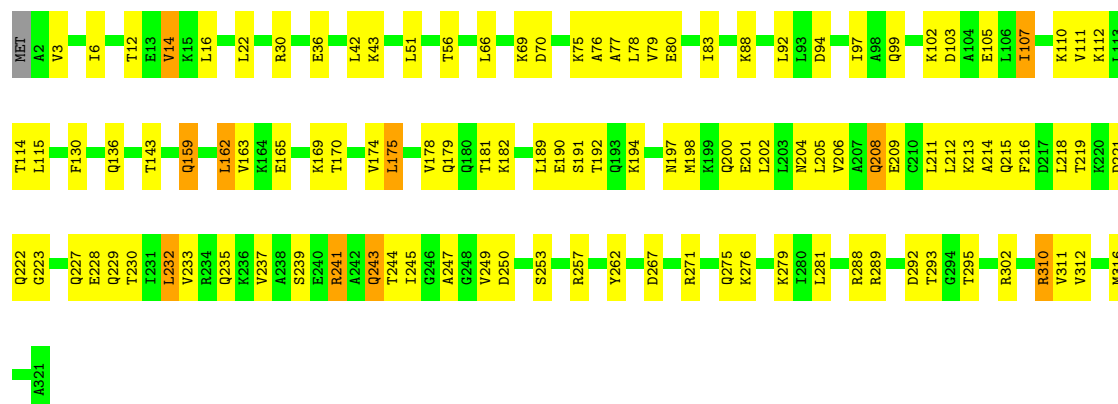
- Molecule 1: gp75 tail tube

Chain K: 70% 27% .



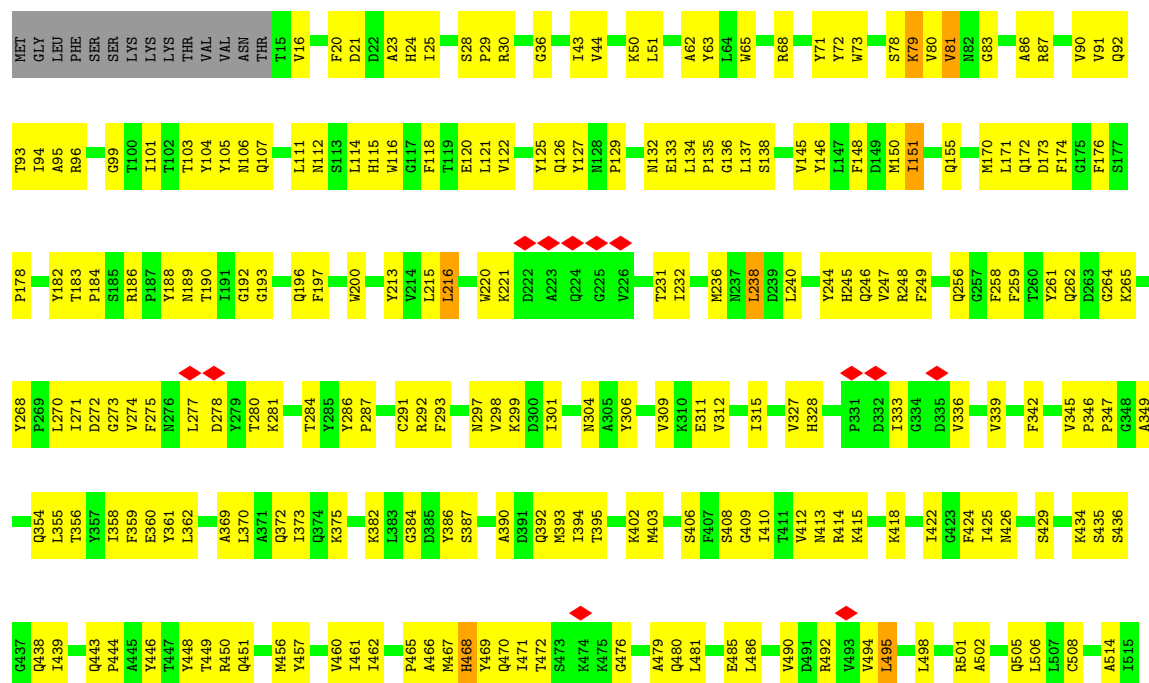
• Molecule 1: gp75 tail tube

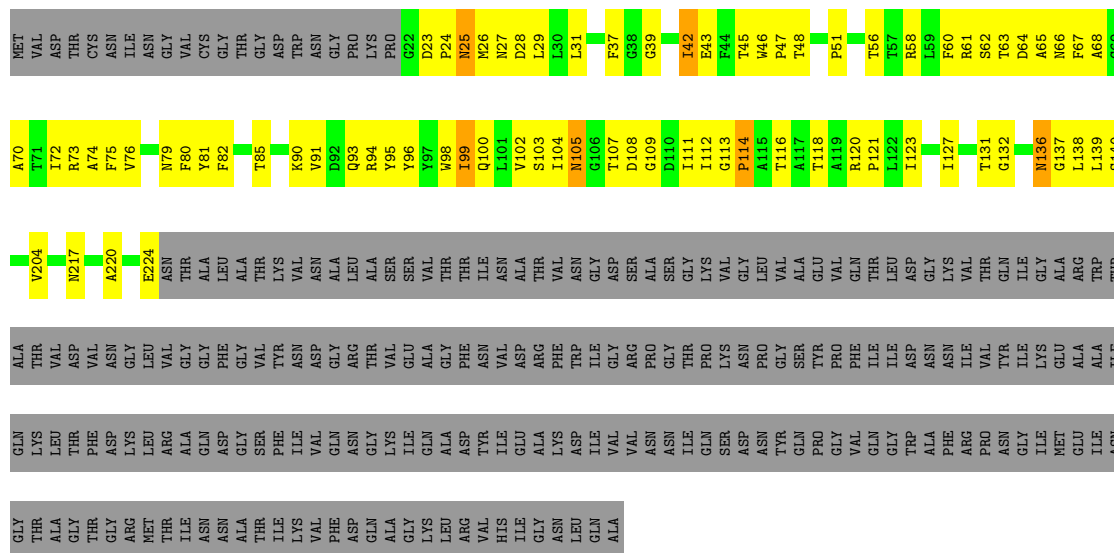
Chain L: 65% 32%



• Molecule 2: N4 gp53-like protein

Chain M: 37% 30% 32%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8241	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.308	Depositor
Minimum map value	-0.109	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0176	Depositor
Map size ($\text{\AA}$)	764.16003, 764.16003, 764.16003	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.194, 1.194, 1.194	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	0.16	0/2346	0.38	0/3172
1	B	0.15	0/2346	0.37	0/3172
1	C	0.14	0/2346	0.37	0/3172
1	D	0.15	0/2346	0.36	0/3172
1	E	0.15	0/2346	0.37	0/3172
1	F	0.15	0/2346	0.35	0/3172
1	G	0.15	0/2346	0.39	0/3172
1	H	0.15	0/2346	0.37	0/3172
1	I	0.19	0/2346	0.40	0/3172
1	J	0.14	0/2346	0.35	0/3172
1	K	0.15	0/2346	0.37	0/3172
1	L	0.15	0/2346	0.38	0/3172
2	M	0.16	0/4085	0.40	0/5545
3	N	0.24	0/1298	0.46	0/1788
3	O	0.26	0/1298	0.44	0/1788
3	P	0.26	0/1298	0.48	0/1788
All	All	0.17	0/36131	0.39	0/48973

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2336	0	2317	92	0
1	B	2336	0	2317	78	0
1	C	2336	0	2317	81	0
1	D	2336	0	2317	90	0
1	E	2336	0	2317	78	0
1	F	2336	0	2317	97	0
1	G	2336	0	2317	85	0
1	H	2336	0	2317	66	0
1	I	2336	0	2317	71	0
1	J	2336	0	2317	89	0
1	K	2336	0	2317	87	0
1	L	2336	0	2317	102	0
2	M	3990	0	3898	195	0
3	N	1277	0	971	92	0
3	O	1277	0	971	98	0
3	P	1277	0	971	84	0
All	All	35853	0	34615	1106	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 16.

All (1106) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:96:TYR:HA	3:N:115:ALA:O	1.56	1.06
2:M:193:GLY:HA3	3:O:202:SER:CB	1.92	1.00
2:M:186:ARG:HB3	2:M:189:ASN:HB2	1.45	0.97
2:M:193:GLY:CA	3:O:202:SER:CB	2.45	0.93
2:M:193:GLY:HA2	3:O:199:ALA:HA	1.55	0.88
1:L:178:VAL:O	1:L:181:THR:HB	1.77	0.85
3:O:58:ARG:HH12	3:O:108:ASP:HB3	1.43	0.82
2:M:197:PHE:CD2	3:O:199:ALA:HB2	2.17	0.80
3:N:102:VAL:HG11	3:O:51:PRO:HG2	1.62	0.80
2:M:197:PHE:CE1	3:O:195:ALA:HB1	2.16	0.80
3:N:91:VAL:HG13	3:N:120:ARG:HA	1.62	0.80
1:A:232:LEU:HG	1:A:236:LYS:HE3	1.64	0.79
1:B:235:GLN:HG2	1:C:241:ARG:HH21	1.46	0.78
1:H:218:LEU:HD13	1:I:223:GLY:HA2	1.65	0.77
3:O:138:LEU:HA	3:P:131:THR:HA	1.66	0.77
2:M:197:PHE:CZ	3:O:195:ALA:O	2.38	0.76
3:N:94:ARG:HA	3:N:117:ALA:O	1.86	0.76
1:H:185:GLU:O	1:H:188:VAL:HB	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:197:ASN:HA	1:J:202:LEU:HD13	1.66	0.76
1:F:235:GLN:HE22	1:G:241:ARG:HE	1.31	0.76
1:A:289:ARG:HE	1:B:288:ARG:HA	1.51	0.75
1:D:165:GLU:HG3	1:E:167:THR:HG23	1.68	0.75
1:C:321:ALA:HB1	1:D:311:VAL:HG22	1.67	0.75
3:O:31:LEU:HD13	3:O:99:ILE:HG12	1.66	0.75
2:M:129:PRO:HG2	2:M:256:GLN:HB2	1.67	0.75
1:A:197:ASN:HA	1:B:202:LEU:HD13	1.68	0.74
1:F:158:PHE:O	1:F:161:LEU:HB3	1.88	0.74
2:M:28:SER:HB3	2:M:50:LYS:HB3	1.70	0.74
1:D:321:ALA:HB1	1:E:311:VAL:HG22	1.69	0.74
1:J:321:ALA:HA	1:K:314:MET:HG2	1.71	0.73
2:M:79:LYS:HE3	2:M:278:ASP:HB2	1.70	0.73
3:N:26:MET:HB3	3:N:101:LEU:HB2	1.70	0.73
3:P:112:ILE:HG22	3:P:113:GLY:H	1.53	0.73
3:P:90:LYS:HB2	3:P:93:GLN:HB2	1.70	0.73
1:F:235:GLN:HE21	1:G:240:GLU:HG3	1.52	0.73
1:E:197:ASN:HA	1:F:202:LEU:HD13	1.70	0.72
2:M:403:MET:HG2	2:M:469:TYR:HA	1.71	0.72
3:P:31:LEU:HD11	3:P:42:ILE:HG23	1.71	0.72
1:C:178:VAL:O	1:C:181:THR:HB	1.89	0.72
2:M:197:PHE:CE2	3:O:195:ALA:O	2.42	0.72
3:N:126:MET:HA	3:O:123:ILE:HA	1.72	0.72
3:P:98:TRP:NE1	3:P:113:GLY:O	2.21	0.72
1:A:170:THR:HG21	1:L:165:GLU:HB3	1.71	0.72
1:G:181:THR:O	1:G:184:MET:HB2	1.91	0.71
2:M:80:VAL:HG22	2:M:394:ILE:HG12	1.72	0.71
1:K:208:GLN:HE21	1:L:212:LEU:HD22	1.56	0.71
2:M:345:VAL:HG23	2:M:490:VAL:HG22	1.72	0.71
3:O:99:ILE:HG13	3:O:112:ILE:HG13	1.72	0.71
2:M:412:VAL:HG22	2:M:460:VAL:HG22	1.73	0.70
1:I:216:PHE:O	1:I:219:THR:HB	1.91	0.70
3:P:63:THR:HA	3:P:95:TYR:HA	1.73	0.70
1:H:216:PHE:O	1:H:219:THR:HB	1.92	0.70
2:M:469:TYR:O	2:M:476:GLY:HA3	1.91	0.70
1:A:238:ALA:HB3	1:B:241:ARG:HH22	1.57	0.70
1:C:232:LEU:HG	1:C:236:LYS:HE3	1.72	0.70
1:H:208:GLN:HG3	1:I:212:LEU:HD13	1.72	0.70
1:A:239:SER:HA	1:B:243:GLN:HG2	1.73	0.70
3:N:132:GLY:H	3:P:138:LEU:HA	1.54	0.70
3:N:60:PHE:HE1	3:N:100:GLN:HB3	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:232:LEU:HG	1:J:236:LYS:HE3	1.74	0.70
3:N:139:LEU:H	3:O:131:THR:HA	1.55	0.70
1:K:181:THR:O	1:K:184:MET:HB2	1.92	0.69
1:C:102:LYS:HE3	1:D:104:ALA:HB1	1.72	0.69
1:A:211:LEU:HG	1:A:215:GLN:HE21	1.56	0.69
3:P:25:ASN:OD1	3:P:25:ASN:N	2.23	0.69
1:G:183:VAL:HG22	1:H:188:VAL:HG22	1.75	0.69
3:N:51:PRO:HD2	3:P:102:VAL:HG11	1.75	0.69
3:N:57:THR:HA	3:N:101:LEU:HA	1.74	0.69
3:O:101:LEU:O	3:O:109:GLY:N	2.22	0.69
1:F:204:ASN:HA	1:G:209:GLU:HG3	1.75	0.69
1:L:179:GLN:HA	1:L:182:LYS:HE3	1.73	0.69
2:M:444:PRO:HB3	2:M:481:LEU:HD22	1.75	0.68
1:C:186:GLN:HE22	1:D:188:VAL:HG22	1.58	0.68
1:A:179:GLN:HA	1:A:182:LYS:HE3	1.73	0.68
1:I:218:LEU:HG	1:I:222:GLN:HE21	1.59	0.68
2:M:193:GLY:CA	3:O:199:ALA:HA	2.22	0.68
1:A:262:TYR:HB3	1:L:257:ARG:HB3	1.74	0.68
3:O:102:VAL:HG11	3:P:51:PRO:HG2	1.76	0.68
2:M:362:LEU:HB3	2:M:460:VAL:HG11	1.75	0.68
2:M:93:THR:HG21	2:M:268:TYR:HB3	1.76	0.67
1:C:218:LEU:HD13	1:D:223:GLY:HA2	1.75	0.67
2:M:112:ASN:HA	2:M:170:MET:HA	1.77	0.67
1:F:190:GLU:HG2	1:G:195:VAL:HG22	1.76	0.67
1:J:232:LEU:HB2	1:K:237:VAL:HG22	1.77	0.67
3:P:39:GLY:HA2	3:P:85:THR:H	1.60	0.67
1:A:243:GLN:HG2	1:L:239:SER:HA	1.74	0.67
1:B:204:ASN:HA	1:C:209:GLU:HG3	1.76	0.67
1:A:190:GLU:HG2	1:B:195:VAL:HG22	1.77	0.67
1:B:179:GLN:HA	1:B:182:LYS:HE3	1.76	0.67
1:G:197:ASN:HA	1:H:202:LEU:HD13	1.77	0.67
1:K:197:ASN:HA	1:L:202:LEU:HD13	1.77	0.66
1:K:232:LEU:HG	1:K:236:LYS:HE3	1.76	0.66
3:P:99:ILE:HG13	3:P:112:ILE:HG13	1.77	0.66
1:A:181:THR:HG21	1:L:175:LEU:HD21	1.77	0.66
1:B:257:ARG:HB3	1:C:262:TYR:HB3	1.77	0.66
3:O:92:ASP:HA	3:O:118:THR:HG23	1.77	0.66
1:A:99:GLN:HA	1:A:102:LYS:HE2	1.77	0.66
1:A:321:ALA:HA	1:B:314:MET:HG2	1.77	0.66
1:C:257:ARG:HB3	1:D:262:TYR:HB3	1.76	0.66
3:O:96:TYR:CD2	3:O:116:THR:HB	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:96:TYR:HD2	3:P:114:PRO:HB2	1.61	0.66
1:J:216:PHE:O	1:J:219:THR:HB	1.95	0.66
1:K:233:VAL:HA	1:K:236:LYS:HD2	1.76	0.66
1:F:179:GLN:HA	1:F:182:LYS:HE3	1.78	0.66
2:M:101:ILE:HB	2:M:249:PHE:HB2	1.77	0.66
2:M:148:PHE:HA	2:M:186:ARG:HH22	1.61	0.66
1:B:211:LEU:HG	1:B:215:GLN:HE21	1.60	0.65
3:O:96:TYR:HD2	3:O:114:PRO:HB2	1.61	0.65
3:O:46:TRP:NE1	3:O:51:PRO:O	2.29	0.65
2:M:395:THR:HG23	2:M:402:LYS:HE3	1.76	0.65
1:D:232:LEU:HG	1:D:236:LYS:HE3	1.78	0.65
1:L:218:LEU:HG	1:L:222:GLN:HE21	1.62	0.65
2:M:336:VAL:HG11	2:M:339:VAL:HG23	1.79	0.65
3:N:113:GLY:O	3:N:115:ALA:N	2.29	0.65
1:F:165:GLU:HB3	1:G:170:THR:HG21	1.77	0.65
1:J:191:SER:O	1:J:194:LYS:HB3	1.97	0.65
1:B:36:GLU:HB3	1:B:41:ARG:HE	1.62	0.65
1:L:191:SER:O	1:L:194:LYS:HB3	1.96	0.65
1:L:209:GLU:HA	1:L:212:LEU:HG	1.79	0.65
3:N:24:PRO:HB2	3:N:47:PRO:HG2	1.79	0.65
3:O:58:ARG:HH21	3:P:51:PRO:HG3	1.63	0.64
2:M:298:VAL:HA	2:M:301:ILE:HD12	1.78	0.64
1:F:218:LEU:HG	1:F:222:GLN:HE21	1.63	0.64
2:M:386:TYR:HB2	2:M:409:GLY:HA3	1.80	0.64
3:N:101:LEU:O	3:N:109:GLY:N	2.31	0.64
1:K:232:LEU:HD13	1:L:237:VAL:HG22	1.80	0.64
1:C:283:ASP:HA	1:C:286:ASN:HD22	1.62	0.64
3:O:28:ASP:N	3:O:28:ASP:OD1	2.31	0.64
1:A:211:LEU:HD13	1:B:216:PHE:HA	1.78	0.64
1:L:209:GLU:O	1:L:212:LEU:HB2	1.98	0.64
1:D:211:LEU:HD13	1:E:216:PHE:HA	1.80	0.63
1:H:211:LEU:HG	1:H:215:GLN:HE21	1.63	0.63
1:C:211:LEU:HD13	1:D:216:PHE:HA	1.81	0.63
2:M:216:LEU:HD23	2:M:232:ILE:HB	1.81	0.63
3:N:34:THR:HB	3:N:41:ASP:HB2	1.81	0.63
1:H:321:ALA:HA	1:I:314:MET:HG2	1.78	0.63
1:F:178:VAL:O	1:F:181:THR:HB	1.98	0.63
1:J:232:LEU:HD13	1:K:237:VAL:HA	1.79	0.63
1:A:204:ASN:HA	1:B:209:GLU:HG3	1.80	0.63
1:F:182:LYS:HD2	1:G:188:VAL:HG21	1.81	0.63
3:O:37:PHE:HB3	3:O:122:LEU:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:LEU:HB3	1:D:47:TYR:HE1	1.63	0.63
1:E:78:LEU:HD13	1:F:83:ILE:HG12	1.81	0.63
1:E:257:ARG:HB3	1:F:262:TYR:HB3	1.81	0.63
1:C:241:ARG:HA	1:C:243:GLN:HE21	1.64	0.62
1:H:102:LYS:HG3	1:I:108:ALA:HB2	1.81	0.62
2:M:184:PRO:HB3	2:M:221:LYS:HE3	1.79	0.62
2:M:262:GLN:HB3	2:M:265:LYS:HB2	1.81	0.62
1:C:211:LEU:HG	1:C:215:GLN:HE21	1.63	0.62
1:C:233:VAL:HA	1:C:236:LYS:HD2	1.81	0.62
1:G:257:ARG:HB3	1:H:262:TYR:HB3	1.81	0.62
1:K:208:GLN:HE22	1:K:211:LEU:HD23	1.65	0.62
2:M:125:TYR:HB2	2:M:134:LEU:HD22	1.80	0.62
2:M:146:TYR:HB2	2:M:184:PRO:HD3	1.81	0.62
3:O:100:GLN:HB2	3:O:111:ILE:HD13	1.82	0.62
2:M:192:GLY:H	2:M:196:GLN:HB3	1.64	0.62
2:M:426:ASN:O	2:M:448:TYR:HA	1.99	0.62
3:O:23:ASP:OD1	3:O:105:ASN:ND2	2.32	0.62
3:O:94:ARG:HG2	3:O:96:TYR:CE1	2.34	0.62
3:P:96:TYR:CD2	3:P:116:THR:HB	2.34	0.62
1:F:197:ASN:HA	1:G:202:LEU:HD13	1.82	0.62
1:H:181:THR:O	1:H:184:MET:HB2	2.00	0.62
1:H:209:GLU:O	1:H:212:LEU:HB2	2.00	0.62
1:G:190:GLU:HG2	1:H:195:VAL:HG22	1.82	0.61
1:K:211:LEU:HG	1:K:215:GLN:HE21	1.65	0.61
1:F:12:THR:HB	1:F:22:LEU:HB2	1.81	0.61
1:J:195:VAL:HG12	1:J:199:LYS:HE3	1.82	0.61
2:M:346:PRO:HG2	2:M:349:ALA:HB2	1.82	0.61
3:N:48:THR:O	3:P:58:ARG:NH2	2.33	0.61
1:E:186:GLN:HE22	1:F:188:VAL:HG22	1.64	0.61
1:J:233:VAL:HA	1:J:236:LYS:HD2	1.81	0.61
1:E:211:LEU:HG	1:E:215:GLN:HE21	1.65	0.61
1:J:218:LEU:HD13	1:K:223:GLY:HA2	1.82	0.61
3:N:31:LEU:HD13	3:N:44:PHE:HB3	1.83	0.61
3:O:58:ARG:HH22	3:O:108:ASP:CG	2.08	0.61
3:P:66:ASN:HD21	3:P:68:ALA:HB3	1.65	0.61
1:J:257:ARG:HB3	1:K:262:TYR:HB3	1.82	0.61
2:M:90:VAL:HB	2:M:106:ASN:HD21	1.66	0.60
1:F:225:ASN:HD22	1:G:230:THR:HA	1.65	0.60
1:A:223:GLY:HA2	1:L:218:LEU:HD13	1.83	0.60
1:A:270:LYS:HD3	1:A:271:ARG:HH22	1.66	0.60
1:L:211:LEU:HG	1:L:215:GLN:HE21	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:73:ARG:O	3:P:73:ARG:NH1	2.27	0.60
1:B:197:ASN:HA	1:C:202:LEU:HD13	1.83	0.60
1:I:102:LYS:HE3	1:J:104:ALA:HB1	1.84	0.60
1:J:161:LEU:HD22	1:K:163:VAL:HG12	1.82	0.60
2:M:197:PHE:HD2	3:O:199:ALA:HB2	1.64	0.60
1:L:312:VAL:HG12	1:L:316:MET:HE2	1.84	0.60
2:M:418:LYS:HA	2:M:451:GLN:HE22	1.67	0.60
2:M:291:CYS:HB2	2:M:339:VAL:HG12	1.83	0.60
2:M:197:PHE:CE2	3:O:199:ALA:HB2	2.37	0.59
1:A:212:LEU:HD22	1:L:208:GLN:HE21	1.67	0.59
2:M:438:GLN:H	3:O:188:ILE:CB	2.14	0.59
2:M:466:ALA:HB2	2:M:480:GLN:HE21	1.66	0.59
3:N:37:PHE:HA	3:N:120:ARG:HB2	1.83	0.59
3:O:57:THR:HA	3:O:101:LEU:HA	1.84	0.59
1:A:115:LEU:HD11	1:L:112:LYS:HE3	1.84	0.59
1:H:44:GLY:HA2	1:H:47:TYR:HD2	1.66	0.59
2:M:86:ALA:HA	2:M:274:VAL:HG21	1.84	0.59
2:M:438:GLN:HG3	3:O:185:ASN:HA	1.84	0.59
3:O:98:TRP:HD1	3:O:112:ILE:O	1.84	0.59
1:B:181:THR:O	1:B:184:MET:HB2	2.03	0.59
1:F:218:LEU:HD13	1:G:223:GLY:HA2	1.84	0.59
1:D:235:GLN:HE22	1:E:241:ARG:HE	1.48	0.59
1:J:161:LEU:HD23	1:K:167:THR:HG21	1.84	0.59
2:M:72:TYR:HB2	2:M:304:ASN:HB2	1.85	0.59
3:N:39:GLY:HA2	3:N:85:THR:HG23	1.85	0.59
1:F:99:GLN:HA	1:F:102:LYS:HE2	1.84	0.59
1:I:181:THR:O	1:I:184:MET:HB2	2.03	0.58
1:H:218:LEU:HG	1:H:222:GLN:HE21	1.67	0.58
1:K:289:ARG:HE	1:L:288:ARG:HA	1.68	0.58
1:K:290:THR:HG21	2:M:44:VAL:HG21	1.86	0.58
2:M:469:TYR:O	2:M:476:GLY:CA	2.52	0.58
1:I:16:LEU:HG	1:J:31:LEU:HB3	1.85	0.58
3:O:31:LEU:H	3:O:112:ILE:HG21	1.68	0.58
1:C:238:ALA:HB3	1:D:241:ARG:HH22	1.68	0.58
2:M:170:MET:HE3	2:M:238:LEU:HD13	1.86	0.58
1:A:148:ARG:HA	1:L:143:THR:HA	1.86	0.58
1:A:188:VAL:HG21	1:L:182:LYS:HD2	1.85	0.58
1:B:258:GLN:HB2	1:C:262:TYR:HE2	1.69	0.58
1:F:279:LYS:HD3	1:G:280:ILE:HG12	1.85	0.58
3:P:46:TRP:NE1	3:P:51:PRO:O	2.30	0.58
1:F:36:GLU:HB2	1:F:42:LEU:HG	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:168:ALA:HA	1:K:171:LYS:HD2	1.85	0.57
1:K:179:GLN:HA	1:K:182:LYS:HE3	1.86	0.57
3:N:132:GLY:N	3:P:138:LEU:HA	2.20	0.57
2:M:114:LEU:HD23	2:M:150:MET:HE3	1.86	0.57
2:M:151:ILE:HD12	2:M:215:LEU:HD23	1.85	0.57
1:E:208:GLN:HE21	1:F:212:LEU:HD22	1.70	0.57
1:F:211:LEU:HG	1:F:215:GLN:HE21	1.69	0.57
2:M:62:ALA:HB1	2:M:312:VAL:HG13	1.86	0.57
2:M:105:TYR:CZ	2:M:174:PHE:HB3	2.40	0.57
1:G:176:THR:HA	1:G:179:GLN:HG2	1.86	0.57
1:L:216:PHE:O	1:L:219:THR:HB	2.05	0.57
3:P:111:ILE:HG22	3:P:112:ILE:H	1.68	0.57
1:B:165:GLU:HB3	1:C:170:THR:HG21	1.85	0.57
1:D:213:LYS:O	1:D:216:PHE:HB3	2.04	0.57
2:M:86:ALA:O	2:M:90:VAL:HG23	2.04	0.57
3:O:55:GLY:O	3:O:77:ASN:ND2	2.37	0.57
1:B:208:GLN:HG2	1:C:212:LEU:HD13	1.87	0.57
1:H:36:GLU:HB2	1:H:42:LEU:HG	1.87	0.57
1:I:196:LEU:HA	1:I:199:LYS:HD2	1.86	0.57
3:P:76:VAL:HG11	3:P:81:TYR:HB2	1.87	0.57
1:A:255:ILE:HD12	1:B:244:THR:HA	1.86	0.57
1:F:235:GLN:NE2	1:G:241:ARG:HE	2.02	0.57
1:H:11:LEU:HG	1:H:12:THR:HG22	1.86	0.57
1:A:202:LEU:HD13	1:L:197:ASN:HA	1.86	0.57
1:K:211:LEU:HD13	1:L:216:PHE:HA	1.86	0.57
1:B:267:ASP:O	1:B:271:ARG:HG2	2.05	0.56
1:J:218:LEU:HG	1:J:222:GLN:HE21	1.69	0.56
2:M:86:ALA:HB1	2:M:245:HIS:CE1	2.40	0.56
2:M:213:TYR:HA	2:M:236:MET:HG3	1.87	0.56
2:M:356:THR:O	2:M:360:GLU:HG2	2.04	0.56
1:E:176:THR:O	1:E:179:GLN:HB2	2.05	0.56
2:M:126:GLN:O	2:M:135:PRO:HD2	2.04	0.56
2:M:135:PRO:HA	2:M:138:SER:HB2	1.87	0.56
2:M:197:PHE:HE2	3:O:199:ALA:N	2.02	0.56
2:M:328:HIS:HA	2:M:333:ILE:HG12	1.87	0.56
1:A:211:LEU:HA	1:B:216:PHE:HD2	1.70	0.56
1:D:56:THR:O	1:D:59:LEU:HB3	2.05	0.56
1:E:52:THR:HG21	1:F:33:LEU:HD11	1.86	0.56
1:E:165:GLU:HB3	1:F:170:THR:HG21	1.87	0.56
1:G:211:LEU:HG	1:G:215:GLN:HE21	1.71	0.56
1:L:245:ILE:HG22	1:L:247:ALA:H	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:94:ILE:HG12	2:M:259:PHE:CG	2.40	0.56
2:M:196:GLN:NE2	3:O:198:THR:CB	2.68	0.56
3:N:35:PRO:HG3	3:N:118:THR:H	1.69	0.56
3:N:79:ASN:CG	3:P:75:PHE:H	2.14	0.56
1:A:97:ILE:O	1:A:100:ALA:HB3	2.05	0.56
1:G:12:THR:HB	1:G:22:LEU:HB2	1.86	0.56
1:A:170:THR:O	1:A:174:VAL:HG23	2.05	0.56
1:B:211:LEU:HD13	1:C:216:PHE:HA	1.88	0.56
1:D:275:GLN:HE22	1:E:273:ALA:HA	1.69	0.56
1:E:204:ASN:HA	1:F:209:GLU:HG3	1.85	0.56
1:D:216:PHE:O	1:D:219:THR:HB	2.04	0.56
1:J:189:LEU:HB2	1:K:195:VAL:HG21	1.88	0.56
3:N:38:GLY:N	3:N:120:ARG:O	2.30	0.56
1:K:235:GLN:HE22	1:L:241:ARG:NH2	2.04	0.56
3:N:31:LEU:HD11	3:N:42:ILE:HG23	1.87	0.56
3:N:31:LEU:HD22	3:N:99:ILE:HG23	1.88	0.56
1:D:102:LYS:HE3	1:E:104:ALA:HB1	1.88	0.55
1:D:218:LEU:HD13	1:E:223:GLY:HA2	1.89	0.55
1:E:190:GLU:HG2	1:F:195:VAL:HG22	1.88	0.55
1:I:271:ARG:HD3	1:J:273:ALA:HB2	1.88	0.55
2:M:65:TRP:HA	2:M:68:ARG:HD2	1.87	0.55
2:M:438:GLN:CG	3:O:185:ASN:HA	2.35	0.55
3:O:65:ALA:HA	3:O:96:TYR:CD2	2.41	0.55
3:O:54:VAL:HG11	3:O:101:LEU:HD23	1.87	0.55
1:K:124:GLN:HA	1:L:130:PHE:HA	1.87	0.55
1:K:165:GLU:HB3	1:L:170:THR:HG21	1.88	0.55
1:L:12:THR:HB	1:L:22:LEU:HB2	1.87	0.55
2:M:86:ALA:HB1	2:M:245:HIS:HE1	1.72	0.55
1:F:223:GLY:O	1:F:226:THR:HB	2.07	0.55
2:M:193:GLY:C	3:O:199:ALA:HA	2.31	0.55
2:M:193:GLY:N	3:O:202:SER:CB	2.70	0.55
1:F:52:THR:HG21	1:G:33:LEU:HD21	1.89	0.55
1:H:281:LEU:HD12	1:H:311:VAL:HG21	1.88	0.55
1:I:170:THR:O	1:I:174:VAL:HG23	2.05	0.55
1:I:232:LEU:HG	1:I:236:LYS:HE3	1.87	0.55
1:A:174:VAL:HG22	1:L:169:LYS:HB2	1.88	0.55
1:G:211:LEU:HD13	1:H:216:PHE:HA	1.89	0.55
1:A:186:GLN:O	1:A:190:GLU:HG3	2.07	0.55
1:F:175:LEU:HD21	1:G:181:THR:HG21	1.88	0.55
3:N:104:ILE:HG21	3:P:104:ILE:HG21	1.88	0.55
1:A:31:LEU:HD13	1:L:16:LEU:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:ALA:HA	1:F:171:LYS:HD2	1.86	0.55
1:I:249:VAL:HG22	1:J:244:THR:HB	1.88	0.55
2:M:29:PRO:HG2	2:M:501:ARG:HB2	1.89	0.55
3:O:29:LEU:HD11	3:O:47:PRO:HD3	1.89	0.55
1:F:208:GLN:HE21	1:G:212:LEU:HD22	1.72	0.55
1:I:218:LEU:HD13	1:J:223:GLY:HA2	1.89	0.55
1:C:175:LEU:HD21	1:D:181:THR:HG21	1.87	0.55
2:M:414:ARG:HA	2:M:457:TYR:O	2.07	0.55
1:B:179:GLN:OE1	1:C:185:GLU:HG3	2.07	0.54
1:D:179:GLN:HB2	1:E:184:MET:HG2	1.88	0.54
1:F:225:ASN:HA	1:F:228:GLU:HB2	1.89	0.54
2:M:173:ASP:HB3	2:M:200:TRP:CE2	2.43	0.54
2:M:373:ILE:HG13	2:M:382:LYS:HD3	1.89	0.54
3:N:94:ARG:HH11	3:N:118:THR:HG23	1.72	0.54
3:N:94:ARG:NH1	3:N:118:THR:HG23	2.21	0.54
3:N:104:ILE:HD13	3:P:104:ILE:HD12	1.89	0.54
1:G:180:GLN:HG2	1:G:184:MET:HE1	1.90	0.54
1:E:218:LEU:HD13	1:F:223:GLY:HA2	1.89	0.54
1:J:197:ASN:HA	1:K:202:LEU:HD13	1.88	0.54
2:M:467:MET:HB2	2:M:486:LEU:HD12	1.89	0.54
3:N:44:PHE:HE2	3:N:101:LEU:HD21	1.72	0.54
3:N:90:LYS:HB2	3:N:93:GLN:HB2	1.89	0.54
1:A:181:THR:O	1:A:184:MET:HB2	2.07	0.54
1:A:240:GLU:HG3	1:L:235:GLN:HE21	1.72	0.54
1:B:185:GLU:O	1:B:188:VAL:HB	2.08	0.54
3:P:37:PHE:HA	3:P:120:ARG:HB2	1.90	0.54
3:P:43:GLU:OE2	3:P:79:ASN:ND2	2.41	0.54
1:A:178:VAL:O	1:A:181:THR:HB	2.08	0.54
1:H:170:THR:O	1:H:174:VAL:HG23	2.08	0.54
1:K:281:LEU:HD12	1:K:311:VAL:HG21	1.89	0.54
3:N:42:ILE:HB	3:N:81:TYR:O	2.07	0.54
1:E:161:LEU:HD23	1:F:163:VAL:HG12	1.90	0.54
1:H:190:GLU:HG2	1:I:195:VAL:HG22	1.89	0.54
1:J:169:LYS:HG3	1:K:174:VAL:HG22	1.90	0.54
3:O:81:TYR:HE1	3:P:80:PHE:CG	2.25	0.54
3:O:112:ILE:HG22	3:O:113:GLY:H	1.73	0.54
2:M:178:PRO:HD3	2:M:200:TRP:CE3	2.43	0.53
1:A:280:ILE:HG12	1:L:279:LYS:HD3	1.89	0.53
1:G:169:LYS:HB2	1:H:174:VAL:HG22	1.90	0.53
1:J:319:VAL:HG11	1:K:277:ALA:HB2	1.90	0.53
1:K:209:GLU:O	1:K:212:LEU:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:29:LEU:HD13	3:N:45:THR:O	2.08	0.53
1:K:179:GLN:HG3	1:L:181:THR:HG23	1.91	0.53
1:G:77:ALA:O	1:G:80:GLU:HG3	2.07	0.53
2:M:111:LEU:HB2	2:M:244:TYR:CE1	2.44	0.53
1:I:281:LEU:HD13	1:I:311:VAL:HG21	1.89	0.53
1:L:170:THR:O	1:L:174:VAL:HG23	2.09	0.53
3:N:93:GLN:HG3	3:N:95:TYR:CE2	2.43	0.53
2:M:91:VAL:HA	2:M:101:ILE:HD11	1.90	0.53
3:N:220:ALA:HB2	3:P:217:ASN:HA	1.89	0.53
3:P:67:PHE:HB2	3:P:98:TRP:CD1	2.44	0.53
1:J:30:ARG:HG2	1:J:47:TYR:HE1	1.73	0.53
3:N:139:LEU:HA	3:O:132:GLY:H	1.74	0.53
1:F:105:GLU:HB2	1:G:111:VAL:HG11	1.90	0.52
1:L:30:ARG:HE	1:L:51:LEU:HD22	1.73	0.52
3:P:58:ARG:HG2	3:P:75:PHE:CE2	2.44	0.52
1:C:191:SER:O	1:C:194:LYS:HB3	2.09	0.52
2:M:150:MET:HB2	2:M:178:PRO:HG2	1.91	0.52
2:M:298:VAL:O	2:M:306:TYR:HB2	2.09	0.52
3:N:48:THR:HA	3:N:51:PRO:HB3	1.91	0.52
1:B:321:ALA:HA	1:C:314:MET:HG2	1.91	0.52
1:K:267:ASP:O	1:K:271:ARG:HG2	2.09	0.52
3:O:91:VAL:HG11	3:O:121:PRO:HD3	1.91	0.52
1:A:233:VAL:HA	1:A:236:LYS:HD2	1.91	0.52
1:L:281:LEU:HD12	1:L:311:VAL:HG21	1.90	0.52
3:N:27:ASN:OD1	3:N:110:ASP:N	2.41	0.52
3:N:139:LEU:CA	3:O:132:GLY:H	2.22	0.52
3:P:93:GLN:NE2	3:P:94:ARG:O	2.42	0.52
1:A:180:GLN:HG2	1:A:184:MET:HE1	1.90	0.52
1:K:249:VAL:HG13	1:L:244:THR:HB	1.90	0.52
1:K:284:THR:O	1:K:288:ARG:HG3	2.10	0.52
2:M:81:VAL:HG11	2:M:275:PHE:HA	1.92	0.52
3:N:57:THR:OG1	3:N:101:LEU:HG	2.10	0.52
3:O:26:MET:HG2	3:O:54:VAL:HG22	1.92	0.52
1:I:195:VAL:HG12	1:I:199:LYS:HE3	1.90	0.52
1:J:209:GLU:O	1:J:212:LEU:HB2	2.08	0.52
3:N:224:GLU:HA	3:P:224:GLU:HA	1.92	0.52
3:O:86:ASP:HB2	3:O:89:SER:HB3	1.92	0.52
1:B:256:GLY:HA2	1:B:259:LYS:HD3	1.92	0.52
2:M:145:VAL:HA	2:M:220:TRP:HB3	1.91	0.52
1:F:161:LEU:O	1:F:164:LYS:HB2	2.10	0.52
2:M:264:GLY:H	2:M:272:ASP:CG	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:43:GLU:OE2	3:O:79:ASN:ND2	2.43	0.52
1:A:280:ILE:HG23	1:L:279:LYS:HD3	1.92	0.52
1:C:197:ASN:HA	1:D:202:LEU:HD13	1.92	0.52
1:D:235:GLN:HE22	1:E:241:ARG:NE	2.08	0.52
1:E:170:THR:O	1:E:174:VAL:HG23	2.09	0.52
2:M:425:ILE:HG12	2:M:450:ARG:HB2	1.91	0.52
1:B:6:ILE:HD12	1:B:66:LEU:HD23	1.92	0.51
1:D:52:THR:HA	1:D:55:ILE:HD11	1.91	0.51
1:E:218:LEU:HG	1:E:222:GLN:HE21	1.74	0.51
1:G:267:ASP:O	1:G:271:ARG:HG2	2.10	0.51
1:H:136:GLN:HA	1:I:141:VAL:HA	1.92	0.51
2:M:182:TYR:HB2	2:M:190:THR:HG22	1.91	0.51
3:P:67:PHE:CG	3:P:111:ILE:HG21	2.45	0.51
1:C:239:SER:HA	1:D:243:GLN:HG2	1.93	0.51
1:F:211:LEU:HD13	1:G:216:PHE:HA	1.91	0.51
1:I:267:ASP:O	1:I:271:ARG:HG2	2.10	0.51
3:P:26:MET:HE1	3:P:107:THR:HG22	1.92	0.51
1:E:99:GLN:HA	1:E:102:LYS:HE2	1.92	0.51
1:I:168:ALA:HA	1:I:171:LYS:HD2	1.92	0.51
1:J:196:LEU:HA	1:J:199:LYS:HD2	1.91	0.51
1:J:289:ARG:NH2	1:K:293:THR:H	2.07	0.51
1:K:189:LEU:O	1:K:192:THR:HB	2.11	0.51
2:M:216:LEU:O	2:M:231:THR:HA	2.10	0.51
1:J:179:GLN:HA	1:J:182:LYS:HE3	1.91	0.51
3:N:60:PHE:CG	3:N:67:PHE:HE1	2.28	0.51
3:O:24:PRO:HB3	3:O:50:ASN:O	2.10	0.51
3:P:67:PHE:HB2	3:P:98:TRP:NE1	2.25	0.51
1:F:189:LEU:HB3	1:G:195:VAL:HG11	1.93	0.51
2:M:104:TYR:HD2	2:M:248:ARG:HG2	1.76	0.51
1:B:97:ILE:O	1:B:100:ALA:HB3	2.10	0.51
1:D:178:VAL:O	1:D:181:THR:HB	2.11	0.51
1:C:257:ARG:CZ	1:D:263:LYS:HD2	2.41	0.51
1:E:191:SER:O	1:E:194:LYS:HB3	2.10	0.51
1:H:254:VAL:HG11	1:I:258:GLN:CD	2.36	0.51
1:I:257:ARG:HB3	1:J:262:TYR:HB3	1.93	0.51
1:A:141:VAL:HA	1:L:136:GLN:HA	1.92	0.51
1:D:197:ASN:HA	1:E:202:LEU:HD13	1.93	0.51
1:E:179:GLN:HG3	1:F:181:THR:HG23	1.93	0.51
1:I:179:GLN:HA	1:I:182:LYS:HE3	1.93	0.51
1:K:218:LEU:HG	1:K:222:GLN:HE21	1.75	0.51
3:N:25:ASN:HD21	3:N:47:PRO:HA	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLN:HE22	1:B:188:VAL:HG13	1.75	0.51
1:D:208:GLN:HG3	1:E:212:LEU:HD13	1.93	0.51
1:F:170:THR:O	1:F:174:VAL:HG23	2.10	0.51
1:G:209:GLU:O	1:G:212:LEU:HB2	2.11	0.51
1:J:281:LEU:HD12	1:J:311:VAL:HG21	1.93	0.51
1:L:267:ASP:O	1:L:271:ARG:HG2	2.10	0.51
3:O:26:MET:HB3	3:O:101:LEU:HD22	1.93	0.51
1:C:232:LEU:HD13	1:D:237:VAL:HG22	1.93	0.51
1:G:284:THR:O	1:G:288:ARG:HG3	2.10	0.51
1:I:164:LYS:O	1:I:167:THR:HB	2.10	0.51
1:I:186:GLN:NE2	1:J:188:VAL:HG22	2.25	0.51
1:I:321:ALA:HB1	1:J:311:VAL:HA	1.93	0.51
3:N:70:ALA:HB2	3:N:98:TRP:CZ3	2.46	0.51
3:P:99:ILE:H	3:P:112:ILE:CG1	2.24	0.51
1:B:196:LEU:HA	1:B:199:LYS:HD2	1.93	0.50
1:G:289:ARG:HD3	1:H:295:THR:O	2.10	0.50
1:I:211:LEU:HG	1:I:215:GLN:HE21	1.76	0.50
2:M:91:VAL:HG22	2:M:103:THR:HG21	1.93	0.50
3:P:31:LEU:HD13	3:P:99:ILE:HG12	1.93	0.50
1:F:202:LEU:HA	1:F:205:LEU:HD12	1.93	0.50
2:M:429:SER:HB3	2:M:446:TYR:CZ	2.46	0.50
2:M:471:ILE:HG12	2:M:516:ASN:HB3	1.92	0.50
1:A:195:VAL:HG22	1:L:190:GLU:HG2	1.92	0.50
1:F:232:LEU:HB2	1:G:237:VAL:HG22	1.93	0.50
1:H:245:ILE:HG22	1:H:247:ALA:H	1.76	0.50
3:N:60:PHE:CE1	3:N:100:GLN:HB3	2.43	0.50
3:O:70:ALA:HB2	3:O:98:TRP:CZ3	2.46	0.50
1:B:170:THR:O	1:B:174:VAL:HG23	2.12	0.50
1:H:175:LEU:O	1:H:179:GLN:HG2	2.10	0.50
3:N:40:ILE:HD13	3:N:117:ALA:HB3	1.94	0.50
1:D:12:THR:HB	1:D:22:LEU:HB2	1.93	0.50
1:E:167:THR:O	1:E:170:THR:HB	2.11	0.50
1:F:225:ASN:HD21	1:G:233:VAL:HG21	1.75	0.50
1:H:172:GLN:HE21	1:I:177:ALA:HB1	1.76	0.50
1:H:179:GLN:HB2	1:I:184:MET:HG2	1.92	0.50
1:K:117:GLN:O	1:K:121:PRO:HD3	2.12	0.50
1:K:176:THR:O	1:K:179:GLN:HB2	2.11	0.50
1:L:229:GLN:O	1:L:233:VAL:HG23	2.12	0.50
2:M:94:ILE:HB	2:M:101:ILE:HD13	1.92	0.50
3:O:31:LEU:HD22	3:O:99:ILE:HG23	1.94	0.50
1:G:107:ILE:O	1:G:111:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:218:LEU:HD13	1:L:223:GLY:HA2	1.93	0.50
1:L:94:ASP:O	1:L:97:ILE:HG12	2.11	0.50
2:M:65:TRP:CZ2	2:M:311:GLU:HG2	2.47	0.50
2:M:115:HIS:CD2	2:M:246:GLN:HB3	2.46	0.50
3:N:139:LEU:O	3:N:143:LEU:N	2.35	0.50
2:M:498:LEU:HB3	2:M:502:ALA:HB3	1.94	0.50
3:N:25:ASN:O	3:N:47:PRO:HG3	2.10	0.50
3:P:102:VAL:HG22	3:P:108:ASP:HA	1.94	0.50
1:I:106:LEU:HA	1:J:111:VAL:HG22	1.93	0.50
3:N:64:ASP:O	3:N:98:TRP:HH2	1.95	0.50
3:O:31:LEU:HD11	3:O:42:ILE:HG22	1.94	0.50
3:P:100:GLN:HG3	3:P:109:GLY:C	2.35	0.50
1:E:216:PHE:O	1:E:219:THR:HB	2.12	0.50
2:M:114:LEU:HD13	2:M:200:TRP:CE3	2.47	0.50
3:P:31:LEU:HD22	3:P:99:ILE:HG23	1.93	0.50
1:G:218:LEU:HG	1:G:222:GLN:HE21	1.77	0.49
1:D:297:ALA:HB1	1:D:304:ASP:HA	1.93	0.49
2:M:121:LEU:HD21	2:M:216:LEU:HD22	1.94	0.49
3:N:53:ALA:HA	3:P:104:ILE:HG22	1.93	0.49
1:A:244:THR:HB	1:L:249:VAL:HG22	1.93	0.49
1:D:159:GLN:O	1:D:163:VAL:HB	2.12	0.49
1:C:281:LEU:HD12	1:C:311:VAL:HG21	1.95	0.49
1:D:314:MET:HG3	1:D:315:LEU:N	2.25	0.49
2:M:342:PHE:HE1	2:M:514:ALA:HB2	1.77	0.49
2:M:369:ALA:HA	2:M:392:GLN:HE22	1.76	0.49
3:P:31:LEU:HB3	3:P:112:ILE:HG21	1.93	0.49
3:P:65:ALA:HA	3:P:96:TYR:CD2	2.48	0.49
1:J:112:LYS:HE3	1:J:113:LEU:HD22	1.95	0.49
2:M:415:LYS:HB2	2:M:457:TYR:CE1	2.47	0.49
3:O:138:LEU:C	3:P:132:GLY:H	2.21	0.49
3:P:96:TYR:CD2	3:P:114:PRO:HB2	2.45	0.49
1:B:186:GLN:NE2	1:C:188:VAL:HG13	2.28	0.49
2:M:196:GLN:HE22	3:O:198:THR:CB	2.25	0.49
2:M:438:GLN:HE21	3:O:185:ASN:CB	2.25	0.49
3:O:96:TYR:HB2	3:O:98:TRP:CH2	2.48	0.49
3:P:91:VAL:HG13	3:P:120:ARG:C	2.37	0.49
1:A:235:GLN:NE2	1:B:240:GLU:HG3	2.28	0.49
1:A:289:ARG:HG3	1:B:287:VAL:HG12	1.94	0.49
1:D:232:LEU:HD13	1:E:237:VAL:HG22	1.95	0.49
1:H:214:ALA:HB1	1:I:219:THR:HG21	1.94	0.49
2:M:451:GLN:HA	2:M:457:TYR:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:73:ARG:NH2	3:O:83:ASP:OD1	2.44	0.49
1:A:292:ASP:HA	1:L:289:ARG:NH2	2.28	0.49
1:C:254:VAL:HG11	1:D:258:GLN:CD	2.38	0.49
1:E:283:ASP:O	1:E:287:VAL:HG23	2.13	0.49
3:O:40:ILE:HD12	3:O:95:TYR:HB2	1.95	0.49
1:G:275:GLN:HE22	1:H:273:ALA:HB1	1.78	0.49
2:M:438:GLN:NE2	3:O:185:ASN:CB	2.76	0.49
1:I:176:THR:O	1:I:179:GLN:HB2	2.13	0.48
1:L:227:GLN:O	1:L:230:THR:HB	2.13	0.48
1:B:180:GLN:HG2	1:B:184:MET:HE1	1.93	0.48
1:C:209:GLU:HA	1:C:212:LEU:HG	1.95	0.48
1:I:214:ALA:HB1	1:J:219:THR:HG21	1.94	0.48
1:J:201:GLU:O	1:J:205:LEU:HG	2.13	0.48
1:L:211:LEU:HG	1:L:215:GLN:NE2	2.28	0.48
2:M:173:ASP:HB3	2:M:200:TRP:CD2	2.48	0.48
2:M:293:PHE:HD2	2:M:301:ILE:HD13	1.79	0.48
3:N:135:ASP:N	3:P:138:LEU:O	2.39	0.48
1:B:283:ASP:O	1:B:287:VAL:HG23	2.13	0.48
1:B:312:VAL:HG12	1:B:316:MET:HE2	1.95	0.48
2:M:424:PHE:O	2:M:450:ARG:HA	2.13	0.48
3:P:70:ALA:HB2	3:P:98:TRP:CZ3	2.48	0.48
2:M:132:ASN:O	2:M:146:TYR:HA	2.13	0.48
3:N:54:VAL:HG11	3:N:101:LEU:HD23	1.96	0.48
1:D:289:ARG:HD3	1:E:295:THR:O	2.13	0.48
1:E:229:GLN:HG2	1:F:233:VAL:HG11	1.95	0.48
1:F:191:SER:O	1:F:194:LYS:HB3	2.12	0.48
1:G:99:GLN:HA	1:G:102:LYS:HE2	1.95	0.48
2:M:79:LYS:HA	2:M:280:THR:O	2.14	0.48
2:M:94:ILE:HD11	2:M:247:VAL:HG21	1.94	0.48
3:N:24:PRO:HB2	3:N:47:PRO:CG	2.42	0.48
3:O:75:PHE:H	3:P:79:ASN:CG	2.21	0.48
1:F:6:ILE:HD12	1:F:66:LEU:HD23	1.94	0.48
1:K:257:ARG:HB3	1:L:262:TYR:HB3	1.95	0.48
2:M:193:GLY:O	2:M:196:GLN:HG2	2.14	0.48
3:N:79:ASN:HD21	3:P:74:ALA:HA	1.79	0.48
3:O:24:PRO:HG2	3:O:26:MET:SD	2.53	0.48
1:D:227:GLN:O	1:D:230:THR:HB	2.14	0.48
1:E:105:GLU:HG3	1:F:111:VAL:HG21	1.95	0.48
1:F:14:VAL:HA	1:G:28:VAL:HB	1.94	0.48
1:F:106:LEU:HB2	1:G:111:VAL:HG22	1.95	0.48
1:G:162:LEU:HG	1:G:166:GLN:NE2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:ARG:HE	1:E:51:LEU:HD22	1.79	0.48
1:G:208:GLN:HG3	1:H:212:LEU:HD13	1.96	0.48
3:P:123:ILE:O	3:P:127:ILE:N	2.45	0.48
1:A:216:PHE:HA	1:L:211:LEU:HD13	1.96	0.48
1:C:112:LYS:HE2	1:C:112:LYS:HB3	1.65	0.48
1:C:289:ARG:HH21	1:D:288:ARG:HA	1.79	0.48
1:D:225:ASN:HB2	1:E:230:THR:OG1	2.13	0.48
1:E:106:LEU:HA	1:F:111:VAL:HG22	1.96	0.48
1:H:180:GLN:HG2	1:H:184:MET:HE1	1.95	0.48
1:H:186:GLN:OE1	1:I:188:VAL:HA	2.14	0.48
1:I:88:LYS:HB3	1:J:93:LEU:HD23	1.95	0.48
1:I:201:GLU:HG3	1:J:205:LEU:HD13	1.95	0.48
1:B:94:ASP:O	1:B:97:ILE:HG12	2.14	0.48
1:D:218:LEU:HG	1:D:222:GLN:HE21	1.79	0.48
1:G:102:LYS:O	1:G:106:LEU:HB2	2.14	0.48
1:J:289:ARG:HA	1:K:295:THR:HB	1.95	0.48
1:K:99:GLN:HA	1:K:102:LYS:HE2	1.96	0.48
2:M:79:LYS:HE2	2:M:81:VAL:HG22	1.95	0.48
3:P:63:THR:HG22	3:P:95:TYR:CD1	2.49	0.48
1:A:267:ASP:O	1:A:271:ARG:HG2	2.14	0.47
1:C:185:GLU:O	1:C:188:VAL:HB	2.13	0.47
1:D:193:GLN:HG2	1:E:198:MET:HB3	1.96	0.47
1:D:279:LYS:HD2	1:E:280:ILE:HG23	1.96	0.47
1:H:191:SER:O	1:H:194:LYS:HB3	2.14	0.47
1:L:211:LEU:HD12	1:L:214:ALA:HB3	1.96	0.47
1:B:200:GLN:NE2	1:C:206:VAL:HA	2.29	0.47
1:E:65:PHE:HD1	1:E:66:LEU:HD12	1.79	0.47
1:F:105:GLU:HG3	1:G:111:VAL:HG21	1.96	0.47
1:L:218:LEU:HD12	1:L:221:ASP:HB2	1.97	0.47
2:M:249:PHE:CE1	2:M:259:PHE:HB2	2.49	0.47
1:B:160:ASP:O	1:B:163:VAL:HB	2.13	0.47
1:E:106:LEU:HD21	1:F:110:LYS:HG3	1.96	0.47
1:F:39:ALA:HB3	1:F:41:ARG:HH11	1.79	0.47
1:H:232:LEU:HG	1:H:236:LYS:HE3	1.96	0.47
2:M:116:TRP:O	2:M:120:GLU:HG2	2.15	0.47
2:M:133:GLU:C	2:M:135:PRO:HD3	2.40	0.47
2:M:425:ILE:HA	2:M:449:THR:O	2.13	0.47
3:O:40:ILE:HD13	3:O:117:ALA:HB3	1.96	0.47
1:A:243:GLN:HB3	1:A:245:ILE:HG12	1.97	0.47
1:C:187:GLN:O	1:C:191:SER:HB3	2.15	0.47
1:C:216:PHE:O	1:C:219:THR:HB	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:99:GLN:OE1	1:I:107:ILE:HD11	2.14	0.47
2:M:244:TYR:HA	2:M:262:GLN:HA	1.97	0.47
2:M:422:ILE:HA	2:M:451:GLN:O	2.13	0.47
1:D:229:GLN:O	1:D:233:VAL:HG23	2.15	0.47
1:K:200:GLN:NE2	1:L:206:VAL:HA	2.28	0.47
2:M:359:PHE:HB2	2:M:425:ILE:HG21	1.96	0.47
3:N:60:PHE:CE2	3:N:72:ILE:HG12	2.48	0.47
1:A:241:ARG:HA	1:L:235:GLN:HE22	1.79	0.47
1:I:99:GLN:HA	1:I:102:LYS:HE2	1.97	0.47
1:I:194:LYS:HE2	1:I:198:MET:SD	2.54	0.47
2:M:361:TYR:HD1	2:M:494:VAL:HG21	1.80	0.47
1:B:208:GLN:HE21	1:C:212:LEU:HB3	1.79	0.47
1:C:235:GLN:HE22	1:D:241:ARG:HA	1.80	0.47
1:C:312:VAL:HG12	1:C:316:MET:HE2	1.96	0.47
1:D:196:LEU:HA	1:D:199:LYS:HD2	1.97	0.47
1:D:229:GLN:HG2	1:E:233:VAL:HG11	1.97	0.47
1:F:97:ILE:O	1:F:100:ALA:HB3	2.14	0.47
1:F:186:GLN:NE2	1:G:188:VAL:HG13	2.29	0.47
1:F:267:ASP:O	1:F:271:ARG:HG2	2.15	0.47
1:F:316:MET:HE3	1:F:316:MET:HB2	1.69	0.47
1:G:102:LYS:HB3	1:H:107:ILE:HG13	1.97	0.47
1:H:103:ASP:O	1:H:107:ILE:HG12	2.15	0.47
1:K:78:LEU:HD13	1:L:83:ILE:HG12	1.97	0.47
3:N:35:PRO:HB2	3:N:120:ARG:NH2	2.30	0.47
3:N:75:PHE:H	3:O:79:ASN:CG	2.22	0.47
3:P:29:LEU:HD11	3:P:47:PRO:HD3	1.97	0.47
1:A:186:GLN:NE2	1:B:188:VAL:HG13	2.30	0.47
1:D:213:LYS:H	1:D:213:LYS:HD2	1.80	0.47
1:F:179:GLN:HG3	1:G:181:THR:HG23	1.96	0.47
1:K:204:ASN:HA	1:L:209:GLU:HG3	1.97	0.47
2:M:104:TYR:CD2	2:M:248:ARG:HG2	2.50	0.47
2:M:111:LEU:HD21	2:M:116:TRP:CD1	2.50	0.47
1:B:312:VAL:HB	1:C:302:ARG:HB2	1.97	0.47
1:G:209:GLU:HA	1:G:212:LEU:HG	1.97	0.47
1:H:312:VAL:HG12	1:H:316:MET:HE2	1.96	0.47
1:J:102:LYS:HE3	1:K:104:ALA:HB1	1.97	0.47
1:J:289:ARG:HH21	1:K:288:ARG:HA	1.80	0.47
1:L:103:ASP:O	1:L:107:ILE:HG12	2.15	0.47
2:M:107:GLN:O	2:M:245:HIS:HA	2.15	0.47
2:M:249:PHE:HE1	2:M:259:PHE:HB2	1.80	0.47
3:N:95:TYR:O	3:N:116:THR:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:56:THR:OG1	3:O:57:THR:N	2.47	0.47
1:B:254:VAL:HG22	1:C:259:LYS:HG3	1.96	0.47
1:G:178:VAL:O	1:G:181:THR:HB	2.15	0.47
1:J:78:LEU:HD13	1:K:83:ILE:HG12	1.96	0.47
2:M:83:GLY:O	2:M:87:ARG:HG3	2.15	0.47
2:M:402:LYS:HD3	2:M:470:GLN:NE2	2.30	0.47
3:O:29:LEU:HD13	3:O:45:THR:O	2.15	0.47
3:P:64:ASP:O	3:P:98:TRP:HH2	1.98	0.47
3:P:67:PHE:CD2	3:P:111:ILE:HG21	2.50	0.47
1:B:195:VAL:HG12	1:B:199:LYS:HE3	1.97	0.46
1:C:165:GLU:HG3	1:D:167:THR:HG23	1.97	0.46
1:C:289:ARG:HG2	1:D:287:VAL:HG12	1.97	0.46
2:M:188:TYR:OH	3:P:204:VAL:HA	2.15	0.46
2:M:384:GLY:HA2	2:M:435:SER:O	2.15	0.46
3:O:60:PHE:CG	3:O:67:PHE:HE1	2.33	0.46
3:O:83:ASP:OD2	3:O:97:TYR:OH	2.24	0.46
1:B:261:LEU:HD13	1:C:265:GLN:HB3	1.97	0.46
1:E:180:GLN:HE21	1:E:184:MET:HE1	1.81	0.46
1:G:112:LYS:HB3	1:G:112:LYS:HE2	1.60	0.46
1:G:232:LEU:HD13	1:H:237:VAL:HG22	1.96	0.46
1:K:169:LYS:HB2	1:L:174:VAL:HG22	1.95	0.46
3:P:62:SER:H	3:P:98:TRP:HZ3	1.64	0.46
1:A:108:ALA:HB2	1:L:102:LYS:HG2	1.96	0.46
1:E:232:LEU:HD13	1:F:237:VAL:HG22	1.98	0.46
1:J:106:LEU:HG	1:K:111:VAL:HG22	1.97	0.46
1:J:187:GLN:O	1:J:191:SER:HB3	2.15	0.46
2:M:492:ARG:HA	2:M:495:LEU:HD23	1.97	0.46
1:D:102:LYS:HG2	1:E:108:ALA:HB2	1.98	0.46
1:J:178:VAL:O	1:J:181:THR:HB	2.15	0.46
1:K:174:VAL:O	1:K:178:VAL:HG23	2.15	0.46
2:M:36:GLY:HA3	2:M:43:ILE:HA	1.96	0.46
2:M:373:ILE:HA	2:M:382:LYS:HG2	1.97	0.46
3:N:35:PRO:HA	3:N:118:THR:O	2.15	0.46
1:B:190:GLU:HG3	1:C:195:VAL:HG22	1.97	0.46
1:E:168:ALA:HA	1:E:171:LYS:HD2	1.97	0.46
1:J:209:GLU:HA	1:J:212:LEU:HD12	1.96	0.46
2:M:327:VAL:HG21	2:M:339:VAL:HG11	1.97	0.46
2:M:406:SER:O	2:M:465:PRO:HA	2.16	0.46
1:B:289:ARG:HD3	1:C:295:THR:O	2.16	0.46
1:D:14:VAL:HA	1:E:28:VAL:HB	1.98	0.46
1:E:307:ASN:O	1:E:311:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:VAL:HG12	1:F:199:LYS:HE3	1.98	0.46
2:M:95:ALA:HA	2:M:99:GLY:O	2.16	0.46
1:D:175:LEU:O	1:D:179:GLN:HG2	2.15	0.46
1:F:16:LEU:HG	1:G:31:LEU:HB3	1.97	0.46
1:F:249:VAL:HG22	1:G:244:THR:HB	1.98	0.46
1:H:178:VAL:O	1:H:181:THR:HB	2.16	0.46
3:N:25:ASN:ND2	3:N:47:PRO:HA	2.31	0.46
1:A:312:VAL:HB	1:B:302:ARG:HB2	1.97	0.46
1:C:168:ALA:HA	1:C:171:LYS:HD2	1.97	0.46
2:M:410:ILE:HG12	2:M:462:ILE:HG13	1.98	0.46
3:N:31:LEU:HD12	3:N:32:LYS:H	1.81	0.46
3:N:33:ALA:N	3:N:115:ALA:HB1	2.30	0.46
1:D:190:GLU:HG3	1:E:195:VAL:HG22	1.97	0.46
1:D:288:ARG:NH1	1:D:297:ALA:HB2	2.31	0.46
1:G:241:ARG:HA	1:G:243:GLN:HE21	1.79	0.46
1:I:185:GLU:O	1:I:188:VAL:HB	2.16	0.46
1:I:211:LEU:HD12	1:I:214:ALA:HB3	1.97	0.46
2:M:90:VAL:O	2:M:94:ILE:HG13	2.15	0.46
2:M:125:TYR:HA	2:M:136:GLY:HA3	1.96	0.46
2:M:236:MET:HE2	2:M:238:LEU:HG	1.97	0.46
1:F:200:GLN:NE2	1:G:206:VAL:HA	2.31	0.46
2:M:299:LYS:HG2	2:M:306:TYR:CZ	2.50	0.46
1:A:243:GLN:CD	1:A:244:THR:H	2.23	0.45
1:D:223:GLY:O	1:D:226:THR:HB	2.16	0.45
1:J:211:LEU:HG	1:J:215:GLN:HE21	1.81	0.45
1:L:107:ILE:O	1:L:111:VAL:HG23	2.16	0.45
3:N:100:GLN:HG3	3:N:109:GLY:O	2.16	0.45
1:K:159:GLN:O	1:K:163:VAL:HG23	2.17	0.45
2:M:471:ILE:HG23	2:M:516:ASN:HB3	1.97	0.45
1:A:293:THR:OG1	1:L:289:ARG:HD2	2.16	0.45
1:B:112:LYS:HB3	1:B:112:LYS:HE2	1.67	0.45
1:B:192:THR:O	1:B:195:VAL:HG23	2.15	0.45
2:M:393:MET:HE2	2:M:393:MET:HB3	1.83	0.45
3:N:26:MET:HA	3:N:29:LEU:HD11	1.98	0.45
3:P:60:PHE:CG	3:P:67:PHE:HE1	2.34	0.45
1:C:183:VAL:HA	1:C:186:GLN:CD	2.42	0.45
1:D:170:THR:O	1:D:174:VAL:HG23	2.17	0.45
1:D:308:VAL:O	1:D:312:VAL:HG23	2.17	0.45
1:J:33:LEU:HD13	1:J:47:TYR:CD1	2.51	0.45
2:M:501:ARG:O	2:M:505:GLN:HG2	2.17	0.45
1:A:195:VAL:HG22	1:L:190:GLU:CG	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:SER:O	1:B:194:LYS:HB3	2.16	0.45
1:C:218:LEU:HG	1:C:222:GLN:HE21	1.82	0.45
1:H:16:LEU:HG	1:I:31:LEU:HB3	1.98	0.45
1:H:239:SER:OG	1:I:241:ARG:HA	2.17	0.45
1:I:316:MET:SD	1:J:307:ASN:HB3	2.56	0.45
1:K:105:GLU:HG3	1:L:111:VAL:HG21	1.99	0.45
1:K:312:VAL:HG12	1:K:316:MET:HE2	1.98	0.45
1:L:99:GLN:HA	1:L:102:LYS:HE2	1.98	0.45
2:M:78:SER:O	2:M:281:LYS:HA	2.17	0.45
2:M:105:TYR:CZ	2:M:248:ARG:HB2	2.51	0.45
2:M:284:THR:HG22	2:M:492:ARG:HD3	1.98	0.45
3:N:74:ALA:HB1	3:O:79:ASN:OD1	2.16	0.45
3:P:60:PHE:CE2	3:P:72:ILE:HG12	2.52	0.45
3:P:120:ARG:HB3	3:P:121:PRO:HD2	1.97	0.45
1:F:186:GLN:HE22	1:G:188:VAL:HG13	1.81	0.45
1:F:235:GLN:HE22	1:G:241:ARG:NE	2.08	0.45
1:J:161:LEU:O	1:J:164:LYS:HB2	2.15	0.45
1:K:163:VAL:O	1:K:167:THR:HB	2.17	0.45
1:K:289:ARG:NH1	1:L:293:THR:H	2.13	0.45
2:M:192:GLY:O	3:O:198:THR:O	2.34	0.45
2:M:386:TYR:O	2:M:434:LYS:HE3	2.17	0.45
2:M:470:GLN:HG2	2:M:472:THR:O	2.16	0.45
3:N:59:LEU:O	3:N:73:ARG:N	2.50	0.45
3:O:31:LEU:HD12	3:O:31:LEU:HA	1.62	0.45
1:A:305:ASP:OD1	1:B:301:ASN:HB3	2.17	0.45
1:C:279:LYS:HD3	1:D:280:ILE:HG12	1.99	0.45
1:E:186:GLN:NE2	1:F:188:VAL:HG22	2.32	0.45
1:H:77:ALA:O	1:H:80:GLU:HG3	2.16	0.45
1:I:229:GLN:O	1:I:233:VAL:HG23	2.17	0.45
1:K:321:ALA:HB3	1:L:310:ARG:HD3	1.97	0.45
3:O:96:TYR:CD2	3:O:114:PRO:HB2	2.47	0.45
1:A:312:VAL:HG12	1:A:316:MET:HE2	1.99	0.45
1:F:102:LYS:HE3	1:G:104:ALA:HB1	1.99	0.45
1:F:254:VAL:HG22	1:G:259:LYS:HG3	1.99	0.45
1:K:321:ALA:HB1	1:L:311:VAL:HA	1.99	0.45
2:M:21:ASP:HB3	2:M:24:HIS:ND1	2.31	0.45
2:M:369:ALA:HA	2:M:392:GLN:NE2	2.32	0.45
1:A:37:HIS:HB2	1:A:42:LEU:HD13	1.98	0.45
1:B:190:GLU:CG	1:C:195:VAL:HG22	2.47	0.45
1:D:193:GLN:NE2	1:E:199:LYS:HA	2.32	0.45
1:F:199:LYS:O	1:F:202:LEU:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:96:TYR:CG	3:P:116:THR:HB	2.51	0.45
1:C:161:LEU:HD23	1:D:163:VAL:HG13	1.99	0.45
1:F:37:HIS:HB2	1:F:42:LEU:HD12	1.99	0.45
1:G:172:GLN:HE21	1:H:177:ALA:HB1	1.82	0.45
1:A:209:GLU:HG3	1:L:204:ASN:HA	1.98	0.44
1:B:251:ALA:HA	1:B:256:GLY:HA3	1.97	0.44
1:C:249:VAL:HG11	1:C:259:LYS:HD3	1.99	0.44
1:J:191:SER:O	1:J:195:VAL:HG23	2.16	0.44
1:D:264:ALA:HB1	1:E:269:PHE:HB2	1.99	0.44
1:E:76:ALA:O	1:E:79:VAL:HB	2.17	0.44
2:M:63:TYR:CD2	2:M:287:PRO:HD3	2.52	0.44
1:C:242:ALA:H	1:D:243:GLN:HE22	1.64	0.44
1:I:218:LEU:HG	1:I:222:GLN:NE2	2.29	0.44
1:I:310:ARG:HD2	1:I:311:VAL:HG23	1.99	0.44
1:J:190:GLU:H	1:J:190:GLU:HG3	1.54	0.44
2:M:73:TRP:HH2	2:M:301:ILE:HD13	1.80	0.44
3:O:99:ILE:HG13	3:O:112:ILE:CG1	2.46	0.44
1:D:107:ILE:O	1:D:111:VAL:HG23	2.17	0.44
1:E:232:LEU:O	1:E:235:GLN:HB3	2.18	0.44
1:E:252:ASP:HA	1:E:257:ARG:HH21	1.82	0.44
1:H:201:GLU:HG3	1:I:205:LEU:HD13	2.00	0.44
1:J:267:ASP:O	1:J:271:ARG:HG2	2.17	0.44
2:M:25:ILE:HG12	2:M:508:CYS:HB3	1.98	0.44
2:M:29:PRO:HG3	2:M:51:LEU:HD21	1.98	0.44
1:A:83:ILE:HG12	1:L:78:LEU:HD13	1.99	0.44
1:A:228:GLU:HG2	1:B:234:ARG:NH2	2.32	0.44
1:C:103:ASP:O	1:C:106:LEU:HB3	2.18	0.44
1:F:136:GLN:HA	1:G:144:ALA:HB3	2.00	0.44
1:G:170:THR:O	1:G:174:VAL:HG23	2.18	0.44
1:H:44:GLY:HA2	1:H:47:TYR:CD2	2.48	0.44
2:M:370:LEU:HB2	2:M:375:LYS:HG3	1.99	0.44
1:A:229:GLN:O	1:A:233:VAL:HG23	2.18	0.44
1:B:107:ILE:O	1:B:110:LYS:HB3	2.18	0.44
1:C:289:ARG:NH2	1:D:292:ASP:HA	2.33	0.44
1:G:6:ILE:HD12	1:G:66:LEU:HD23	1.98	0.44
1:H:190:GLU:CD	1:I:194:LYS:HD3	2.42	0.44
1:K:289:ARG:HD3	1:L:295:THR:O	2.16	0.44
1:L:77:ALA:O	1:L:80:GLU:HG3	2.18	0.44
2:M:286:TYR:CE2	2:M:492:ARG:HG2	2.52	0.44
3:N:46:TRP:CZ2	3:N:54:VAL:HB	2.53	0.44
1:A:209:GLU:HA	1:A:212:LEU:HG	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:GLU:OE2	1:G:194:LYS:HD3	2.18	0.44
1:F:213:LYS:H	1:F:213:LYS:HD2	1.82	0.44
1:J:172:GLN:HE21	1:K:177:ALA:HB1	1.83	0.44
1:J:255:ILE:H	1:J:255:ILE:HG13	1.49	0.44
2:M:133:GLU:HA	2:M:145:VAL:O	2.17	0.44
2:M:355:LEU:HD23	2:M:358:ILE:HD12	2.00	0.44
1:C:179:GLN:HA	1:C:182:LYS:HE3	1.99	0.44
1:G:249:VAL:HG13	1:H:244:THR:HB	1.99	0.44
1:J:170:THR:O	1:J:174:VAL:HG23	2.16	0.44
1:J:211:LEU:HA	1:K:216:PHE:HD2	1.83	0.44
3:N:27:ASN:HA	3:N:112:ILE:HD11	2.00	0.44
3:O:46:TRP:CZ2	3:O:54:VAL:HB	2.53	0.44
1:F:77:ALA:O	1:F:80:GLU:HG3	2.18	0.44
1:H:71:GLU:H	1:H:71:GLU:HG3	1.59	0.44
2:M:118:PHE:HB3	2:M:258:PHE:CZ	2.53	0.44
3:P:99:ILE:H	3:P:112:ILE:HG13	1.82	0.44
1:A:28:VAL:HG23	1:L:14:VAL:HA	2.00	0.43
1:B:209:GLU:HA	1:B:212:LEU:HG	2.00	0.43
1:C:124:GLN:HA	1:D:130:PHE:HA	2.00	0.43
1:C:235:GLN:NE2	1:D:240:GLU:HG3	2.33	0.43
1:E:197:ASN:ND2	1:F:202:LEU:HB2	2.33	0.43
1:J:77:ALA:O	1:J:80:GLU:HG3	2.18	0.43
2:M:87:ARG:HG2	2:M:106:ASN:O	2.17	0.43
3:N:102:VAL:HA	3:N:107:THR:O	2.18	0.43
1:H:106:LEU:HG	1:I:111:VAL:HG22	2.00	0.43
2:M:261:TYR:CE1	2:M:265:LYS:HB3	2.53	0.43
3:P:61:ARG:HB3	3:P:73:ARG:HB2	2.01	0.43
1:A:77:ALA:O	1:A:80:GLU:HG3	2.18	0.43
1:A:176:THR:HA	1:A:179:GLN:HG3	1.99	0.43
1:J:179:GLN:OE1	1:K:185:GLU:HG3	2.18	0.43
1:L:162:LEU:HD12	1:L:162:LEU:HA	1.83	0.43
3:P:91:VAL:HG22	3:P:121:PRO:HA	2.00	0.43
3:P:111:ILE:HG22	3:P:112:ILE:N	2.32	0.43
1:I:52:THR:HG21	1:J:33:LEU:HD21	1.99	0.43
2:M:99:GLY:O	2:M:101:ILE:HG23	2.19	0.43
2:M:116:TRP:CG	2:M:236:MET:HE3	2.54	0.43
3:N:139:LEU:N	3:O:132:GLY:H	2.16	0.43
3:O:57:THR:OG1	3:O:101:LEU:HG	2.18	0.43
3:P:24:PRO:O	3:P:26:MET:HG3	2.18	0.43
1:A:276:LYS:HB3	1:L:275:GLN:HG2	1.99	0.43
1:C:48:ALA:HA	1:C:51:LEU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:227:GLN:O	1:I:230:THR:HB	2.18	0.43
1:L:110:LYS:O	1:L:114:THR:HG23	2.19	0.43
1:L:159:GLN:O	1:L:163:VAL:HG23	2.18	0.43
1:L:250:ASP:HB2	1:L:253:SER:HB2	2.01	0.43
2:M:122:VAL:HA	2:M:127:TYR:HB3	2.00	0.43
3:P:136:ASN:N	3:P:139:LEU:O	2.51	0.43
1:A:6:ILE:HD11	1:A:67:LEU:HD23	2.01	0.43
1:B:102:LYS:O	1:B:105:GLU:HB3	2.18	0.43
1:D:99:GLN:HA	1:D:102:LYS:HE2	1.99	0.43
1:D:289:ARG:CZ	1:E:293:THR:H	2.31	0.43
1:D:315:LEU:O	1:D:319:VAL:HG22	2.17	0.43
1:E:255:ILE:HD12	1:F:244:THR:HA	2.00	0.43
1:L:175:LEU:HG	1:L:179:GLN:HE21	1.84	0.43
2:M:299:LYS:HG2	2:M:306:TYR:CE2	2.53	0.43
2:M:311:GLU:O	2:M:315:ILE:HG13	2.19	0.43
3:O:41:ASP:HB3	3:O:80:PHE:CE1	2.54	0.43
1:A:194:LYS:HD3	1:L:190:GLU:OE2	2.19	0.43
1:A:237:VAL:HG22	1:L:232:LEU:HD13	2.00	0.43
1:F:275:GLN:HG2	1:G:276:LYS:HB3	1.99	0.43
1:G:92:LEU:O	1:G:96:GLN:HG2	2.19	0.43
1:I:271:ARG:HD3	1:J:273:ALA:CB	2.49	0.43
1:J:214:ALA:HB1	1:K:219:THR:HG21	2.00	0.43
1:C:71:GLU:H	1:C:71:GLU:HG3	1.63	0.43
1:D:52:THR:HG21	1:E:33:LEU:HD21	2.00	0.43
1:D:211:LEU:HD12	1:D:214:ALA:HB3	2.01	0.43
1:G:307:ASN:O	1:G:311:VAL:HG23	2.18	0.43
1:H:232:LEU:HD13	1:I:237:VAL:HA	2.00	0.43
3:N:62:SER:OG	3:N:63:THR:N	2.51	0.43
1:A:289:ARG:HD3	1:B:295:THR:O	2.17	0.43
1:B:14:VAL:HA	1:C:28:VAL:HB	2.00	0.43
1:C:30:ARG:HG2	1:C:51:LEU:HD21	2.01	0.43
1:F:184:MET:O	1:F:188:VAL:HG23	2.19	0.43
1:J:200:GLN:HG2	1:K:205:LEU:HB2	2.01	0.43
2:M:16:VAL:HG22	2:M:485:GLU:HG3	2.00	0.43
2:M:116:TRP:CZ3	2:M:236:MET:HG2	2.53	0.43
3:N:96:TYR:CA	3:N:115:ALA:O	2.47	0.43
3:O:61:ARG:HD2	3:O:95:TYR:CG	2.54	0.43
3:O:81:TYR:HE1	3:P:80:PHE:CD2	2.37	0.43
1:A:111:VAL:HG21	1:L:105:GLU:CD	2.44	0.43
1:J:267:ASP:HB3	1:J:271:ARG:HH11	1.84	0.43
2:M:292:ARG:CZ	2:M:333:ILE:HG13	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:THR:HB	1:L:289:ARG:HA	2.01	0.42
1:C:298:ASN:HD21	1:C:301:ASN:HD21	1.67	0.42
1:E:180:GLN:HG3	1:E:184:MET:HE1	1.99	0.42
1:G:194:LYS:O	1:G:198:MET:HG3	2.18	0.42
1:G:200:GLN:NE2	1:H:206:VAL:HA	2.34	0.42
1:K:232:LEU:O	1:K:235:GLN:HB3	2.19	0.42
2:M:116:TRP:CD2	2:M:236:MET:HE3	2.54	0.42
3:O:59:LEU:HD11	3:O:97:TYR:HD2	1.84	0.42
3:P:64:ASP:O	3:P:96:TYR:HB2	2.18	0.42
1:A:93:LEU:HD23	1:L:88:LYS:HB3	2.01	0.42
1:C:285:TRP:CZ2	1:C:289:ARG:HD3	2.55	0.42
1:H:194:LYS:O	1:H:198:MET:HG3	2.19	0.42
1:I:174:VAL:O	1:I:178:VAL:HG23	2.18	0.42
2:M:125:TYR:CD1	2:M:137:LEU:HG	2.54	0.42
2:M:137:LEU:HB3	2:M:145:VAL:HG21	2.01	0.42
3:N:100:GLN:HG3	3:N:109:GLY:C	2.44	0.42
1:A:195:VAL:HG13	1:L:190:GLU:HA	2.01	0.42
1:B:174:VAL:O	1:B:178:VAL:HG23	2.19	0.42
1:E:77:ALA:O	1:E:80:GLU:HG3	2.19	0.42
1:F:209:GLU:HG2	1:F:213:LYS:NZ	2.35	0.42
1:I:171:LYS:H	1:I:171:LYS:HG3	1.63	0.42
1:J:235:GLN:CG	1:K:240:GLU:HG2	2.49	0.42
1:K:240:GLU:O	1:K:240:GLU:HG3	2.18	0.42
3:O:58:ARG:HG2	3:O:75:PHE:CE2	2.54	0.42
3:O:74:ALA:HA	3:P:79:ASN:HD21	1.83	0.42
3:O:94:ARG:NH1	3:O:118:THR:HB	2.34	0.42
1:A:31:LEU:HD22	1:L:16:LEU:HG	2.01	0.42
1:B:211:LEU:HG	1:B:215:GLN:NE2	2.32	0.42
1:D:289:ARG:HE	1:E:288:ARG:HA	1.82	0.42
2:M:297:ASN:O	2:M:301:ILE:HG13	2.19	0.42
3:N:24:PRO:CB	3:N:54:VAL:HG22	2.49	0.42
3:N:132:GLY:HA2	3:P:137:GLY:O	2.18	0.42
1:A:250:ASP:HB2	1:A:253:SER:HB2	2.01	0.42
1:G:106:LEU:HG	1:H:111:VAL:HG22	2.02	0.42
1:I:85:LEU:HD22	1:J:86:THR:HB	2.02	0.42
1:I:179:GLN:CD	1:J:181:THR:HG23	2.44	0.42
1:J:199:LYS:O	1:J:202:LEU:HB3	2.19	0.42
1:J:289:ARG:NE	1:K:288:ARG:HG2	2.33	0.42
3:P:39:GLY:HA3	3:P:82:PHE:CZ	2.55	0.42
1:A:185:GLU:O	1:A:188:VAL:HB	2.20	0.42
1:D:261:LEU:HG	1:D:265:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:225:ASN:HA	1:H:230:THR:HG23	2.02	0.42
1:I:315:LEU:O	1:I:319:VAL:HG22	2.20	0.42
1:J:112:LYS:HE2	1:J:112:LYS:HB3	1.73	0.42
1:K:6:ILE:HD11	1:L:69:LYS:HA	2.01	0.42
1:K:235:GLN:HE22	1:L:241:ARG:HH21	1.67	0.42
1:K:242:ALA:HB2	1:L:243:GLN:HE22	1.85	0.42
2:M:79:LYS:HD3	2:M:81:VAL:HG22	2.01	0.42
3:N:58:ARG:HH12	3:N:108:ASP:CG	2.27	0.42
1:D:183:VAL:HA	1:D:186:GLN:OE1	2.20	0.42
1:K:16:LEU:HD23	1:K:16:LEU:HA	1.84	0.42
1:K:316:MET:HB3	1:L:310:ARG:NH1	2.34	0.42
1:L:189:LEU:O	1:L:192:THR:HB	2.20	0.42
2:M:90:VAL:HG22	2:M:271:ILE:HG23	2.00	0.42
3:N:132:GLY:CA	3:P:138:LEU:HA	2.50	0.42
1:C:13:GLU:HG3	1:C:15:LYS:HE2	2.02	0.42
1:C:284:THR:O	1:C:288:ARG:HG3	2.20	0.42
1:D:233:VAL:O	1:D:237:VAL:HG23	2.20	0.42
1:F:211:LEU:HG	1:F:215:GLN:NE2	2.34	0.42
1:G:179:GLN:HG3	1:H:181:THR:HG23	2.01	0.42
1:G:204:ASN:HA	1:H:209:GLU:HG3	2.02	0.42
1:G:281:LEU:HD12	1:G:311:VAL:HG21	2.02	0.42
2:M:92:GLN:O	2:M:96:ARG:HG3	2.20	0.42
2:M:390:ALA:HA	2:M:408:SER:HA	2.02	0.42
3:N:40:ILE:HG12	3:N:118:THR:O	2.20	0.42
3:N:99:ILE:H	3:N:99:ILE:HG13	1.69	0.42
3:O:86:ASP:OD1	3:O:86:ASP:N	2.52	0.42
3:O:100:GLN:HG3	3:O:109:GLY:O	2.19	0.42
3:P:25:ASN:ND2	3:P:48:THR:H	2.18	0.42
1:B:232:LEU:HD13	1:C:237:VAL:HG22	2.02	0.42
1:D:218:LEU:O	1:D:221:ASP:HB2	2.20	0.42
1:D:225:ASN:HA	1:D:228:GLU:HB3	2.01	0.42
1:D:235:GLN:HG3	1:E:240:GLU:HG2	2.01	0.42
1:J:180:GLN:HE22	1:J:187:GLN:HE22	1.68	0.42
3:N:55:GLY:O	3:N:77:ASN:ND2	2.53	0.42
3:N:98:TRP:CZ2	3:N:114:PRO:HB3	2.55	0.42
3:P:112:ILE:HG22	3:P:113:GLY:N	2.27	0.42
1:A:190:GLU:HG2	1:B:195:VAL:CG2	2.49	0.42
1:E:6:ILE:O	1:F:69:LYS:HD2	2.20	0.42
1:I:321:ALA:HA	1:J:314:MET:HG2	2.01	0.42
1:J:14:VAL:HA	1:K:28:VAL:HB	2.02	0.42
1:K:92:LEU:O	1:K:96:GLN:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:241:ARG:N	1:K:241:ARG:HD2	2.35	0.42
1:K:258:GLN:HB2	1:L:262:TYR:HE2	1.85	0.42
1:K:275:GLN:OE1	1:L:276:LYS:HD3	2.20	0.42
1:A:174:VAL:HG22	1:L:169:LYS:CB	2.50	0.41
1:C:192:THR:O	1:C:195:VAL:HG23	2.20	0.41
1:E:251:ALA:HA	1:E:256:GLY:HA3	2.00	0.41
1:G:185:GLU:O	1:G:188:VAL:HB	2.20	0.41
1:I:43:LYS:HE3	1:I:43:LYS:HB2	1.92	0.41
1:J:235:GLN:HG3	1:K:240:GLU:HG2	2.01	0.41
3:N:30:LEU:O	3:N:44:PHE:HA	2.20	0.41
3:P:60:PHE:HB3	3:P:70:ALA:HB1	2.01	0.41
1:A:208:GLN:HE21	1:B:212:LEU:HD22	1.85	0.41
1:D:77:ALA:O	1:D:80:GLU:HG3	2.20	0.41
1:D:186:GLN:HA	1:D:189:LEU:HG	2.02	0.41
1:D:209:GLU:HG2	1:D:213:LYS:NZ	2.35	0.41
1:E:258:GLN:HG3	1:E:262:TYR:CE2	2.55	0.41
1:F:196:LEU:HA	1:F:199:LYS:HD2	2.02	0.41
1:J:201:GLU:HG3	1:K:205:LEU:HD13	2.02	0.41
1:L:201:GLU:O	1:L:205:LEU:HG	2.20	0.41
3:N:48:THR:O	3:N:51:PRO:HD3	2.21	0.41
3:N:220:ALA:HB1	3:P:220:ALA:HB3	2.02	0.41
3:P:23:ASP:OD1	3:P:103:SER:OG	2.38	0.41
1:A:200:GLN:NE2	1:B:206:VAL:HA	2.36	0.41
1:A:257:ARG:CZ	1:B:263:LYS:HD2	2.50	0.41
1:H:14:VAL:HA	1:I:28:VAL:HB	2.02	0.41
2:M:71:TYR:CZ	2:M:73:TRP:HD1	2.38	0.41
2:M:114:LEU:HD12	2:M:172:GLN:O	2.19	0.41
2:M:336:VAL:CG1	2:M:339:VAL:HG23	2.49	0.41
3:N:67:PHE:CE2	3:N:111:ILE:HG13	2.55	0.41
3:O:35:PRO:HB3	3:O:118:THR:O	2.20	0.41
1:A:319:VAL:HG11	1:B:277:ALA:HB2	2.03	0.41
1:C:258:GLN:HB2	1:D:262:TYR:HE2	1.86	0.41
1:F:279:LYS:HA	1:F:279:LYS:HD2	1.84	0.41
1:I:107:ILE:O	1:I:111:VAL:HG23	2.20	0.41
1:J:29:THR:HG21	1:J:51:LEU:HD13	2.02	0.41
2:M:479:ALA:HB2	2:M:485:GLU:HB2	2.02	0.41
3:N:46:TRP:HZ3	3:N:78:GLY:H	1.68	0.41
3:N:75:PHE:HB2	3:O:79:ASN:HB3	2.02	0.41
1:A:107:ILE:O	1:A:111:VAL:HG23	2.20	0.41
1:B:83:ILE:O	1:B:87:GLU:HG2	2.20	0.41
1:E:209:GLU:O	1:E:212:LEU:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:289:ARG:HD3	1:G:295:THR:O	2.19	0.41
1:L:194:LYS:HE2	1:L:198:MET:SD	2.60	0.41
2:M:80:VAL:HA	2:M:394:ILE:HA	2.03	0.41
2:M:122:VAL:HG22	2:M:127:TYR:HB3	2.02	0.41
3:O:91:VAL:HG13	3:O:120:ARG:HA	2.02	0.41
1:F:44:GLY:HA2	1:F:47:TYR:CE2	2.55	0.41
1:F:159:GLN:O	1:F:163:VAL:HG23	2.21	0.41
1:F:232:LEU:HD13	1:G:237:VAL:HA	2.02	0.41
1:G:98:ALA:O	1:G:101:ASP:HB2	2.20	0.41
2:M:403:MET:SD	2:M:467:MET:HE3	2.60	0.41
1:H:39:ALA:HB3	1:H:41:ARG:HH11	1.84	0.41
1:H:291:THR:HG22	2:M:23:ALA:O	2.20	0.41
1:I:77:ALA:O	1:I:80:GLU:HG3	2.21	0.41
1:I:255:ILE:HD12	1:J:244:THR:HA	2.01	0.41
1:K:83:ILE:O	1:K:87:GLU:HG2	2.20	0.41
2:M:349:ALA:HB1	2:M:354:GLN:OE1	2.20	0.41
2:M:415:LYS:O	2:M:456:MET:HA	2.21	0.41
3:N:52:GLY:HA2	3:P:56:THR:HB	2.03	0.41
1:A:174:VAL:O	1:A:178:VAL:HG23	2.21	0.41
1:A:192:THR:O	1:A:195:VAL:HG23	2.21	0.41
1:B:39:ALA:HB3	1:B:41:ARG:HD2	2.03	0.41
1:E:225:ASN:HD22	1:F:230:THR:HG23	1.85	0.41
1:J:176:THR:O	1:J:179:GLN:HB2	2.21	0.41
1:J:208:GLN:HG3	1:K:212:LEU:HD13	2.02	0.41
1:J:275:GLN:CD	1:K:276:LYS:HD3	2.46	0.41
2:M:176:PHE:H	2:M:248:ARG:NH1	2.19	0.41
3:N:139:LEU:H	3:O:132:GLY:H	1.68	0.41
3:P:25:ASN:HB2	3:P:28:ASP:CG	2.46	0.41
1:A:205:LEU:HB2	1:L:200:GLN:HG2	2.02	0.41
1:B:229:GLN:O	1:B:233:VAL:HG23	2.21	0.41
1:B:310:ARG:HD2	1:B:311:VAL:HG23	2.02	0.41
1:C:16:LEU:HG	1:D:31:LEU:HB3	2.02	0.41
1:C:232:LEU:HD13	1:D:237:VAL:HA	2.03	0.41
1:C:242:ALA:N	1:D:243:GLN:HE22	2.18	0.41
1:C:289:ARG:CZ	1:D:288:ARG:HG2	2.50	0.41
1:E:13:GLU:HG3	1:E:15:LYS:HE2	2.03	0.41
1:E:289:ARG:HD3	1:F:295:THR:O	2.20	0.41
1:F:316:MET:HA	1:F:319:VAL:HG22	2.02	0.41
1:G:186:GLN:O	1:G:190:GLU:HG3	2.21	0.41
1:H:251:ALA:HA	1:H:256:GLY:HA3	2.03	0.41
1:I:92:LEU:O	1:I:96:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:229:GLN:O	1:J:233:VAL:HG23	2.21	0.41
2:M:28:SER:HB2	2:M:29:PRO:HD3	2.03	0.41
2:M:94:ILE:HG12	2:M:259:PHE:CD1	2.55	0.41
2:M:273:GLY:O	2:M:277:LEU:HB2	2.21	0.41
2:M:495:LEU:HD13	2:M:506:LEU:HD22	2.03	0.41
3:N:40:ILE:HD12	3:N:95:TYR:HB2	2.03	0.41
3:N:42:ILE:HD11	3:N:97:TYR:CE1	2.56	0.41
3:O:24:PRO:HG3	3:O:53:ALA:C	2.46	0.41
3:P:31:LEU:HA	3:P:31:LEU:HD12	1.81	0.41
1:B:186:GLN:HE22	1:C:188:VAL:HG13	1.85	0.41
1:B:257:ARG:HA	1:B:257:ARG:HD3	1.89	0.41
1:C:194:LYS:O	1:C:198:MET:HG3	2.21	0.41
1:E:181:THR:O	1:E:184:MET:HB2	2.21	0.41
1:E:321:ALA:HB1	1:F:311:VAL:HA	2.03	0.41
1:F:79:VAL:O	1:F:83:ILE:HG13	2.20	0.41
1:F:288:ARG:NH1	1:F:297:ALA:HB2	2.35	0.41
1:H:233:VAL:O	1:H:237:VAL:HG23	2.21	0.41
1:H:283:ASP:O	1:H:287:VAL:HG23	2.21	0.41
1:I:289:ARG:HH21	1:J:288:ARG:HA	1.86	0.41
1:J:107:ILE:O	1:J:111:VAL:HG23	2.21	0.41
1:J:201:GLU:O	1:J:204:ASN:HB2	2.21	0.41
2:M:116:TRP:CZ2	2:M:120:GLU:HG3	2.56	0.41
2:M:372:GLN:OE1	2:M:375:LYS:HB2	2.22	0.41
3:O:31:LEU:HD11	3:O:42:ILE:CG2	2.51	0.41
3:P:23:ASP:OD1	3:P:105:ASN:ND2	2.54	0.41
3:P:29:LEU:HD22	3:P:45:THR:C	2.46	0.41
1:A:176:THR:O	1:A:179:GLN:HB2	2.22	0.40
1:A:265:GLN:HG3	1:B:269:PHE:CZ	2.57	0.40
1:D:275:GLN:HE22	1:E:273:ALA:CA	2.33	0.40
1:H:254:VAL:HG13	1:I:259:LYS:HA	2.03	0.40
1:I:230:THR:HG22	1:I:234:ARG:NH2	2.36	0.40
1:J:16:LEU:HA	1:J:16:LEU:HD23	1.89	0.40
3:O:29:LEU:HD12	3:O:101:LEU:HD11	2.02	0.40
1:D:249:VAL:HG22	1:E:244:THR:HB	2.04	0.40
1:F:107:ILE:H	1:F:107:ILE:HG12	1.42	0.40
1:G:162:LEU:HA	1:G:162:LEU:HD12	1.88	0.40
1:J:214:ALA:HA	1:J:217:ASP:OD2	2.21	0.40
2:M:403:MET:HA	2:M:468:HIS:O	2.21	0.40
1:C:107:ILE:O	1:C:111:VAL:HG23	2.22	0.40
1:F:99:GLN:OE1	1:G:104:ALA:HA	2.21	0.40
1:J:193:GLN:NE2	1:K:199:LYS:HA	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:77:ALA:O	1:K:80:GLU:HG3	2.22	0.40
1:L:43:LYS:H	1:L:43:LYS:HG2	1.69	0.40
1:L:76:ALA:O	1:L:79:VAL:HB	2.20	0.40
2:M:213:TYR:HE2	2:M:215:LEU:HB2	1.85	0.40
2:M:436:SER:HB2	2:M:439:ILE:HB	2.03	0.40
3:N:103:SER:O	3:O:52:GLY:HA3	2.21	0.40
1:A:19:LYS:HB3	1:A:24:GLN:HE21	1.86	0.40
1:A:264:ALA:HB1	1:B:269:PHE:CG	2.57	0.40
1:C:252:ASP:HA	1:C:257:ARG:CZ	2.51	0.40
1:G:105:GLU:O	1:G:108:ALA:HB3	2.21	0.40
1:J:249:VAL:CG1	1:J:255:ILE:HB	2.52	0.40
1:K:200:GLN:HG2	1:L:205:LEU:HB2	2.03	0.40
1:L:69:LYS:HB3	1:L:70:ASP:H	1.69	0.40
2:M:356:THR:HA	2:M:425:ILE:CD1	2.52	0.40
1:A:284:THR:O	1:A:288:ARG:HG3	2.21	0.40
1:D:179:GLN:HG3	1:E:181:THR:HG23	2.03	0.40
1:E:164:LYS:O	1:E:167:THR:HB	2.22	0.40
1:G:165:GLU:O	1:G:166:GLN:C	2.65	0.40
1:J:252:ASP:O	1:K:259:LYS:HE3	2.21	0.40
1:L:6:ILE:HD13	1:L:66:LEU:HB3	2.04	0.40
2:M:346:PRO:HA	2:M:347:PRO:HD3	1.97	0.40
3:O:39:GLY:HA2	3:O:85:THR:H	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	A	318/321 (99%)	304 (96%)	13 (4%)	1 (0%)	36	72
1	B	318/321 (99%)	304 (96%)	14 (4%)	0	100	100
1	C	318/321 (99%)	305 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	318/321 (99%)	308 (97%)	10 (3%)	0	100	100
1	E	318/321 (99%)	305 (96%)	13 (4%)	0	100	100
1	F	318/321 (99%)	307 (96%)	11 (4%)	0	100	100
1	G	318/321 (99%)	303 (95%)	15 (5%)	0	100	100
1	H	318/321 (99%)	299 (94%)	19 (6%)	0	100	100
1	I	318/321 (99%)	304 (96%)	14 (4%)	0	100	100
1	J	318/321 (99%)	297 (93%)	21 (7%)	0	100	100
1	K	318/321 (99%)	305 (96%)	12 (4%)	1 (0%)	36	72
1	L	318/321 (99%)	303 (95%)	15 (5%)	0	100	100
2	M	500/740 (68%)	477 (95%)	23 (5%)	0	100	100
3	N	201/429 (47%)	186 (92%)	14 (7%)	1 (0%)	24	63
3	O	201/429 (47%)	188 (94%)	13 (6%)	0	100	100
3	P	201/429 (47%)	180 (90%)	18 (9%)	3 (2%)	8	40
All	All	4919/5879 (84%)	4675 (95%)	238 (5%)	6 (0%)	49	83

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	P	114	PRO
3	P	140	SER
1	A	42	LEU
1	K	42	LEU
3	P	136	ASN
3	N	134	ILE

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	227/264 (86%)	203 (89%)	24 (11%)	6	21
1	B	227/264 (86%)	211 (93%)	16 (7%)	14	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	227/264 (86%)	207 (91%)	20 (9%)	9	28
1	D	227/264 (86%)	203 (89%)	24 (11%)	6	21
1	E	227/264 (86%)	203 (89%)	24 (11%)	6	21
1	F	227/264 (86%)	202 (89%)	25 (11%)	6	20
1	G	227/264 (86%)	205 (90%)	22 (10%)	8	24
1	H	227/264 (86%)	206 (91%)	21 (9%)	8	26
1	I	227/264 (86%)	202 (89%)	25 (11%)	6	20
1	J	227/264 (86%)	203 (89%)	24 (11%)	6	21
1	K	227/264 (86%)	207 (91%)	20 (9%)	9	28
1	L	227/264 (86%)	206 (91%)	21 (9%)	8	26
2	M	431/623 (69%)	412 (96%)	19 (4%)	25	47
3	N	79/345 (23%)	72 (91%)	7 (9%)	9	28
3	O	79/345 (23%)	69 (87%)	10 (13%)	4	16
3	P	79/345 (23%)	73 (92%)	6 (8%)	12	33
All	All	3392/4826 (70%)	3084 (91%)	308 (9%)	11	27

All (308) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	29	THR
1	A	32	HIS
1	A	75	LYS
1	A	92	LEU
1	A	112	LYS
1	A	115	LEU
1	A	178	VAL
1	A	183	VAL
1	A	184	MET
1	A	185	GLU
1	A	189	LEU
1	A	195	VAL
1	A	211	LEU
1	A	218	LEU
1	A	228	GLU
1	A	240	GLU
1	A	241	ARG

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Mol	Chain	Res	Type
1	A	243	GLN
1	A	245	ILE
1	A	258	GLN
1	A	290	THR
1	A	310	ARG
1	A	314	MET
1	B	3	VAL
1	B	75	LYS
1	B	115	LEU
1	B	160	ASP
1	B	163	VAL
1	B	184	MET
1	B	189	LEU
1	B	191	SER
1	B	195	VAL
1	B	218	LEU
1	B	232	LEU
1	B	241	ARG
1	B	243	GLN
1	B	249	VAL
1	B	258	GLN
1	B	310	ARG
1	C	3	VAL
1	C	22	LEU
1	C	75	LYS
1	C	112	LYS
1	C	175	LEU
1	C	184	MET
1	C	189	LEU
1	C	190	GLU
1	C	191	SER
1	C	195	VAL
1	C	211	LEU
1	C	228	GLU
1	C	232	LEU
1	C	240	GLU
1	C	241	ARG
1	C	254	VAL
1	C	258	GLN
1	C	292	ASP
1	C	310	ARG
1	C	313	ASN

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Mol	Chain	Res	Type
1	D	4	GLU
1	D	41	ARG
1	D	42	LEU
1	D	50	VAL
1	D	56	THR
1	D	75	LYS
1	D	105	GLU
1	D	113	LEU
1	D	159	GLN
1	D	163	VAL
1	D	167	THR
1	D	175	LEU
1	D	176	THR
1	D	183	VAL
1	D	184	MET
1	D	195	VAL
1	D	211	LEU
1	D	220	LYS
1	D	232	LEU
1	D	241	ARG
1	D	272	ASP
1	D	279	LYS
1	D	311	VAL
1	D	314	MET
1	E	3	VAL
1	E	14	VAL
1	E	36	GLU
1	E	56	THR
1	E	75	LYS
1	E	106	LEU
1	E	113	LEU
1	E	162	LEU
1	E	167	THR
1	E	175	LEU
1	E	176	THR
1	E	183	VAL
1	E	184	MET
1	E	185	GLU
1	E	189	LEU
1	E	190	GLU
1	E	195	VAL
1	E	220	LYS

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Mol	Chain	Res	Type
1	E	228	GLU
1	E	254	VAL
1	E	258	GLN
1	E	275	GLN
1	E	302	ARG
1	E	310	ARG
1	F	4	GLU
1	F	12	THR
1	F	13	GLU
1	F	42	LEU
1	F	51	LEU
1	F	56	THR
1	F	75	LYS
1	F	92	LEU
1	F	107	ILE
1	F	159	GLN
1	F	166	GLN
1	F	167	THR
1	F	175	LEU
1	F	184	MET
1	F	191	SER
1	F	195	VAL
1	F	208	GLN
1	F	217	ASP
1	F	228	GLU
1	F	243	GLN
1	F	262	TYR
1	F	275	GLN
1	F	305	ASP
1	F	310	ARG
1	F	314	MET
1	G	3	VAL
1	G	36	GLU
1	G	42	LEU
1	G	56	THR
1	G	75	LYS
1	G	92	LEU
1	G	105	GLU
1	G	112	LYS
1	G	115	LEU
1	G	163	VAL
1	G	166	GLN

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Mol	Chain	Res	Type
1	G	172	GLN
1	G	175	LEU
1	G	183	VAL
1	G	184	MET
1	G	189	LEU
1	G	195	VAL
1	G	237	VAL
1	G	241	ARG
1	G	282	ILE
1	G	305	ASP
1	G	314	MET
1	H	4	GLU
1	H	12	THR
1	H	16	LEU
1	H	36	GLU
1	H	42	LEU
1	H	47	TYR
1	H	51	LEU
1	H	56	THR
1	H	71	GLU
1	H	75	LYS
1	H	92	LEU
1	H	172	GLN
1	H	175	LEU
1	H	183	VAL
1	H	184	MET
1	H	191	SER
1	H	195	VAL
1	H	208	GLN
1	H	228	GLU
1	H	254	VAL
1	H	314	MET
1	I	3	VAL
1	I	16	LEU
1	I	22	LEU
1	I	42	LEU
1	I	47	TYR
1	I	56	THR
1	I	69	LYS
1	I	75	LYS
1	I	105	GLU
1	I	112	LYS

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Mol	Chain	Res	Type
1	I	115	LEU
1	I	167	THR
1	I	171	LYS
1	I	175	LEU
1	I	176	THR
1	I	180	GLN
1	I	189	LEU
1	I	195	VAL
1	I	206	VAL
1	I	218	LEU
1	I	228	GLU
1	I	243	GLN
1	I	258	GLN
1	I	272	ASP
1	I	310	ARG
1	J	3	VAL
1	J	47	TYR
1	J	56	THR
1	J	75	LYS
1	J	92	LEU
1	J	105	GLU
1	J	115	LEU
1	J	159	GLN
1	J	165	GLU
1	J	167	THR
1	J	175	LEU
1	J	184	MET
1	J	190	GLU
1	J	191	SER
1	J	195	VAL
1	J	203	LEU
1	J	218	LEU
1	J	228	GLU
1	J	254	VAL
1	J	255	ILE
1	J	258	GLN
1	J	275	GLN
1	J	292	ASP
1	J	295	THR
1	K	42	LEU
1	K	56	THR
1	K	71	GLU

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Mol	Chain	Res	Type
1	K	75	LYS
1	K	92	LEU
1	K	99	GLN
1	K	106	LEU
1	K	114	THR
1	K	160	ASP
1	K	167	THR
1	K	183	VAL
1	K	186	GLN
1	K	218	LEU
1	K	228	GLU
1	K	232	LEU
1	K	240	GLU
1	K	245	ILE
1	K	254	VAL
1	K	258	GLN
1	K	310	ARG
1	L	3	VAL
1	L	14	VAL
1	L	36	GLU
1	L	42	LEU
1	L	56	THR
1	L	75	LYS
1	L	92	LEU
1	L	107	ILE
1	L	115	LEU
1	L	159	GLN
1	L	162	LEU
1	L	175	LEU
1	L	208	GLN
1	L	213	LYS
1	L	228	GLU
1	L	232	LEU
1	L	241	ARG
1	L	243	GLN
1	L	292	ASP
1	L	302	ARG
1	L	310	ARG
2	M	20	PHE
2	M	30	ARG
2	M	79	LYS
2	M	81	VAL

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Mol	Chain	Res	Type
2	M	151	ILE
2	M	155	GLN
2	M	171	LEU
2	M	183	THR
2	M	216	LEU
2	M	238	LEU
2	M	240	LEU
2	M	270	LEU
2	M	309	VAL
2	M	387	SER
2	M	413	ASN
2	M	443	GLN
2	M	461	ILE
2	M	468	HIS
2	M	495	LEU
3	N	54	VAL
3	N	77	ASN
3	N	94	ARG
3	N	99	ILE
3	N	111	ILE
3	N	112	ILE
3	N	118	THR
3	O	27	ASN
3	O	28	ASP
3	O	43	GLU
3	O	86	ASP
3	O	96	TYR
3	O	99	ILE
3	O	102	VAL
3	O	108	ASP
3	O	112	ILE
3	O	118	THR
3	P	25	ASN
3	P	27	ASN
3	P	42	ILE
3	P	99	ILE
3	P	105	ASN
3	P	118	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	GLN
1	A	215	GLN
1	A	235	GLN
1	A	258	GLN
1	A	296	GLN
1	A	301	ASN
1	B	74	ASN
1	B	193	GLN
1	B	225	ASN
1	B	229	GLN
1	C	74	ASN
1	C	96	GLN
1	C	186	GLN
1	C	222	GLN
1	C	235	GLN
1	C	286	ASN
1	C	301	ASN
1	D	24	GLN
1	D	74	ASN
1	D	96	GLN
1	D	225	ASN
1	D	229	GLN
1	D	235	GLN
1	D	243	GLN
1	D	275	GLN
1	D	301	ASN
1	E	32	HIS
1	E	96	GLN
1	E	186	GLN
1	E	208	GLN
1	E	222	GLN
1	E	275	GLN
1	F	32	HIS
1	F	159	GLN
1	F	208	GLN
1	F	222	GLN
1	F	225	ASN
1	F	229	GLN
1	F	235	GLN
1	F	243	GLN
1	F	301	ASN
1	G	159	GLN
1	G	172	GLN

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Mol	Chain	Res	Type
1	G	215	GLN
1	G	222	GLN
1	G	243	GLN
1	H	74	ASN
1	H	96	GLN
1	H	200	GLN
1	H	204	ASN
1	H	215	GLN
1	H	286	ASN
1	H	296	GLN
1	H	313	ASN
1	I	68	GLN
1	I	96	GLN
1	I	179	GLN
1	I	229	GLN
1	I	235	GLN
1	I	275	GLN
1	J	68	GLN
1	J	74	ASN
1	J	96	GLN
1	J	159	GLN
1	J	172	GLN
1	J	180	GLN
1	K	208	GLN
1	K	235	GLN
1	K	298	ASN
1	L	74	ASN
1	L	172	GLN
1	L	208	GLN
1	L	222	GLN
1	L	235	GLN
1	L	243	GLN
2	M	276	ASN
2	M	392	GLN
2	M	468	HIS
2	M	470	GLN
3	N	105	ASN
3	O	93	GLN

5.3.3 RNA ⓘ

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-74091. These allow visual inspection of the internal detail of the map and identification of artifacts.

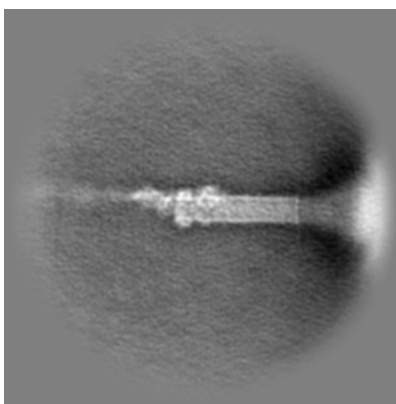
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

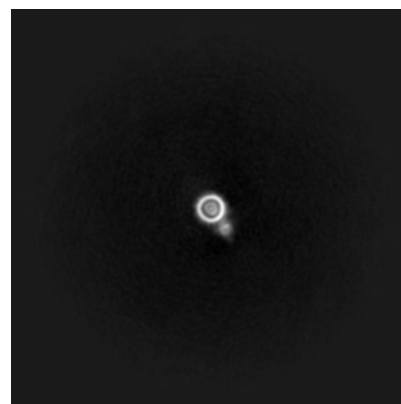
6.1.1 Primary map



X

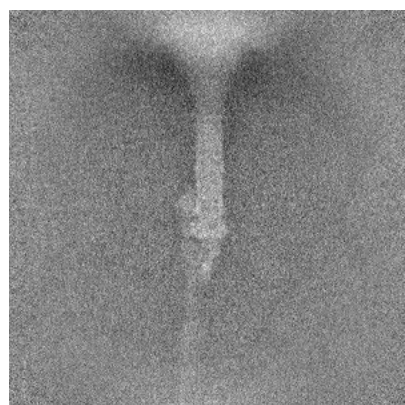


Y

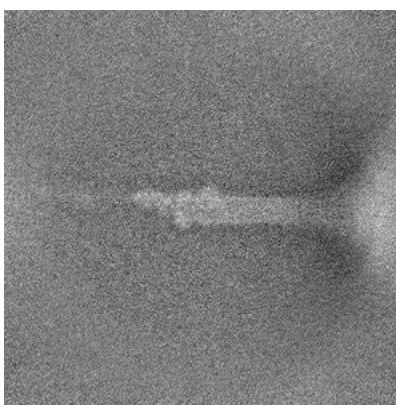


Z

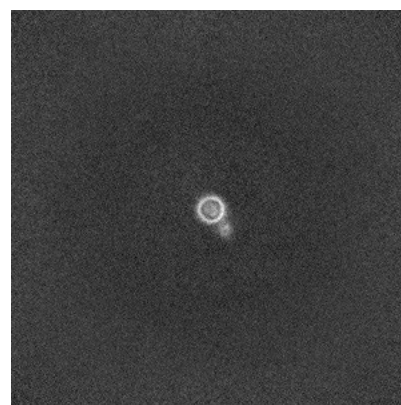
6.1.2 Raw map



X



Y

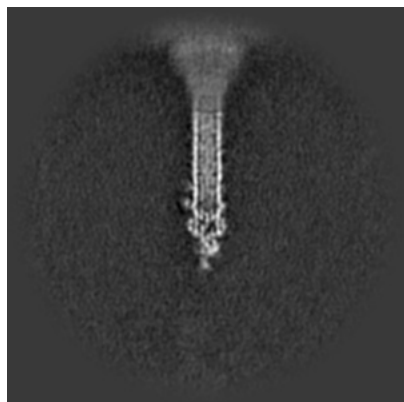


Z

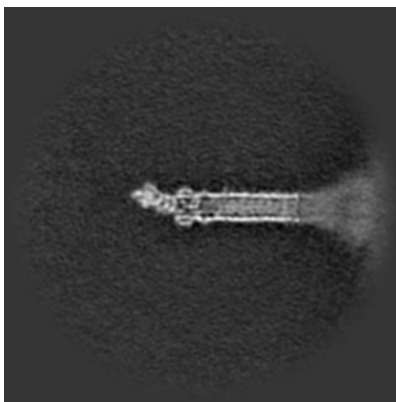
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

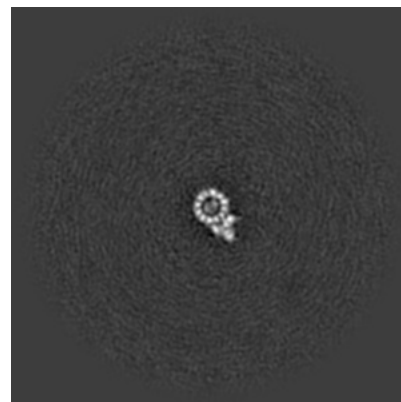
6.2.1 Primary map



X Index: 320

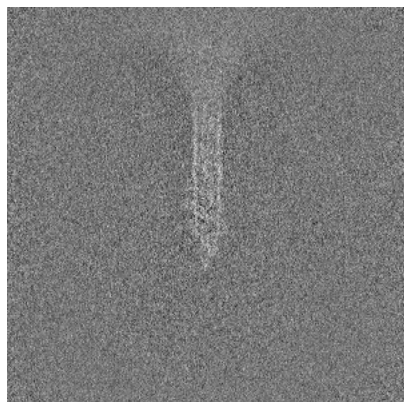


Y Index: 320

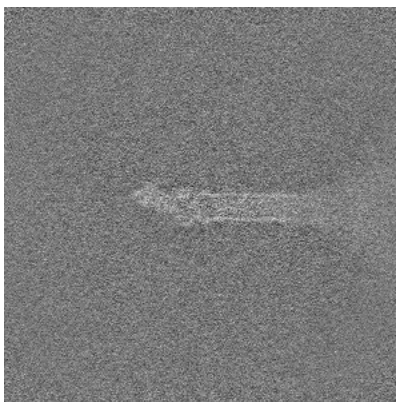


Z Index: 320

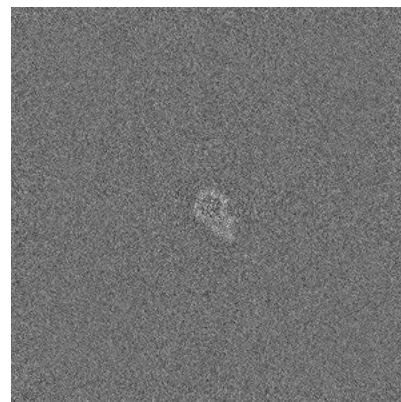
6.2.2 Raw map



X Index: 320



Y Index: 320

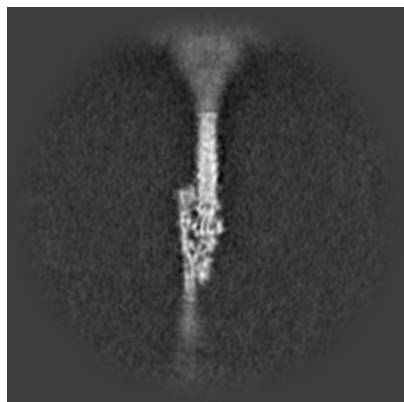


Z Index: 320

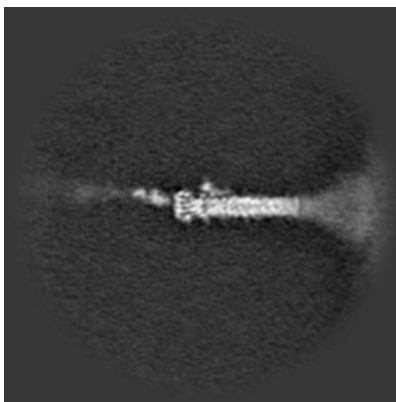
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

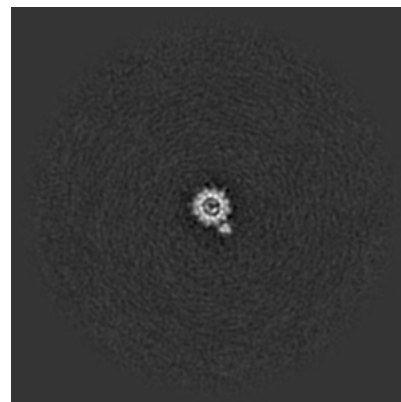
6.3.1 Primary map



X Index: 337

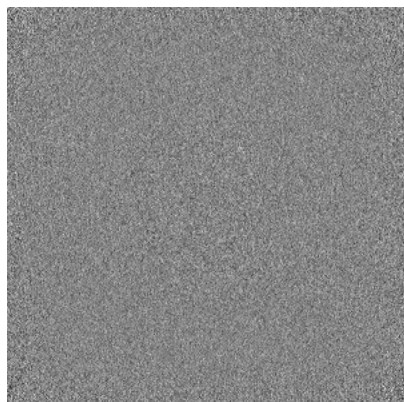


Y Index: 303

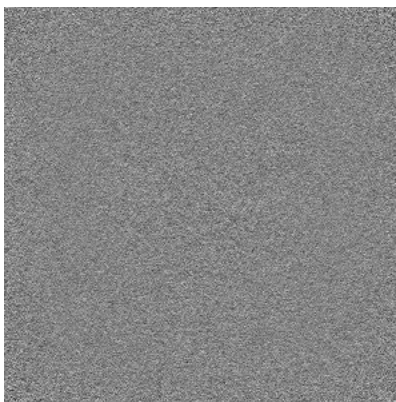


Z Index: 280

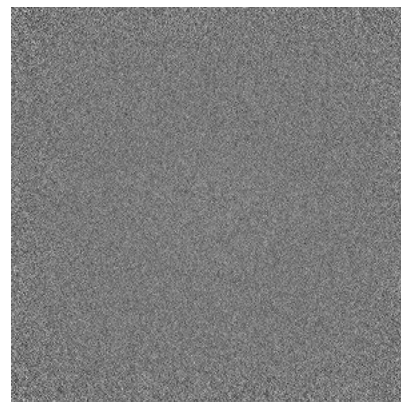
6.3.2 Raw map



X Index: 0



Y Index: 0

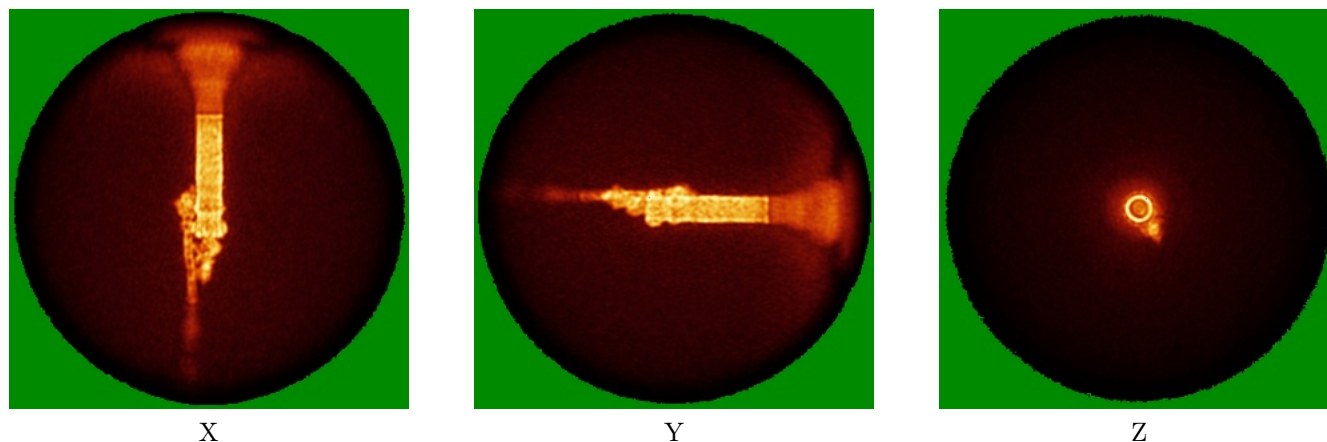


Z Index: 0

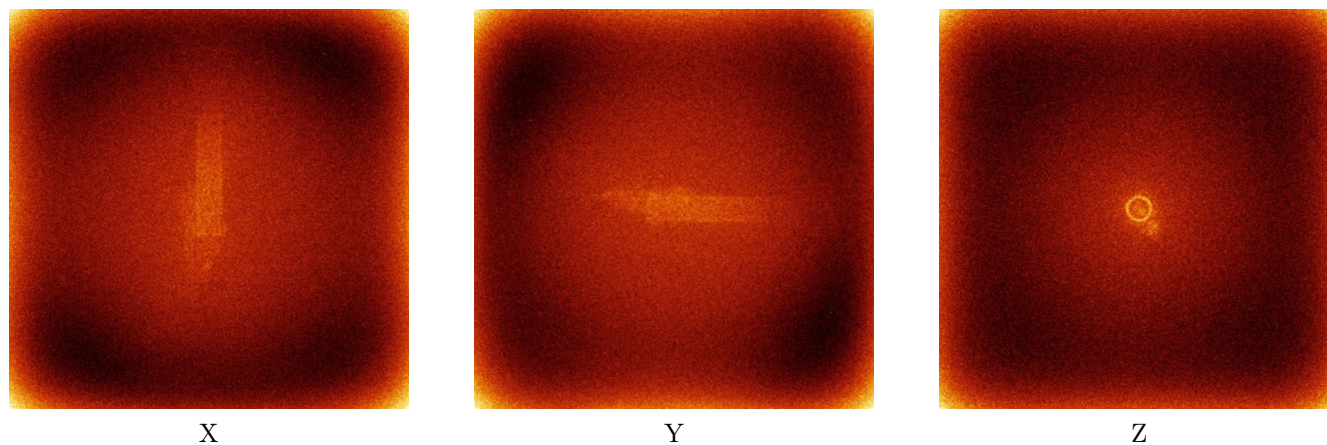
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



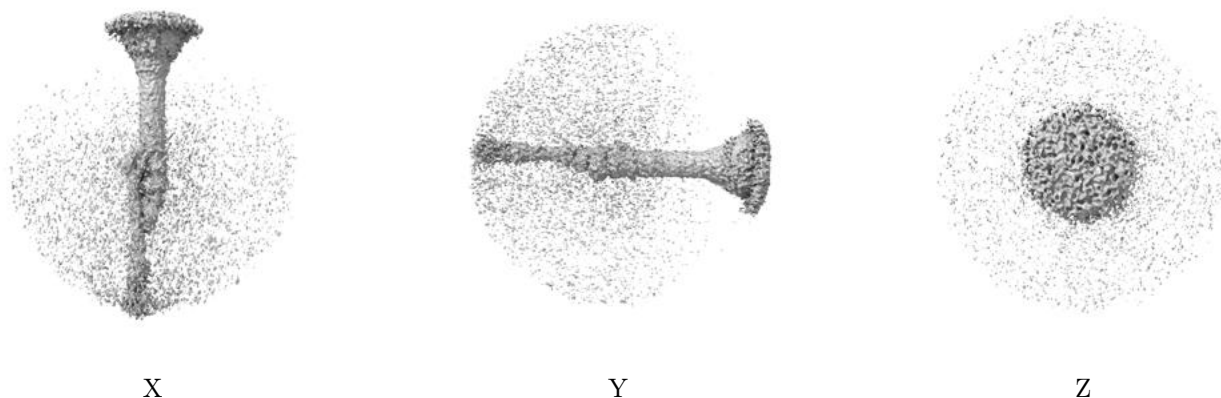
6.4.2 Raw map



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.

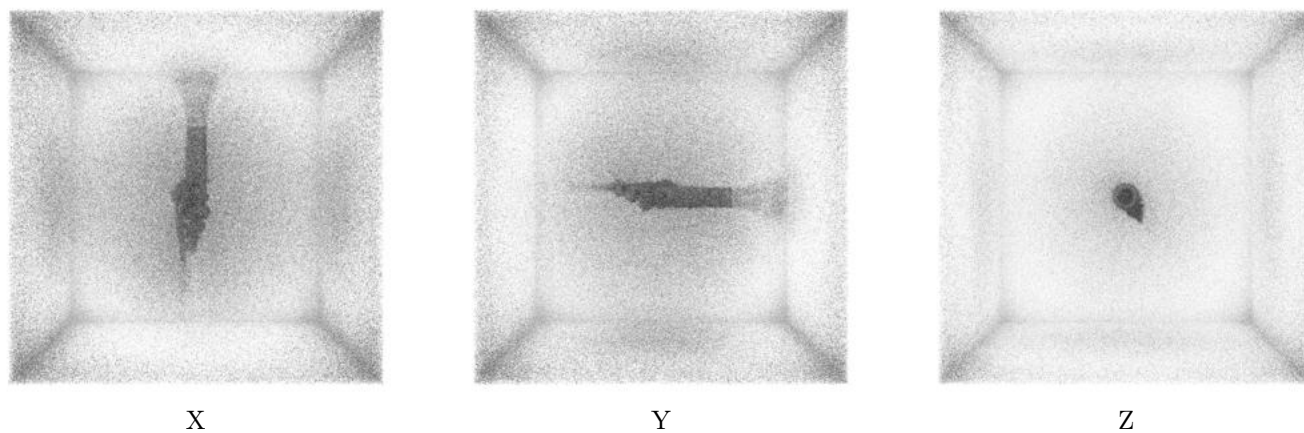
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0176. 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.

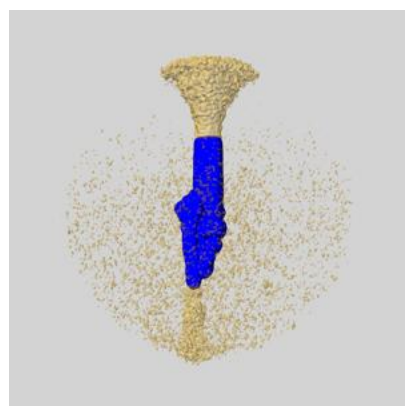
6.6 Mask visualisation [i](#)

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

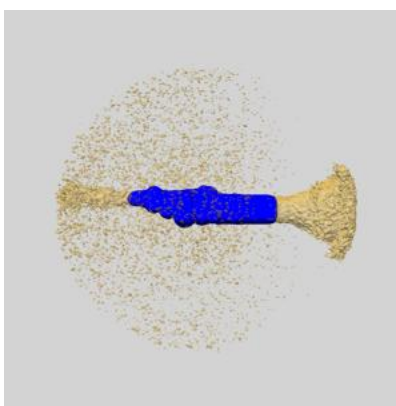
A mask typically either:

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

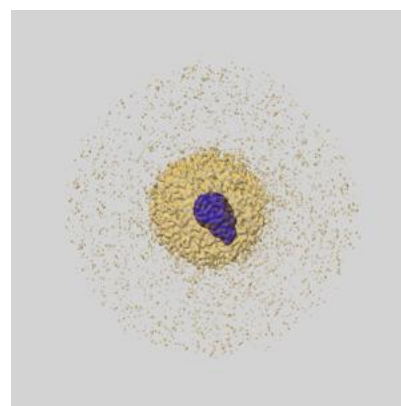
6.6.1 emd_74091_msk_1.map [i](#)



X



Y

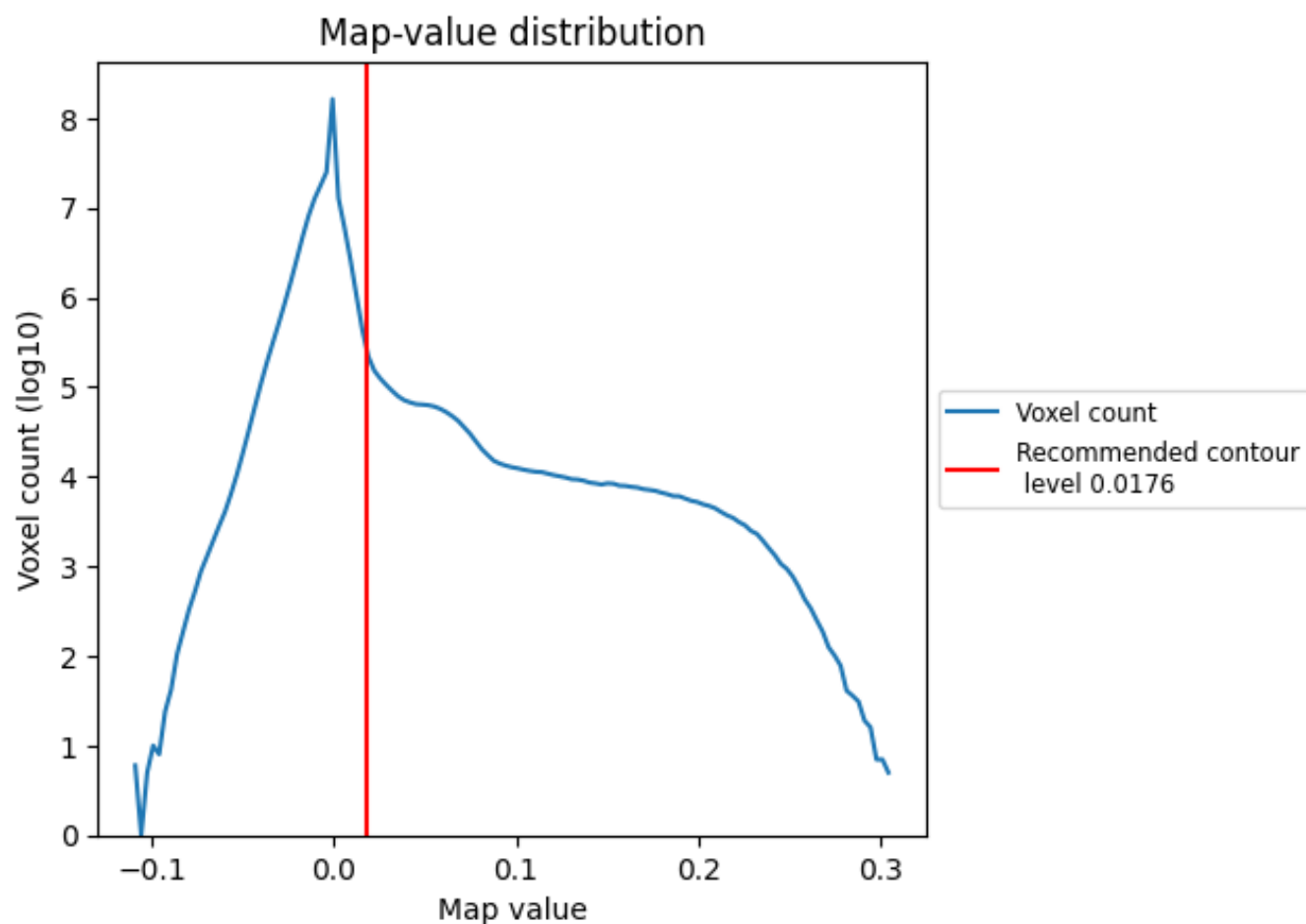


Z

7 Map analysis [i](#)

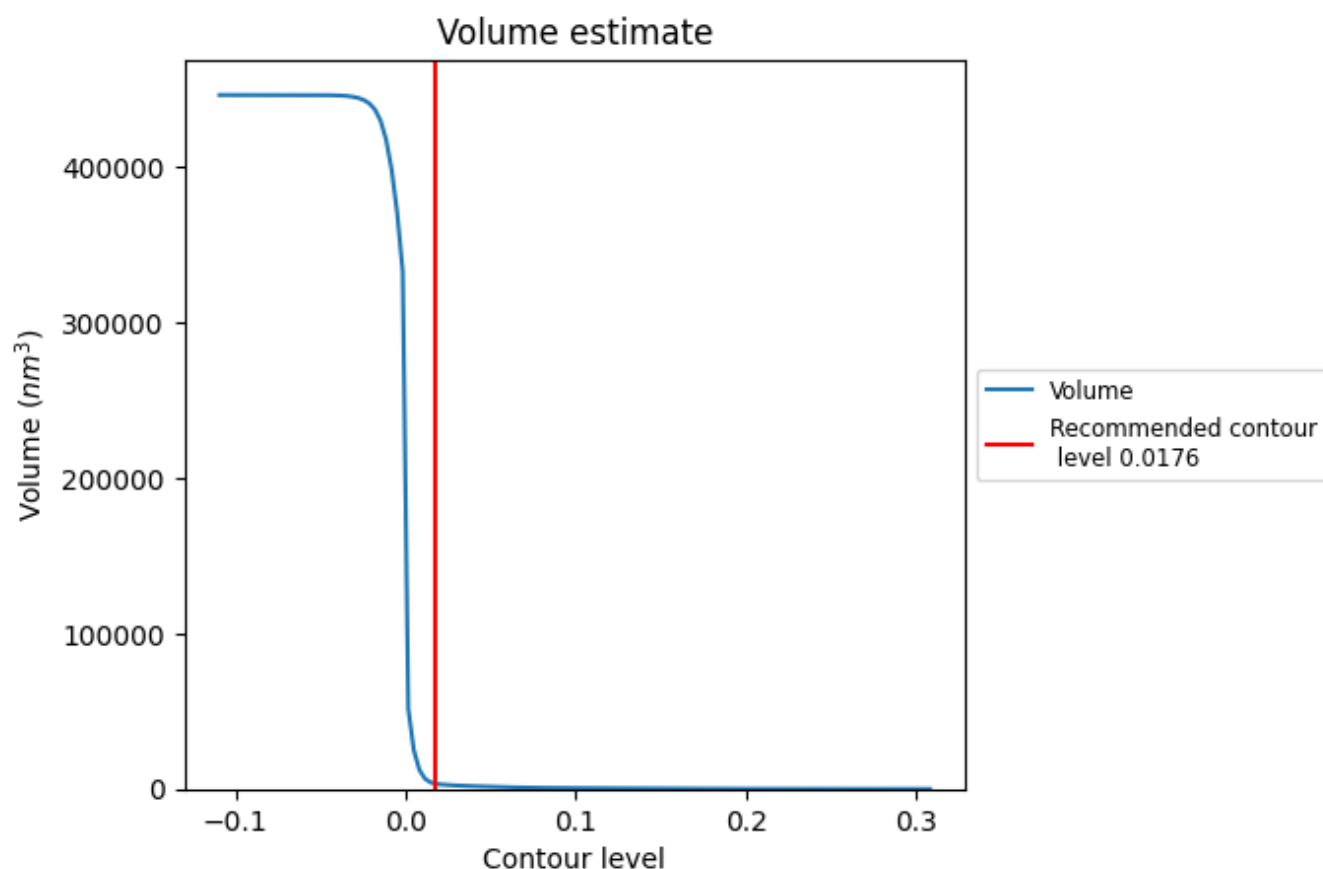
This section contains the results of statistical analysis of the map.

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.

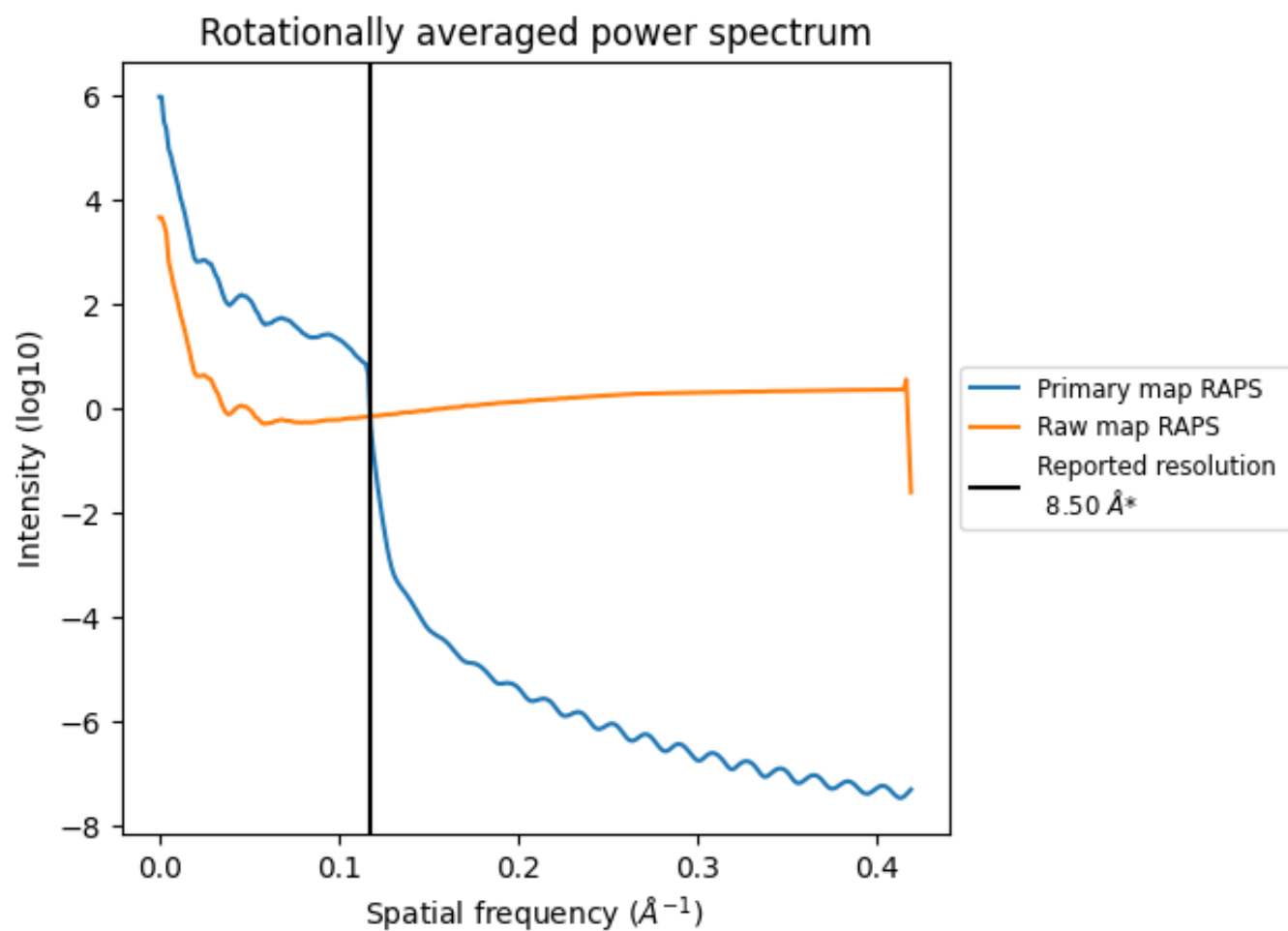
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3366 nm^3 ; this corresponds to an approximate mass of 3040 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 ⓘ

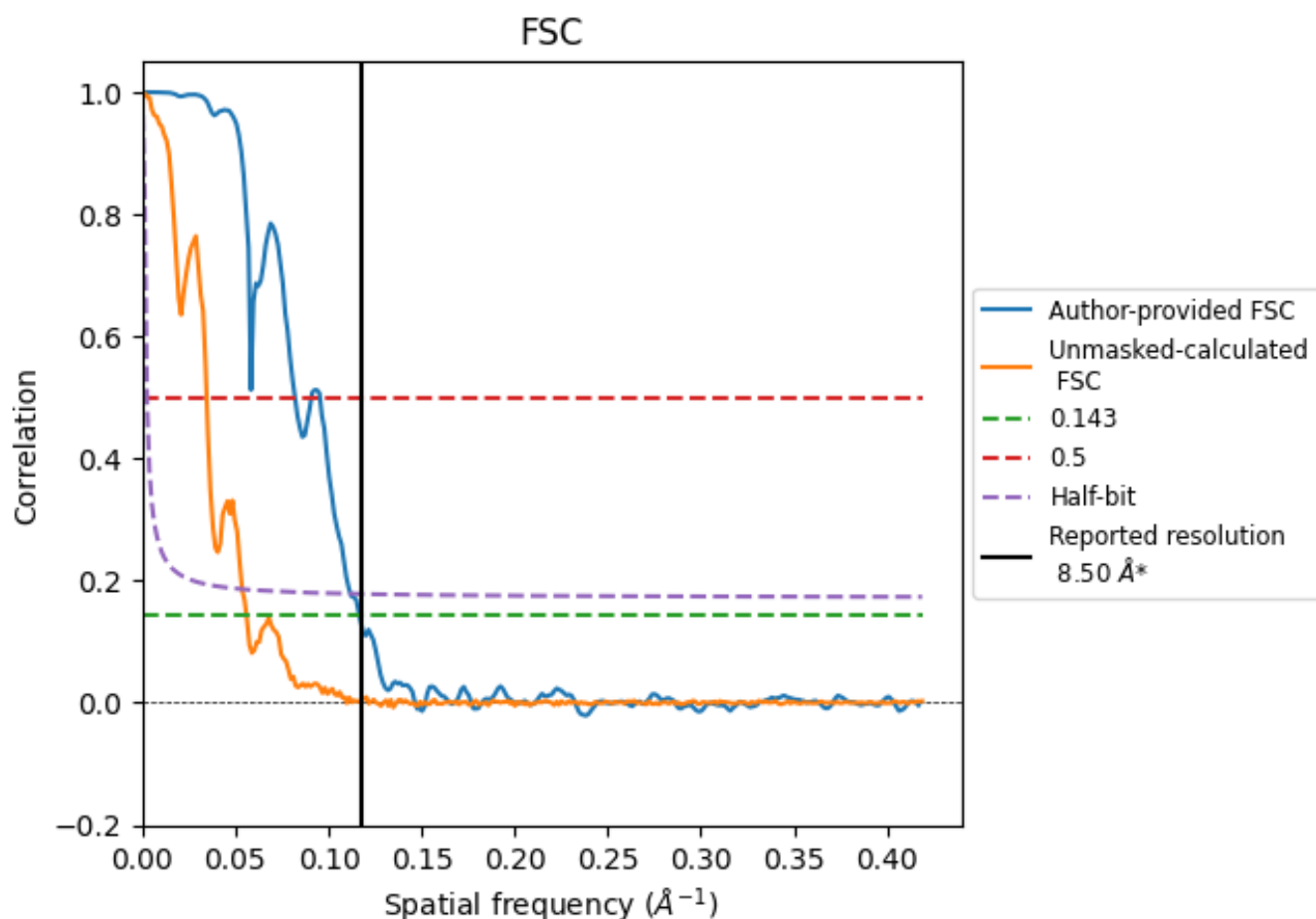


*Reported resolution corresponds to spatial frequency of $0.118 \text{ \AA}^{-1}$

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 0.118 Å⁻¹

8.2 Resolution estimates [i](#)

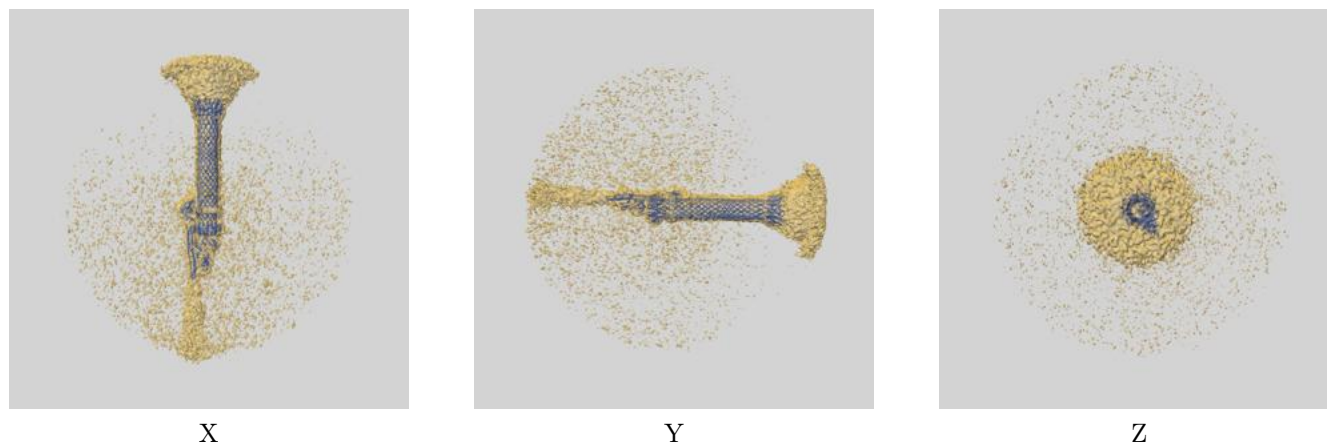
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.50	-	-
Author-provided FSC curve	8.58	12.20	8.94
Unmasked-calculated*	17.89	28.90	18.66

*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 17.89 differs from the reported value 8.5 by more than 10 %

9 Map-model fit [i](#)

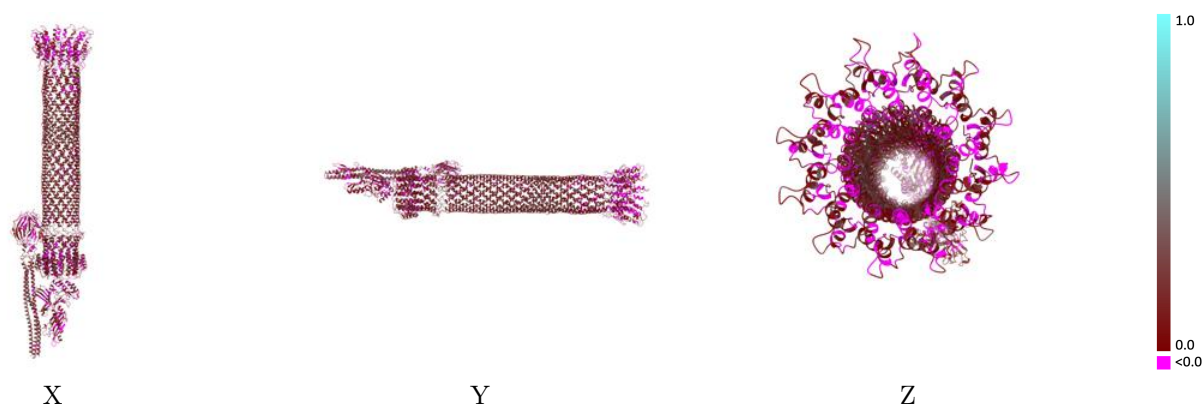
This section contains information regarding the fit between EMDB map EMD-74091 and PDB model 9ZE4. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



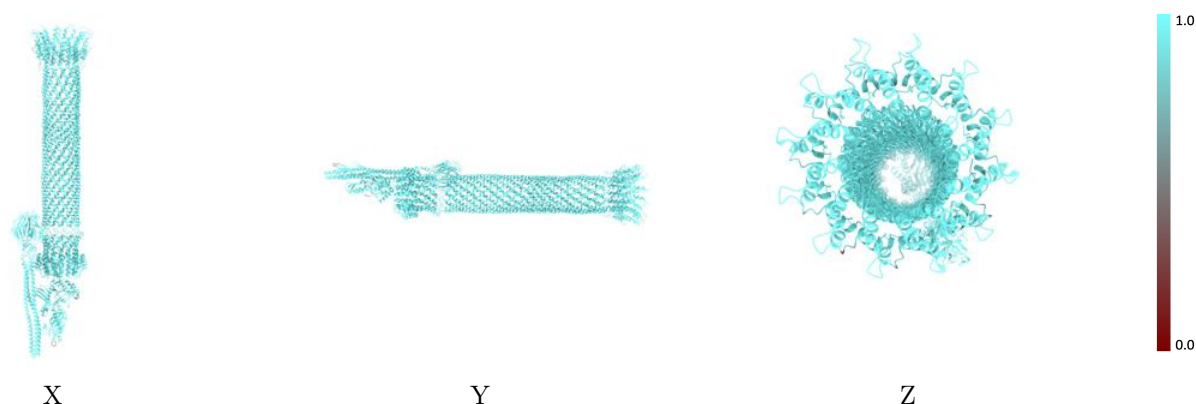
The images above show the 3D surface view of the map at the recommended contour level 0.0176 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



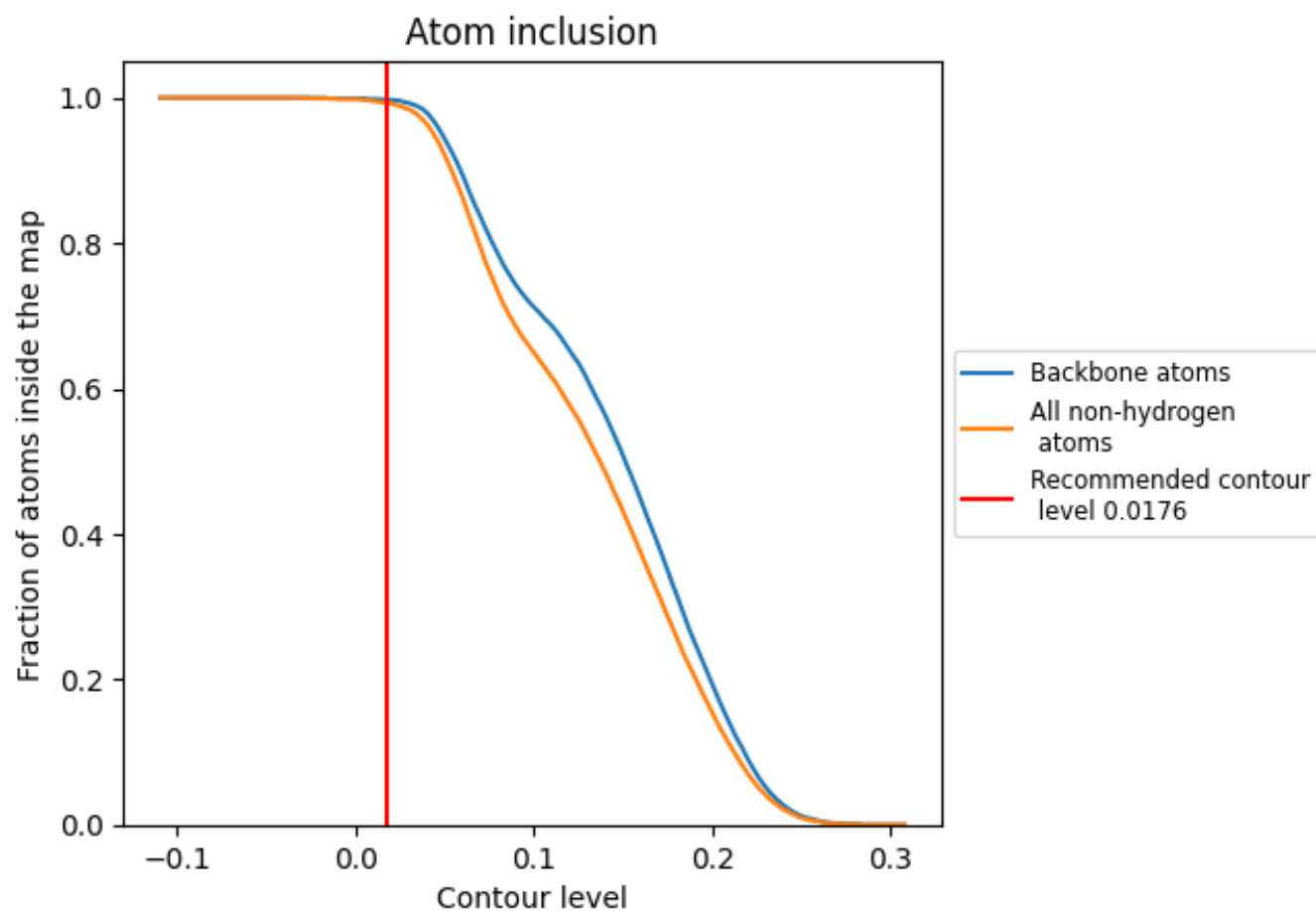
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0176).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.0176) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9930	 0.1130
A	 0.9970	 0.1060
B	 0.9980	 0.1320
C	 0.9980	 0.1170
D	 0.9990	 0.1280
E	 0.9970	 0.1200
F	 0.9940	 0.0990
G	 0.9910	 0.1040
H	 0.9940	 0.1100
I	 0.9890	 0.1190
J	 0.9930	 0.1190
K	 0.9950	 0.1110
L	 0.9980	 0.1170
M	 0.9730	 0.0730
N	 0.9990	 0.1420
O	 0.9940	 0.1380
P	 0.9940	 0.1240

