



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:00 PM UTC

PDB ID : 8Z5Q / pdb_00008z5q
EMDB ID : EMD-39778
Title : human phosphorylase kinase - inactive state
Authors : Ma, R.; Yan, K.
Deposited on : 2024-04-18
Resolution : 4.24 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:

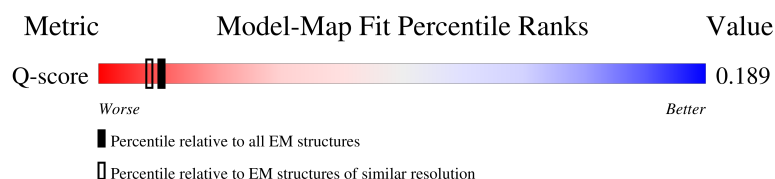
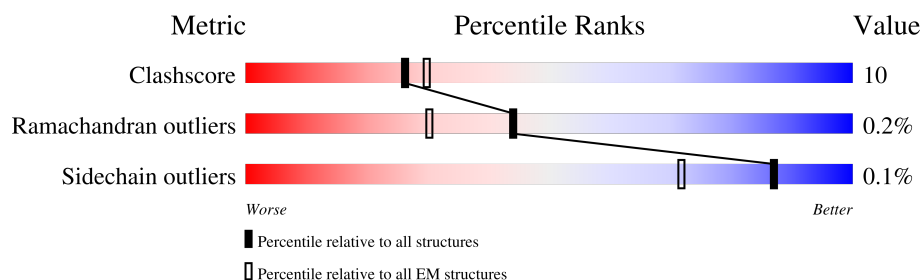
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.24 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.



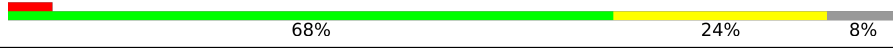
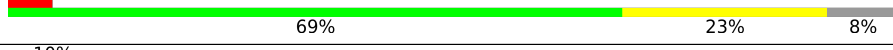
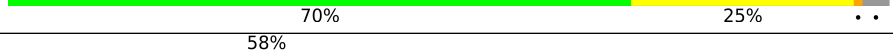
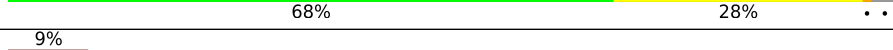
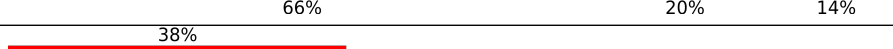
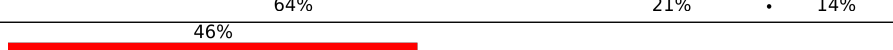
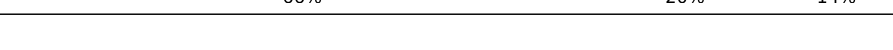
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4688 (3.74 - 4.74)

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	1223	
1	E	1223	
1	I	1223	
1	M	1223	

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Mol	Chain	Length	Quality of chain
2	B	1093	
2	F	1093	
2	J	1093	
2	N	1093	
3	C	387	
3	G	387	
3	K	387	
3	O	387	
4	D	168	
4	H	168	
4	L	168	
4	P	168	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 80239 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 Phosphorylase b kinase regulatory subunit alpha, skeletal muscle isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	995	Total	C	N	O	S	0	0
			7852	5004	1327	1475	46		
1	E	995	Total	C	N	O	S	0	0
			7852	5004	1327	1475	46		
1	I	995	Total	C	N	O	S	0	0
			7852	5004	1327	1475	46		
1	M	995	Total	C	N	O	S	0	0
			7852	5004	1327	1475	46		

- Molecule 2 is a protein called Phosphorylase b kinase regulatory subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1001	Total	C	N	O	S	0	0
			8049	5159	1378	1476	36		
2	F	1001	Total	C	N	O	S	0	0
			8049	5159	1378	1476	36		
2	J	1001	Total	C	N	O	S	0	0
			8049	5159	1378	1476	36		
2	N	1001	Total	C	N	O	S	0	0
			8049	5159	1378	1476	36		

- Molecule 3 is a protein called Phosphorylase b kinase gamma catalytic chain, skeletal muscle/heart isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	376	Total	C	N	O	S	0	0
			3065	1965	527	558	15		
3	G	376	Total	C	N	O	S	0	0
			3065	1965	527	558	15		
3	K	376	Total	C	N	O	S	0	0
			3052	1953	527	557	15		
3	O	376	Total	C	N	O	S	0	0
			3065	1965	527	558	15		

- Molecule 4 is a protein called Calmodulin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	144	Total	C	N	O	S	0	0
			1097	674	178	236	9		
4	H	144	Total	C	N	O	S	0	0
			1097	674	178	236	9		
4	L	144	Total	C	N	O	S	0	0
			1097	674	178	236	9		
4	P	144	Total	C	N	O	S	0	0
			1097	674	178	236	9		

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	ASP	-	expression tag	UNP P0DP25
D	-17	TYR	-	expression tag	UNP P0DP25
D	-16	LYS	-	expression tag	UNP P0DP25
D	-15	ASP	-	expression tag	UNP P0DP25
D	-14	ASP	-	expression tag	UNP P0DP25
D	-13	ASP	-	expression tag	UNP P0DP25
D	-12	ASP	-	expression tag	UNP P0DP25
D	-11	LYS	-	expression tag	UNP P0DP25
D	-10	SER	-	expression tag	UNP P0DP25
D	-9	GLY	-	expression tag	UNP P0DP25
D	-8	PRO	-	expression tag	UNP P0DP25
D	-7	ASP	-	expression tag	UNP P0DP25
D	-6	GLU	-	expression tag	UNP P0DP25
D	-5	VAL	-	expression tag	UNP P0DP25
D	-4	ASP	-	expression tag	UNP P0DP25
D	-3	ALA	-	expression tag	UNP P0DP25
D	-2	SER	-	expression tag	UNP P0DP25
D	-1	GLY	-	expression tag	UNP P0DP25
D	0	ARG	-	expression tag	UNP P0DP25
H	-18	ASP	-	expression tag	UNP P0DP25
H	-17	TYR	-	expression tag	UNP P0DP25
H	-16	LYS	-	expression tag	UNP P0DP25
H	-15	ASP	-	expression tag	UNP P0DP25
H	-14	ASP	-	expression tag	UNP P0DP25
H	-13	ASP	-	expression tag	UNP P0DP25
H	-12	ASP	-	expression tag	UNP P0DP25
H	-11	LYS	-	expression tag	UNP P0DP25
H	-10	SER	-	expression tag	UNP P0DP25
H	-9	GLY	-	expression tag	UNP P0DP25
H	-8	PRO	-	expression tag	UNP P0DP25

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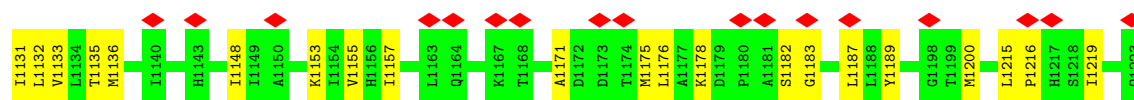
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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASP	-	expression tag	UNP P0DP25
H	-6	GLU	-	expression tag	UNP P0DP25
H	-5	VAL	-	expression tag	UNP P0DP25
H	-4	ASP	-	expression tag	UNP P0DP25
H	-3	ALA	-	expression tag	UNP P0DP25
H	-2	SER	-	expression tag	UNP P0DP25
H	-1	GLY	-	expression tag	UNP P0DP25
H	0	ARG	-	expression tag	UNP P0DP25
L	-18	ASP	-	expression tag	UNP P0DP25
L	-17	TYR	-	expression tag	UNP P0DP25
L	-16	LYS	-	expression tag	UNP P0DP25
L	-15	ASP	-	expression tag	UNP P0DP25
L	-14	ASP	-	expression tag	UNP P0DP25
L	-13	ASP	-	expression tag	UNP P0DP25
L	-12	ASP	-	expression tag	UNP P0DP25
L	-11	LYS	-	expression tag	UNP P0DP25
L	-10	SER	-	expression tag	UNP P0DP25
L	-9	GLY	-	expression tag	UNP P0DP25
L	-8	PRO	-	expression tag	UNP P0DP25
L	-7	ASP	-	expression tag	UNP P0DP25
L	-6	GLU	-	expression tag	UNP P0DP25
L	-5	VAL	-	expression tag	UNP P0DP25
L	-4	ASP	-	expression tag	UNP P0DP25
L	-3	ALA	-	expression tag	UNP P0DP25
L	-2	SER	-	expression tag	UNP P0DP25
L	-1	GLY	-	expression tag	UNP P0DP25
L	0	ARG	-	expression tag	UNP P0DP25
P	-18	ASP	-	expression tag	UNP P0DP25
P	-17	TYR	-	expression tag	UNP P0DP25
P	-16	LYS	-	expression tag	UNP P0DP25
P	-15	ASP	-	expression tag	UNP P0DP25
P	-14	ASP	-	expression tag	UNP P0DP25
P	-13	ASP	-	expression tag	UNP P0DP25
P	-12	ASP	-	expression tag	UNP P0DP25
P	-11	LYS	-	expression tag	UNP P0DP25
P	-10	SER	-	expression tag	UNP P0DP25
P	-9	GLY	-	expression tag	UNP P0DP25
P	-8	PRO	-	expression tag	UNP P0DP25
P	-7	ASP	-	expression tag	UNP P0DP25
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P	-5	VAL	-	expression tag	UNP P0DP25
P	-4	ASP	-	expression tag	UNP P0DP25

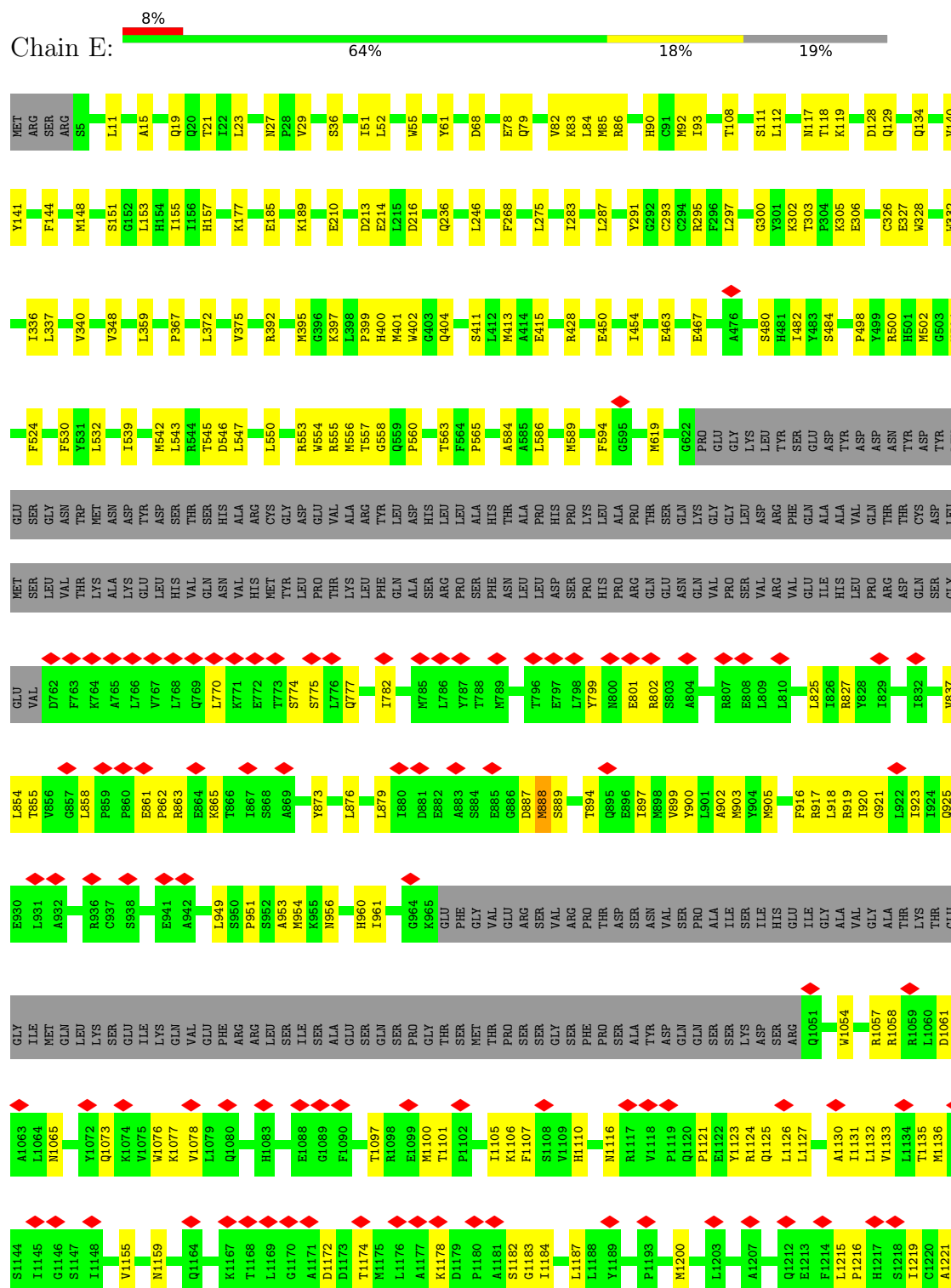
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Chain	Residue	Modelled	Actual	Comment	Reference
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P	-2	SER	-	expression tag	UNP P0DP25
P	-1	GLY	-	expression tag	UNP P0DP25
P	0	ARG	-	expression tag	UNP P0DP25



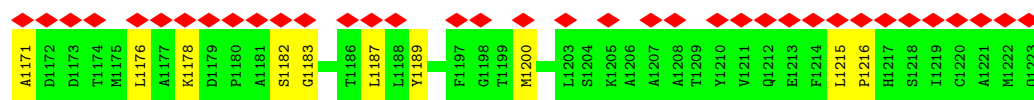
- Molecule 1: Phosphorylase b kinase regulatory subunit alpha, skeletal muscle isoform



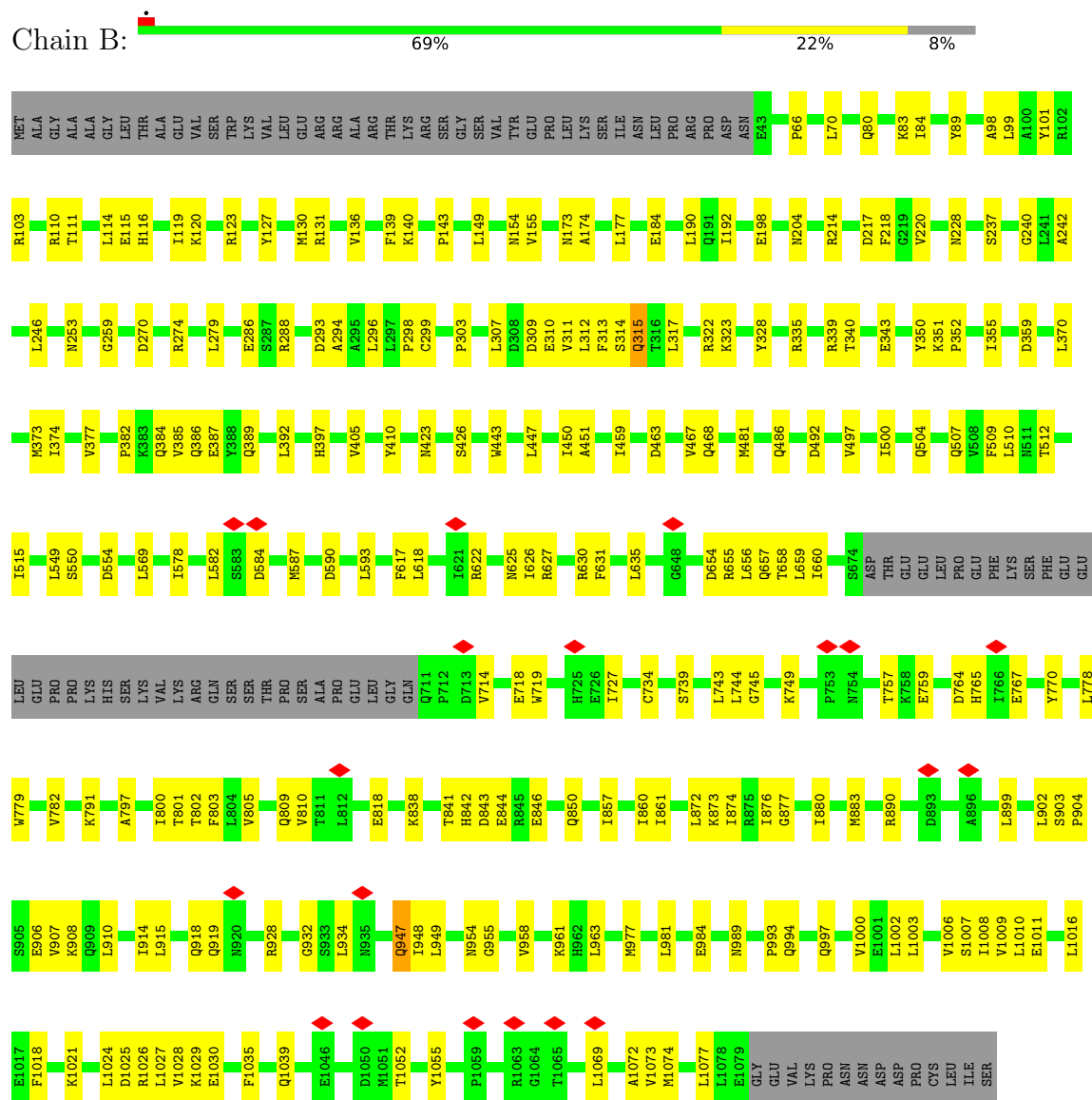
- Molecule 1: Phosphorylase b kinase regulatory subunit alpha, skeletal muscle isoform



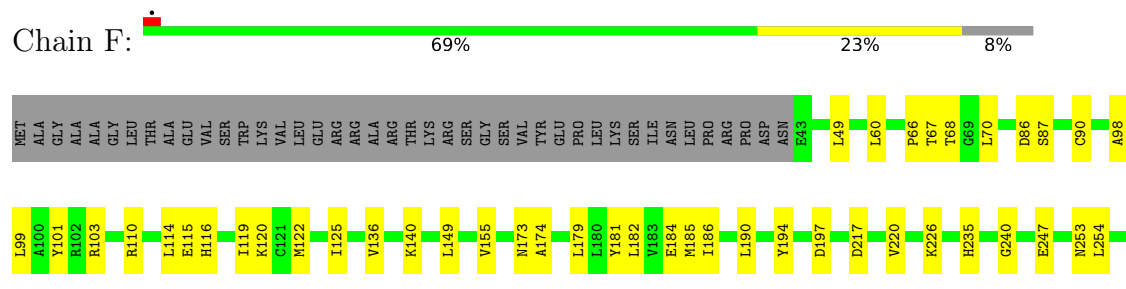


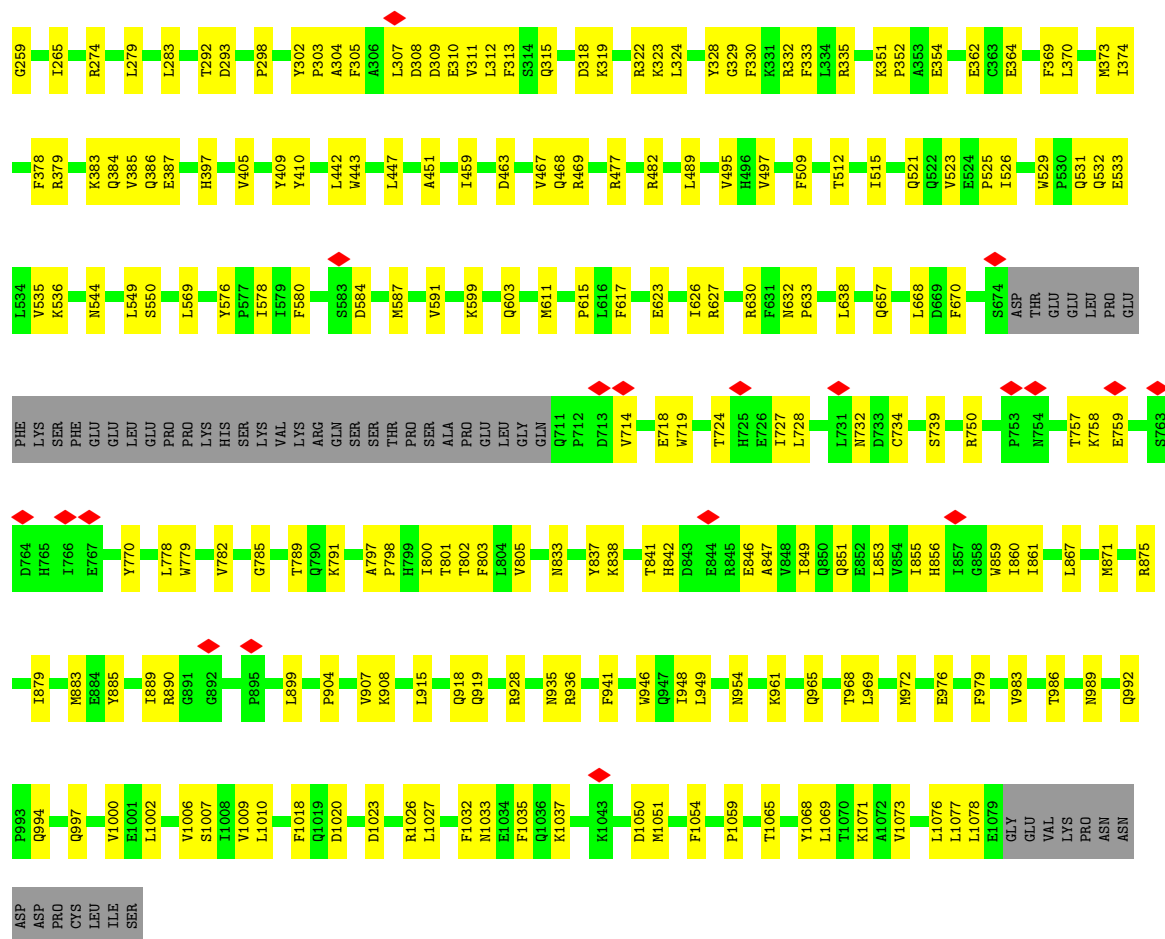


● Molecule 2: Phosphorylase b kinase regulatory subunit beta

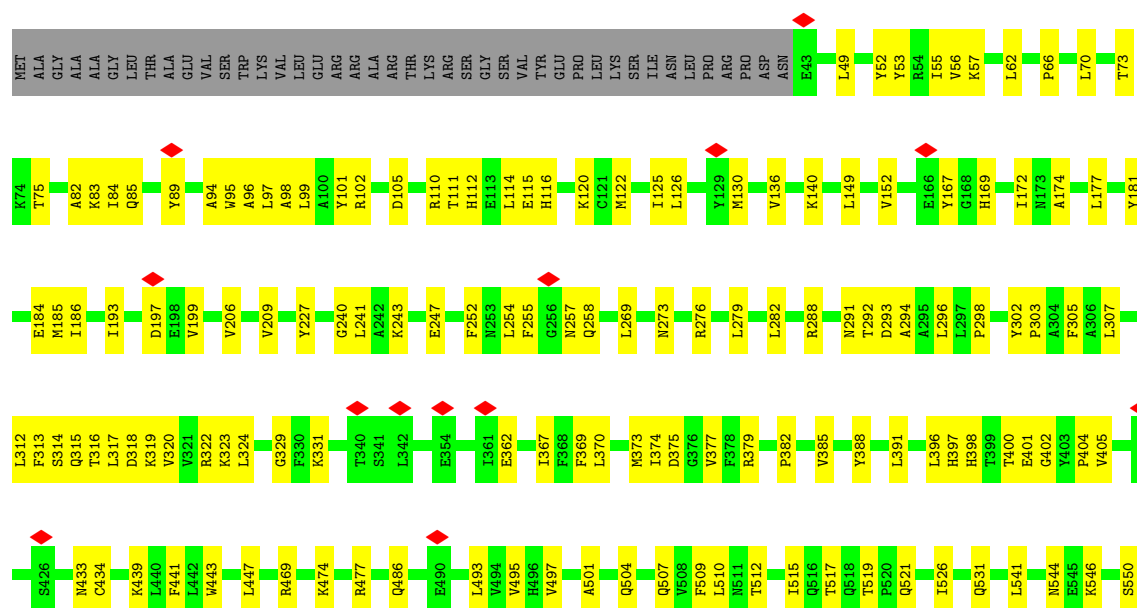


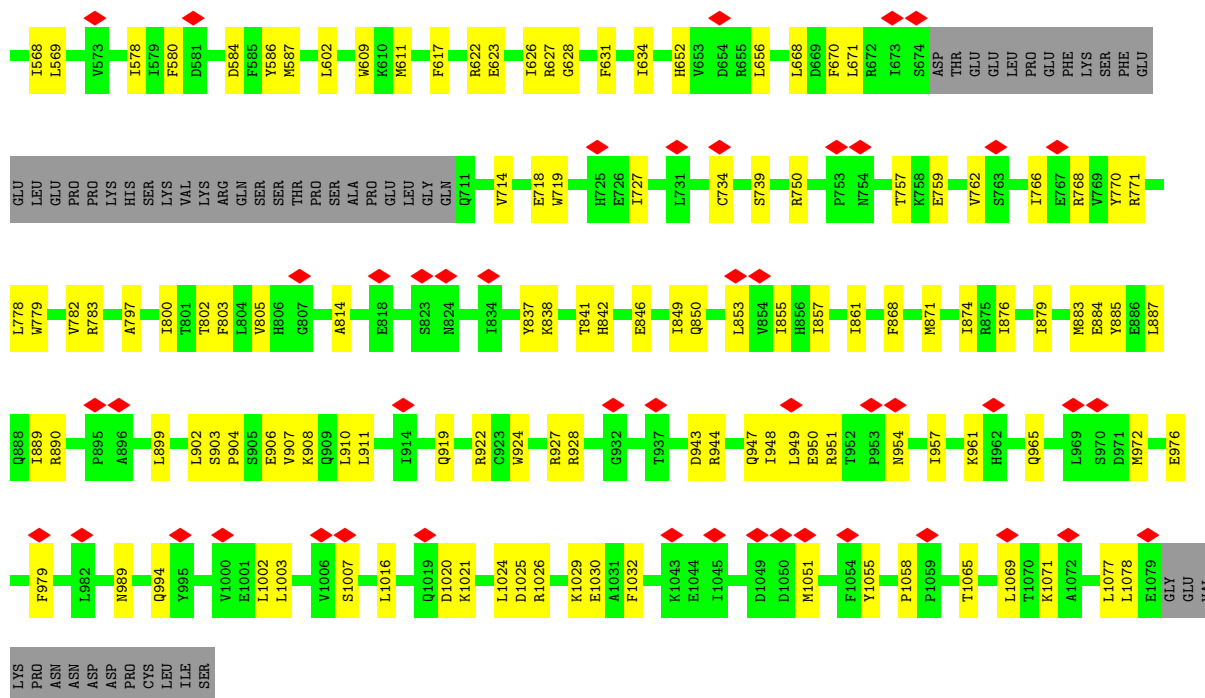
● Molecule 2: Phosphorylase b kinase regulatory subunit beta



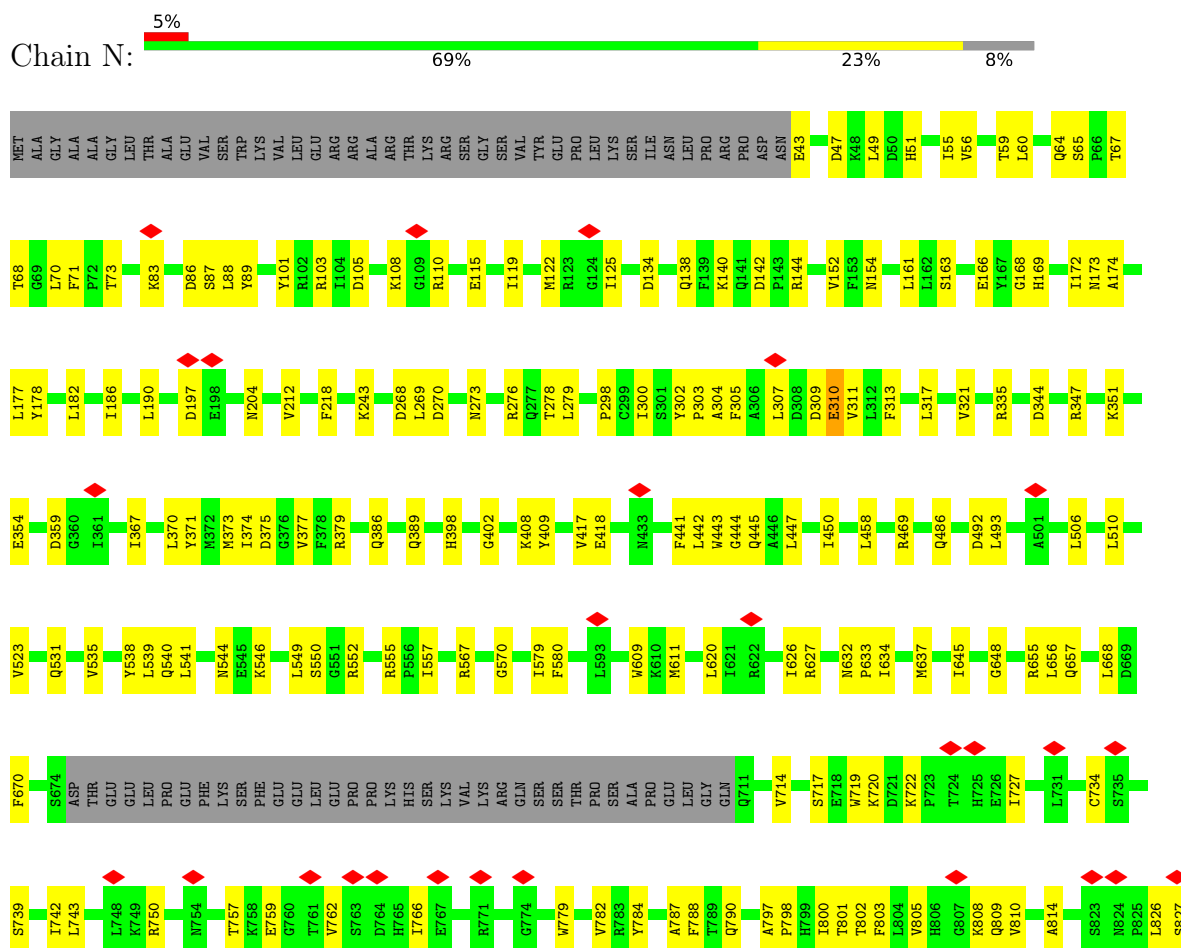


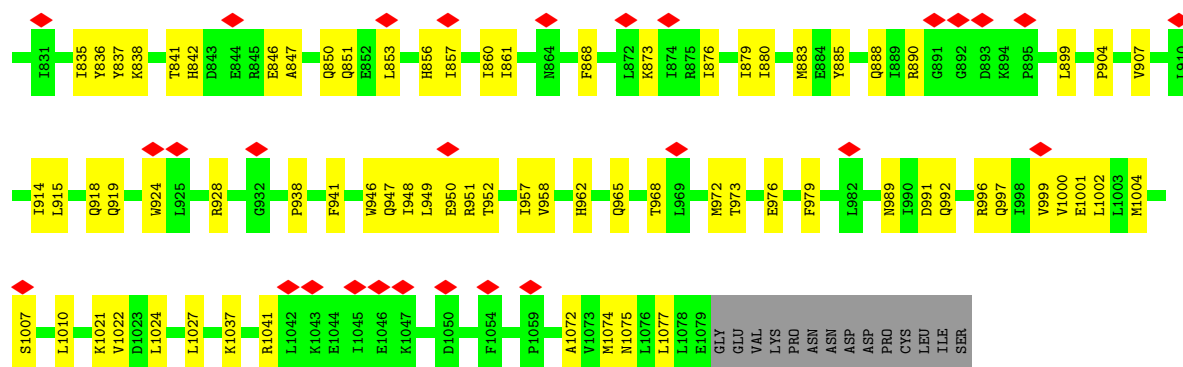
• Molecule 2: Phosphorylase b kinase regulatory subunit beta



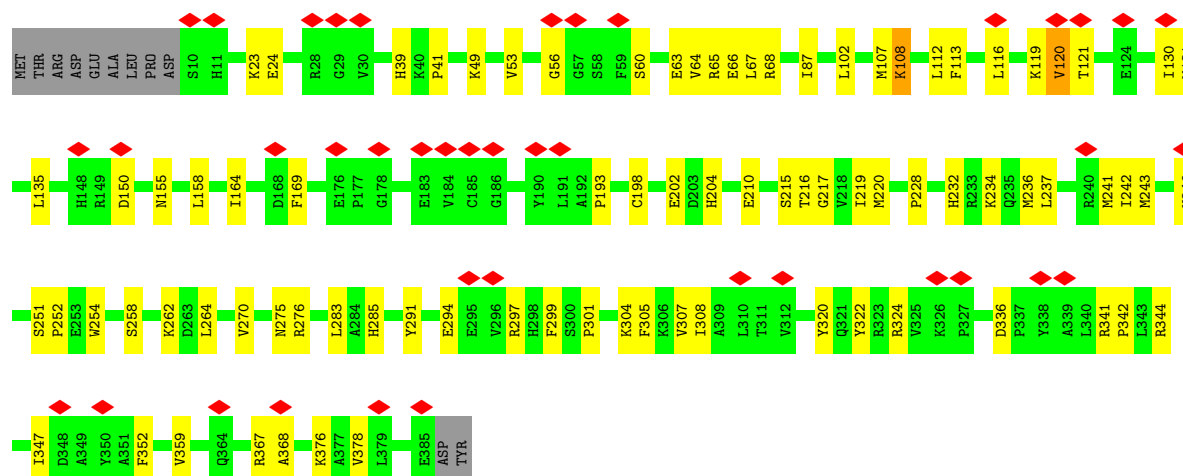
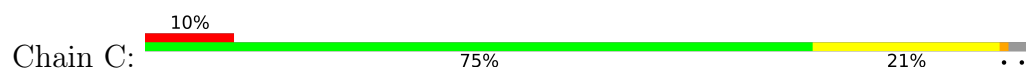


• Molecule 2: Phosphorylase b kinase regulatory subunit beta

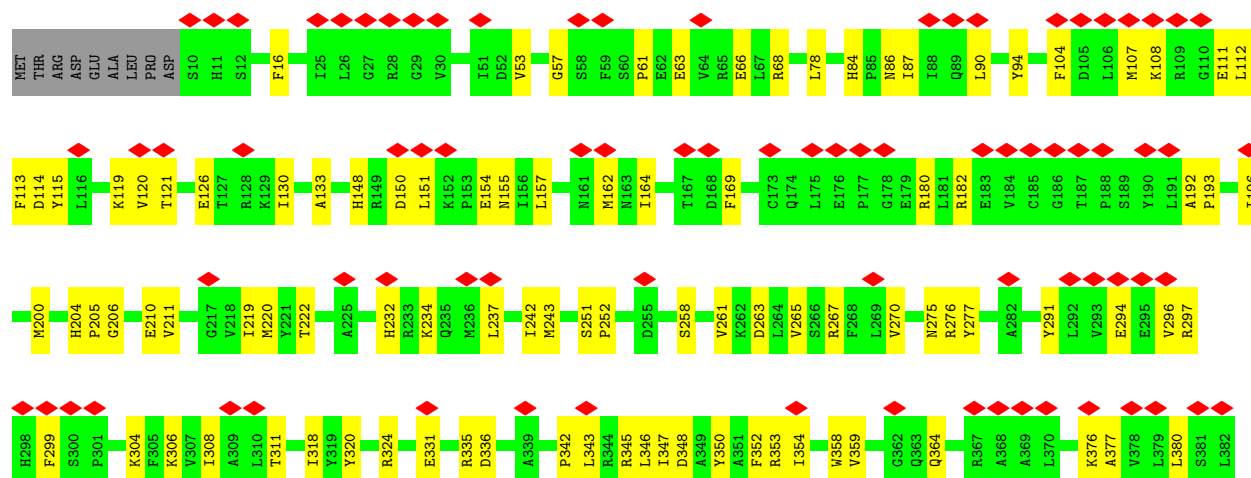


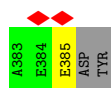


- Molecule 3: Phosphorylase b kinase gamma catalytic chain, skeletal muscle/heart isoform

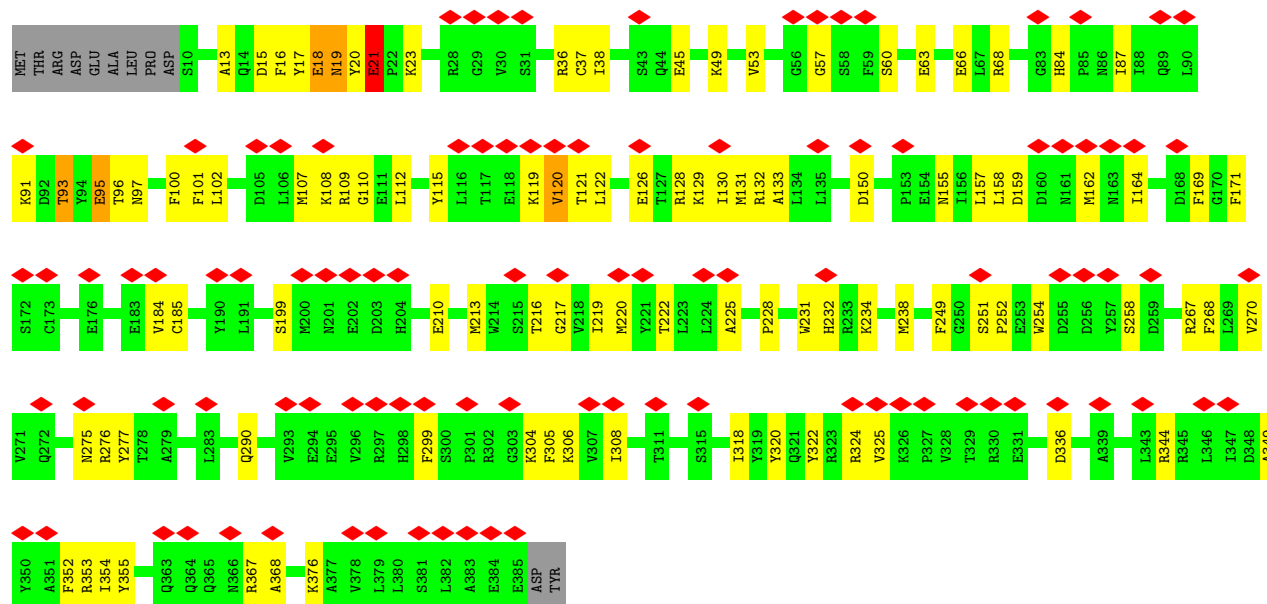


- Molecule 3: Phosphorylase b kinase gamma catalytic chain, skeletal muscle/heart isoform

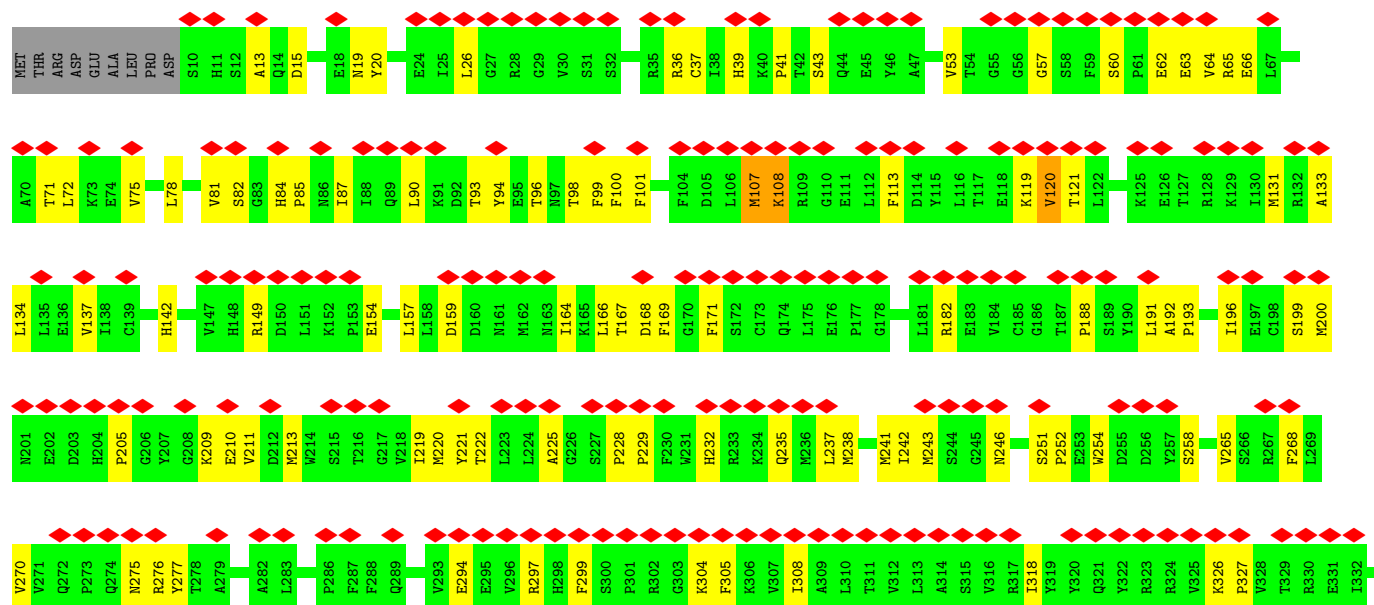


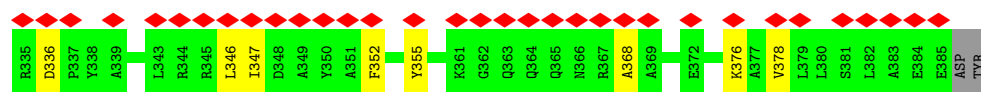


- Molecule 3: Phosphorylase b kinase gamma catalytic chain, skeletal muscle/heart isoform

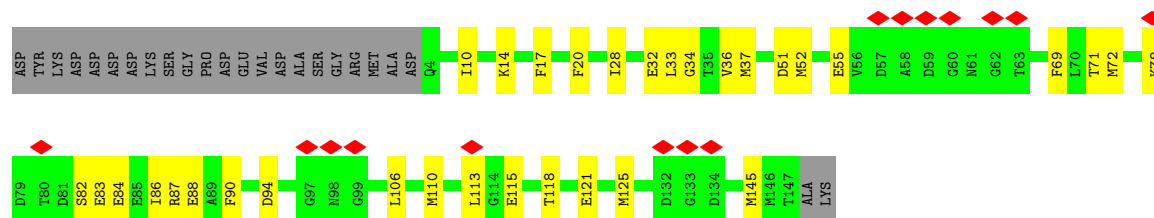


- Molecule 3: Phosphorylase b kinase gamma catalytic chain, skeletal muscle/heart isoform

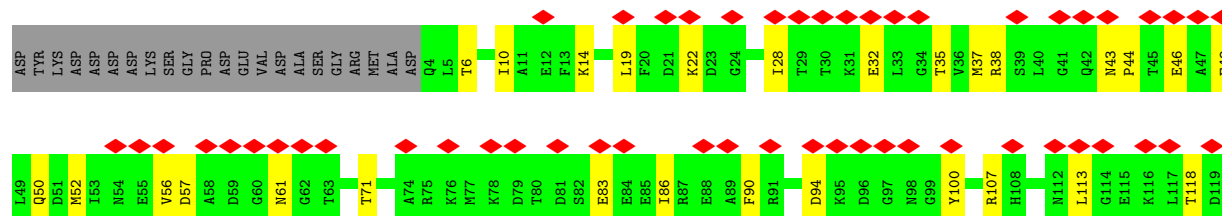
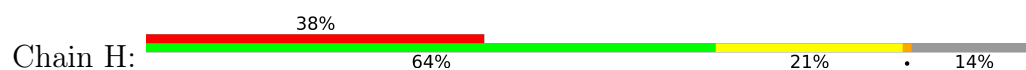




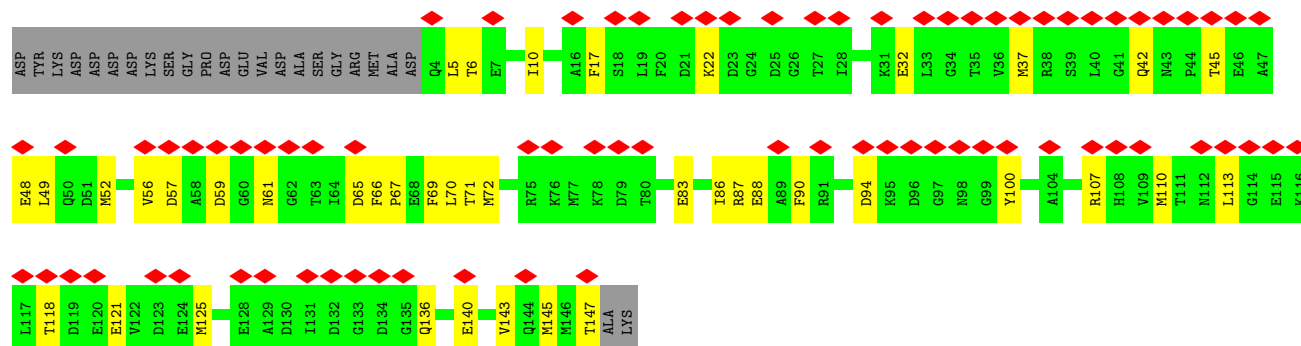
• Molecule 4: Calmodulin-3



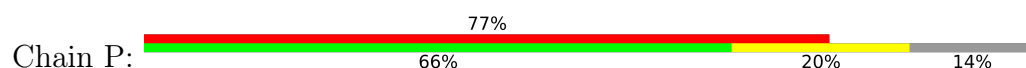
• Molecule 4: Calmodulin-3

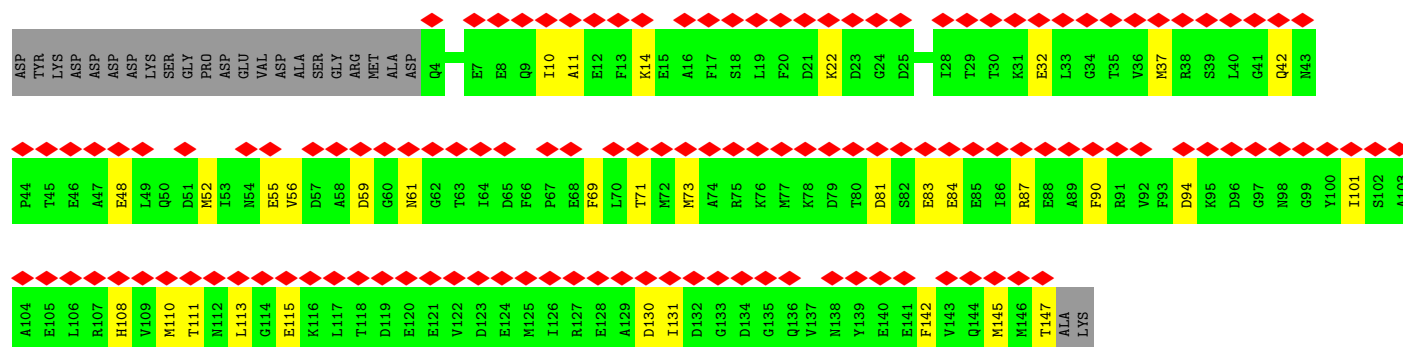


• Molecule 4: Calmodulin-3



• Molecule 4: Calmodulin-3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77068	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.937	Depositor
Minimum map value	-0.557	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.125	Depositor
Map size ($\text{\AA}$)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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	A	0.13	0/8012	0.38	1/10854 (0.0%)
1	E	0.13	0/8012	0.39	0/10854
1	I	0.13	0/8012	0.36	1/10854 (0.0%)
1	M	0.13	0/8012	0.36	0/10854
2	B	0.13	0/8230	0.34	0/11158
2	F	0.13	0/8230	0.34	0/11158
2	J	0.13	0/8230	0.36	0/11158
2	N	0.14	0/8230	0.35	0/11158
3	C	0.12	0/3136	0.33	0/4243
3	G	0.14	0/3136	0.37	1/4243 (0.0%)
3	K	0.19	0/3121	0.44	3/4223 (0.1%)
3	O	0.14	0/3136	0.38	2/4243 (0.0%)
4	D	0.14	0/1109	0.37	0/1493
4	H	0.13	0/1109	0.36	0/1493
4	L	0.14	0/1109	0.40	0/1493
4	P	0.11	0/1109	0.29	0/1493
All	All	0.13	0/81933	0.36	8/110972 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	ILE	N-CA-C	-6.61	106.02	111.91
3	K	21	GLU	CA-C-N	6.31	126.49	120.31
3	K	21	GLU	C-N-CA	6.31	126.49	120.31
3	O	107	MET	CA-C-N	5.95	132.90	121.54
3	O	107	MET	C-N-CA	5.95	132.90	121.54
3	K	15	ASP	N-CA-C	5.53	118.37	111.24
3	G	61	PRO	CA-N-CD	-5.33	104.53	112.00
1	I	155	ILE	N-CA-C	-5.06	108.91	113.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7852	0	7885	137	0
1	E	7852	0	7885	158	0
1	I	7852	0	7885	125	0
1	M	7852	0	7885	141	0
2	B	8049	0	8041	163	0
2	F	8049	0	8041	174	0
2	J	8049	0	8041	184	0
2	N	8049	0	8041	183	0
3	C	3065	0	3063	67	0
3	G	3065	0	3063	72	0
3	K	3052	0	3049	93	0
3	O	3065	0	3063	74	0
4	D	1097	0	1002	30	0
4	H	1097	0	1002	31	0
4	L	1097	0	1002	34	0
4	P	1097	0	1002	22	0
All	All	80239	0	79950	1619	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 10.

All (1619) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:906:ARG:NH1	1:M:907:THR:OG1	2.04	0.91
1:E:1100:MET:HE2	1:E:1107:PHE:H	1.35	0.89
1:I:919:ARG:HH22	1:I:1064:LEU:HA	1.39	0.87
1:I:919:ARG:NH2	1:I:1063:ALA:O	2.08	0.85
1:I:142:LEU:HD11	1:I:165:ILE:HD11	1.59	0.85
3:K:107:MET:HG2	3:K:157:LEU:HB3	1.59	0.84
2:N:531:GLN:HE21	2:N:557:ILE:HG22	1.45	0.82
2:N:367:ILE:HG13	2:N:370:LEU:HD12	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:196:ILE:HG22	3:O:200:MET:HE1	1.62	0.82
3:C:308:ILE:HG12	4:D:110:MET:HE1	1.61	0.80
4:D:84:GLU:OE1	4:D:87:ARG:NE	2.13	0.78
1:A:83:LYS:HE3	2:F:194:TYR:HB2	1.63	0.78
1:E:397:LYS:HG2	1:E:399:PRO:HD2	1.66	0.78
2:N:717:SER:HA	2:N:720:LYS:HE3	1.64	0.78
2:J:874:ILE:HD11	2:J:879:ILE:HD11	1.64	0.77
3:C:217:GLY:HA2	3:C:220:MET:HE2	1.67	0.77
3:G:196:ILE:HG22	3:G:200:MET:HE1	1.65	0.77
1:A:11:LEU:HD13	1:A:61:TYR:HE1	1.50	0.76
3:O:131:MET:HE3	3:O:220:MET:HE2	1.69	0.75
1:A:302:LYS:HB3	1:A:395:MET:HE1	1.67	0.75
1:E:927:MET:HE1	1:E:961:ILE:HG21	1.68	0.74
2:J:85:GLN:HE22	2:J:174:ALA:HB2	1.52	0.74
1:E:1133:VAL:HA	1:E:1136:MET:HE3	1.68	0.74
3:K:305:PHE:HD1	4:L:125:MET:HE2	1.51	0.74
2:F:1035:PHE:HD1	2:F:1068:TYR:HE2	1.35	0.73
3:K:270:VAL:O	3:K:276:ARG:NH1	2.22	0.73
1:M:927:MET:HE1	1:M:961:ILE:HG21	1.70	0.73
1:A:51:ILE:HD13	1:A:84:LEU:HD23	1.71	0.73
2:N:307:LEU:HD22	2:N:313:PHE:HB2	1.71	0.73
1:E:504:VAL:HG13	1:E:550:LEU:HD21	1.71	0.73
2:J:783:ARG:HH21	2:J:849:ILE:HG12	1.54	0.73
1:A:326:CYS:O	1:A:327:GLU:HG3	1.88	0.72
1:E:498:PRO:HD2	1:E:500:ARG:HH22	1.55	0.72
1:E:951:PRO:HA	1:E:954:MET:HE2	1.71	0.72
3:G:148:HIS:CE1	3:G:151:LEU:HG	2.24	0.72
2:B:1035:PHE:O	2:B:1039:GLN:NE2	2.21	0.72
2:F:972:MET:HG2	2:F:979:PHE:HB2	1.71	0.72
3:O:270:VAL:O	3:O:276:ARG:NH1	2.21	0.72
3:K:231:TRP:HA	3:K:238:MET:HE2	1.71	0.72
2:J:948:ILE:HD11	2:J:1007:SER:HB2	1.72	0.72
2:B:322:ARG:HH22	2:B:323:LYS:HE3	1.55	0.71
1:M:1136:MET:HE2	3:O:346:LEU:HD13	1.72	0.71
1:I:837:VAL:HG23	1:I:895:GLN:HE21	1.55	0.71
1:I:894:THR:HG23	1:I:920:ILE:HG12	1.72	0.71
2:F:307:LEU:HD22	2:F:313:PHE:HB2	1.71	0.71
2:N:973:THR:HG22	2:N:976:GLU:HG3	1.71	0.71
2:J:734:CYS:HG	2:J:739:SER:HG	1.39	0.71
3:K:131:MET:HG3	3:K:220:MET:HE1	1.72	0.71
1:M:1200:MET:HG2	3:O:347:ILE:HG23	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:90:LEU:HD21	3:O:93:THR:HG23	1.71	0.71
3:K:18:GLU:O	3:K:19:ASN:C	2.33	0.70
1:A:532:LEU:HD12	1:A:538:MET:HE1	1.73	0.70
2:B:1009:VAL:HG21	2:B:1073:VAL:HG11	1.72	0.70
4:P:59:ASP:OD1	4:P:61:ASN:ND2	2.24	0.70
3:C:252:PRO:O	3:C:344:ARG:NH1	2.25	0.70
1:E:852:LYS:HE3	1:E:918:LEU:HD23	1.74	0.70
2:N:1021:LYS:NZ	2:N:1022:VAL:O	2.24	0.70
1:M:791:GLY:HA2	1:M:794:TRP:CD1	2.26	0.69
1:E:917:ARG:HG3	1:E:919:ARG:HH22	1.57	0.69
2:F:532:GLN:NE2	2:F:533:GLU:OE2	2.25	0.69
1:E:302:LYS:HB3	1:E:395:MET:HE1	1.74	0.69
1:M:570:MET:HE3	1:M:582:ILE:HG13	1.74	0.69
4:H:46:GLU:O	4:H:50:GLN:NE2	2.25	0.69
1:E:852:LYS:NZ	1:E:853:HIS:O	2.26	0.69
1:I:1187:LEU:HD12	3:K:376:LYS:HD3	1.73	0.69
2:N:1027:LEU:HD22	2:N:1072:ALA:HB1	1.73	0.69
3:O:308:ILE:HD11	4:P:113:LEU:HD13	1.75	0.69
1:E:586:LEU:HA	1:E:589:MET:SD	2.32	0.69
1:A:1053:GLN:HG2	1:A:1057:ARG:HH22	1.57	0.68
2:B:727:ILE:HG13	2:B:743:LEU:HD22	1.74	0.68
1:E:326:CYS:O	1:E:327:GLU:HG3	1.94	0.68
2:N:850:GLN:HG2	2:N:876:ILE:HG21	1.75	0.68
1:E:1159:ASN:HD21	1:E:1184:ILE:HA	1.57	0.68
1:M:268:PHE:O	1:M:428:ARG:NH2	2.26	0.68
3:O:308:ILE:HG12	4:P:110:MET:HE1	1.75	0.68
1:A:62:ARG:HH22	1:A:71:LYS:HG2	1.57	0.68
2:F:734:CYS:HG	2:F:739:SER:HG	1.42	0.68
2:J:307:LEU:HD22	2:J:313:PHE:HB2	1.74	0.68
4:P:48:GLU:O	4:P:52:MET:HG3	1.94	0.68
1:A:1078:VAL:HG21	1:A:1135:THR:HG22	1.75	0.67
1:I:310:ARG:HH12	1:I:313:TYR:HD1	1.42	0.67
2:N:802:THR:HA	2:N:805:VAL:HG12	1.75	0.67
3:O:84:HIS:CD2	3:O:85:PRO:HD2	2.30	0.67
1:A:1200:MET:HG2	3:C:347:ILE:HG23	1.77	0.67
3:G:350:TYR:HD1	3:G:353:ARG:HD2	1.58	0.67
2:J:312:LEU:HD12	2:J:315:GLN:HE21	1.59	0.67
1:A:283:ILE:HG13	1:A:287:LEU:HD12	1.76	0.67
2:J:501:ALA:HB2	2:J:517:THR:HG22	1.75	0.67
2:N:408:LYS:HG3	2:N:409:TYR:HD1	1.60	0.67
2:N:197:ASP:OD1	2:N:544:ASN:ND2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:150:ASP:OD2	3:C:155:ASN:ND2	2.28	0.67
4:L:59:ASP:OD1	4:L:61:ASN:ND2	2.29	0.66
1:I:11:LEU:HB2	1:I:61:TYR:HE1	1.59	0.66
3:K:16:PHE:HA	3:K:19:ASN:HB2	1.78	0.66
1:A:156:ILE:HG13	1:A:217:LEU:HD13	1.78	0.66
1:M:1187:LEU:HD12	3:O:376:LYS:HD3	1.78	0.66
2:B:382:PRO:O	2:B:386:GLN:NE2	2.29	0.66
1:E:482:ILE:HG23	1:E:619:MET:HE3	1.77	0.66
1:M:11:LEU:HB3	1:M:61:TYR:HE1	1.60	0.66
3:K:20:TYR:HB3	3:K:37:CYS:HB2	1.77	0.66
2:J:373:MET:HE1	2:J:385:VAL:HG13	1.78	0.66
3:K:210:GLU:OE1	3:K:276:ARG:NH2	2.29	0.66
1:A:523:GLN:OE1	1:A:523:GLN:N	2.29	0.65
1:E:921:GLY:O	1:E:925:GLN:NE2	2.29	0.65
1:I:326:CYS:O	1:I:327:GLU:HG3	1.95	0.65
1:I:538:MET:SD	1:I:952:SER:OG	2.51	0.65
2:F:254:LEU:HD11	2:F:265:ILE:HD11	1.78	0.65
2:J:493:LEU:HD11	2:J:609:TRP:HD1	1.61	0.65
1:E:283:ILE:HG13	1:E:287:LEU:HD12	1.79	0.65
1:E:1106:LYS:O	1:E:1110:HIS:ND1	2.27	0.65
1:I:86:ARG:NH1	1:I:155:ILE:O	2.29	0.65
2:N:567:ARG:HE	2:N:570:GLY:HA2	1.62	0.65
2:N:972:MET:HG3	2:N:979:PHE:HB2	1.79	0.65
2:B:584:ASP:HB2	2:B:770:TYR:HE2	1.61	0.65
1:E:865:LYS:HG3	1:E:879:LEU:HD11	1.79	0.65
2:N:668:LEU:HD22	2:N:670:PHE:HE2	1.62	0.65
2:B:240:GLY:HA2	2:B:279:LEU:HD11	1.79	0.65
1:I:60:ALA:HB2	1:I:418:LEU:HD21	1.78	0.65
3:K:16:PHE:O	3:K:19:ASN:HB2	1.96	0.65
1:A:482:ILE:HG23	1:A:619:MET:HE3	1.79	0.64
3:O:228:PRO:HD2	3:O:368:ALA:HB2	1.79	0.64
2:F:1009:VAL:HG11	2:F:1073:VAL:HG11	1.79	0.64
2:F:803:PHE:HE1	2:F:861:ILE:HG21	1.62	0.64
3:K:130:ILE:HG23	3:K:164:ILE:HD13	1.79	0.64
3:K:150:ASP:OD2	3:K:155:ASN:ND2	2.30	0.64
3:K:210:GLU:HB2	3:K:276:ARG:HE	1.62	0.64
2:J:569:LEU:HD21	2:J:671:LEU:HD22	1.79	0.64
1:M:1076:TRP:NE1	1:M:1097:THR:OG1	2.30	0.64
3:O:107:MET:HG2	3:O:157:LEU:HB3	1.78	0.64
4:D:84:GLU:O	4:D:87:ARG:HG3	1.97	0.64
3:K:213:MET:HE3	3:K:268:PHE:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:846:GLU:OE1	2:N:846:GLU:N	2.27	0.64
2:B:734:CYS:HG	2:B:739:SER:HG	1.45	0.63
3:C:308:ILE:HD11	4:D:113:LEU:HD13	1.80	0.63
2:F:948:ILE:HG12	2:F:1010:LEU:HD21	1.80	0.63
3:O:107:MET:O	3:O:108:LYS:HG2	1.98	0.63
2:B:997:GLN:HA	2:B:1000:VAL:HG12	1.79	0.63
1:I:497:ARG:HH22	1:I:502:MET:HE1	1.63	0.63
2:J:70:LEU:HD22	2:J:125:ILE:HG23	1.79	0.63
2:J:247:GLU:OE2	2:J:469:ARG:NH2	2.28	0.63
3:C:270:VAL:O	3:C:276:ARG:NH1	2.32	0.63
2:J:802:THR:HA	2:J:805:VAL:HG12	1.80	0.63
3:K:305:PHE:HD2	4:L:145:MET:HE1	1.62	0.63
2:J:269:LEU:HD21	2:J:611:MET:HE3	1.80	0.63
2:N:952:THR:O	2:N:965:GLN:NE2	2.31	0.63
3:O:235:GLN:HA	3:O:238:MET:HE2	1.81	0.63
3:G:270:VAL:O	3:G:276:ARG:NH1	2.31	0.63
1:M:233:ASP:O	1:M:237:HIS:ND1	2.28	0.63
1:A:92:MET:HE1	1:A:141:TYR:HE2	1.63	0.63
3:C:135:LEU:HD22	3:C:283:LEU:HD13	1.81	0.63
3:G:261:VAL:O	3:G:265:VAL:HG23	1.99	0.63
2:J:846:GLU:OE1	2:J:846:GLU:N	2.26	0.63
3:K:232:HIS:CD2	3:K:234:LYS:H	2.17	0.62
1:M:895:GLN:NE2	1:M:896:GLU:HG3	2.14	0.62
3:O:210:GLU:HB3	3:O:276:ARG:HH21	1.62	0.62
1:M:1077:LYS:O	1:M:1080:GLN:NE2	2.29	0.62
2:N:948:ILE:HD11	2:N:1007:SER:HB2	1.81	0.62
2:B:593:LEU:HD21	2:B:904:PRO:HB2	1.80	0.62
2:F:67:THR:HG23	2:F:68:THR:HG23	1.82	0.62
2:N:89:TYR:CD2	2:N:443:TRP:CZ3	2.87	0.62
2:N:103:ARG:NH2	2:N:458:LEU:O	2.32	0.62
2:B:655:ARG:HD2	2:B:657:GLN:H	1.64	0.62
1:M:823:TRP:HB3	1:M:827:ARG:HH22	1.65	0.62
4:P:11:ALA:HA	4:P:14:LYS:HE2	1.80	0.62
1:E:246:LEU:HD22	1:E:275:LEU:HD12	1.82	0.62
1:E:900:TYR:HA	1:E:903:MET:SD	2.39	0.62
1:E:1187:LEU:HD12	3:G:376:LYS:HD3	1.79	0.62
1:M:831:GLY:HA2	1:M:888:MET:HE2	1.80	0.62
1:E:887:ASP:O	1:E:889:SER:N	2.32	0.62
2:J:924:TRP:CD1	2:J:927:ARG:HH21	2.18	0.61
1:A:566:ILE:HD12	1:A:570:MET:HE3	1.82	0.61
1:A:763:PHE:HE1	1:A:789:MET:HE3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:ARG:NH2	1:A:881:ASP:OD1	2.33	0.61
2:F:734:CYS:SG	2:F:739:SER:OG	2.58	0.61
2:N:847:ALA:O	2:N:851:GLN:HG2	2.00	0.61
3:K:23:LYS:HB2	3:K:36:ARG:HB3	1.81	0.61
1:M:265:PHE:HB2	1:M:337:LEU:HD13	1.83	0.61
2:F:99:LEU:HD21	2:F:463:ASP:HB3	1.82	0.61
1:I:570:MET:SD	1:I:582:ILE:HG13	2.40	0.61
2:N:70:LEU:HD21	2:N:125:ILE:HG23	1.82	0.61
2:N:538:TYR:HB3	2:N:552:ARG:HD3	1.82	0.61
2:F:197:ASP:OD1	2:F:544:ASN:ND2	2.33	0.61
3:K:109:ARG:HG2	3:K:110:GLY:H	1.66	0.61
2:N:949:LEU:HD21	2:N:968:THR:HG21	1.83	0.61
1:E:36:SER:HB2	1:E:401:MET:HE1	1.82	0.61
1:I:538:MET:HE3	1:I:951:PRO:HB2	1.83	0.61
4:L:83:GLU:O	4:L:87:ARG:HG2	1.99	0.61
1:M:513:ILE:HG23	1:M:619:MET:HE3	1.81	0.61
2:N:826:LEU:HD12	2:N:827:SER:H	1.66	0.61
3:O:39:HIS:CD2	3:O:41:PRO:HD2	2.36	0.61
3:C:112:LEU:HD23	3:C:158:LEU:HD11	1.82	0.61
1:E:268:PHE:O	1:E:428:ARG:NH2	2.33	0.61
2:F:247:GLU:OE2	2:F:482:ARG:NE	2.34	0.61
2:N:523:VAL:HG11	2:N:656:LEU:HD21	1.83	0.61
2:N:949:LEU:O	2:N:965:GLN:NE2	2.34	0.61
1:E:27:ASN:OD1	1:E:119:LYS:NZ	2.34	0.60
1:M:51:ILE:HD11	1:M:81:VAL:HG22	1.83	0.60
1:M:310:ARG:HH12	1:M:313:TYR:HA	1.66	0.60
2:B:872:LEU:HD11	2:B:984:GLU:HG3	1.83	0.60
2:F:532:GLN:HA	2:F:535:VAL:HG12	1.82	0.60
2:J:152:VAL:HB	2:J:169:HIS:HE1	1.66	0.60
1:M:1100:MET:HE2	1:M:1107:PHE:CD1	2.36	0.60
2:B:802:THR:HA	2:B:805:VAL:HG12	1.83	0.60
2:F:948:ILE:HD11	2:F:1007:SER:HB2	1.82	0.60
2:N:928:ARG:NH1	2:N:997:GLN:OE1	2.34	0.60
1:E:1057:ARG:HD2	3:G:358:TRP:CD1	2.37	0.60
2:F:497:VAL:HG22	2:F:617:PHE:HB3	1.84	0.60
1:E:79:GLN:HA	1:E:82:VAL:HG12	1.83	0.60
3:G:111:GLU:HB3	3:G:157:LEU:HD23	1.84	0.60
1:M:326:CYS:O	1:M:327:GLU:HG3	2.00	0.60
1:E:1132:LEU:HD23	3:G:354:ILE:HD11	1.82	0.60
2:F:240:GLY:HA2	2:F:279:LEU:HD11	1.83	0.60
2:N:73:THR:OG1	2:N:83:LYS:NZ	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:883:MET:HB3	2:B:914:ILE:HD13	1.84	0.59
1:I:19:GLN:HA	1:I:23:LEU:HB2	1.83	0.59
1:M:282:GLU:O	1:M:286:LYS:HG3	2.03	0.59
2:J:291:ASN:OD1	2:J:292:THR:N	2.35	0.59
1:M:371:GLU:HB3	1:M:400:HIS:NE2	2.17	0.59
4:H:107:ARG:NH2	4:H:118:THR:O	2.35	0.59
4:L:140:GLU:HA	4:L:143:VAL:HG12	1.84	0.59
2:F:770:TYR:OH	2:F:791:LYS:NZ	2.30	0.59
2:J:227:TYR:OH	2:J:976:GLU:OE2	2.11	0.59
2:J:441:PHE:CE2	2:J:443:TRP:HD1	2.20	0.59
2:N:579:ILE:HG13	2:N:580:PHE:HD1	1.67	0.59
2:F:1068:TYR:HA	2:F:1071:LYS:HD2	1.83	0.59
2:B:846:GLU:OE1	2:B:846:GLU:N	2.25	0.59
1:E:542:MET:HA	1:E:545:THR:HG22	1.83	0.59
3:G:107:MET:HE3	3:G:157:LEU:HB2	1.85	0.59
1:M:584:ALA:O	1:M:588:LYS:HG2	2.03	0.59
2:B:1002:LEU:HD13	2:B:1069:LEU:HD22	1.83	0.59
3:C:270:VAL:HG11	3:C:275:ASN:HB2	1.85	0.59
1:E:1076:TRP:NE1	1:E:1097:THR:OG1	2.35	0.59
1:I:43:TRP:O	1:I:47:ASN:ND2	2.35	0.59
3:K:320:TYR:OH	4:L:88:GLU:OE2	2.19	0.59
1:A:1076:TRP:NE1	1:A:1097:THR:OG1	2.36	0.58
1:E:916:PHE:HZ	1:E:1105:ILE:HG23	1.67	0.58
2:J:296:LEU:HD11	2:J:320:VAL:HG11	1.84	0.58
1:M:43:TRP:O	1:M:47:ASN:ND2	2.36	0.58
2:N:809:GLN:HB3	2:N:873:LYS:HG2	1.85	0.58
2:B:119:ILE:HD11	2:B:190:LEU:HD23	1.85	0.58
2:B:509:PHE:O	2:B:512:THR:OG1	2.21	0.58
2:B:902:LEU:HD22	2:B:906:GLU:HG3	1.85	0.58
2:N:989:ASN:ND2	2:N:989:ASN:O	2.35	0.58
1:A:298:ARG:N	1:A:325:GLU:OE1	2.37	0.58
2:B:500:ILE:HD12	2:B:618:LEU:HD11	1.84	0.58
2:B:759:GLU:OE2	2:B:765:HIS:HB2	2.03	0.58
2:B:803:PHE:HE1	2:B:861:ILE:HG21	1.68	0.58
3:C:299:PHE:HE1	3:C:304:LYS:HG2	1.68	0.58
2:F:292:THR:OG1	2:F:319:LYS:NZ	2.37	0.58
2:F:318:ASP:OD2	2:F:322:ARG:NH2	2.37	0.58
3:G:311:THR:HG21	4:H:19:LEU:HD23	1.86	0.58
2:J:899:LEU:HA	2:J:902:LEU:HD23	1.85	0.58
1:A:854:LEU:HG	1:A:918:LEU:HD11	1.84	0.58
1:E:86:ARG:NH1	1:E:155:ILE:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:302:LYS:HD3	1:E:372:LEU:HD21	1.85	0.58
3:G:210:GLU:HB3	3:G:276:ARG:HH21	1.67	0.58
2:J:370:LEU:HD11	2:J:447:LEU:HB3	1.85	0.58
2:N:154:ASN:HB2	2:N:161:LEU:HG	1.84	0.58
2:F:253:ASN:HD21	2:F:259:GLY:HA3	1.69	0.58
2:J:957:ILE:HD12	2:J:1021:LYS:HE2	1.86	0.58
2:N:140:LYS:NZ	2:N:550:SER:OG	2.37	0.58
2:J:972:MET:HE3	2:J:976:GLU:HB3	1.85	0.58
2:B:590:ASP:HB3	2:B:593:LEU:HD23	1.85	0.58
3:G:294:GLU:OE2	3:G:297:ARG:NH1	2.37	0.58
2:N:951:ARG:HD3	2:N:1010:LEU:HD21	1.85	0.58
1:A:1187:LEU:HD12	3:C:376:LYS:HD3	1.84	0.57
3:G:111:GLU:OE1	3:G:154:GLU:HA	2.03	0.57
1:I:30:THR:HG21	1:I:119:LYS:HA	1.86	0.57
2:N:367:ILE:HD12	2:N:444:GLY:HA2	1.86	0.57
1:A:763:PHE:CE1	1:A:789:MET:HE3	2.39	0.57
1:I:1078:VAL:HG21	1:I:1135:THR:HG22	1.85	0.57
2:N:310:GLU:HG2	2:N:311:VAL:H	1.70	0.57
3:G:150:ASP:OD2	3:G:155:ASN:ND2	2.38	0.57
2:J:842:HIS:CE1	2:J:846:GLU:HG3	2.39	0.57
2:N:375:ASP:OD1	2:N:379:ARG:NH1	2.37	0.57
1:M:584:ALA:HB2	3:O:57:GLY:HA3	1.85	0.57
1:M:837:VAL:HB	1:M:840:LEU:HD13	1.86	0.57
1:E:1116:ASN:OD1	1:E:1124:ARG:NH1	2.38	0.57
1:I:951:PRO:HA	1:I:954:MET:HE2	1.86	0.57
2:J:197:ASP:OD1	2:J:544:ASN:ND2	2.38	0.57
3:K:308:ILE:HD11	4:L:113:LEU:HD13	1.87	0.57
2:N:441:PHE:CE2	2:N:443:TRP:HB3	2.40	0.57
1:E:1058:ARG:HE	1:E:1125:GLN:HE22	1.52	0.57
1:E:1100:MET:HE2	1:E:1107:PHE:N	2.13	0.57
1:I:271:GLU:OE2	1:I:555:ARG:NH2	2.38	0.57
1:A:1131:ILE:O	1:A:1135:THR:HG23	2.05	0.57
2:B:948:ILE:HD11	2:B:1007:SER:HB2	1.87	0.57
2:F:217:ASP:OD1	2:F:235:HIS:ND1	2.38	0.57
1:I:1099:GLU:OE2	1:I:1100:MET:HE2	2.04	0.57
1:E:1159:ASN:ND2	1:E:1184:ILE:HA	2.19	0.57
2:J:928:ARG:NH1	2:J:1055:TYR:O	2.37	0.57
3:K:18:GLU:O	3:K:20:TYR:N	2.38	0.57
1:M:438:VAL:HG21	1:M:554:TRP:CD1	2.40	0.57
2:F:66:PRO:O	2:F:120:LYS:NZ	2.37	0.56
2:F:364:GLU:HB3	2:F:410:TYR:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:803:PHE:HA	2:N:808:LYS:HZ3	1.69	0.56
2:B:904:PRO:HA	2:B:907:VAL:HG22	1.86	0.56
2:F:1035:PHE:CD1	2:F:1068:TYR:HE2	2.19	0.56
3:G:180:ARG:HB3	3:G:206:GLY:HA3	1.87	0.56
3:G:331:GLU:HB3	3:G:335:ARG:NH1	2.20	0.56
1:A:268:PHE:O	1:A:428:ARG:NH2	2.36	0.56
1:A:848:LEU:HD22	1:A:854:LEU:HD13	1.87	0.56
2:B:1074:MET:SD	2:N:1074:MET:HE3	2.46	0.56
2:N:300:ILE:HD12	2:N:307:LEU:HB2	1.87	0.56
2:N:883:MET:HB3	2:N:914:ILE:HD13	1.86	0.56
1:E:923:ILE:O	1:E:927:MET:HG2	2.06	0.56
2:F:302:TYR:HA	2:F:305:PHE:CE2	2.40	0.56
2:J:83:LYS:NZ	2:J:167:TYR:OH	2.39	0.56
1:M:563:THR:HG22	1:M:565:PRO:HD3	1.88	0.56
2:F:928:ARG:HH21	2:F:1059:PRO:HG3	1.71	0.56
3:G:270:VAL:HG11	3:G:275:ASN:HB2	1.88	0.56
1:M:1131:ILE:O	1:M:1135:THR:HG23	2.06	0.56
2:B:500:ILE:HD11	2:B:656:LEU:HD22	1.87	0.56
3:C:301:PRO:HB3	4:D:125:MET:HG2	1.87	0.56
4:D:69:PHE:HA	4:D:72:MET:HE3	1.86	0.56
1:E:11:LEU:HB3	1:E:61:TYR:HE1	1.69	0.56
1:E:189:LYS:NZ	1:E:297:LEU:O	2.27	0.56
3:G:331:GLU:HB3	3:G:335:ARG:HH12	1.70	0.56
3:K:53:VAL:HG21	3:K:68:ARG:HH21	1.71	0.56
2:J:396:LEU:HD21	2:J:404:PRO:HA	1.87	0.56
3:K:95:GLU:HG3	3:K:100:PHE:HE1	1.71	0.56
3:K:112:LEU:HD23	3:K:158:LEU:HD11	1.88	0.56
3:C:297:ARG:HH21	4:D:14:LYS:HD3	1.71	0.56
3:O:213:MET:HE1	3:O:277:TYR:H	1.70	0.56
2:B:99:LEU:HD21	2:B:463:ASP:HB3	1.87	0.56
2:B:883:MET:HE3	2:B:910:LEU:HD22	1.87	0.56
1:E:858:LEU:N	1:E:863:ARG:HH12	2.04	0.56
2:J:509:PHE:O	2:J:512:THR:OG1	2.21	0.56
2:J:950:GLU:OE1	2:J:950:GLU:N	2.36	0.56
3:K:252:PRO:O	3:K:344:ARG:NH1	2.39	0.56
3:C:241:MET:HE1	3:C:246:ASN:HB2	1.87	0.55
1:E:1058:ARG:HE	1:E:1125:GLN:NE2	2.03	0.55
3:G:306:LYS:HZ1	4:H:147:THR:HB	1.71	0.55
1:I:1142:ILE:HG13	1:I:1142:ILE:O	2.06	0.55
2:J:568:ILE:HD11	2:J:668:LEU:HD22	1.89	0.55
3:K:95:GLU:HG3	3:K:100:PHE:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1131:ILE:O	1:I:1135:THR:HG23	2.06	0.55
2:N:941:PHE:CE2	2:N:1000:VAL:HG13	2.40	0.55
3:C:131:MET:HE3	3:C:220:MET:SD	2.47	0.55
1:E:128:ASP:OD1	1:E:129:GLN:NE2	2.40	0.55
1:E:1132:LEU:O	1:E:1135:THR:OG1	2.20	0.55
2:F:309:ASP:O	2:F:311:VAL:N	2.40	0.55
3:G:308:ILE:HD11	4:H:113:LEU:HD13	1.86	0.55
1:M:1142:ILE:O	1:M:1142:ILE:HG13	2.06	0.55
2:N:443:TRP:CZ3	2:N:447:LEU:HD21	2.41	0.55
2:N:957:ILE:HD11	2:N:962:HIS:HD2	1.70	0.55
1:E:917:ARG:HG3	1:E:919:ARG:NH2	2.21	0.55
3:K:21:GLU:O	3:K:21:GLU:HG2	2.06	0.55
3:K:128:ARG:HH21	3:K:132:ARG:HH22	1.53	0.55
2:N:313:PHE:HZ	2:N:379:ARG:HH12	1.54	0.55
2:N:853:LEU:HD21	2:N:876:ILE:HG23	1.87	0.55
2:B:307:LEU:HD22	2:B:313:PHE:HB2	1.88	0.55
2:J:331:LYS:HE2	2:J:362:GLU:HB2	1.87	0.55
3:K:16:PHE:HA	3:K:19:ASN:CB	2.37	0.55
3:K:16:PHE:HA	3:K:19:ASN:CG	2.32	0.55
3:K:107:MET:HE3	3:K:159:ASP:HB2	1.88	0.55
1:E:556:MET:HE3	1:E:557:THR:HG22	1.89	0.55
1:E:852:LYS:HZ1	1:E:918:LEU:H	1.53	0.55
2:F:954:ASN:ND2	2:F:1020:ASP:OD1	2.37	0.55
4:H:48:GLU:O	4:H:52:MET:HG3	2.06	0.55
1:I:584:ALA:HB2	3:K:57:GLY:HA3	1.88	0.55
2:N:172:ILE:HG21	2:N:212:VAL:HG11	1.88	0.55
1:A:1132:LEU:O	1:A:1135:THR:OG1	2.16	0.55
4:D:33:LEU:HD23	4:D:37:MET:HE2	1.89	0.55
2:J:53:TYR:OH	2:J:57:LYS:NZ	2.40	0.55
2:N:417:VAL:HG23	2:N:418:GLU:HG2	1.88	0.55
2:B:584:ASP:HB2	2:B:770:TYR:CE2	2.41	0.55
2:B:1006:VAL:HG12	2:B:1073:VAL:HG22	1.89	0.55
1:E:51:ILE:HD11	1:E:84:LEU:HD13	1.88	0.55
1:E:777:GLN:HA	1:E:825:LEU:HD11	1.89	0.55
2:J:177:LEU:HD13	2:J:241:LEU:HD11	1.89	0.55
1:M:165:ILE:HD13	1:M:168:LEU:HD21	1.88	0.55
2:N:268:ASP:OD2	2:N:555:ARG:NH2	2.35	0.55
2:N:579:ILE:HG13	2:N:580:PHE:CD1	2.42	0.55
3:O:96:THR:OG1	3:O:99:PHE:N	2.37	0.55
1:I:85:MET:HE1	1:I:148:MET:HG3	1.90	0.54
2:N:842:HIS:CE1	2:N:846:GLU:HG3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:10:ILE:O	4:P:14:LYS:HG2	2.05	0.54
4:P:110:MET:HB3	4:P:115:GLU:HB3	1.89	0.54
2:F:495:VAL:HG13	2:F:615:PRO:HG2	1.89	0.54
2:J:367:ILE:O	2:J:370:LEU:HG	2.07	0.54
2:N:115:GLU:O	2:N:119:ILE:HG12	2.07	0.54
2:B:253:ASN:HD21	2:B:259:GLY:HA3	1.73	0.54
1:E:90:HIS:HA	1:E:93:ILE:HG22	1.90	0.54
1:E:563:THR:HG22	1:E:565:PRO:HD3	1.90	0.54
1:E:902:ALA:HA	1:E:905:MET:HE1	1.90	0.54
4:L:5:LEU:HD22	4:L:10:ILE:HG12	1.89	0.54
3:O:53:VAL:HG22	3:O:64:VAL:HG13	1.90	0.54
1:A:890:ILE:HD13	1:A:893:LEU:HD21	1.88	0.54
1:E:539:ILE:O	1:E:543:LEU:HG	2.07	0.54
3:O:149:ARG:HE	3:O:171:PHE:HE2	1.54	0.54
1:E:917:ARG:HB2	1:E:919:ARG:HH12	1.72	0.54
2:F:322:ARG:HB3	2:F:323:LYS:HZ2	1.73	0.54
2:F:384:GLN:HA	2:F:387:GLU:HG2	1.90	0.54
3:G:258:SER:HB3	4:H:71:THR:HG23	1.89	0.54
3:K:228:PRO:HD2	3:K:368:ALA:HB2	1.90	0.54
3:C:23:LYS:HG3	3:C:24:GLU:OE1	2.07	0.54
3:C:120:VAL:HG13	3:C:352:PHE:HE2	1.71	0.54
3:C:210:GLU:HB3	3:C:276:ARG:HH21	1.72	0.54
1:I:563:THR:HG22	1:I:565:PRO:HD3	1.90	0.54
1:I:129:GLN:NE2	1:I:130:TRP:HB2	2.22	0.54
2:J:172:ILE:HD11	2:J:209:VAL:HG23	1.89	0.54
1:M:51:ILE:HD13	1:M:84:LEU:HD21	1.90	0.54
1:M:382:GLU:HA	1:M:385:GLN:HE21	1.72	0.54
1:E:1131:ILE:O	1:E:1135:THR:HG23	2.07	0.54
2:N:168:GLY:HA3	2:N:218:PHE:HE2	1.71	0.54
2:N:946:TRP:NE1	2:N:950:GLU:OE2	2.41	0.54
3:O:219:ILE:HA	3:O:222:THR:HG22	1.89	0.54
1:A:781:ASP:O	1:A:785:MET:HG3	2.08	0.54
2:F:1027:LEU:HD21	2:F:1076:LEU:HD12	1.88	0.54
2:J:584:ASP:HB2	2:J:770:TYR:HE2	1.72	0.54
2:J:954:ASN:ND2	2:J:1020:ASP:OD1	2.39	0.54
1:M:97:ASP:OD1	1:M:98:LYS:N	2.41	0.54
1:A:1126:LEU:HD13	1:A:1155:VAL:HG11	1.89	0.54
2:B:587:MET:SD	2:B:587:MET:N	2.78	0.54
2:F:802:THR:HA	2:F:805:VAL:HG22	1.89	0.54
2:J:329:GLY:HA2	2:J:369:PHE:HE1	1.73	0.54
1:I:944:GLU:OE2	1:I:948:ASN:ND2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:991:ASP:OD1	2:N:992:GLN:N	2.39	0.53
2:B:497:VAL:HG23	2:B:617:PHE:HD2	1.72	0.53
2:B:932:GLY:HA3	2:B:993:PRO:HB2	1.90	0.53
1:E:858:LEU:O	1:E:863:ARG:NH1	2.41	0.53
1:I:1145:ILE:HG21	1:I:1149:ILE:HD11	1.90	0.53
1:A:530:PHE:CD2	1:A:532:LEU:HB2	2.44	0.53
2:F:101:TYR:CE2	2:F:110:ARG:HB2	2.43	0.53
2:F:140:LYS:NZ	2:F:550:SER:OG	2.42	0.53
2:F:182:LEU:O	2:F:186:ILE:HG12	2.08	0.53
2:F:329:GLY:HA2	2:F:369:PHE:CZ	2.44	0.53
2:J:400:THR:OG1	2:J:401:GLU:OE1	2.26	0.53
2:J:580:PHE:O	2:J:622:ARG:NH2	2.42	0.53
3:K:222:THR:OG1	3:K:367:ARG:NH2	2.33	0.53
4:L:118:THR:HG23	4:L:121:GLU:H	1.74	0.53
1:A:418:LEU:HD12	1:A:419:ALA:H	1.72	0.53
2:B:809:GLN:N	2:B:872:LEU:O	2.37	0.53
1:E:1078:VAL:HG21	1:E:1135:THR:HG22	1.88	0.53
1:I:114:ALA:HA	1:I:134:GLN:HE22	1.74	0.53
1:I:833:LEU:C	1:I:834:ARG:HD3	2.34	0.53
2:J:49:LEU:HD23	2:J:101:TYR:CD1	2.43	0.53
2:J:727:ILE:HD12	2:J:750:ARG:HH22	1.74	0.53
1:A:588:LYS:HE2	3:C:56:GLY:HA2	1.91	0.53
1:A:917:ARG:HH21	1:A:1109:VAL:HA	1.74	0.53
2:B:335:ARG:HG3	2:B:359:ASP:HB3	1.89	0.53
3:G:193:PRO:HA	3:G:243:MET:HE1	1.91	0.53
4:H:141:GLU:HG2	4:H:145:MET:CE	2.39	0.53
1:I:62:ARG:O	1:I:62:ARG:NE	2.41	0.53
2:N:1074:MET:HA	2:N:1077:LEU:HG	1.91	0.53
3:C:23:LYS:HG3	3:C:24:GLU:H	1.74	0.53
3:C:241:MET:HE3	3:C:241:MET:O	2.09	0.53
1:I:919:ARG:HE	1:I:922:LEU:HB2	1.74	0.53
2:N:719:TRP:CE3	2:N:722:LYS:HG3	2.43	0.53
2:N:727:ILE:HG23	2:N:743:LEU:HG	1.91	0.53
2:N:958:VAL:HB	2:N:1024:LEU:HD12	1.90	0.53
1:A:583:LEU:HD21	1:A:587:ARG:HE	1.74	0.53
3:C:65:ARG:HH12	3:C:68:ARG:HD2	1.73	0.53
1:E:82:VAL:HG23	1:E:155:ILE:HD13	1.91	0.53
1:E:400:HIS:CE1	1:E:402:TRP:HB3	2.43	0.53
4:P:130:ASP:OD1	4:P:131:ILE:N	2.42	0.53
1:A:413:MET:HE1	1:A:418:LEU:HG	1.90	0.53
1:M:535:ASP:HB3	1:M:538:MET:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:787:ALA:O	2:N:790:GLN:NE2	2.42	0.53
2:B:217:ASP:OD1	2:B:218:PHE:N	2.42	0.53
2:J:374:ILE:HA	2:J:377:VAL:HG12	1.90	0.53
2:J:56:VAL:HG21	2:J:97:LEU:HD22	1.91	0.52
2:J:302:TYR:HA	2:J:305:PHE:CE2	2.44	0.52
2:J:972:MET:HE1	2:J:979:PHE:H	1.74	0.52
1:A:29:VAL:HB	1:A:119:LYS:HE3	1.90	0.52
1:A:1215:LEU:HD21	1:A:1219:ILE:HA	1.91	0.52
1:E:300:GLY:O	1:E:303:THR:OG1	2.20	0.52
1:I:545:THR:HG21	1:I:906:ARG:HH21	1.73	0.52
2:J:95:TRP:CE3	2:J:185:MET:HE1	2.45	0.52
2:N:757:THR:HG23	2:N:759:GLU:H	1.74	0.52
3:C:322:TYR:HB2	4:D:52:MET:HG3	1.91	0.52
3:G:114:ASP:OD1	3:G:115:TYR:N	2.42	0.52
3:K:267:ARG:NH1	3:K:277:TYR:OH	2.42	0.52
1:M:859:PRO:O	1:M:863:ARG:NH2	2.42	0.52
1:A:104:TYR:HE1	1:A:498:PRO:HB3	1.75	0.52
1:A:859:PRO:O	1:A:863:ARG:NH2	2.43	0.52
2:F:374:ILE:HG23	2:F:378:PHE:HE2	1.75	0.52
4:H:100:TYR:HB3	4:H:136:GLN:NE2	2.23	0.52
1:I:45:ARG:NH1	1:I:136:ASP:OD2	2.41	0.52
4:L:90:PHE:O	4:L:94:ASP:N	2.43	0.52
3:O:82:SER:HA	3:O:87:ILE:HD11	1.90	0.52
2:B:123:ARG:HH12	2:B:192:ILE:HG23	1.73	0.52
2:B:140:LYS:NZ	2:B:550:SER:OG	2.43	0.52
2:B:309:ASP:O	2:B:311:VAL:N	2.43	0.52
2:J:319:LYS:HB3	2:J:323:LYS:NZ	2.25	0.52
2:N:89:TYR:HD2	2:N:443:TRP:CZ3	2.27	0.52
1:A:11:LEU:HD13	1:A:61:TYR:CE1	2.39	0.52
4:D:87:ARG:NH1	4:D:88:GLU:OE1	2.42	0.52
4:D:118:THR:HG23	4:D:121:GLU:H	1.73	0.52
2:N:868:PHE:HE1	2:N:915:LEU:HD13	1.75	0.52
2:N:957:ILE:HD12	2:N:1021:LYS:HE3	1.91	0.52
2:B:66:PRO:O	2:B:120:LYS:NZ	2.41	0.52
2:B:963:LEU:O	2:B:963:LEU:HD12	2.09	0.52
1:I:282:GLU:HA	1:I:285:THR:HG22	1.91	0.52
2:J:904:PRO:HA	2:J:907:VAL:HG22	1.92	0.52
1:M:538:MET:SD	1:M:542:MET:HE2	2.50	0.52
3:O:241:MET:HE1	3:O:246:ASN:HB3	1.92	0.52
1:A:79:GLN:HA	1:A:82:VAL:HG12	1.92	0.52
1:A:563:THR:HG22	1:A:565:PRO:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:918:LEU:O	1:A:919:ARG:NH1	2.41	0.52
2:F:972:MET:SD	2:F:976:GLU:HB2	2.50	0.52
3:G:53:VAL:HG21	3:G:68:ARG:HH21	1.75	0.52
1:I:542:MET:HE3	1:I:542:MET:HA	1.92	0.52
1:I:823:TRP:O	1:I:948:ASN:HA	2.10	0.52
2:J:757:THR:HG23	2:J:759:GLU:H	1.75	0.52
3:C:215:SER:O	3:C:219:ILE:HG12	2.10	0.52
2:F:1032:PHE:HA	2:F:1054:PHE:CZ	2.45	0.52
2:J:382:PRO:O	2:J:385:VAL:HB	2.10	0.52
2:J:922:ARG:HG2	2:J:927:ARG:NH1	2.25	0.52
4:L:5:LEU:HD23	4:L:6:THR:H	1.73	0.52
2:B:89:TYR:HE1	2:B:177:LEU:HD21	1.74	0.52
3:K:20:TYR:CE1	3:K:91:LYS:NZ	2.78	0.52
1:M:245:LEU:HD23	1:M:245:LEU:O	2.09	0.52
1:M:824:GLY:HA2	1:M:947:MET:HE1	1.91	0.52
1:I:859:PRO:O	1:I:863:ARG:NH2	2.43	0.51
2:N:101:TYR:CE1	2:N:110:ARG:HB2	2.45	0.51
3:O:213:MET:HE2	3:O:268:PHE:HA	1.92	0.51
1:E:899:VAL:HG12	1:E:903:MET:HE1	1.92	0.51
4:H:83:GLU:HA	4:H:86:ILE:HG12	1.91	0.51
1:I:310:ARG:HD2	1:I:311:LEU:O	2.09	0.51
3:C:258:SER:HB3	4:D:71:THR:HG23	1.91	0.51
1:E:1215:LEU:HD21	1:E:1219:ILE:HA	1.91	0.51
1:I:337:LEU:HA	1:I:340:VAL:HG12	1.91	0.51
1:I:1085:LEU:HD11	1:I:1151:VAL:HG13	1.92	0.51
1:A:572:ASP:OD1	1:A:575:GLY:N	2.43	0.51
2:B:443:TRP:CD1	2:B:447:LEU:HD23	2.45	0.51
3:C:193:PRO:HA	3:C:243:MET:HE1	1.92	0.51
4:D:87:ARG:HD2	4:D:88:GLU:N	2.25	0.51
1:I:1121:PRO:HA	1:I:1124:ARG:NE	2.25	0.51
2:J:320:VAL:O	2:J:324:LEU:HB2	2.11	0.51
2:F:1050:ASP:OD1	2:F:1051:MET:N	2.44	0.51
1:I:336:ILE:HG13	1:I:348:VAL:HG13	1.93	0.51
2:J:519:THR:HG22	2:J:521:GLN:H	1.75	0.51
3:K:16:PHE:C	3:K:19:ASN:HB2	2.35	0.51
3:K:20:TYR:O	3:K:21:GLU:O	2.28	0.51
1:M:318:LEU:HD23	1:M:1098:ARG:HG3	1.92	0.51
1:A:1128:VAL:O	1:A:1132:LEU:HD23	2.10	0.51
2:F:871:MET:HE1	2:F:936:ARG:HG2	1.93	0.51
2:J:838:LYS:O	2:J:841:THR:OG1	2.23	0.51
2:B:809:GLN:HB3	2:B:873:LYS:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:116:LEU:HB3	3:C:367:ARG:HH22	1.75	0.51
1:E:140:VAL:HG22	1:E:144:PHE:CE2	2.46	0.51
2:F:330:PHE:N	2:F:364:GLU:OE2	2.44	0.51
1:I:827:ARG:HH21	1:I:947:MET:HE3	1.76	0.51
2:N:880:ILE:HA	2:N:883:MET:HE3	1.93	0.51
2:N:1037:LYS:O	2:N:1041:ARG:HG2	2.10	0.51
1:A:92:MET:HE1	1:A:141:TYR:CE2	2.44	0.51
3:K:349:ALA:O	3:K:353:ARG:HG2	2.11	0.51
1:M:341:PHE:HZ	1:M:429:ARG:HG2	1.76	0.51
3:O:192:ALA:HB3	3:O:211:VAL:HG12	1.93	0.51
2:F:928:ARG:NH2	2:F:1059:PRO:HG3	2.26	0.51
1:M:149:THR:OG1	1:M:155:ILE:HD12	2.11	0.51
3:O:193:PRO:HA	3:O:243:MET:HE1	1.93	0.51
3:G:126:GLU:O	3:G:130:ILE:HG12	2.10	0.51
1:A:1122:GLU:O	1:A:1125:GLN:HG3	2.11	0.50
2:F:1035:PHE:HB3	2:F:1054:PHE:CE2	2.46	0.50
3:G:318:ILE:HD11	4:H:56:VAL:HG21	1.93	0.50
1:I:70:ASP:HA	1:I:73:LYS:HD2	1.91	0.50
2:J:312:LEU:HD12	2:J:315:GLN:NE2	2.25	0.50
2:J:469:ARG:HE	2:J:469:ARG:HA	1.76	0.50
2:J:497:VAL:HG12	2:J:617:PHE:HB3	1.93	0.50
3:C:53:VAL:HG11	3:C:68:ARG:HH21	1.74	0.50
1:I:293:CYS:HG	1:I:332:TRP:CD1	2.29	0.50
3:O:210:GLU:HB3	3:O:276:ARG:HE	1.76	0.50
1:A:538:MET:O	1:A:541:GLU:HG2	2.11	0.50
4:D:20:PHE:HD2	4:D:28:ILE:HD12	1.76	0.50
2:J:66:PRO:O	2:J:120:LYS:NZ	2.42	0.50
3:K:131:MET:CG	3:K:220:MET:HE1	2.40	0.50
4:L:65:ASP:CG	4:L:66:PHE:H	2.19	0.50
1:M:455:LEU:HB3	1:M:460:ILE:HB	1.94	0.50
3:G:133:ALA:HB3	3:G:164:ILE:HD11	1.92	0.50
1:I:75:TYR:O	1:I:79:GLN:HG2	2.12	0.50
1:I:257:ALA:HB3	1:I:331:PHE:CE2	2.47	0.50
2:J:57:LYS:O	2:J:62:LEU:HG	2.11	0.50
2:J:871:MET:HE2	2:J:874:ILE:HD13	1.94	0.50
2:B:312:LEU:HA	2:B:315:GLN:HG3	1.92	0.50
2:B:569:LEU:HD23	2:B:569:LEU:O	2.12	0.50
2:B:903:SER:N	2:B:906:GLU:OE2	2.37	0.50
2:F:324:LEU:HD11	2:F:333:PHE:HA	1.93	0.50
2:F:757:THR:HG23	2:F:759:GLU:H	1.75	0.50
3:G:306:LYS:HZ1	4:H:147:THR:CB	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1215:LEU:HD12	1:I:1216:PRO:HD2	1.93	0.50
2:N:714:VAL:HG13	2:N:719:TRP:CD1	2.46	0.50
3:O:270:VAL:HG11	3:O:275:ASN:HB3	1.93	0.50
1:A:543:LEU:O	1:A:547:LEU:HD23	2.12	0.50
2:B:582:LEU:HD21	2:B:622:ARG:HH12	1.77	0.50
1:E:52:LEU:HD11	1:E:144:PHE:CE1	2.46	0.50
1:E:917:ARG:O	1:E:919:ARG:NH2	2.44	0.50
3:G:232:HIS:HD2	3:G:237:LEU:HB2	1.77	0.50
2:J:95:TRP:CD2	2:J:185:MET:HE1	2.46	0.50
2:J:373:MET:CE	2:J:385:VAL:HG13	2.40	0.50
3:K:20:TYR:HA	3:K:38:ILE:O	2.11	0.50
1:A:1132:LEU:O	1:A:1136:MET:HE3	2.11	0.50
2:B:130:MET:SD	1:E:29:VAL:HG22	2.52	0.50
3:G:291:TYR:HB3	4:H:14:LYS:HE2	1.94	0.50
2:N:904:PRO:HA	2:N:907:VAL:HG12	1.94	0.50
2:B:298:PRO:O	2:B:303:PRO:HG2	2.10	0.50
2:B:443:TRP:HD1	2:B:447:LEU:HD23	1.77	0.50
2:B:584:ASP:OD2	2:B:791:LYS:HD3	2.12	0.50
1:M:165:ILE:HA	1:M:168:LEU:HG	1.94	0.50
3:O:318:ILE:HD11	4:P:56:VAL:HG21	1.94	0.50
1:A:1132:LEU:C	1:A:1136:MET:HE3	2.37	0.50
2:F:797:ALA:HA	2:F:800:ILE:HG12	1.92	0.50
4:H:10:ILE:HG22	4:H:14:LYS:HD2	1.93	0.50
1:M:282:GLU:HG2	1:M:286:LYS:NZ	2.27	0.50
1:M:585:ALA:O	1:M:589:MET:HG2	2.11	0.50
2:N:853:LEU:HD11	2:N:876:ILE:HG23	1.92	0.50
2:B:214:ARG:HD2	2:B:801:THR:HG21	1.94	0.49
3:C:53:VAL:HG22	3:C:64:VAL:HG13	1.93	0.49
1:E:1054:TRP:O	1:E:1058:ARG:HG2	2.12	0.49
2:F:304:ALA:O	2:F:469:ARG:NH2	2.39	0.49
2:F:626:ILE:HG13	2:F:627:ARG:N	2.27	0.49
1:I:400:HIS:CE1	1:I:402:TRP:HB3	2.46	0.49
1:E:1062:GLY:HA3	1:E:1121:PRO:HB3	1.92	0.49
1:I:585:ALA:O	1:I:589:MET:HG2	2.11	0.49
2:J:98:ALA:O	2:J:102:ARG:HG3	2.12	0.49
2:J:919:GLN:O	2:J:927:ARG:NH1	2.44	0.49
2:N:67:THR:HG23	2:N:68:THR:HG23	1.94	0.49
2:N:310:GLU:HG2	2:N:311:VAL:N	2.26	0.49
2:B:288:ARG:HD3	2:B:977:MET:HE2	1.94	0.49
2:B:1027:LEU:HD22	2:B:1072:ALA:HB1	1.94	0.49
2:B:1052:THR:HA	2:B:1055:TYR:HD2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:332:TRP:HA	1:I:335:PHE:HD2	1.78	0.49
2:J:370:LEU:CD1	2:J:447:LEU:HB3	2.42	0.49
1:M:68:ASP:OD1	1:M:69:GLU:N	2.45	0.49
4:D:83:GLU:HA	4:D:86:ILE:HG12	1.93	0.49
1:E:92:MET:HE3	1:E:92:MET:HA	1.92	0.49
3:G:192:ALA:HB3	3:G:211:VAL:HG12	1.94	0.49
1:I:1145:ILE:HD12	1:I:1214:PHE:HE1	1.77	0.49
3:K:120:VAL:HG13	3:K:352:PHE:HE2	1.76	0.49
1:M:337:LEU:HA	1:M:340:VAL:HG12	1.95	0.49
2:N:441:PHE:HE2	2:N:443:TRP:HD1	1.60	0.49
4:P:83:GLU:O	4:P:87:ARG:HG2	2.12	0.49
2:B:173:ASN:OD1	2:B:174:ALA:N	2.45	0.49
2:B:339:ARG:N	2:B:343:GLU:OE2	2.46	0.49
3:G:342:PRO:O	3:G:345:ARG:HG2	2.12	0.49
3:G:343:LEU:HD23	3:G:346:LEU:HD21	1.94	0.49
1:M:514:ARG:HG3	1:M:619:MET:HE1	1.94	0.49
2:N:541:LEU:HB2	2:N:670:PHE:CE1	2.47	0.49
1:A:1171:ALA:HA	3:C:378:VAL:HG13	1.94	0.49
2:F:274:ARG:HH12	2:F:798:PRO:HB3	1.76	0.49
2:F:509:PHE:O	2:F:512:THR:OG1	2.31	0.49
2:J:319:LYS:HG2	2:J:322:ARG:HH21	1.76	0.49
2:J:587:MET:HE1	2:J:855:ILE:HD11	1.95	0.49
1:M:114:ALA:HA	1:M:134:GLN:HE22	1.75	0.49
2:N:374:ILE:HA	2:N:377:VAL:HG12	1.95	0.49
1:A:1215:LEU:HD12	1:A:1216:PRO:HD2	1.95	0.49
2:B:237:SER:HA	2:B:299:CYS:SG	2.53	0.49
2:B:958:VAL:HA	2:B:1024:LEU:HD21	1.95	0.49
1:E:1215:LEU:HD12	1:E:1216:PRO:HD2	1.95	0.49
2:F:335:ARG:N	2:F:362:GLU:OE2	2.45	0.49
2:F:972:MET:HE2	2:F:972:MET:HA	1.95	0.49
2:J:902:LEU:HD12	2:J:906:GLU:HB3	1.94	0.49
1:M:931:LEU:HD12	1:M:946:LEU:HD12	1.95	0.49
3:O:119:LYS:O	3:O:121:THR:N	2.45	0.49
1:A:1068:PRO:HG2	1:A:1071:PHE:HB2	1.95	0.49
3:C:305:PHE:CE2	4:D:145:MET:HE2	2.48	0.49
2:F:591:VAL:H	2:F:630:ARG:HH12	1.61	0.49
2:F:949:LEU:O	2:F:965:GLN:NE2	2.46	0.49
3:G:220:MET:CE	3:G:265:VAL:HG22	2.43	0.49
1:I:72:ALA:O	1:I:76:GLU:HG3	2.13	0.49
1:M:892:ILE:O	1:M:895:GLN:HG3	2.13	0.49
2:N:370:LEU:HA	2:N:373:MET:SD	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:540:GLN:HE22	2:N:670:PHE:HD1	1.61	0.49
3:O:221:TYR:HE2	3:O:229:PRO:HA	1.78	0.49
3:O:294:GLU:HB3	3:O:297:ARG:CZ	2.43	0.49
2:B:928:ARG:HD2	2:B:1055:TYR:HD1	1.78	0.49
4:D:90:PHE:O	4:D:94:ASP:N	2.45	0.49
1:E:554:TRP:NE1	1:E:558:GLY:O	2.40	0.49
2:F:173:ASN:OD1	2:F:174:ALA:N	2.46	0.49
2:F:727:ILE:HD12	2:F:750:ARG:HH22	1.77	0.49
4:H:90:PHE:O	4:H:94:ASP:N	2.45	0.49
2:J:375:ASP:O	2:J:379:ARG:HG2	2.13	0.49
3:K:13:ALA:HB2	3:K:96:THR:HG22	1.95	0.49
3:K:219:ILE:HA	3:K:222:THR:HG22	1.95	0.49
1:M:1129:GLU:OE2	3:O:355:TYR:OH	2.30	0.49
2:B:286:GLU:HB2	2:B:296:LEU:HD21	1.94	0.49
2:B:810:VAL:HG22	2:B:874:ILE:HB	1.94	0.49
1:E:480:SER:HB2	1:E:502:MET:CE	2.43	0.49
1:M:69:GLU:O	1:M:73:LYS:HG3	2.12	0.49
1:M:1052:GLY:O	1:M:1056:ARG:NH1	2.46	0.49
2:B:370:LEU:O	2:B:374:ILE:HG12	2.13	0.48
2:B:880:ILE:HA	2:B:883:MET:HG2	1.94	0.48
1:E:1130:ALA:O	1:E:1133:VAL:HG12	2.12	0.48
2:F:838:LYS:O	2:F:841:THR:OG1	2.24	0.48
3:G:232:HIS:CD2	3:G:237:LEU:HB2	2.48	0.48
1:I:584:ALA:O	1:I:588:LYS:HD3	2.12	0.48
1:M:129:GLN:NE2	1:M:130:TRP:HB2	2.28	0.48
3:O:220:MET:HG3	3:O:265:VAL:HG12	1.95	0.48
3:C:291:TYR:HB3	4:D:14:LYS:HE2	1.94	0.48
1:E:1178:LYS:HD2	1:E:1183:GLY:HA2	1.94	0.48
2:J:83:LYS:HG3	2:J:85:GLN:H	1.77	0.48
3:K:93:THR:HB	3:K:102:LEU:HD13	1.95	0.48
1:M:55:TRP:NE1	1:M:148:MET:HE1	2.28	0.48
1:M:1100:MET:HG3	1:M:1107:PHE:HB2	1.94	0.48
3:O:299:PHE:HE1	3:O:304:LYS:HG2	1.78	0.48
1:A:85:MET:HE2	1:A:85:MET:HA	1.94	0.48
1:A:435:LYS:HD2	1:A:436:PRO:HD2	1.96	0.48
2:B:467:VAL:HG12	2:B:467:VAL:O	2.13	0.48
3:C:322:TYR:CE1	4:D:51:ASP:HB3	2.49	0.48
1:E:291:TYR:HB2	1:E:327:GLU:OE2	2.14	0.48
3:G:385:GLU:OE2	3:G:385:GLU:N	2.46	0.48
2:J:883:MET:HE1	2:J:911:LEU:HB3	1.95	0.48
2:J:890:ARG:O	2:J:890:ARG:NE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ASP:OD1	1:A:68:ASP:N	2.46	0.48
1:E:894:THR:HG23	1:E:920:ILE:HG21	1.95	0.48
1:I:291:TYR:HB2	1:I:327:GLU:OE2	2.13	0.48
2:J:1002:LEU:HD12	2:J:1069:LEU:HD22	1.96	0.48
1:M:837:VAL:O	1:M:873:TYR:OH	2.24	0.48
2:N:51:HIS:O	2:N:55:ILE:HG12	2.12	0.48
2:N:826:LEU:HD12	2:N:827:SER:N	2.27	0.48
3:O:258:SER:HB3	4:P:71:THR:HG23	1.95	0.48
1:A:585:ALA:HA	1:A:588:LYS:HD2	1.94	0.48
2:B:947:GLN:NE2	2:B:947:GLN:C	2.72	0.48
1:E:480:SER:HB2	1:E:502:MET:HE1	1.96	0.48
1:E:844:CYS:SG	1:E:876:LEU:HD21	2.53	0.48
2:J:111:THR:O	2:J:115:GLU:HG3	2.13	0.48
2:J:857:ILE:HG23	2:J:868:PHE:CZ	2.48	0.48
4:L:57:ASP:OD2	4:L:61:ASN:ND2	2.47	0.48
1:M:320:LEU:O	1:M:324:ILE:HD11	2.13	0.48
1:M:1215:LEU:HD12	1:M:1216:PRO:HD2	1.96	0.48
2:N:304:ALA:O	2:N:469:ARG:NH2	2.43	0.48
2:N:868:PHE:CE1	2:N:915:LEU:HD13	2.48	0.48
3:O:39:HIS:O	3:O:43:SER:N	2.44	0.48
1:A:1062:GLY:HA3	1:A:1121:PRO:HB3	1.94	0.48
2:B:745:GLY:O	2:B:749:LYS:HG2	2.13	0.48
1:E:21:THR:HG21	1:E:404:GLN:HE21	1.78	0.48
1:E:861:GLU:HG2	1:E:862:PRO:HA	1.96	0.48
1:E:1106:LYS:HE2	1:E:1110:HIS:HE1	1.78	0.48
2:F:587:MET:SD	2:F:587:MET:N	2.83	0.48
2:F:847:ALA:O	2:F:851:GLN:HG2	2.13	0.48
2:F:1068:TYR:HD1	2:F:1071:LYS:HD2	1.79	0.48
4:H:122:VAL:HA	4:H:125:MET:HG2	1.95	0.48
2:B:915:LEU:HD23	2:B:934:LEU:HD21	1.96	0.48
2:N:302:TYR:HA	2:N:305:PHE:CE2	2.48	0.48
2:N:493:LEU:HD11	2:N:609:TRP:HD1	1.78	0.48
4:P:90:PHE:O	4:P:94:ASP:N	2.47	0.48
1:A:99:VAL:HG23	1:A:171:TYR:CD1	2.48	0.48
1:A:291:TYR:HB2	1:A:327:GLU:OE2	2.14	0.48
1:E:1121:PRO:O	1:E:1124:ARG:HG2	2.14	0.48
2:F:623:GLU:O	2:F:626:ILE:HG12	2.14	0.48
2:F:842:HIS:CE1	2:F:846:GLU:HG3	2.48	0.48
2:J:112:HIS:O	2:J:116:HIS:ND1	2.46	0.48
2:J:928:ARG:HG2	2:J:994:GLN:HA	1.94	0.48
3:K:336:ASP:OD1	3:K:336:ASP:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:583:LEU:HD12	1:M:586:LEU:HD11	1.95	0.48
1:M:1076:TRP:CD1	1:M:1100:MET:HE1	2.49	0.48
2:N:270:ASP:OD1	2:N:270:ASP:N	2.47	0.48
3:C:336:ASP:OD1	3:C:336:ASP:N	2.47	0.48
4:D:34:GLY:HA2	4:D:37:MET:CE	2.44	0.48
2:J:257:ASN:OD1	2:J:258:GLN:HG3	2.14	0.48
2:J:884:GLU:HA	2:J:887:LEU:HG	1.95	0.48
1:M:1171:ALA:HA	3:O:378:VAL:HG13	1.96	0.48
3:O:336:ASP:OD1	3:O:336:ASP:N	2.47	0.48
1:E:887:ASP:C	1:E:888:MET:HG3	2.39	0.48
3:G:220:MET:HE1	3:G:265:VAL:HG22	1.94	0.48
3:K:16:PHE:CA	3:K:19:ASN:HB2	2.43	0.48
3:K:270:VAL:HG11	3:K:275:ASN:HB2	1.96	0.48
2:N:122:MET:HG2	2:N:178:TYR:HE1	1.79	0.48
2:N:204:ASN:HD21	2:N:549:LEU:HB3	1.77	0.48
2:N:441:PHE:CE2	2:N:443:TRP:HD1	2.32	0.48
2:N:1001:GLU:O	2:N:1004:MET:HG3	2.13	0.48
3:O:213:MET:SD	3:O:276:ARG:HB3	2.54	0.48
1:A:786:LEU:O	1:A:791:GLY:N	2.43	0.47
3:C:39:HIS:CE1	3:C:41:PRO:HD2	2.48	0.47
1:E:134:GLN:NE2	1:E:185:GLU:OE2	2.46	0.47
1:E:1100:MET:HE3	1:E:1101:THR:O	2.14	0.47
1:I:460:ILE:HG13	1:I:586:LEU:HD13	1.96	0.47
2:J:504:GLN:O	2:J:507:GLN:HG3	2.14	0.47
2:J:714:VAL:HG13	2:J:719:TRP:CD2	2.49	0.47
3:K:93:THR:HA	3:K:101:PHE:O	2.13	0.47
3:K:162:MET:HE2	3:K:162:MET:HA	1.96	0.47
4:P:81:ASP:O	4:P:84:GLU:HG3	2.14	0.47
3:G:294:GLU:HG2	3:G:296:VAL:HG22	1.96	0.47
2:J:924:TRP:CE2	2:J:1058:PRO:HG3	2.48	0.47
1:M:293:CYS:O	1:M:328:TRP:N	2.47	0.47
1:M:570:MET:CE	1:M:582:ILE:HG13	2.43	0.47
1:M:1123:TYR:OH	1:M:1182:SER:HA	2.14	0.47
2:N:278:THR:HG23	2:N:805:VAL:HG21	1.95	0.47
1:E:148:MET:SD	1:E:153:LEU:HD12	2.54	0.47
1:E:543:LEU:O	1:E:547:LEU:HD23	2.14	0.47
2:F:968:THR:O	2:F:972:MET:HB3	2.15	0.47
3:G:219:ILE:HA	3:G:222:THR:HG22	1.97	0.47
1:M:785:MET:O	1:M:789:MET:HG2	2.15	0.47
3:O:26:LEU:HD11	3:O:36:ARG:HB2	1.96	0.47
1:A:336:ILE:HG13	1:A:348:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:THR:HG21	1:E:404:GLN:HG2	1.96	0.47
1:E:140:VAL:HG22	1:E:144:PHE:HE2	1.79	0.47
1:E:530:PHE:HD2	1:E:532:LEU:H	1.61	0.47
1:E:546:ASP:O	1:E:550:LEU:HG	2.14	0.47
2:F:992:GLN:HG3	2:F:994:GLN:HG2	1.95	0.47
1:M:51:ILE:HD12	1:M:54:VAL:HB	1.96	0.47
1:M:145:LEU:HD12	1:M:155:ILE:HG21	1.96	0.47
1:A:300:GLY:O	1:A:303:THR:OG1	2.20	0.47
3:C:210:GLU:HB3	3:C:276:ARG:HE	1.80	0.47
1:E:68:ASP:OD1	1:E:68:ASP:N	2.48	0.47
1:E:837:VAL:O	1:E:873:TYR:OH	2.26	0.47
1:I:1215:LEU:HD21	1:I:1219:ILE:HA	1.97	0.47
2:J:803:PHE:HZ	2:J:857:ILE:HG22	1.80	0.47
1:M:282:GLU:HG2	1:M:286:LYS:HZ2	1.78	0.47
1:A:79:GLN:HB3	2:F:194:TYR:HB3	1.96	0.47
2:B:631:PHE:CE2	2:B:635:LEU:HD11	2.49	0.47
2:B:850:GLN:HG2	2:B:876:ILE:HG21	1.96	0.47
2:B:890:ARG:O	2:B:890:ARG:NE	2.45	0.47
2:B:1003:LEU:HA	2:B:1006:VAL:HG22	1.96	0.47
1:E:413:MET:HA	1:E:413:MET:HE2	1.96	0.47
2:F:86:ASP:OD1	2:F:87:SER:N	2.47	0.47
2:F:1018:PHE:HE1	2:F:1077:LEU:HD21	1.79	0.47
2:J:510:LEU:HD22	2:J:515:ILE:HB	1.96	0.47
1:M:291:TYR:HB2	1:M:327:GLU:OE2	2.14	0.47
1:A:1178:LYS:HD2	1:A:1183:GLY:HA2	1.96	0.47
2:B:204:ASN:HD21	2:B:549:LEU:HB3	1.79	0.47
2:B:351:LYS:HG3	2:B:352:PRO:HD2	1.97	0.47
1:E:295:ARG:HG3	1:E:328:TRP:CD1	2.49	0.47
1:E:799:TYR:CE2	1:E:801:GLU:HB2	2.50	0.47
2:F:569:LEU:O	2:F:569:LEU:HD23	2.14	0.47
2:F:714:VAL:HG13	2:F:719:TRP:CD2	2.50	0.47
1:I:148:MET:HB3	1:I:155:ILE:HD11	1.97	0.47
2:J:961:LYS:HG3	2:J:989:ASN:ND2	2.29	0.47
3:K:217:GLY:O	3:K:220:MET:HB2	2.14	0.47
1:M:927:MET:HE2	1:M:927:MET:N	2.29	0.47
2:N:626:ILE:HG13	2:N:627:ARG:N	2.30	0.47
2:N:879:ILE:HG22	2:N:883:MET:CE	2.44	0.47
3:O:142:HIS:CE1	3:O:209:LYS:HB2	2.50	0.47
1:A:19:GLN:OE1	1:A:23:LEU:HD22	2.15	0.47
4:D:51:ASP:O	4:D:55:GLU:HG2	2.15	0.47
2:F:226:LYS:NZ	2:F:976:GLU:OE2	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:119:LYS:O	3:G:121:THR:N	2.47	0.47
1:I:28:PRO:O	1:I:29:VAL:HB	2.15	0.47
2:J:319:LYS:O	2:J:323:LYS:HG2	2.15	0.47
2:J:797:ALA:HA	2:J:800:ILE:HG22	1.97	0.47
1:M:11:LEU:HB3	1:M:61:TYR:CE1	2.46	0.47
2:N:803:PHE:HA	2:N:808:LYS:NZ	2.28	0.47
1:A:204:MET:HE2	1:A:204:MET:HA	1.97	0.47
1:A:884:SER:HB2	1:A:890:ILE:HB	1.97	0.47
1:E:463:GLU:OE2	1:E:467:GLU:HB3	2.14	0.47
3:G:251:SER:HB3	3:G:252:PRO:HD3	1.97	0.47
1:I:1133:VAL:HA	1:I:1136:MET:HG2	1.96	0.47
2:J:140:LYS:NZ	2:J:550:SER:OG	2.47	0.47
1:A:90:HIS:HA	1:A:93:ILE:HG22	1.95	0.47
1:A:418:LEU:HD11	1:A:422:GLU:HB2	1.97	0.47
2:B:593:LEU:HD21	2:B:908:LYS:HZ3	1.80	0.47
2:B:818:GLU:CD	2:B:842:HIS:HE2	2.22	0.47
1:E:293:CYS:HG	1:E:332:TRP:CD1	2.32	0.47
1:E:337:LEU:HA	1:E:340:VAL:HG12	1.96	0.47
1:E:1140:ILE:HG22	1:E:1221:ALA:HB1	1.97	0.47
2:F:544:ASN:H	2:F:549:LEU:HB2	1.80	0.47
4:H:142:PHE:O	4:H:146:MET:HG2	2.15	0.47
1:I:330:LEU:HD21	1:I:400:HIS:CE1	2.50	0.47
2:J:52:TYR:HA	2:J:55:ILE:HG12	1.97	0.47
2:J:273:ASN:O	2:J:276:ARG:HG2	2.15	0.47
2:J:282:LEU:HD11	2:J:288:ARG:HH12	1.80	0.47
2:J:947:GLN:HA	2:J:950:GLU:OE1	2.15	0.47
3:K:225:ALA:HB2	3:K:254:TRP:HZ2	1.80	0.47
2:N:182:LEU:O	2:N:186:ILE:HG12	2.15	0.47
3:O:225:ALA:HB2	3:O:254:TRP:HZ2	1.80	0.47
3:O:305:PHE:CE2	4:P:145:MET:HE2	2.50	0.47
2:B:744:LEU:HD21	2:B:765:HIS:ND1	2.30	0.46
3:C:232:HIS:CE1	3:C:237:LEU:HD12	2.50	0.46
1:E:85:MET:SD	1:E:141:TYR:HE1	2.38	0.46
3:G:263:ASP:O	3:G:267:ARG:HG2	2.14	0.46
1:M:398:LEU:N	1:M:399:PRO:HD3	2.30	0.46
1:M:509:LYS:HG3	1:M:612:CYS:HB3	1.96	0.46
2:N:89:TYR:CE1	2:N:177:LEU:HD21	2.49	0.46
3:O:251:SER:HB3	3:O:252:PRO:HD3	1.97	0.46
2:B:103:ARG:HH22	2:B:459:ILE:HA	1.79	0.46
2:F:312:LEU:O	2:F:315:GLN:HG3	2.16	0.46
2:F:885:TYR:CE2	2:F:889:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:267:ARG:HD2	3:G:277:TYR:HE2	1.81	0.46
1:I:1178:LYS:HD2	1:I:1183:GLY:HA2	1.95	0.46
2:J:626:ILE:HG13	2:J:627:ARG:N	2.30	0.46
2:J:1032:PHE:CE1	2:J:1051:MET:HA	2.50	0.46
3:K:109:ARG:HG2	3:K:110:GLY:N	2.28	0.46
2:N:398:HIS:HB3	2:N:402:GLY:HA2	1.97	0.46
2:N:885:TYR:O	2:N:888:GLN:HG3	2.15	0.46
2:N:999:VAL:HA	2:N:1002:LEU:HG	1.96	0.46
3:O:188:PRO:HA	3:O:191:LEU:HG	1.95	0.46
2:B:204:ASN:ND2	2:B:549:LEU:HD22	2.31	0.46
1:E:584:ALA:HB2	3:G:57:GLY:HA3	1.98	0.46
1:E:1057:ARG:HB3	1:E:1058:ARG:NH1	2.30	0.46
3:G:16:PHE:HB2	3:G:94:TYR:CG	2.50	0.46
3:G:364:GLN:OE1	3:G:364:GLN:N	2.42	0.46
3:G:377:ALA:H	3:G:380:LEU:HD23	1.80	0.46
2:J:96:ALA:O	2:J:99:LEU:HG	2.15	0.46
2:J:122:MET:HE1	2:J:185:MET:HG3	1.96	0.46
2:J:1065:THR:O	2:J:1069:LEU:HG	2.16	0.46
3:K:128:ARG:HG2	3:K:129:LYS:NZ	2.30	0.46
1:M:141:TYR:O	1:M:145:LEU:HD23	2.15	0.46
2:N:803:PHE:HD2	2:N:810:VAL:HG11	1.81	0.46
2:B:757:THR:HG23	2:B:759:GLU:HG3	1.98	0.46
3:C:234:LYS:HB3	3:C:236:MET:SD	2.55	0.46
4:D:20:PHE:CE1	4:D:36:VAL:HG11	2.50	0.46
2:F:890:ARG:O	2:F:890:ARG:NE	2.42	0.46
3:G:299:PHE:HE1	3:G:304:LYS:HG2	1.80	0.46
3:G:336:ASP:N	3:G:336:ASP:OD1	2.48	0.46
1:I:99:VAL:HG23	1:I:112:LEU:HD21	1.97	0.46
3:K:352:PHE:HB2	3:K:353:ARG:NH1	2.31	0.46
2:N:119:ILE:HD11	2:N:190:LEU:HD23	1.98	0.46
3:O:107:MET:HE3	3:O:159:ASP:HB2	1.96	0.46
3:O:137:VAL:HG11	3:O:166:LEU:HD22	1.96	0.46
1:A:1123:TYR:OH	1:A:1182:SER:HA	2.15	0.46
2:B:228:ASN:HB3	2:B:350:TYR:HD2	1.81	0.46
2:B:578:ILE:H	2:B:578:ILE:HD12	1.79	0.46
4:D:10:ILE:HG22	4:D:14:LYS:HD2	1.97	0.46
2:F:611:MET:HA	2:F:611:MET:HE2	1.96	0.46
2:B:389:GLN:HA	2:B:392:LEU:HG	1.98	0.46
2:B:843:ASP:HB3	2:B:846:GLU:CD	2.40	0.46
4:D:32:GLU:OE1	4:D:32:GLU:N	2.48	0.46
1:E:148:MET:O	1:E:151:SER:OG	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:336:ILE:HG13	1:E:348:VAL:HG13	1.97	0.46
4:H:57:ASP:OD2	4:H:61:ASN:ND2	2.49	0.46
3:K:109:ARG:HH12	3:K:162:MET:HE1	1.80	0.46
1:M:1178:LYS:HD2	1:M:1183:GLY:HA2	1.97	0.46
2:B:447:LEU:HA	2:B:450:ILE:HG22	1.97	0.46
2:B:626:ILE:HG13	2:B:627:ARG:N	2.31	0.46
2:B:764:ASP:O	2:B:767:GLU:HG3	2.15	0.46
3:C:359:VAL:HG11	3:C:367:ARG:HD3	1.98	0.46
2:F:668:LEU:HD23	2:F:670:PHE:HE1	1.81	0.46
1:I:554:TRP:NE1	1:I:556:MET:SD	2.89	0.46
1:I:823:TRP:C	1:I:827:ARG:HH12	2.23	0.46
1:I:1123:TYR:O	1:I:1127:LEU:HG	2.15	0.46
2:J:885:TYR:CE2	2:J:889:ILE:HD11	2.50	0.46
4:L:17:PHE:CZ	4:L:69:PHE:HD2	2.33	0.46
1:M:52:LEU:HB3	1:M:409:LEU:HD22	1.97	0.46
1:E:108:THR:O	1:E:111:SER:OG	2.24	0.46
2:F:115:GLU:O	2:F:119:ILE:HG12	2.15	0.46
1:I:11:LEU:HB2	1:I:61:TYR:CE1	2.47	0.46
1:I:856:VAL:HG12	1:I:920:ILE:HD13	1.97	0.46
3:C:63:GLU:O	3:C:66:GLU:HG2	2.16	0.46
2:F:364:GLU:O	2:F:409:TYR:HA	2.16	0.46
2:F:856:HIS:O	2:F:860:ILE:HG12	2.16	0.46
2:F:965:GLN:HG2	2:F:969:LEU:HD23	1.97	0.46
4:H:6:THR:O	4:H:10:ILE:HG12	2.16	0.46
2:J:883:MET:SD	2:J:910:LEU:HB3	2.55	0.46
3:K:20:TYR:O	3:K:21:GLU:HG2	2.15	0.46
1:M:479:LEU:HB2	1:M:520:PHE:CE2	2.51	0.46
2:N:309:ASP:O	2:N:311:VAL:N	2.49	0.46
1:A:539:ILE:O	1:A:543:LEU:HD23	2.16	0.46
2:B:654:ASP:HB3	2:B:659:LEU:HD21	1.98	0.46
2:F:293:ASP:HA	2:F:333:PHE:HB3	1.97	0.46
2:F:918:GLN:O	2:F:919:GLN:NE2	2.46	0.46
3:G:162:MET:HE2	3:G:162:MET:HA	1.97	0.46
1:I:138:THR:O	1:I:142:LEU:HD23	2.16	0.46
1:I:207:ALA:HB1	1:I:428:ARG:NH1	2.30	0.46
2:J:105:ASP:OD1	2:N:486:GLN:NE2	2.49	0.46
2:J:255:PHE:HB2	2:J:258:GLN:O	2.16	0.46
2:N:344:ASP:OD1	2:N:344:ASP:N	2.48	0.46
1:A:140:VAL:HG22	1:A:144:PHE:CE2	2.52	0.45
2:B:423:ASN:OD1	2:B:426:SER:HB3	2.16	0.45
2:B:655:ARG:HE	2:B:658:THR:H	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:961:LYS:HG3	2:B:989:ASN:ND2	2.31	0.45
1:E:539:ILE:HA	1:E:542:MET:HE3	1.97	0.45
2:F:997:GLN:HA	2:F:1000:VAL:HG12	1.98	0.45
1:I:319:LYS:O	1:I:384:TYR:OH	2.29	0.45
2:J:779:TRP:HA	2:J:782:VAL:HG22	1.98	0.45
2:J:1003:LEU:HD21	2:J:1024:LEU:HD21	1.98	0.45
3:K:131:MET:SD	3:K:220:MET:HE1	2.56	0.45
4:L:5:LEU:HD23	4:L:6:THR:N	2.31	0.45
1:M:1124:ARG:O	1:M:1128:VAL:HG23	2.15	0.45
2:N:742:ILE:HD12	2:N:784:TYR:OH	2.16	0.45
2:N:924:TRP:HE1	2:N:928:ARG:CZ	2.29	0.45
3:O:131:MET:HA	3:O:134:LEU:HG	1.96	0.45
2:B:843:ASP:CG	2:B:844:GLU:H	2.23	0.45
1:E:359:LEU:HD21	1:E:367:PRO:HB3	1.97	0.45
1:E:1123:TYR:OH	1:E:1182:SER:HA	2.17	0.45
2:J:305:PHE:HB2	2:J:469:ARG:HG3	1.98	0.45
3:K:352:PHE:HB2	3:K:353:ARG:HH12	1.79	0.45
1:M:566:ILE:HG23	1:M:570:MET:HG2	1.97	0.45
1:M:592:GLY:HA2	1:M:599:VAL:O	2.16	0.45
2:N:125:ILE:HD11	2:N:178:TYR:CE1	2.51	0.45
2:N:734:CYS:SG	2:N:739:SER:OG	2.63	0.45
3:O:131:MET:SD	3:O:134:LEU:HD21	2.56	0.45
3:O:242:ILE:HG22	3:O:243:MET:HE2	1.99	0.45
1:A:1171:ALA:HB3	1:A:1176:LEU:HD11	1.99	0.45
2:B:115:GLU:O	2:B:119:ILE:HG12	2.17	0.45
2:F:525:PRO:HG2	2:F:526:ILE:HD12	1.98	0.45
1:I:880:ILE:HD11	1:I:894:THR:HG21	1.99	0.45
2:J:53:TYR:O	2:J:57:LYS:HG2	2.16	0.45
2:J:184:GLU:HG3	2:J:185:MET:HE2	1.98	0.45
2:J:298:PRO:O	2:J:303:PRO:HG2	2.17	0.45
3:K:251:SER:HB3	3:K:252:PRO:HD3	1.98	0.45
1:M:85:MET:SD	1:M:155:ILE:HG23	2.56	0.45
1:M:1078:VAL:HG21	1:M:1135:THR:HG22	1.97	0.45
2:N:64:GLN:OE1	2:N:65:SER:N	2.50	0.45
2:B:714:VAL:HG13	2:B:719:TRP:CD2	2.52	0.45
2:B:797:ALA:HA	2:B:800:ILE:HG12	1.96	0.45
2:F:846:GLU:OE1	2:F:846:GLU:N	2.30	0.45
1:I:97:ASP:OD1	1:I:98:LYS:N	2.49	0.45
1:I:140:VAL:HG22	1:I:144:PHE:CE2	2.51	0.45
2:N:351:LYS:HB2	2:N:354:GLU:HG3	1.99	0.45
2:N:788:PHE:O	2:N:790:GLN:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:355:ILE:HD12	2:B:355:ILE:H	1.81	0.45
3:C:198:CYS:SG	3:C:204:HIS:ND1	2.81	0.45
3:C:228:PRO:HD2	3:C:368:ALA:HB2	1.99	0.45
3:G:204:HIS:NE2	3:G:206:GLY:O	2.49	0.45
4:H:122:VAL:HA	4:H:125:MET:HE2	1.99	0.45
2:J:73:THR:HG23	2:J:82:ALA:HA	1.97	0.45
2:J:441:PHE:CE2	2:J:443:TRP:CD1	3.03	0.45
3:K:126:GLU:H	3:K:126:GLU:CD	2.25	0.45
1:M:29:VAL:H	1:M:83:LYS:HZ3	1.65	0.45
2:N:367:ILE:HD13	2:N:443:TRP:NE1	2.32	0.45
2:N:442:LEU:HD23	2:N:442:LEU:H	1.81	0.45
1:A:386:ASN:O	1:A:389:THR:OG1	2.30	0.45
1:A:887:ASP:O	1:A:889:SER:N	2.49	0.45
2:B:374:ILE:HD11	2:B:451:ALA:HA	1.97	0.45
3:C:251:SER:HB3	3:C:252:PRO:HD3	1.98	0.45
1:M:286:LYS:HB2	1:M:286:LYS:HE2	1.78	0.45
2:N:49:LEU:HD23	2:N:101:TYR:CD2	2.52	0.45
3:O:167:THR:OG1	3:O:168:ASP:N	2.49	0.45
1:A:177:LYS:NZ	1:A:841:ASP:OD2	2.41	0.45
2:B:89:TYR:CE1	2:B:177:LEU:HD21	2.52	0.45
2:B:101:TYR:HB3	2:B:111:THR:HG22	1.99	0.45
3:G:210:GLU:HB3	3:G:276:ARG:HE	1.82	0.45
1:I:799:TYR:CE2	1:I:801:GLU:HB2	2.51	0.45
2:J:526:ILE:CD1	2:J:656:LEU:HD22	2.47	0.45
2:J:1016:LEU:HB3	2:J:1077:LEU:HD12	1.99	0.45
3:K:290:GLN:HA	4:L:66:PHE:CD2	2.51	0.45
1:M:255:VAL:HG21	1:M:286:LYS:NZ	2.31	0.45
3:O:20:TYR:HB3	3:O:37:CYS:SG	2.56	0.45
1:A:554:TRP:NE1	1:A:558:GLY:O	2.45	0.45
2:F:122:MET:HA	2:F:125:ILE:HG22	1.99	0.45
2:F:308:ASP:OD1	2:F:308:ASP:N	2.49	0.45
2:F:531:GLN:HG2	2:F:578:ILE:HG22	1.98	0.45
2:F:657:GLN:O	2:F:657:GLN:NE2	2.49	0.45
2:F:879:ILE:O	2:F:883:MET:HG3	2.16	0.45
1:I:785:MET:O	1:I:789:MET:HG2	2.17	0.45
3:K:36:ARG:HG3	3:K:45:GLU:OE2	2.16	0.45
3:K:133:ALA:HB3	3:K:164:ILE:HD11	1.97	0.45
1:M:15:ALA:HB2	1:M:61:TYR:OH	2.17	0.45
1:M:82:VAL:HG12	1:M:86:ARG:HE	1.82	0.45
1:M:375:VAL:HA	1:M:392:ARG:HG3	1.99	0.45
1:M:524:PHE:HB2	1:M:542:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:486:GLN:NE2	2:N:492:ASP:OD1	2.50	0.45
2:B:103:ARG:HD3	2:F:477:ARG:HH12	1.81	0.45
2:B:1010:LEU:HD11	2:B:1018:PHE:HE2	1.82	0.45
1:E:847:LEU:HB3	1:E:854:LEU:HD21	1.99	0.45
2:F:599:LYS:O	2:F:603:GLN:HG2	2.17	0.45
4:H:32:GLU:N	4:H:32:GLU:OE1	2.49	0.45
1:I:295:ARG:HA	1:I:331:PHE:HE2	1.80	0.45
1:I:513:ILE:HB	1:I:518:PHE:CE1	2.51	0.45
3:K:225:ALA:HB2	3:K:254:TRP:CZ2	2.52	0.45
3:K:305:PHE:CD2	4:L:145:MET:HE1	2.47	0.45
1:M:538:MET:O	1:M:542:MET:HG2	2.17	0.45
2:N:88:LEU:HD21	2:N:178:TYR:HA	1.98	0.45
2:N:837:TYR:O	2:N:841:THR:HG23	2.17	0.45
1:A:213:ASP:HA	1:A:230:VAL:HG12	1.99	0.45
2:F:374:ILE:HG23	2:F:378:PHE:CE2	2.51	0.45
2:F:859:TRP:HZ3	2:F:908:LYS:HD2	1.82	0.45
2:F:1006:VAL:HG12	2:F:1010:LEU:HD23	1.99	0.45
4:L:66:PHE:CE2	4:L:70:LEU:HD11	2.51	0.45
1:M:102:PHE:HB2	1:M:110:ASP:O	2.17	0.45
1:M:373:TYR:CE2	1:M:394:PRO:HG3	2.52	0.45
2:N:857:ILE:HG23	2:N:868:PHE:CE2	2.52	0.45
3:O:232:HIS:CE1	3:O:237:LEU:HD12	2.52	0.45
1:A:418:LEU:HD12	1:A:419:ALA:N	2.32	0.44
1:A:1055:GLN:HA	1:A:1058:ARG:NH1	2.32	0.44
3:C:242:ILE:HG22	3:C:243:MET:HE2	1.98	0.44
1:E:78:GLU:OE2	1:E:153:LEU:HD13	2.17	0.44
1:E:1126:LEU:HD13	1:E:1155:VAL:HG11	1.98	0.44
2:F:523:VAL:HG12	2:F:523:VAL:O	2.16	0.44
2:F:1035:PHE:HD1	2:F:1068:TYR:CE2	2.25	0.44
4:H:32:GLU:HA	4:H:35:THR:HG22	2.00	0.44
2:J:541:LEU:HD12	2:J:670:PHE:CD1	2.52	0.44
2:J:546:LYS:HE3	1:M:28:PRO:HG2	2.00	0.44
3:K:49:LYS:HB3	3:K:102:LEU:HB2	1.99	0.44
3:K:68:ARG:NH2	3:K:97:ASN:O	2.50	0.44
4:L:32:GLU:OE1	4:L:32:GLU:N	2.47	0.44
1:M:139:SER:OG	1:M:204:MET:HG3	2.17	0.44
2:N:163:SER:OG	2:N:166:GLU:OE1	2.33	0.44
1:A:30:THR:OG1	1:A:119:LYS:HD3	2.16	0.44
4:D:110:MET:HB3	4:D:115:GLU:HB3	1.99	0.44
3:G:111:GLU:OE1	3:G:112:LEU:N	2.50	0.44
2:J:83:LYS:HG3	2:J:84:ILE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:119:LYS:O	3:K:121:THR:N	2.50	0.44
4:L:17:PHE:CZ	4:L:69:PHE:HB3	2.52	0.44
1:M:386:ASN:O	1:M:389:THR:OG1	2.29	0.44
1:M:532:LEU:HB3	1:M:538:MET:HE3	1.99	0.44
1:M:588:LYS:NZ	3:O:98:THR:HB	2.32	0.44
2:N:838:LYS:O	2:N:841:THR:OG1	2.24	0.44
2:N:890:ARG:O	2:N:890:ARG:NE	2.46	0.44
1:A:1130:ALA:O	1:A:1133:VAL:HG12	2.18	0.44
2:B:779:TRP:HA	2:B:782:VAL:HG22	1.98	0.44
2:B:899:LEU:H	2:B:899:LEU:HD23	1.82	0.44
2:F:328:TYR:HB2	2:F:364:GLU:HG2	1.99	0.44
2:J:199:VAL:HG22	2:J:254:LEU:HD23	1.98	0.44
2:J:768:ARG:O	2:J:771:ARG:HG3	2.16	0.44
1:M:504:VAL:HG11	1:M:546:ASP:OD1	2.16	0.44
2:N:173:ASN:OD1	2:N:174:ALA:N	2.50	0.44
4:P:52:MET:HA	4:P:55:GLU:HG2	1.99	0.44
1:A:305:LYS:O	1:A:306:GLU:HB3	2.18	0.44
1:A:311:LEU:H	1:A:311:LEU:HD23	1.82	0.44
2:B:857:ILE:HA	2:B:860:ILE:HG12	2.00	0.44
3:C:216:THR:HG22	3:C:220:MET:SD	2.58	0.44
1:E:852:LYS:HZ3	1:E:917:ARG:HA	1.82	0.44
2:F:515:ILE:HD13	2:F:638:LEU:HD12	1.98	0.44
2:F:904:PRO:HA	2:F:907:VAL:HG22	1.98	0.44
1:I:1123:TYR:OH	1:I:1182:SER:HA	2.17	0.44
2:J:318:ASP:O	2:J:322:ARG:HG2	2.16	0.44
2:J:433:ASN:OD1	2:J:434:CYS:N	2.51	0.44
2:J:474:LYS:O	2:J:477:ARG:NH2	2.39	0.44
3:K:171:PHE:CE2	3:K:185:CYS:HB2	2.53	0.44
4:L:66:PHE:HB3	4:L:67:PRO:HD3	1.98	0.44
1:A:134:GLN:NE2	1:A:185:GLU:OE2	2.49	0.44
1:A:589:MET:HA	1:A:594:PHE:HB2	1.99	0.44
3:C:87:ILE:HD11	3:C:169:PHE:CE1	2.52	0.44
1:E:799:TYR:HD2	1:E:802:ARG:H	1.64	0.44
2:J:837:TYR:O	2:J:841:THR:HG23	2.17	0.44
2:J:876:ILE:HA	2:J:879:ILE:HD12	2.00	0.44
3:K:318:ILE:HD12	4:L:72:MET:HE1	2.00	0.44
1:M:167:ASN:OD1	1:M:494:LEU:HD12	2.17	0.44
2:B:504:GLN:O	2:B:507:GLN:HG3	2.18	0.44
2:B:510:LEU:HB3	2:B:515:ILE:HB	2.00	0.44
2:B:657:GLN:O	2:B:657:GLN:NE2	2.44	0.44
3:C:130:ILE:HG23	3:C:164:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:398:LEU:N	1:I:399:PRO:HD3	2.33	0.44
1:I:545:THR:HG21	1:I:906:ARG:NH2	2.32	0.44
1:I:1052:GLY:O	1:I:1056:ARG:NH1	2.50	0.44
1:I:1132:LEU:O	1:I:1135:THR:OG1	2.29	0.44
1:M:1132:LEU:O	1:M:1135:THR:OG1	2.27	0.44
2:N:347:ARG:CZ	2:N:351:LYS:HG2	2.47	0.44
2:N:835:ILE:HG13	2:N:836:TYR:HD1	1.82	0.44
1:E:530:PHE:CE2	1:E:532:LEU:HB2	2.53	0.44
1:E:774:SER:OG	1:E:775:SER:N	2.51	0.44
2:F:1023:ASP:HB3	2:F:1026:ARG:HB2	1.99	0.44
3:G:78:LEU:HD11	3:G:169:PHE:HB2	2.00	0.44
1:I:28:PRO:HG2	2:N:546:LYS:NZ	2.33	0.44
3:K:128:ARG:HE	3:K:132:ARG:NH2	2.16	0.44
3:K:290:GLN:HA	4:L:66:PHE:HD2	1.82	0.44
1:A:1058:ARG:NH1	1:A:1189:TYR:HB3	2.32	0.44
2:B:838:LYS:O	2:B:841:THR:OG1	2.30	0.44
3:C:294:GLU:HG3	3:C:297:ARG:NE	2.33	0.44
1:E:852:LYS:HA	1:E:852:LYS:HD2	1.82	0.44
1:E:861:GLU:CG	1:E:862:PRO:HA	2.48	0.44
1:I:926:VAL:O	1:I:930:GLU:HG2	2.18	0.44
3:K:87:ILE:HD11	3:K:169:PHE:CE1	2.52	0.44
3:K:184:VAL:HG21	3:K:199:SER:HB3	2.00	0.44
3:O:94:TYR:HB2	3:O:101:PHE:HB2	2.00	0.44
4:P:37:MET:SD	4:P:42:GLN:HB2	2.58	0.44
1:E:92:MET:HE1	1:E:112:LEU:HG	2.00	0.44
2:J:944:ARG:HA	2:J:947:GLN:OE1	2.18	0.44
1:M:90:HIS:HA	1:M:93:ILE:HG22	2.00	0.44
2:N:655:ARG:HB3	2:N:657:GLN:OE1	2.18	0.44
1:E:213:ASP:OD1	1:E:214:GLU:N	2.51	0.43
1:E:949:LEU:HB3	1:E:953:ALA:HB3	2.00	0.43
1:E:1106:LYS:HE2	1:E:1110:HIS:CE1	2.52	0.43
1:I:535:ASP:HB3	1:I:538:MET:HE2	2.00	0.43
1:I:583:LEU:HD12	1:I:586:LEU:HD11	1.99	0.43
2:N:634:ILE:HA	2:N:637:MET:HG3	2.00	0.43
2:N:856:HIS:O	2:N:860:ILE:HG12	2.18	0.43
1:A:1086:SER:HB2	1:A:1148:ILE:HD11	1.99	0.43
3:C:304:LYS:HA	3:C:307:VAL:HG12	2.00	0.43
2:F:173:ASN:HD22	2:F:220:VAL:HG22	1.83	0.43
2:F:329:GLY:HA2	2:F:369:PHE:CE2	2.53	0.43
1:M:30:THR:HG22	1:M:32:LEU:HD23	2.00	0.43
2:N:386:GLN:HA	2:N:389:GLN:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:1074:MET:SD	2:N:1075:ASN:N	2.92	0.43
1:A:445:LEU:HD21	1:A:565:PRO:HG3	2.00	0.43
3:C:301:PRO:HB3	4:D:125:MET:CG	2.48	0.43
3:G:113:PHE:CZ	3:G:359:VAL:HG22	2.53	0.43
1:I:15:ALA:HB2	1:I:61:TYR:OH	2.17	0.43
1:I:1095:SER:HA	1:I:1098:ARG:HE	1.82	0.43
3:K:318:ILE:HD11	4:L:56:VAL:HG21	2.01	0.43
2:N:335:ARG:HG3	2:N:359:ASP:HB3	2.00	0.43
1:A:538:MET:HA	1:A:541:GLU:HG2	2.00	0.43
3:C:119:LYS:O	3:C:121:THR:N	2.51	0.43
3:G:111:GLU:CD	3:G:154:GLU:HA	2.43	0.43
1:I:1121:PRO:O	1:I:1124:ARG:HG2	2.19	0.43
2:J:943:ASP:O	2:J:947:GLN:OE1	2.36	0.43
2:N:797:ALA:HA	2:N:800:ILE:HG12	1.98	0.43
3:C:107:MET:O	3:C:108:LYS:HB2	2.18	0.43
1:E:55:TRP:CG	1:E:148:MET:HE1	2.54	0.43
2:F:961:LYS:HG3	2:F:989:ASN:ND2	2.32	0.43
3:G:87:ILE:HD11	3:G:169:PHE:CZ	2.52	0.43
4:H:141:GLU:HG2	4:H:145:MET:HE3	2.00	0.43
1:I:1210:TYR:CE2	1:I:1214:PHE:HE2	2.36	0.43
2:J:243:LYS:HE2	2:J:279:LEU:HD13	2.01	0.43
2:J:885:TYR:O	2:J:889:ILE:HG13	2.19	0.43
2:N:938:PRO:HG2	2:N:941:PHE:HB2	2.00	0.43
4:P:108:HIS:HA	4:P:111:THR:HG22	2.00	0.43
1:A:1053:GLN:O	1:A:1057:ARG:NH1	2.51	0.43
2:B:139:PHE:HE1	2:B:143:PRO:HB3	1.84	0.43
2:B:270:ASP:O	2:B:274:ARG:HG3	2.18	0.43
2:B:880:ILE:HD12	2:B:883:MET:SD	2.59	0.43
2:B:1025:ASP:HA	2:B:1028:VAL:HG12	2.01	0.43
1:E:375:VAL:HA	1:E:392:ARG:HG3	2.00	0.43
1:E:827:ARG:HH22	1:E:954:MET:HE1	1.83	0.43
2:F:576:TYR:CD2	2:F:580:PHE:HB2	2.54	0.43
2:F:983:VAL:HA	2:F:986:THR:HG22	2.01	0.43
2:F:1032:PHE:HA	2:F:1054:PHE:CE2	2.53	0.43
3:G:242:ILE:HG22	3:G:243:MET:HE2	2.00	0.43
3:K:18:GLU:H	3:K:18:GLU:HG3	1.61	0.43
2:N:779:TRP:HA	2:N:782:VAL:HG22	1.99	0.43
3:O:72:LEU:HA	3:O:75:VAL:HG22	2.00	0.43
1:A:538:MET:HB3	1:A:542:MET:HE1	2.01	0.43
2:B:98:ALA:HB2	2:B:114:LEU:HB2	2.00	0.43
2:B:328:TYR:HB3	2:B:410:TYR:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:340:THR:HG22	2:B:343:GLU:HG3	2.00	0.43
2:F:181:TYR:O	2:F:184:GLU:HB3	2.18	0.43
3:G:182:ARG:NH2	3:G:205:PRO:O	2.51	0.43
1:I:117:ASN:OD1	1:I:118:THR:N	2.43	0.43
1:I:903:MET:HA	1:I:906:ARG:NH1	2.34	0.43
2:J:89:TYR:HE1	2:J:181:TYR:HE2	1.67	0.43
2:J:762:VAL:O	2:J:766:ILE:HG12	2.19	0.43
3:K:249:PHE:HB3	3:K:254:TRP:CD1	2.53	0.43
1:M:142:LEU:HD11	1:M:168:LEU:HD11	2.01	0.43
2:N:89:TYR:HE1	2:N:177:LEU:HD11	1.83	0.43
2:N:152:VAL:HB	2:N:169:HIS:HE1	1.83	0.43
3:O:62:GLU:O	3:O:65:ARG:HG2	2.19	0.43
3:O:63:GLU:O	3:O:66:GLU:HG3	2.19	0.43
1:A:41:ASP:OD1	1:A:42:ALA:N	2.51	0.43
2:B:127:TYR:OH	2:B:131:ARG:NH2	2.51	0.43
2:B:1069:LEU:O	2:B:1072:ALA:HB3	2.19	0.43
1:E:524:PHE:HB2	1:E:542:MET:SD	2.58	0.43
3:G:126:GLU:CD	3:G:126:GLU:H	2.26	0.43
2:J:83:LYS:HG3	2:J:84:ILE:H	1.82	0.43
2:J:469:ARG:HA	2:J:469:ARG:NE	2.34	0.43
2:J:903:SER:HB2	2:J:906:GLU:OE1	2.19	0.43
2:J:947:GLN:O	2:J:951:ARG:HG3	2.18	0.43
2:J:1026:ARG:O	2:J:1030:GLU:OE1	2.36	0.43
1:M:139:SER:HB2	1:M:205:ALA:HA	2.01	0.43
1:M:255:VAL:HG11	1:M:286:LYS:HE3	2.01	0.43
1:M:777:GLN:HA	1:M:825:LEU:HD11	2.00	0.43
1:A:253:LYS:HD2	1:A:256:ASP:HB2	1.99	0.43
2:B:184:GLU:OE1	2:B:467:VAL:HG23	2.19	0.43
2:B:374:ILE:O	2:B:377:VAL:HG12	2.19	0.43
2:B:384:GLN:HA	2:B:387:GLU:HG2	2.00	0.43
2:B:977:MET:SD	2:B:981:LEU:HD23	2.59	0.43
3:C:202:GLU:OE1	3:C:202:GLU:N	2.51	0.43
1:E:19:GLN:HA	1:E:23:LEU:HB2	2.00	0.43
1:E:177:LYS:NZ	1:E:841:ASP:OD2	2.42	0.43
2:F:529:TRP:HB3	2:F:533:GLU:HG3	2.01	0.43
2:F:623:GLU:OE1	2:F:623:GLU:N	2.51	0.43
4:H:38:ARG:HD3	4:H:43:ASN:OD1	2.19	0.43
2:J:626:ILE:HG22	2:J:634:ILE:HD11	2.01	0.43
1:M:371:GLU:OE2	1:M:372:LEU:HG	2.19	0.43
2:N:243:LYS:HE2	2:N:279:LEU:HD13	2.00	0.43
2:N:634:ILE:O	2:N:637:MET:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:71:THR:HG21	3:O:100:PHE:CD2	2.54	0.43
3:O:81:VAL:HG12	3:O:87:ILE:HD13	2.00	0.43
2:B:397:HIS:HB2	2:B:405:VAL:HB	2.00	0.43
4:D:82:SER:O	4:D:86:ILE:HG23	2.19	0.43
1:E:1057:ARG:HB3	1:E:1058:ARG:HH12	1.84	0.43
4:H:46:GLU:C	4:H:50:GLN:HE22	2.27	0.43
1:I:119:LYS:O	1:I:120:THR:OG1	2.34	0.43
2:J:397:HIS:NE2	2:J:398:HIS:O	2.52	0.43
3:K:320:TYR:O	3:K:324:ARG:HG3	2.19	0.43
2:N:134:ASP:O	2:N:138:GLN:HG2	2.19	0.43
1:A:586:LEU:HA	1:A:589:MET:HG3	2.01	0.42
4:D:17:PHE:CE1	4:D:28:ILE:HD11	2.54	0.42
1:E:855:THR:HG23	1:E:865:LYS:O	2.19	0.42
2:F:103:ARG:HH22	2:F:459:ILE:HA	1.83	0.42
2:F:370:LEU:HD12	2:F:451:ALA:HB3	1.99	0.42
2:F:467:VAL:C	2:F:468:GLN:HG3	2.44	0.42
2:F:724:THR:O	2:F:728:LEU:HG	2.19	0.42
2:F:849:ILE:O	2:F:853:LEU:HD23	2.19	0.42
2:F:871:MET:HA	2:F:871:MET:HE2	2.01	0.42
1:M:781:ASP:O	1:M:785:MET:HG3	2.19	0.42
2:N:552:ARG:NH2	2:N:555:ARG:HE	2.16	0.42
2:N:996:ARG:O	2:N:999:VAL:HG12	2.18	0.42
1:A:356:GLU:HA	1:A:359:LEU:HD23	2.00	0.42
2:B:994:GLN:HB2	2:B:1055:TYR:CE1	2.55	0.42
3:C:113:PHE:HZ	3:C:359:VAL:HG12	1.84	0.42
4:D:106:LEU:O	4:D:110:MET:HG2	2.20	0.42
2:F:298:PRO:O	2:F:303:PRO:HG2	2.18	0.42
1:I:80:SER:O	1:I:84:LEU:HG	2.19	0.42
1:I:877:THR:O	1:I:880:ILE:HG22	2.19	0.42
2:J:718:GLU:HB3	2:J:719:TRP:CE3	2.54	0.42
1:M:157:HIS:N	1:M:161:GLU:OE2	2.46	0.42
1:M:255:VAL:HG21	1:M:286:LYS:HZ1	1.84	0.42
3:O:113:PHE:HB2	3:O:154:GLU:HG2	2.01	0.42
2:B:136:VAL:HG22	2:B:149:LEU:HD21	2.01	0.42
3:C:53:VAL:HG23	3:C:67:LEU:HD22	2.01	0.42
2:F:60:LEU:HD22	2:F:90:CYS:SG	2.60	0.42
2:F:1078:LEU:HD13	2:J:1071:LYS:HZ2	1.84	0.42
3:G:63:GLU:O	3:G:66:GLU:HG3	2.19	0.42
1:I:306:GLU:O	1:I:310:ARG:NH2	2.50	0.42
2:J:388:TYR:CD1	2:J:391:LEU:HD12	2.54	0.42
2:J:814:ALA:HB2	2:J:842:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:107:ARG:O	4:L:110:MET:HG2	2.19	0.42
1:M:52:LEU:HD21	1:M:144:PHE:CE1	2.54	0.42
2:N:370:LEU:O	2:N:373:MET:HG2	2.19	0.42
2:N:879:ILE:HG22	2:N:883:MET:HE2	2.00	0.42
1:A:213:ASP:OD1	1:A:214:GLU:N	2.51	0.42
1:A:479:LEU:HB2	1:A:520:PHE:CE1	2.54	0.42
2:B:949:LEU:HA	2:B:949:LEU:HD12	1.79	0.42
3:C:264:LEU:HD13	3:C:285:HIS:CG	2.54	0.42
1:E:236:GLN:OE1	1:E:553:ARG:HD3	2.19	0.42
2:F:49:LEU:HD13	2:F:101:TYR:CE1	2.54	0.42
2:F:467:VAL:O	2:F:467:VAL:HG12	2.20	0.42
2:F:785:GLY:O	2:F:789:THR:HG23	2.20	0.42
1:I:28:PRO:HG2	2:N:546:LYS:HZ2	1.84	0.42
1:I:1172:ASP:OD1	1:I:1174:THR:OG1	2.32	0.42
4:L:45:THR:HG23	4:L:48:GLU:H	1.84	0.42
4:L:49:LEU:HA	4:L:52:MET:HE3	2.02	0.42
4:L:86:ILE:HD12	4:L:86:ILE:HA	1.95	0.42
1:M:927:MET:SD	1:M:961:ILE:HG13	2.59	0.42
3:O:326:LYS:HE3	3:O:327:PRO:HD2	2.02	0.42
1:A:233:ASP:OD1	1:A:234:GLU:N	2.53	0.42
2:B:173:ASN:HD22	2:B:220:VAL:HG22	1.84	0.42
2:B:373:MET:SD	2:B:385:VAL:HG13	2.59	0.42
2:B:486:GLN:OE1	2:B:492:ASP:N	2.52	0.42
2:B:625:ASN:O	2:B:630:ARG:NE	2.50	0.42
1:E:305:LYS:O	1:E:306:GLU:HB3	2.18	0.42
1:E:897:ILE:HG21	1:E:920:ILE:HG23	2.01	0.42
1:E:1172:ASP:OD1	1:E:1174:THR:OG1	2.35	0.42
2:F:279:LEU:O	2:F:283:LEU:HB2	2.20	0.42
2:F:283:LEU:HD11	2:F:307:LEU:HD12	2.02	0.42
2:F:332:ARG:HG2	2:F:333:PHE:CD1	2.55	0.42
2:J:292:THR:HG21	2:J:320:VAL:HG12	2.00	0.42
2:J:1051:MET:SD	2:J:1051:MET:N	2.92	0.42
4:L:49:LEU:HA	4:L:52:MET:CE	2.49	0.42
1:A:65:ALA:HA	1:A:70:ASP:OD2	2.19	0.42
1:A:406:LEU:HD23	1:A:406:LEU:HA	1.78	0.42
2:B:657:GLN:HA	2:B:660:ILE:HG22	2.02	0.42
1:E:484:SER:O	1:E:484:SER:OG	2.37	0.42
1:E:502:MET:SD	1:E:502:MET:N	2.93	0.42
1:E:1133:VAL:CA	1:E:1136:MET:HE3	2.42	0.42
2:F:98:ALA:HB2	2:F:114:LEU:HB2	2.00	0.42
2:F:119:ILE:HD11	2:F:190:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:140:VAL:HG22	1:I:144:PHE:HE2	1.84	0.42
2:N:580:PHE:HE2	2:N:620:LEU:H	1.68	0.42
2:N:957:ILE:HD11	2:N:962:HIS:CD2	2.52	0.42
3:O:13:ALA:HB2	3:O:96:THR:HG22	2.02	0.42
3:O:78:LEU:HD21	3:O:169:PHE:CD1	2.55	0.42
1:A:157:HIS:HB3	2:F:116:HIS:HB3	2.02	0.42
1:A:263:VAL:HG12	1:A:263:VAL:O	2.20	0.42
1:A:398:LEU:N	1:A:399:PRO:HD3	2.34	0.42
2:B:1027:LEU:O	2:B:1030:GLU:HG3	2.19	0.42
3:C:120:VAL:HG22	3:C:352:PHE:HD2	1.85	0.42
1:E:770:LEU:HD13	1:E:782:ILE:HG21	2.01	0.42
2:F:489:LEU:H	2:F:489:LEU:HD23	1.84	0.42
2:F:867:LEU:HG	2:F:915:LEU:HG	2.01	0.42
3:G:113:PHE:HZ	3:G:359:VAL:HG22	1.85	0.42
1:I:138:THR:HG21	1:I:168:LEU:HD11	2.00	0.42
1:I:156:ILE:HG13	1:I:161:GLU:OE1	2.20	0.42
1:I:837:VAL:O	1:I:873:TYR:OH	2.34	0.42
2:N:626:ILE:HG22	2:N:634:ILE:HD11	2.01	0.42
2:N:762:VAL:O	2:N:766:ILE:HG12	2.20	0.42
2:N:924:TRP:HZ2	2:N:928:ARG:HH21	1.68	0.42
1:A:373:TYR:CE2	1:A:394:PRO:HG3	2.54	0.42
1:A:525:ILE:O	1:A:525:ILE:HG22	2.19	0.42
2:B:80:GLN:HB3	2:B:154:ASN:ND2	2.35	0.42
2:B:116:HIS:HB3	1:E:157:HIS:HB3	2.02	0.42
2:B:314:SER:O	2:B:317:LEU:HG	2.20	0.42
3:C:299:PHE:CE1	3:C:304:LYS:HG2	2.53	0.42
2:F:86:ASP:HB2	2:F:442:LEU:HD11	2.02	0.42
2:F:136:VAL:HG22	2:F:149:LEU:HD21	2.01	0.42
2:F:443:TRP:CD1	2:F:447:LEU:HD23	2.55	0.42
1:I:46:ASP:OD1	1:I:47:ASN:N	2.51	0.42
1:I:1118:VAL:HA	1:I:1119:PRO:HD3	1.93	0.42
2:J:186:ILE:HG23	2:J:252:PHE:HE2	1.84	0.42
2:J:441:PHE:HE2	2:J:443:TRP:HD1	1.66	0.42
2:J:668:LEU:HD23	2:J:670:PHE:CE1	2.55	0.42
3:K:60:SER:HB3	3:K:63:GLU:OE1	2.20	0.42
3:K:299:PHE:HE1	3:K:304:LYS:HG2	1.83	0.42
1:M:102:PHE:HB3	1:M:171:TYR:CE1	2.55	0.42
1:M:954:MET:HE1	1:M:957:LEU:HD23	2.00	0.42
2:N:727:ILE:HG12	2:N:743:LEU:HD11	2.01	0.42
2:N:918:GLN:O	2:N:919:GLN:NE2	2.52	0.42
1:E:956:ASN:OD1	1:E:960:HIS:NE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1073:GLN:O	1:E:1077:LYS:HG2	2.19	0.42
2:F:1073:VAL:O	2:F:1077:LEU:HD23	2.20	0.42
1:I:142:LEU:HD12	1:I:212:LEU:HD11	2.02	0.42
1:I:1149:ILE:HG23	1:I:1210:TYR:HE2	1.84	0.42
2:J:193:ILE:HD13	2:J:254:LEU:HG	2.02	0.42
3:K:354:ILE:HG22	3:K:355:TYR:CD1	2.55	0.42
1:M:117:ASN:OD1	1:M:118:THR:N	2.46	0.42
1:M:210:GLU:OE1	1:M:428:ARG:NH1	2.52	0.42
1:M:263:VAL:HG12	1:M:263:VAL:O	2.20	0.42
1:A:6:ASN:O	1:A:10:ARG:HG2	2.19	0.42
1:A:75:TYR:O	1:A:79:GLN:HG2	2.20	0.42
2:B:1008:ILE:O	2:B:1011:GLU:HG3	2.19	0.42
1:E:554:TRP:CE2	1:E:560:PRO:HG3	2.55	0.42
2:F:833:ASN:O	2:F:837:TYR:CD2	2.73	0.42
1:I:1062:GLY:HA3	1:I:1121:PRO:HB3	2.01	0.42
2:J:89:TYR:CE1	2:J:177:LEU:HD21	2.55	0.42
2:J:181:TYR:O	2:J:185:MET:HG2	2.20	0.42
2:J:531:GLN:HG2	2:J:578:ILE:HG22	2.02	0.42
2:J:778:LEU:O	2:J:782:VAL:HG13	2.20	0.42
2:J:861:ILE:HD13	2:J:868:PHE:HB2	2.02	0.42
1:M:36:SER:HB2	1:M:401:MET:HE1	2.01	0.42
1:M:1171:ALA:HB3	1:M:1176:LEU:HD11	2.02	0.42
2:N:56:VAL:HG22	2:N:60:LEU:HD12	2.02	0.42
2:N:64:GLN:NE2	2:N:71:PHE:HE1	2.17	0.42
2:N:161:LEU:HD23	2:N:161:LEU:HA	1.90	0.42
2:N:173:ASN:O	2:N:177:LEU:HB2	2.20	0.42
2:N:861:ILE:HD12	2:N:868:PHE:HD2	1.84	0.42
3:O:15:ASP:O	3:O:19:ASN:HB2	2.20	0.42
3:O:60:SER:HB3	3:O:63:GLU:OE1	2.20	0.42
4:P:69:PHE:O	4:P:73:MET:HG2	2.18	0.42
1:A:143:LEU:HD22	1:A:267:ALA:HB2	2.01	0.41
2:B:1030:GLU:OE2	2:B:1072:ALA:HB2	2.20	0.41
3:C:49:LYS:HB3	3:C:102:LEU:HB2	2.02	0.41
3:C:254:TRP:HB3	3:C:262:LYS:HE2	2.02	0.41
1:E:919:ARG:O	1:E:923:ILE:HG12	2.20	0.41
3:G:84:HIS:CE1	3:G:86:ASN:HB2	2.55	0.41
3:G:204:HIS:ND1	3:G:205:PRO:HD2	2.34	0.41
4:H:46:GLU:OE2	4:H:50:GLN:NE2	2.53	0.41
1:I:768:LEU:O	1:I:771:LYS:N	2.53	0.41
2:J:75:THR:OG1	2:J:439:LYS:HA	2.20	0.41
2:J:136:VAL:HG22	2:J:149:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:63:GLU:O	3:K:66:GLU:HG3	2.19	0.41
3:K:84:HIS:O	3:K:87:ILE:HG22	2.20	0.41
1:M:894:THR:O	1:M:898:MET:HG3	2.19	0.41
2:N:269:LEU:HD11	2:N:611:MET:HE1	2.00	0.41
2:N:317:LEU:O	2:N:321:VAL:HG13	2.20	0.41
2:N:371:TYR:O	2:N:374:ILE:HG22	2.20	0.41
1:A:216:ASP:N	1:A:216:ASP:OD1	2.53	0.41
1:A:530:PHE:CE2	1:A:532:LEU:HB2	2.55	0.41
2:B:101:TYR:CE2	2:B:110:ARG:HB2	2.55	0.41
2:B:778:LEU:O	2:B:782:VAL:HG13	2.20	0.41
1:E:216:ASP:OD1	1:E:216:ASP:N	2.53	0.41
1:E:1200:MET:HG2	3:G:347:ILE:HG23	2.01	0.41
2:F:182:LEU:HA	2:F:185:MET:HE3	2.02	0.41
2:F:779:TRP:HA	2:F:782:VAL:HG22	2.02	0.41
2:F:798:PRO:HA	2:F:801:THR:HG22	2.02	0.41
3:G:350:TYR:HA	3:G:353:ARG:HG2	2.02	0.41
4:H:141:GLU:O	4:H:144:GLN:HG2	2.20	0.41
1:I:442:VAL:HG23	1:I:562:ILE:HG23	2.02	0.41
1:I:445:LEU:HD12	1:I:446:ALA:N	2.35	0.41
2:J:282:LEU:HD11	2:J:288:ARG:NH1	2.35	0.41
2:J:317:LEU:HA	2:J:320:VAL:HG22	2.01	0.41
2:J:497:VAL:HG22	2:J:652:HIS:O	2.20	0.41
1:M:30:THR:OG1	1:M:119:LYS:HG2	2.19	0.41
1:M:843:ALA:O	1:M:847:LEU:HG	2.20	0.41
2:N:447:LEU:HA	2:N:450:ILE:HG22	2.02	0.41
3:O:78:LEU:HD21	3:O:169:PHE:CG	2.55	0.41
4:P:32:GLU:OE1	4:P:32:GLU:N	2.52	0.41
1:A:341:PHE:CZ	1:A:429:ARG:HG2	2.54	0.41
1:A:439:VAL:O	1:A:560:PRO:HD2	2.21	0.41
1:A:841:ASP:N	1:A:841:ASP:OD1	2.52	0.41
2:B:883:MET:HB2	2:B:910:LEU:CD2	2.51	0.41
2:F:122:MET:HE3	2:F:185:MET:HE1	2.02	0.41
2:F:351:LYS:HB3	2:F:354:GLU:HG3	2.03	0.41
2:F:728:LEU:HB3	2:F:758:LYS:NZ	2.34	0.41
2:J:398:HIS:HB3	2:J:402:GLY:HA2	2.02	0.41
2:J:628:GLY:O	2:J:631:PHE:HD1	2.03	0.41
3:K:115:TYR:CE2	3:K:122:LEU:HD21	2.54	0.41
3:K:120:VAL:HG22	3:K:352:PHE:HD2	1.85	0.41
2:N:798:PRO:HA	2:N:801:THR:HG22	2.02	0.41
1:A:1153:LYS:HE3	1:A:1157:ILE:CG1	2.50	0.41
2:B:467:VAL:C	2:B:468:GLN:HG3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:122:MET:CE	2:F:185:MET:HE1	2.50	0.41
2:F:837:TYR:O	2:F:841:THR:HG23	2.20	0.41
2:F:899:LEU:HD23	2:F:899:LEU:H	1.84	0.41
2:F:941:PHE:CE1	2:F:1000:VAL:HG23	2.55	0.41
4:H:22:LYS:NZ	4:H:32:GLU:HG3	2.34	0.41
2:J:94:ALA:HB1	2:J:114:LEU:HD12	2.02	0.41
2:J:623:GLU:O	2:J:626:ILE:HG12	2.20	0.41
4:L:37:MET:HG3	4:L:42:GLN:HB2	2.02	0.41
1:M:778:GLU:O	1:M:782:ILE:HG22	2.20	0.41
2:N:86:ASP:OD1	2:N:87:SER:N	2.52	0.41
2:N:273:ASN:O	2:N:276:ARG:HG2	2.20	0.41
4:P:110:MET:HA	4:P:110:MET:HE3	2.01	0.41
1:A:102:PHE:HB2	1:A:110:ASP:O	2.21	0.41
1:E:589:MET:HA	1:E:594:PHE:HB2	2.03	0.41
2:F:1065:THR:O	2:F:1069:LEU:HD13	2.20	0.41
1:I:899:VAL:O	1:I:903:MET:HG3	2.20	0.41
1:I:1175:MET:SD	1:I:1187:LEU:HG	2.60	0.41
1:I:1200:MET:HE2	1:I:1200:MET:HB3	1.84	0.41
2:J:397:HIS:HB3	2:J:405:VAL:HB	2.02	0.41
4:L:100:TYR:CD1	4:L:136:GLN:HB3	2.55	0.41
1:M:1080:GLN:NE2	1:M:1081:LYS:HG3	2.36	0.41
2:N:269:LEU:HD21	2:N:611:MET:HE3	2.03	0.41
2:N:298:PRO:O	2:N:303:PRO:HG2	2.21	0.41
4:P:101:ILE:HD13	4:P:142:PHE:CE2	2.55	0.41
1:A:109:LYS:NZ	1:A:128:ASP:OD1	2.42	0.41
1:A:318:LEU:O	1:A:319:LYS:HD2	2.20	0.41
1:A:438:VAL:HG11	1:A:554:TRP:CD1	2.55	0.41
2:B:877:GLY:O	2:B:880:ILE:HG22	2.21	0.41
1:E:15:ALA:HB2	1:E:61:TYR:OH	2.21	0.41
1:E:1061:ASP:O	1:E:1065:ASN:N	2.54	0.41
2:F:70:LEU:HB3	2:F:155:VAL:HG23	2.03	0.41
2:F:383:LYS:O	2:F:386:GLN:HG3	2.19	0.41
2:F:875:ARG:NH2	2:F:935:ASN:OD1	2.53	0.41
3:G:348:ASP:O	3:G:352:PHE:HD2	2.03	0.41
2:J:206:VAL:HA	2:J:209:VAL:HG12	2.02	0.41
1:M:19:GLN:HA	1:M:23:LEU:HB2	2.02	0.41
1:M:60:ALA:HB2	1:M:418:LEU:HD21	2.02	0.41
3:O:133:ALA:HB3	3:O:164:ILE:HD11	2.02	0.41
1:A:139:SER:HB2	1:A:204:MET:HG3	2.01	0.41
1:A:897:ILE:HD11	1:A:924:ILE:HD11	2.02	0.41
2:B:554:ASP:OD1	2:B:554:ASP:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:232:HIS:CD2	3:G:234:LYS:H	2.38	0.41
1:I:1120:GLN:HB2	1:I:1123:TYR:CD2	2.55	0.41
1:M:774:SER:OG	1:M:775:SER:N	2.53	0.41
1:M:1062:GLY:HA3	1:M:1121:PRO:HB3	2.03	0.41
4:P:22:LYS:NZ	4:P:32:GLU:HG3	2.36	0.41
2:B:83:LYS:HG3	2:B:84:ILE:H	1.85	0.41
1:E:210:GLU:OE1	1:E:428:ARG:NH1	2.53	0.41
2:F:373:MET:SD	2:F:385:VAL:HG13	2.61	0.41
2:F:846:GLU:O	2:F:849:ILE:N	2.53	0.41
2:F:1002:LEU:HA	2:F:1069:LEU:HD23	2.03	0.41
2:F:1033:ASN:O	2:F:1037:LYS:HG2	2.21	0.41
1:I:592:GLY:HA2	1:I:599:VAL:O	2.20	0.41
2:N:89:TYR:CE1	2:N:177:LEU:HD11	2.56	0.41
2:N:89:TYR:CZ	2:N:177:LEU:HD21	2.56	0.41
2:N:371:TYR:HA	2:N:374:ILE:HG22	2.03	0.41
2:N:535:VAL:O	2:N:539:LEU:HG	2.20	0.41
2:N:996:ARG:O	2:N:1000:VAL:HG23	2.21	0.41
3:O:221:TYR:HE1	3:O:254:TRP:CZ2	2.39	0.41
1:A:285:THR:HG23	1:A:286:LYS:HG3	2.03	0.41
2:B:123:ARG:NE	2:B:123:ARG:HA	2.36	0.41
2:B:198:GLU:OE2	1:E:83:LYS:NZ	2.53	0.41
2:B:655:ARG:NE	2:B:657:GLN:HB3	2.36	0.41
2:B:955:GLY:C	2:B:1021:LYS:HZ2	2.29	0.41
2:B:1016:LEU:HB3	2:B:1077:LEU:HD12	2.02	0.41
2:F:533:GLU:O	2:F:536:LYS:HG2	2.21	0.41
3:G:232:HIS:NE2	3:G:237:LEU:HD12	2.36	0.41
4:H:28:ILE:O	4:H:32:GLU:HB2	2.20	0.41
1:I:148:MET:HE3	1:I:148:MET:HA	2.03	0.41
1:I:216:ASP:OD1	1:I:216:ASP:N	2.54	0.41
1:I:786:LEU:O	1:I:791:GLY:N	2.53	0.41
2:J:89:TYR:CE1	2:J:181:TYR:HE2	2.39	0.41
2:J:486:GLN:NE2	2:N:105:ASP:HB3	2.35	0.41
2:J:495:VAL:HG21	2:J:602:LEU:HD11	2.03	0.41
2:J:586:TYR:HB3	2:J:782:VAL:HG21	2.03	0.41
3:K:216:THR:O	3:K:220:MET:HG2	2.21	0.41
3:K:222:THR:HG1	3:K:367:ARG:HH22	1.63	0.41
3:K:258:SER:HB3	4:L:71:THR:HG23	2.02	0.41
1:M:554:TRP:NE1	1:M:558:GLY:O	2.40	0.41
1:M:786:LEU:HD11	1:M:794:TRP:HZ2	1.86	0.41
2:N:142:ASP:OD2	2:N:144:ARG:NH1	2.54	0.41
2:N:506:LEU:O	2:N:510:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:814:ALA:HB2	2:N:842:HIS:CE1	2.56	0.41
2:N:899:LEU:H	2:N:899:LEU:HD23	1.86	0.41
1:A:542:MET:HA	1:A:545:THR:HG22	2.03	0.41
1:A:592:GLY:HA2	1:A:599:VAL:O	2.21	0.41
2:B:70:LEU:HB3	2:B:155:VAL:HG23	2.03	0.41
2:B:718:GLU:HB3	2:B:719:TRP:CE3	2.56	0.41
3:C:341:ARG:HB3	3:C:342:PRO:HD3	2.03	0.41
1:E:293:CYS:O	1:E:328:TRP:N	2.53	0.41
1:E:411:SER:O	1:E:415:GLU:HG2	2.21	0.41
1:E:498:PRO:HB2	1:E:500:ARG:HH12	1.85	0.41
1:I:207:ALA:HB1	1:I:428:ARG:HH12	1.84	0.41
1:I:224:PRO:HD3	2:N:108:LYS:HE3	2.02	0.41
2:J:477:ARG:HD3	2:N:103:ARG:HH12	1.86	0.41
1:M:265:PHE:HA	1:M:268:PHE:CZ	2.56	0.41
1:M:336:ILE:HG13	1:M:337:LEU:N	2.36	0.41
1:M:554:TRP:CE2	1:M:560:PRO:HG3	2.56	0.41
1:M:1055:GLN:HE21	1:M:1189:TYR:HB2	1.85	0.41
2:N:727:ILE:HD12	2:N:750:ARG:HH22	1.86	0.41
1:A:57:LEU:HG	1:A:61:TYR:CE2	2.56	0.40
1:A:337:LEU:HA	1:A:340:VAL:HG12	2.02	0.40
1:A:451:ILE:HD11	1:A:571:LEU:HD11	2.03	0.40
1:A:1053:GLN:HG2	1:A:1057:ARG:NH2	2.32	0.40
2:B:242:ALA:O	2:B:246:LEU:HD23	2.21	0.40
2:B:1026:ARG:NH2	2:B:1029:LYS:HD2	2.35	0.40
1:E:117:ASN:OD1	1:E:118:THR:N	2.46	0.40
1:E:450:GLU:O	1:E:454:ILE:HG12	2.21	0.40
2:F:313:PHE:HZ	2:F:379:ARG:HH12	1.68	0.40
4:H:46:GLU:CD	4:H:50:GLN:HE22	2.28	0.40
2:J:849:ILE:O	2:J:853:LEU:HD23	2.21	0.40
3:K:322:TYR:O	3:K:325:VAL:HG23	2.21	0.40
2:N:645:ILE:HD11	2:N:648:GLY:HA2	2.03	0.40
2:N:885:TYR:HD1	2:N:888:GLN:HE21	1.69	0.40
3:O:196:ILE:O	3:O:199:SER:OG	2.31	0.40
1:A:335:PHE:HB3	1:A:351:TYR:CE2	2.56	0.40
1:A:1175:MET:HE1	3:C:378:VAL:HA	2.04	0.40
2:B:293:ASP:OD1	2:B:294:ALA:N	2.54	0.40
2:B:954:ASN:HB3	2:B:1021:LYS:HG3	2.03	0.40
2:F:632:ASN:HB2	2:F:633:PRO:HD3	2.03	0.40
3:G:320:TYR:O	3:G:324:ARG:HG3	2.22	0.40
4:H:37:MET:SD	4:H:44:PRO:HG2	2.62	0.40
2:J:846:GLU:HA	2:J:849:ILE:HD12	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:22:LYS:NZ	4:L:32:GLU:HG3	2.36	0.40
1:M:823:TRP:C	1:M:827:ARG:HH12	2.29	0.40
2:N:59:THR:HG21	2:N:445:GLN:HG3	2.03	0.40
3:O:120:VAL:HG13	3:O:352:PHE:CE2	2.55	0.40
3:O:182:ARG:NH2	3:O:205:PRO:O	2.55	0.40
1:A:879:LEU:O	1:A:882:GLU:HG3	2.22	0.40
2:B:481:MET:HE3	2:B:481:MET:HB3	1.91	0.40
2:B:486:GLN:HE22	2:B:492:ASP:H	1.70	0.40
2:B:918:GLN:O	2:B:919:GLN:NE2	2.52	0.40
2:B:928:ARG:HD2	2:B:1055:TYR:CD1	2.56	0.40
1:E:555:ARG:HA	1:E:555:ARG:CZ	2.51	0.40
2:F:179:LEU:O	2:F:182:LEU:HG	2.21	0.40
2:F:584:ASP:N	2:F:584:ASP:OD1	2.53	0.40
2:F:946:TRP:O	2:F:949:LEU:HG	2.21	0.40
2:F:1035:PHE:HB3	2:F:1054:PHE:CZ	2.56	0.40
2:F:1071:LYS:NZ	2:J:1078:LEU:HD13	2.37	0.40
2:J:101:TYR:CE2	2:J:110:ARG:HB2	2.57	0.40
2:J:293:ASP:OD1	2:J:294:ALA:N	2.54	0.40
1:M:216:ASP:OD1	1:M:216:ASP:N	2.54	0.40
2:N:43:GLU:OE2	2:N:47:ASP:HB2	2.22	0.40
2:N:784:TYR:CZ	2:N:788:PHE:CZ	3.10	0.40
1:A:331:PHE:HA	1:A:334:TYR:CD2	2.57	0.40
2:B:1006:VAL:HA	2:B:1009:VAL:HG22	2.04	0.40
3:C:320:TYR:O	3:C:324:ARG:HG3	2.22	0.40
2:F:351:LYS:HD2	2:F:352:PRO:HD2	2.03	0.40
2:F:373:MET:HE1	2:F:385:VAL:O	2.21	0.40
2:F:397:HIS:HB2	2:F:405:VAL:HB	2.04	0.40
2:F:732:ASN:ND2	2:F:758:LYS:HE3	2.36	0.40
2:F:778:LEU:O	2:F:782:VAL:HG13	2.22	0.40
3:G:90:LEU:HD13	3:G:104:PHE:HE1	1.86	0.40
2:J:240:GLY:HA2	2:J:279:LEU:HD12	2.03	0.40
2:J:315:GLN:NE2	2:J:316:THR:HG23	2.36	0.40
2:J:850:GLN:HG2	2:J:876:ILE:HD12	2.04	0.40
2:J:908:LYS:O	2:J:911:LEU:HG	2.20	0.40
3:K:306:LYS:NZ	4:L:147:THR:HA	2.37	0.40
1:M:500:ARG:HE	1:M:501:HIS:CD2	2.39	0.40
2:N:632:ASN:HB2	2:N:633:PRO:HD3	2.03	0.40
1:A:14:TYR:CD1	1:A:408:ILE:HD11	2.56	0.40
1:A:55:TRP:HZ3	1:A:153:LEU:HD11	1.87	0.40
3:C:60:SER:HB3	3:C:63:GLU:OE1	2.21	0.40
3:C:65:ARG:CZ	3:C:65:ARG:HA	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:131:MET:HE1	3:C:219:ILE:HG22	2.03	0.40
4:D:33:LEU:HD23	4:D:37:MET:CE	2.51	0.40
1:E:1127:LEU:O	1:E:1131:ILE:HG12	2.22	0.40
2:F:718:GLU:HB3	2:F:719:TRP:CE3	2.56	0.40
2:F:851:GLN:O	2:F:855:ILE:HG22	2.20	0.40
1:I:1096:THR:O	1:I:1100:MET:HE3	2.21	0.40
2:J:126:LEU:O	2:J:130:MET:HG2	2.21	0.40
2:J:314:SER:O	2:J:317:LEU:HG	2.20	0.40
2:J:367:ILE:HD13	2:J:443:TRP:NE1	2.36	0.40
2:J:949:LEU:HG	2:J:965:GLN:HE22	1.85	0.40
2:J:1025:ASP:O	2:J:1029:LYS:HG2	2.22	0.40
3:K:23:LYS:N	3:K:36:ARG:O	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	989/1223 (81%)	926 (94%)	63 (6%)	0	100	100
1	E	989/1223 (81%)	924 (93%)	64 (6%)	1 (0%)	48	82
1	I	989/1223 (81%)	917 (93%)	71 (7%)	1 (0%)	48	82
1	M	989/1223 (81%)	914 (92%)	75 (8%)	0	100	100
2	B	997/1093 (91%)	965 (97%)	31 (3%)	1 (0%)	48	82
2	F	997/1093 (91%)	964 (97%)	32 (3%)	1 (0%)	48	82
2	J	997/1093 (91%)	960 (96%)	37 (4%)	0	100	100
2	N	997/1093 (91%)	961 (96%)	35 (4%)	1 (0%)	48	82
3	C	374/387 (97%)	358 (96%)	14 (4%)	2 (0%)	24	62
3	G	374/387 (97%)	352 (94%)	20 (5%)	2 (0%)	24	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	374/387 (97%)	353 (94%)	16 (4%)	5 (1%)	9	41
3	O	374/387 (97%)	356 (95%)	16 (4%)	2 (0%)	24	62
4	D	142/168 (84%)	138 (97%)	3 (2%)	1 (1%)	18	55
4	H	142/168 (84%)	137 (96%)	5 (4%)	0	100	100
4	L	142/168 (84%)	138 (97%)	4 (3%)	0	100	100
4	P	142/168 (84%)	138 (97%)	4 (3%)	0	100	100
All	All	10008/11484 (87%)	9501 (95%)	490 (5%)	17 (0%)	44	77

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	310	GLU
1	E	888	MET
2	F	310	GLU
3	G	108	LYS
3	C	108	LYS
3	K	17	TYR
3	K	19	ASN
3	K	108	LYS
2	N	310	GLU
3	O	108	LYS
3	K	21	GLU
4	D	78	LYS
1	I	66	ASP
3	C	120	VAL
3	K	120	VAL
3	O	120	VAL
3	G	120	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	864/1068 (81%)	864 (100%)	0	100	100
1	E	864/1068 (81%)	864 (100%)	0	100	100
1	I	864/1068 (81%)	864 (100%)	0	100	100
1	M	864/1068 (81%)	864 (100%)	0	100	100
2	B	885/975 (91%)	883 (100%)	2 (0%)	87	85
2	F	885/975 (91%)	884 (100%)	1 (0%)	88	88
2	J	885/975 (91%)	885 (100%)	0	100	100
2	N	885/975 (91%)	884 (100%)	1 (0%)	88	88
3	C	336/349 (96%)	336 (100%)	0	100	100
3	G	336/349 (96%)	336 (100%)	0	100	100
3	K	334/349 (96%)	331 (99%)	3 (1%)	70	76
3	O	336/349 (96%)	336 (100%)	0	100	100
4	D	114/143 (80%)	114 (100%)	0	100	100
4	H	114/143 (80%)	113 (99%)	1 (1%)	70	76
4	L	114/143 (80%)	114 (100%)	0	100	100
4	P	114/143 (80%)	113 (99%)	1 (1%)	70	76
All	All	8794/10140 (87%)	8785 (100%)	9 (0%)	87	88

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	315	GLN
2	B	947	GLN
2	F	521	GLN
4	H	147	THR
3	K	18	GLU
3	K	93	THR
3	K	95	GLU
2	N	947	GLN
4	P	147	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	90	HIS
1	A	106	GLN
1	A	288	GLN
1	A	1051	GLN
1	A	1125	GLN
2	B	51	HIS
2	B	171	GLN
2	B	191	GLN
2	B	204	ASN
2	B	228	ASN
2	B	386	GLN
2	B	740	GLN
2	B	864	ASN
2	B	962	HIS
2	B	1019	GLN
2	B	1039	GLN
3	C	321	GLN
1	E	129	GLN
1	E	147	GLN
1	E	288	GLN
1	E	364	ASN
1	E	925	GLN
1	E	948	ASN
1	E	959	HIS
1	E	1053	GLN
1	E	1159	ASN
2	F	51	HIS
2	F	85	GLN
2	F	171	GLN
2	F	191	GLN
2	F	422	ASN
2	F	478	ASN
2	F	607	GLN
2	F	842	HIS
2	F	1019	GLN
3	G	19	ASN
3	G	232	HIS
3	G	298	HIS
3	G	321	GLN
4	H	50	GLN
1	I	129	GLN
1	I	167	ASN

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Mol	Chain	Res	Type
1	I	288	GLN
1	I	404	GLN
1	I	590	GLN
1	I	895	GLN
1	I	1080	GLN
1	I	1110	HIS
2	J	85	GLN
2	J	229	ASN
2	J	272	HIS
2	J	315	GLN
2	J	381	ASN
2	J	486	GLN
2	J	522	GLN
2	J	632	ASN
2	J	652	HIS
2	J	732	ASN
2	J	776	GLN
2	J	842	HIS
2	J	965	GLN
2	J	1019	GLN
3	K	19	ASN
3	K	39	HIS
3	K	204	HIS
3	K	232	HIS
3	K	298	HIS
3	K	321	GLN
1	M	27	ASN
1	M	288	GLN
1	M	349	GLN
1	M	386	ASN
1	M	404	GLN
1	M	536	ASN
1	M	1110	HIS
2	N	51	HIS
2	N	204	ASN
2	N	228	ASN
2	N	397	HIS
2	N	527	GLN
2	N	531	GLN
2	N	540	GLN
2	N	842	HIS
3	O	84	HIS

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Mol	Chain	Res	Type
3	O	89	GLN
3	O	204	HIS
3	O	246	ASN
3	O	248	GLN
3	O	298	HIS
3	O	364	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

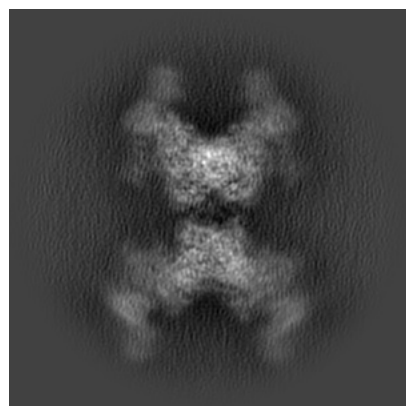
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39778. These allow visual inspection of the internal detail of the map and identification of artifacts.

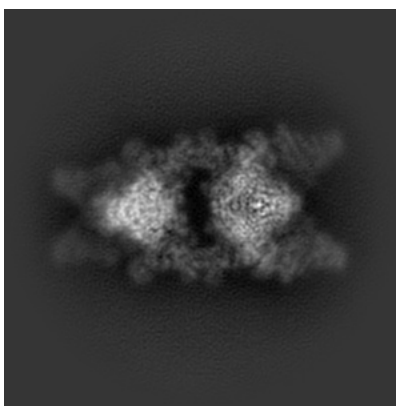
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

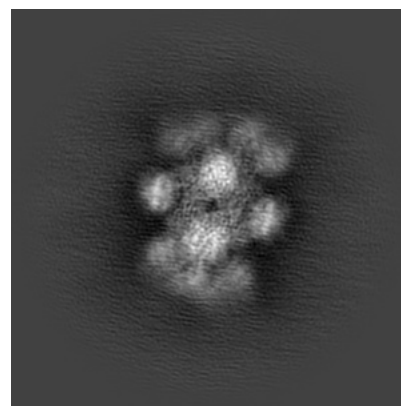
6.1.1 Primary map



X

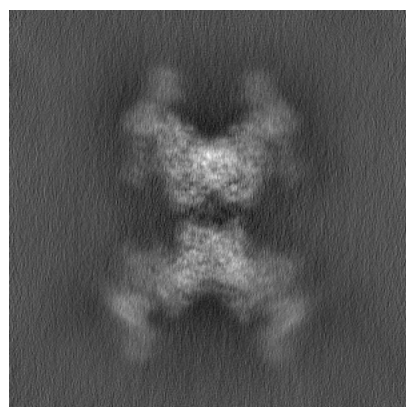


Y

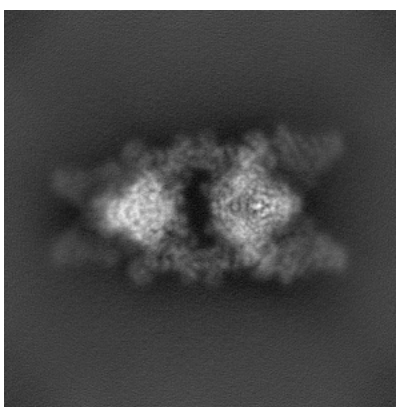


Z

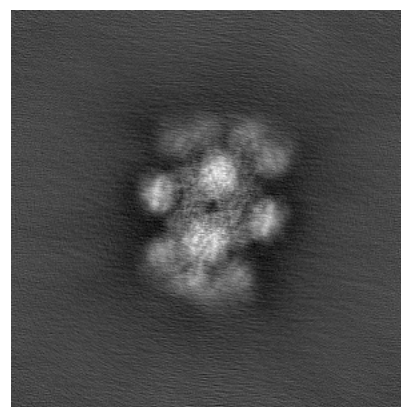
6.1.2 Raw map



X



Y

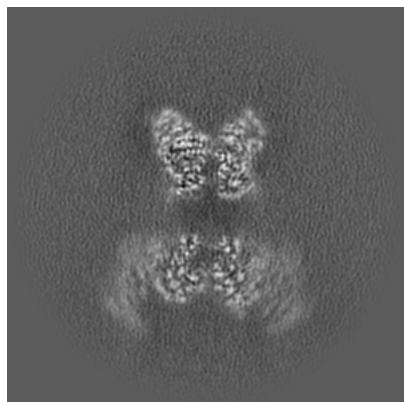


Z

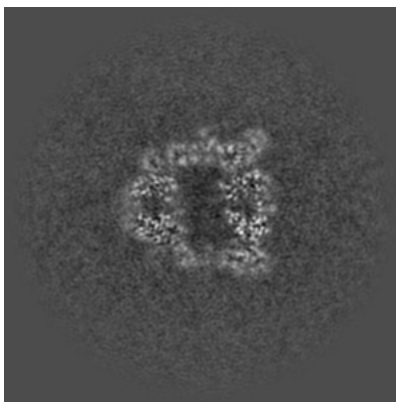
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

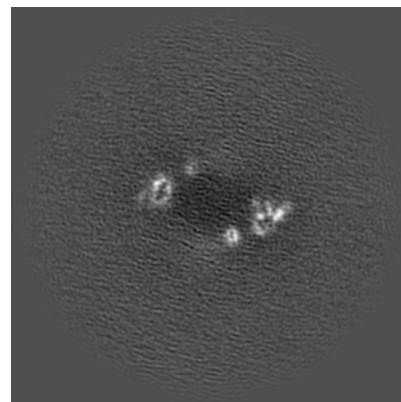
6.2.1 Primary map



X Index: 200

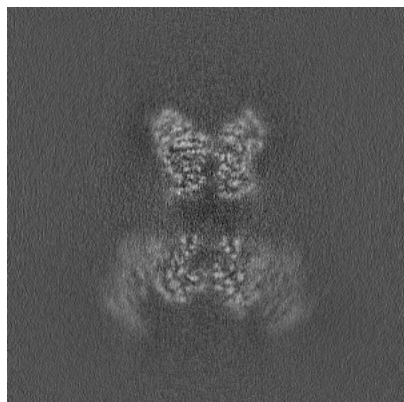


Y Index: 200

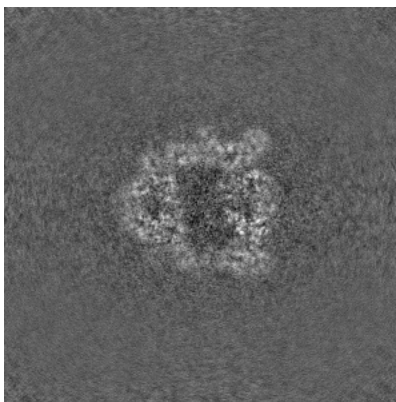


Z Index: 200

6.2.2 Raw map



X Index: 200



Y Index: 200

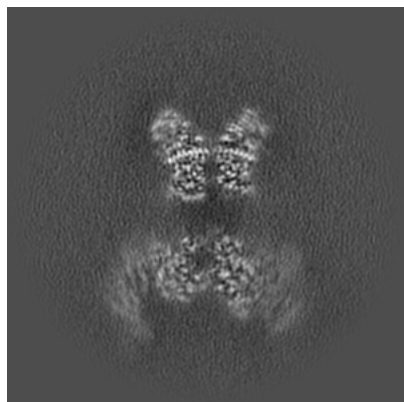


Z Index: 200

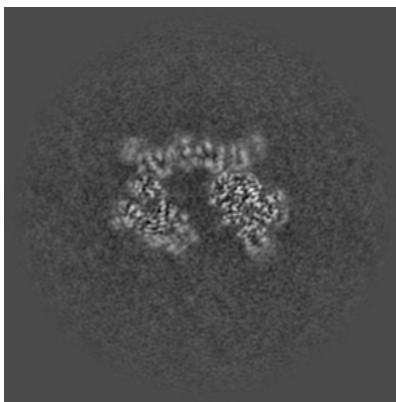
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

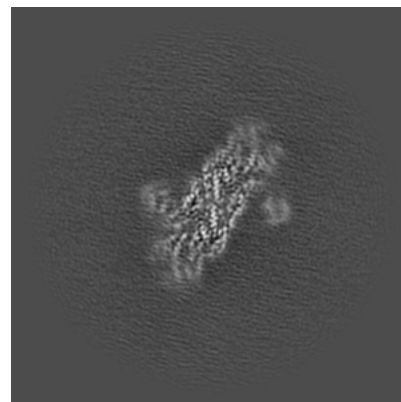
6.3.1 Primary map



X Index: 203

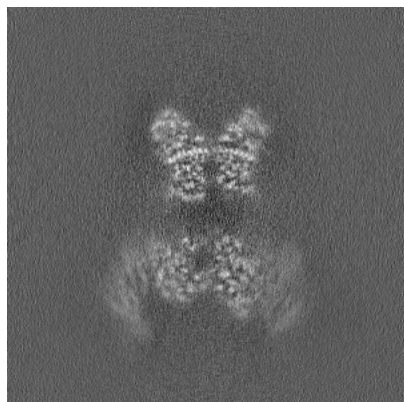


Y Index: 185

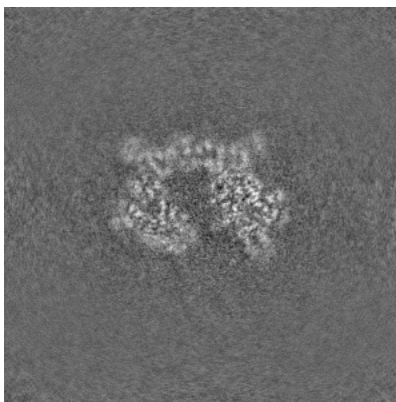


Z Index: 255

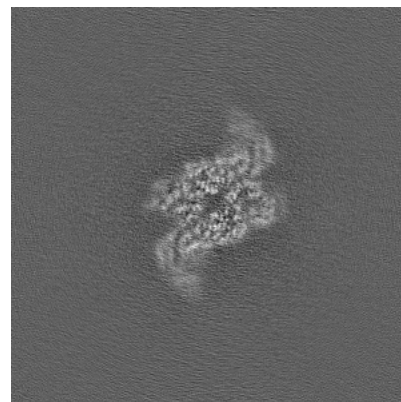
6.3.2 Raw map



X Index: 203



Y Index: 185

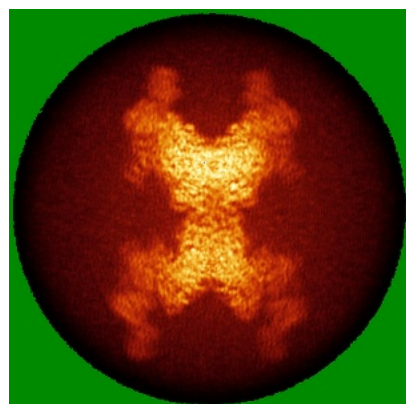


Z Index: 239

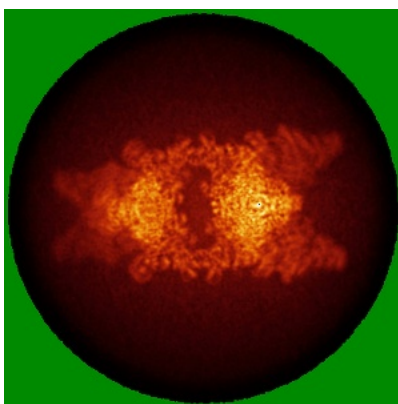
The images above show the largest variance slices of the map in three orthogonal directions.

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

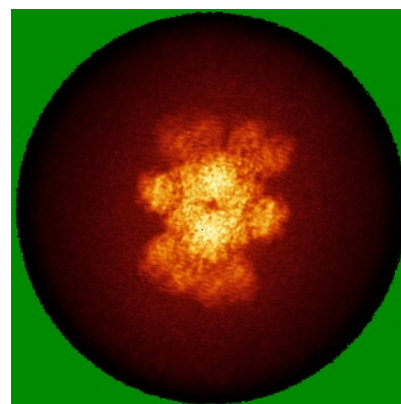
6.4.1 Primary map



X

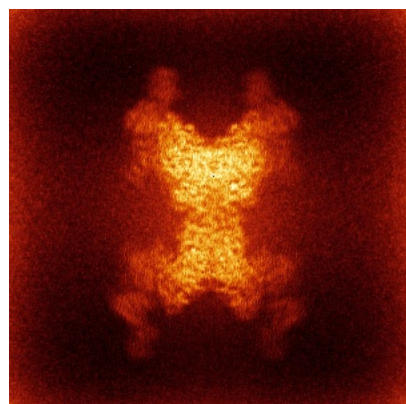


Y

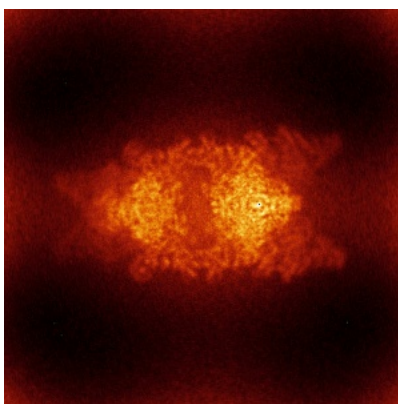


Z

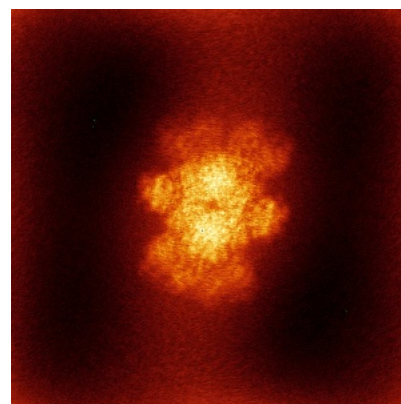
6.4.2 Raw map



X



Y



Z

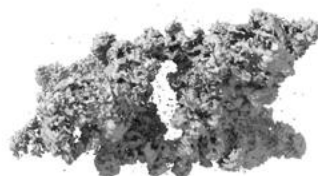
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



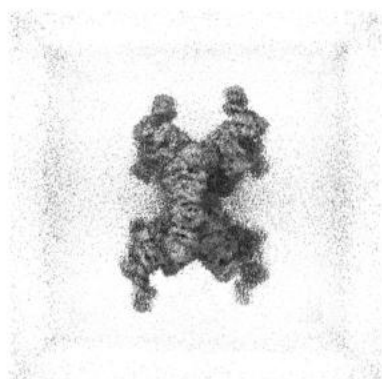
Y



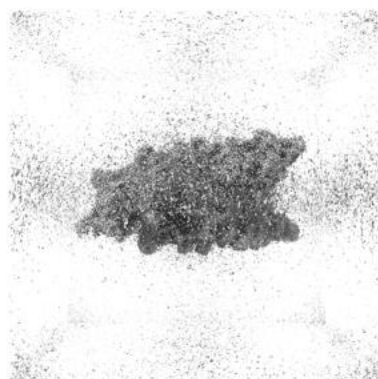
Z

The images above show the 3D surface view of the map at the recommended contour level 0.125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

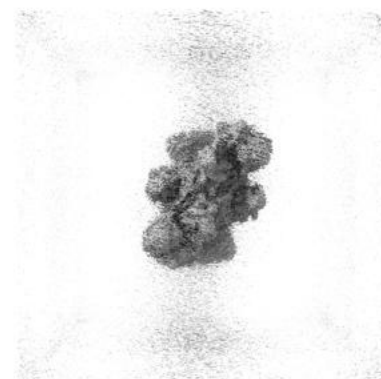
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

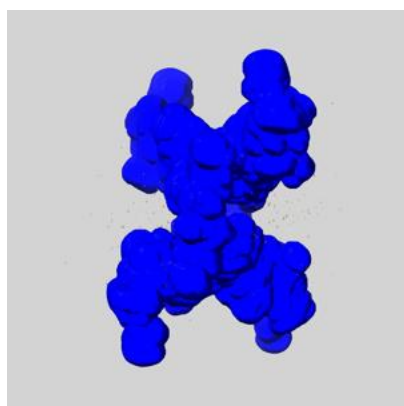
6.6 Mask visualisation [i](#)

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

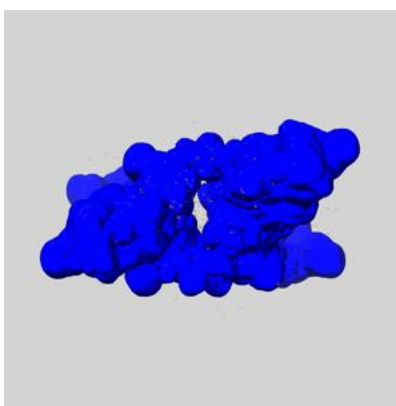
A mask typically either:

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

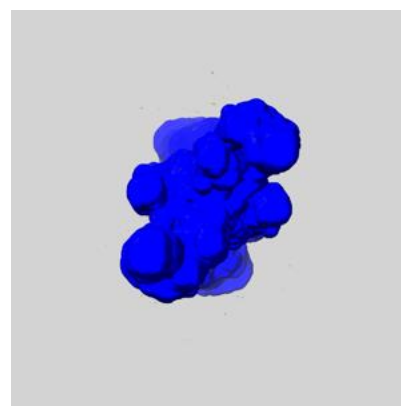
6.6.1 emd_39778_msk_1.map [i](#)



X



Y

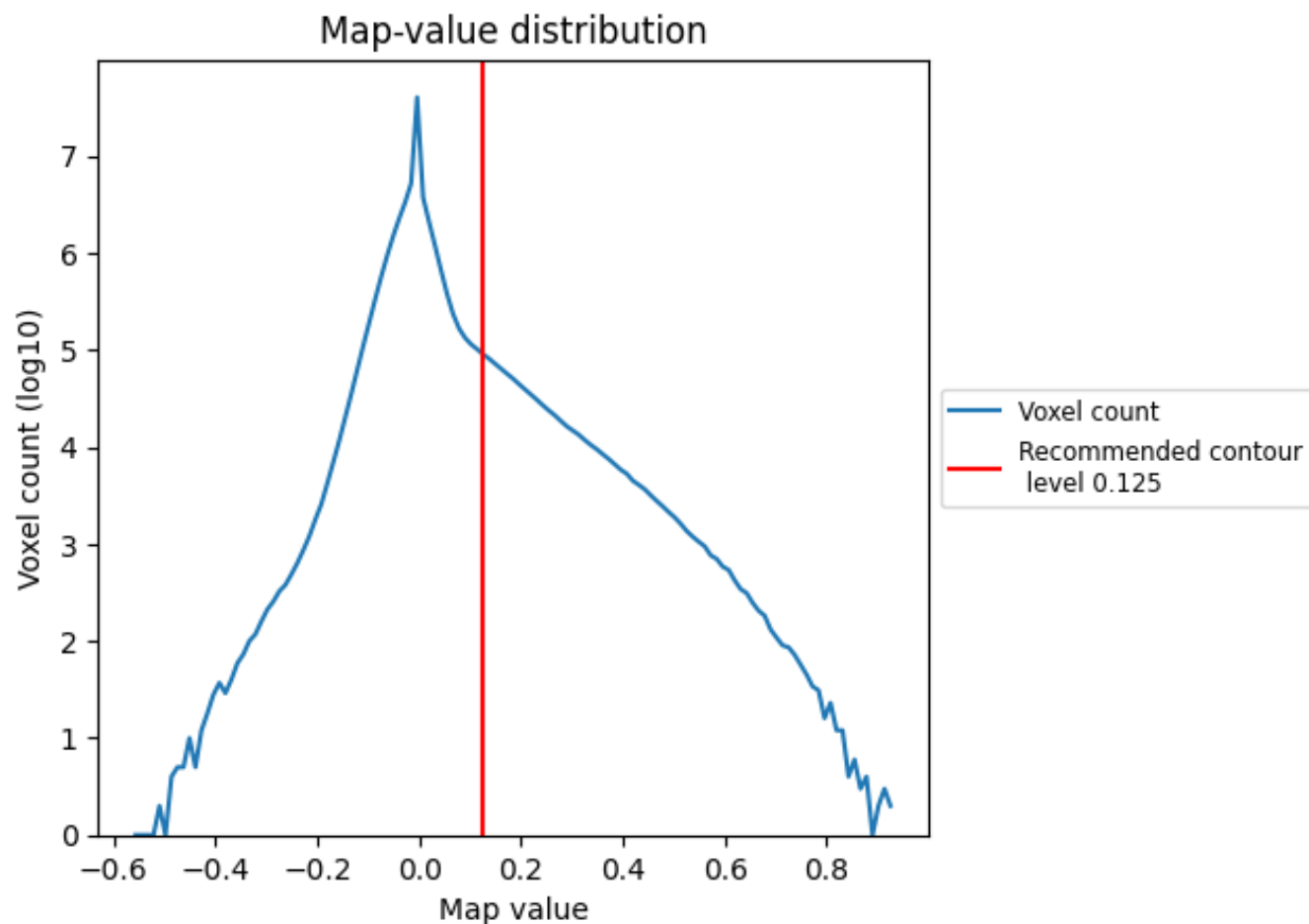


Z

7 Map analysis [i](#)

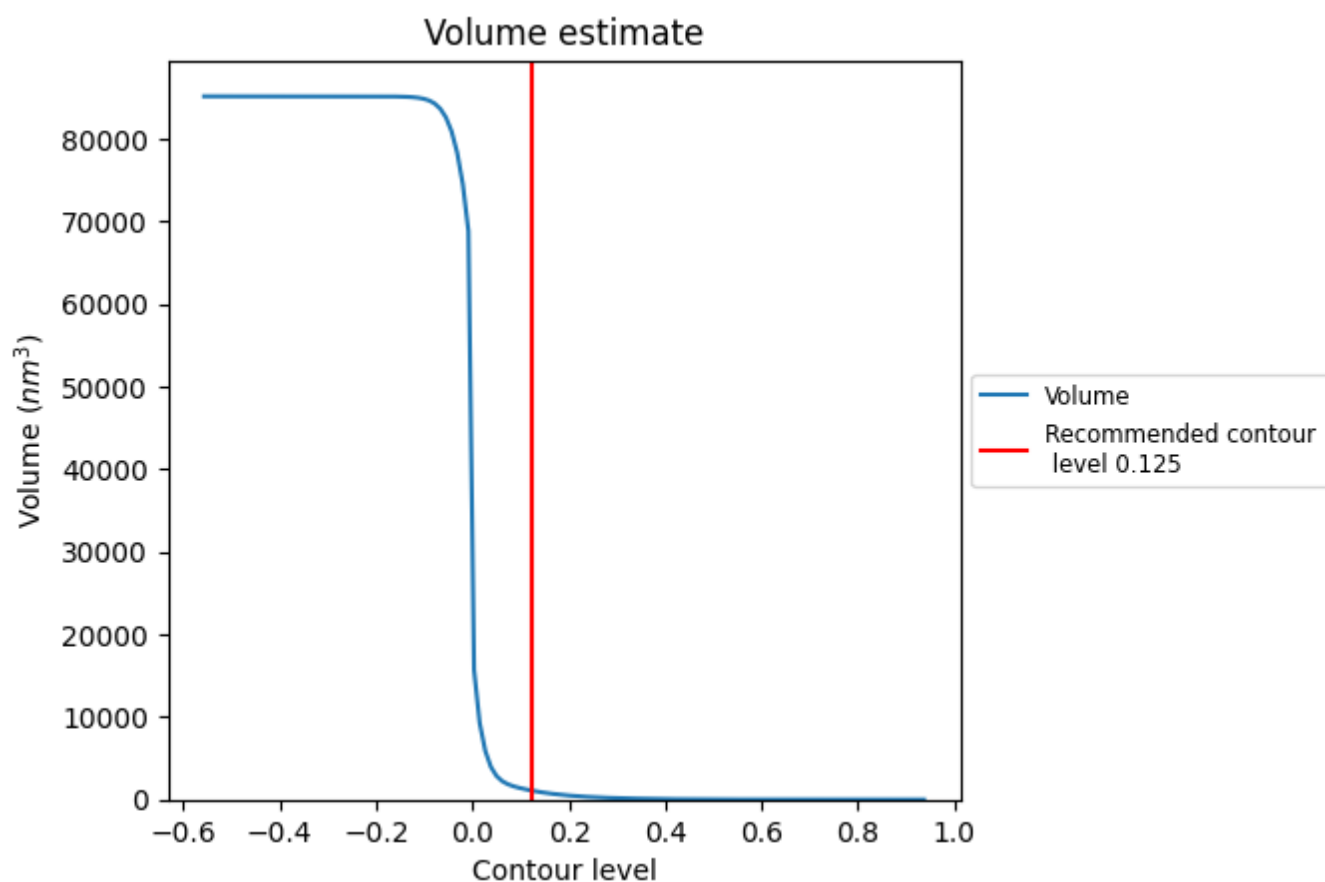
This section contains the results of statistical analysis of the map.

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.

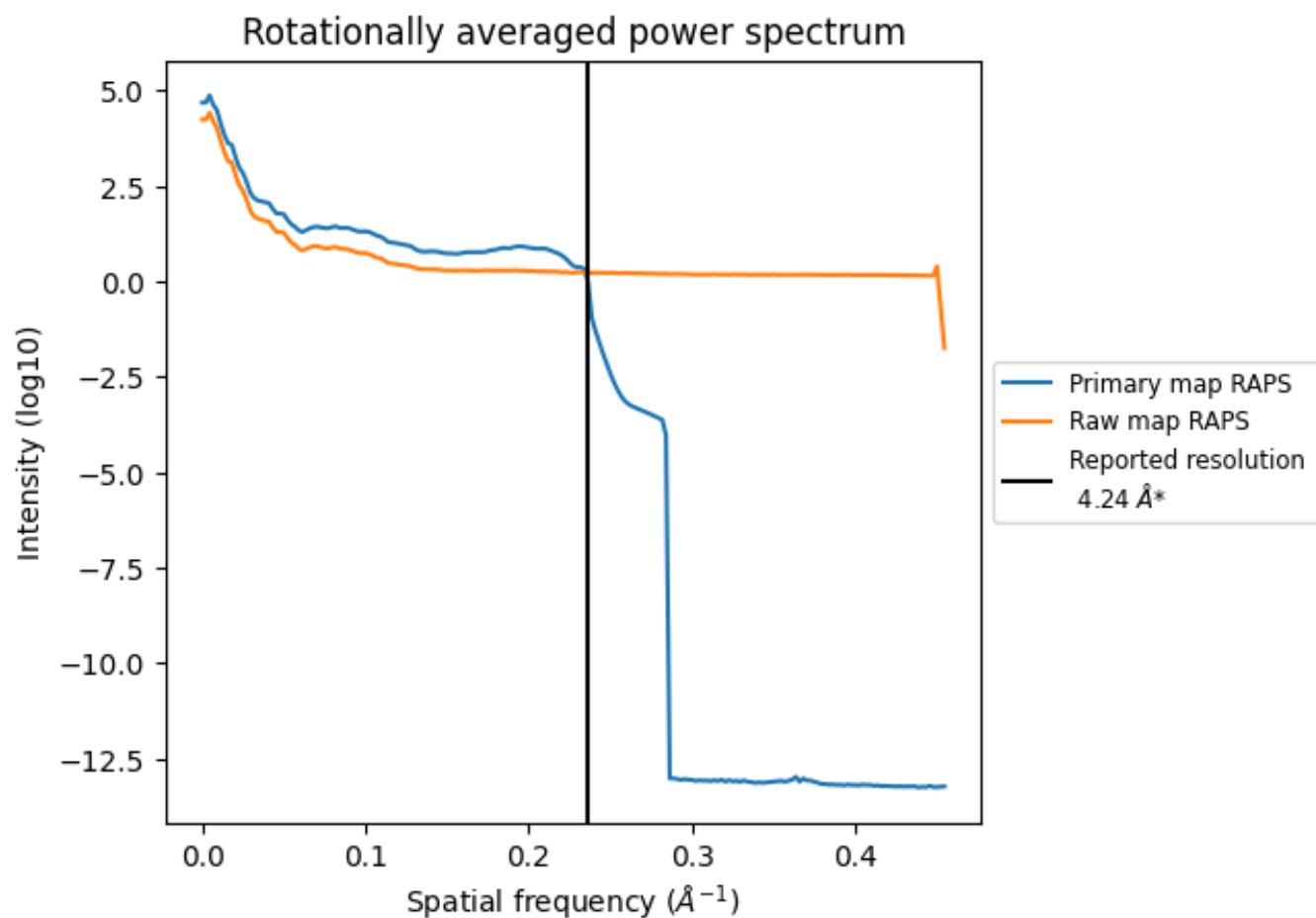
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1066 nm³; this corresponds to an approximate mass of 963 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 ⓘ

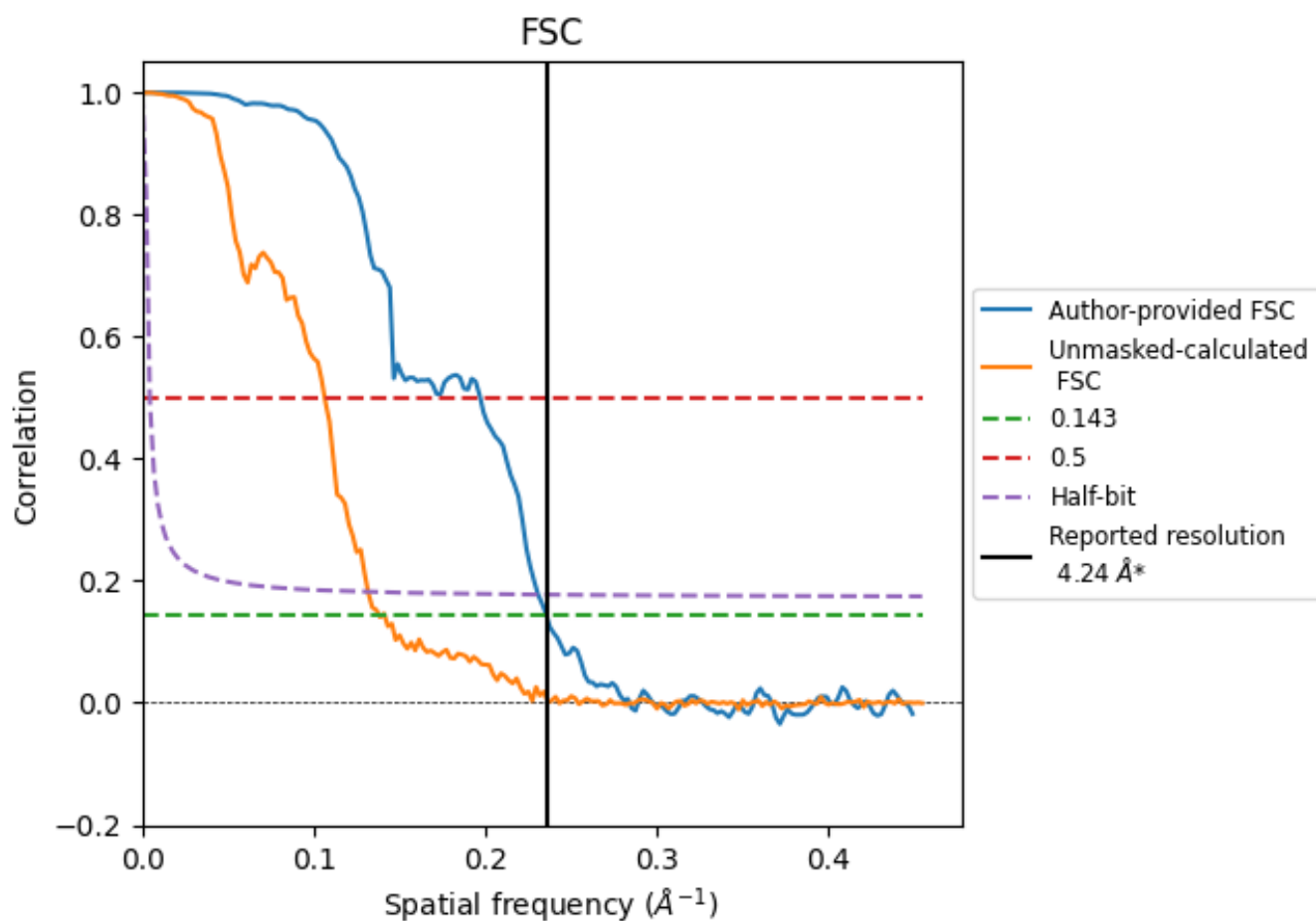


*Reported resolution corresponds to spatial frequency of 0.236 Å⁻¹

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 $0.236 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

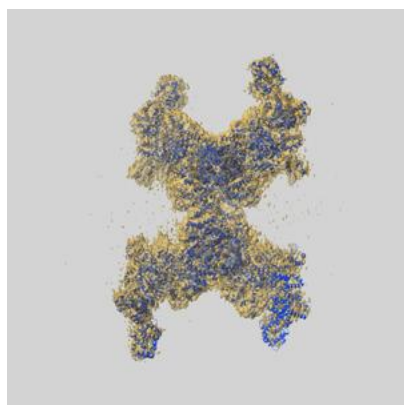
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.24	-	-
Author-provided FSC curve	4.24	5.08	4.33
Unmasked-calculated*	7.24	9.40	7.59

*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 7.24 differs from the reported value 4.24 by more than 10 %

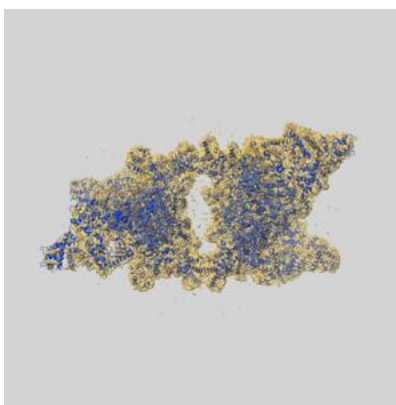
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39778 and PDB model 8Z5Q. Per-residue inclusion information can be found in section [3](#) on page [8](#).

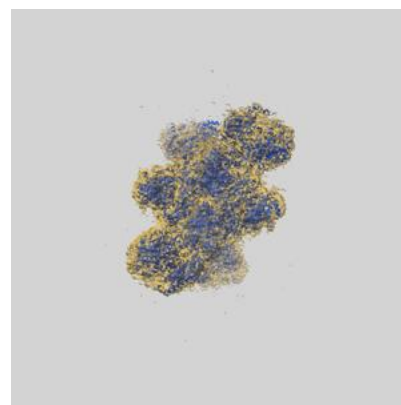
9.1 Map-model overlay [i](#)



X



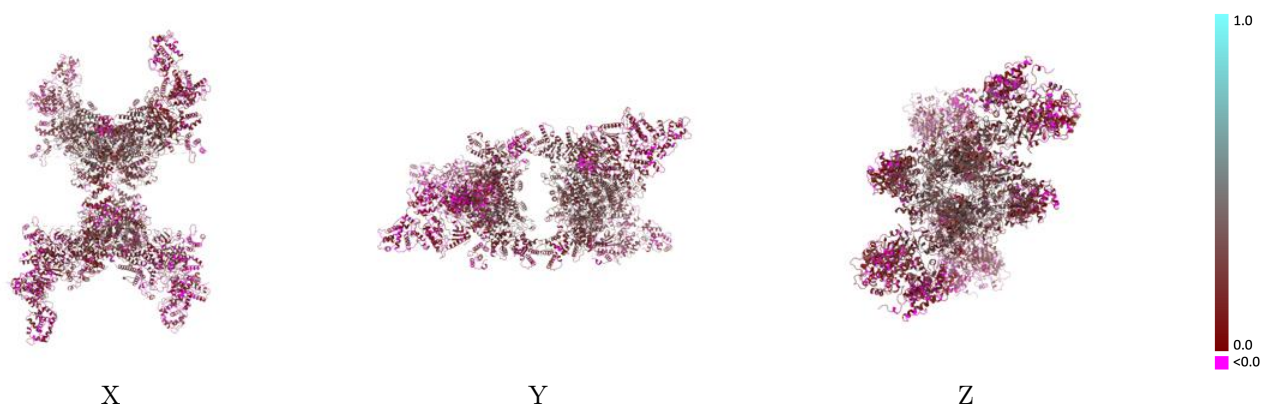
Y



Z

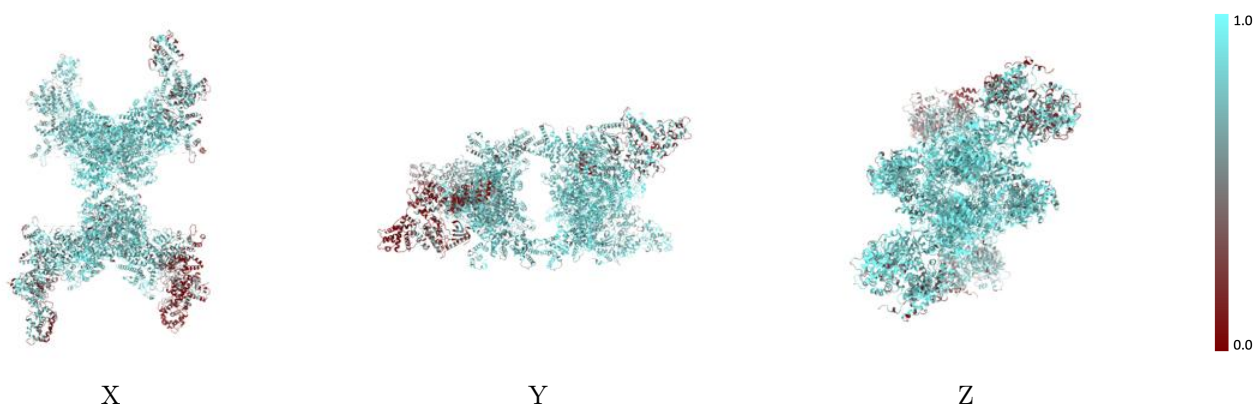
The images above show the 3D surface view of the map at the recommended contour level 0.125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



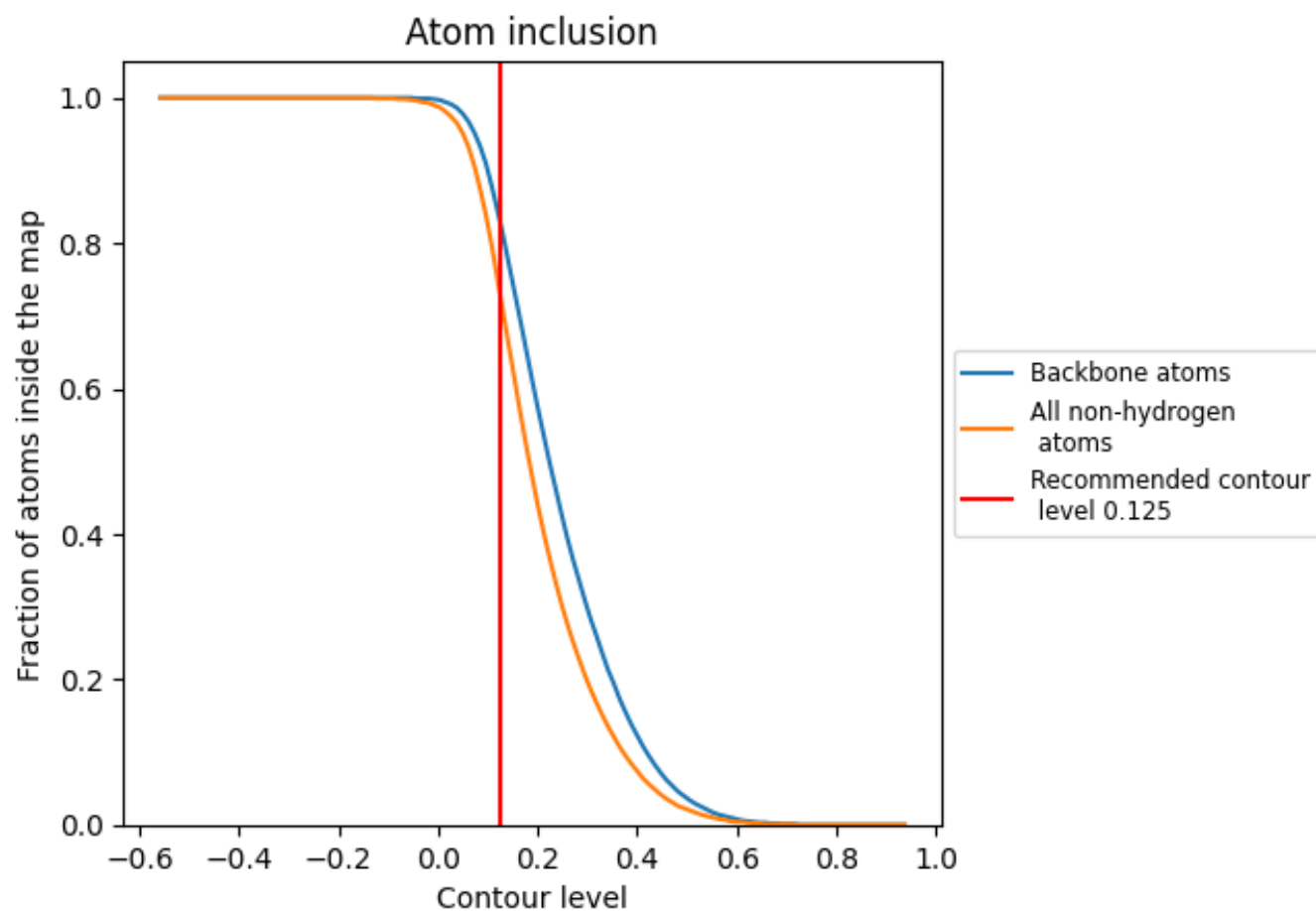
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.125).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 73% 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 (0.125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7290	 0.1890
A	 0.8380	 0.2270
B	 0.8670	 0.2500
C	 0.7650	 0.1470
D	 0.7730	 0.1250
E	 0.7770	 0.2150
F	 0.8670	 0.2660
G	 0.6290	 0.1470
H	 0.5130	 0.0960
I	 0.6860	 0.1340
J	 0.8000	 0.2070
K	 0.5980	 0.1180
L	 0.4130	 0.1060
M	 0.5630	 0.1230
N	 0.8110	 0.2290
O	 0.3340	 0.1030
P	 0.1220	 0.0960

