



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 10:46 AM UTC

PDB ID : 7B70 / pdb_00007b70
EMDB ID : EMD-12063
Title : TRAPPCore plus C8 (355-596) and C11 (1-718) from MiniTRAPPIII
Authors : Galindo, A.; Munro, S.; Planelles-Herrero, V.J.
Deposited on : 2020-12-09
Resolution : 4.00 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

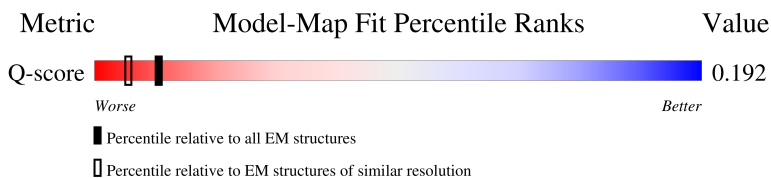
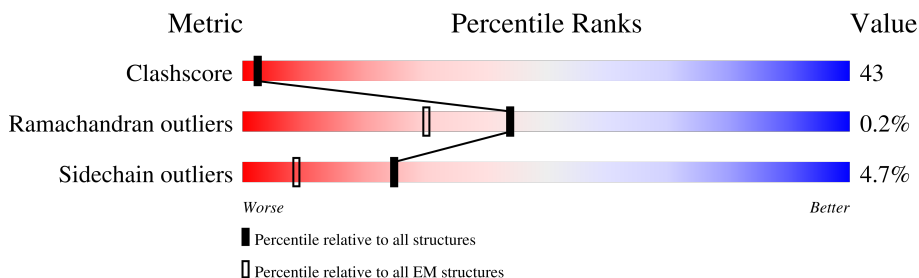
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	7587 (3.50 - 4.50)

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	178	
1	G	178	
2	B	152	
3	C	145	

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Mol	Chain	Length	Quality of chain
4	D	219	38% 62%
5	E	139	35% 65%
6	F	194	26% 57% 15%
7	H	138	20% 77%
8	I	246	11% 37% 29% 17% 15%
9	J	718	38% 47% 14%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 17084 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 Trafficking protein particle complex subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	165	Total	C	N	O	S	0	0
			1337	847	229	253	8		
1	G	169	Total	C	N	O	S	0	0
			1363	861	233	261	8		

- Molecule 2 is a protein called GEO08327p1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	151	Total	C	N	O	S	0	0
			1226	780	211	227	8		

- Molecule 3 is a protein called Trafficking protein particle complex subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	145	Total	C	N	O	S	0	0
			1204	792	194	216	2		

- Molecule 4 is a protein called Trafficking protein particle complex subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	219	Total	C	N	O	S	0	0
			1741	1125	279	330	7		

- Molecule 5 is a protein called Probable trafficking protein particle complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	139	Total	C	N	O	S	0	0
			1177	759	199	214	5		

- Molecule 6 is a protein called Trafficking protein particle complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	164	Total	C	N	O	S	0	0
			1333	852	225	250	6		

- Molecule 7 is a protein called TRAPPC2L.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	138	Total	C	N	O	S	0	0
			1089	697	179	207	6		

- Molecule 8 is a protein called FI18195p1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	208	Total	C	N	O	S	0	0
			1710	1096	301	301	12		

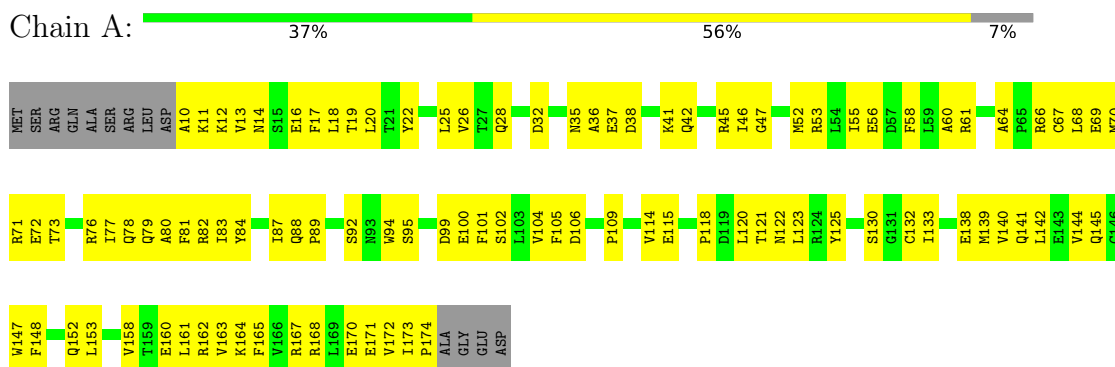
- Molecule 9 is a protein called Trafficking protein particle complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	614	Total	C	N	O	S	0	0
			4904	3125	864	882	33		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

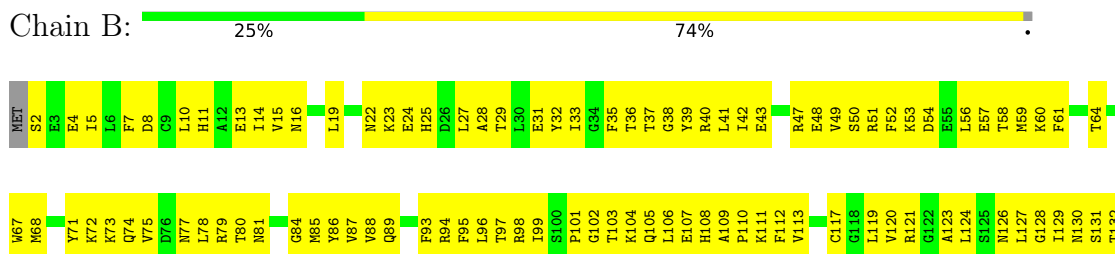
- Molecule 1: Trafficking protein particle complex subunit



- Molecule 1: Trafficking protein particle complex subunit



- Molecule 2: GEO08327p1



V133
T134
A135
E136
V137
Q138
S139
I140
P141
A142
C143
K144
F145
H146
I147
E148
V149
M150
R151
M152

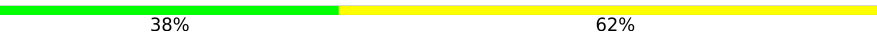
- Molecule 3: Trafficking protein particle complex subunit

Chain C:  41% 59%

K1 T2 T3 F4 N5 L6 Y7 D10 K11 F12 L16 H17 Y18 A19 E20 V21 T24 K25 S27 T30 R31 E32 E33 M41 L42 L43 F43 S44 L45 K46 S47 F48 K51 I52 S53 P54 H55 D56 F57 K58 E59 L62 Y63 Y64 K65 T66 N67 R68 L71 H72 Y73 L74

F77 S78 G79 L80 K81 F82 F83 L84 M85 T86 D87 T88 T89 A90 Y91 N92 V93 K94 E95 L96 Q98 Q99 I100 Y101 K102 K103 V104 M105 V106 E107 F108 M109 V110 R111 D112 P117 S123 E124 L125 F126 K129 R135 Q136 S137 F138 I139 F140 G141 I142 R143 N144 I145

- Molecule 4: Trafficking protein particle complex subunit

Chain D:  38% 62%

M1 I2 I3 Y4 G5 V6 Y7 I8 V9 S10 K11 L15 I16 F17 M18 N21 N22 V23 P24 R25 H28 E29 K30 K31 F32 L36 M37 D37 L40 D41 Y42 Y47 S50 F51 N52 R53 K54 D55 G56 I57 N58 V59 G60 H61 V62 L63 V64 A65 V66 V71 T75 L76

D77 D78 G79 R80 D81 V82 R83 T84 T85 L86 D87 A88 N91 Y92 P93 I94 N95 L96 K97 S99 R100 K102 M103 T104 T105 M106 E107 K108 I109 F110 L111 F115 Y116 P117 L118 F119 A120 I121 A122 S123 Q124 L125 S126 P127 E128 P129 K130 S131 S132 G133 I134 E135 I136 L137 E138 A139

D140 T143 C146 F147 Q148 T149 L150 T151 G152 G153 K154 F155 I157 T161 G162 L163 D167 L168 L169 R171 K172 V173 Y174 E175 L176 Y177 S178 D179 V180 L181 L182 K183 M184 F186 Y187 S188 L189 E190 M191 P192 I193 R194 L197 F198 D199 N200 Q203 V209 T212

G213 I214 S215 N216 D217 I218 K219

- Molecule 5: Probable trafficking protein particle complex subunit 2

Chain E:  35% 65%

H1 S2 T3 Y4 Y5 F6 V7 I8 V9 G10 Q11 Q12 D13 M14 P15 I16 P17 E18 K19 E20 F21 V24 N25 K26 E27 L28 R29 K30 E31 D32 H33 R34 T37 Q38 F39 I40 A41 H42 L45 D46 L47 V48 D49 E50 K52 K53 K54 T55 A56 N57 M58 Q59 L60 K61 S62 I63

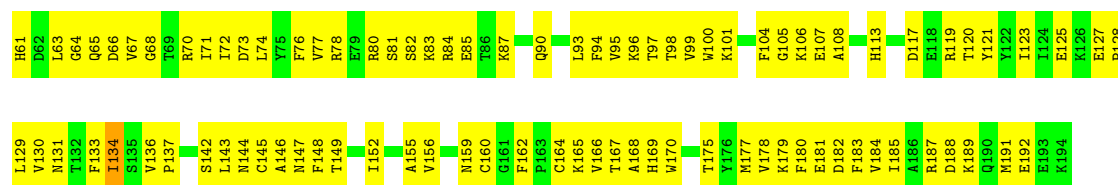
D64 R65 Q68 W69 F70 V71 S72 A73 F74 T75 I76 A77 S76 Q79 I80 R81 F82 R83 I84 V85 H86 D87 K88 K89 R90 D91 E92 G93 I94 K95 K96 F97 F98 N99 E100 M101 Y102 M110 N111 A112 F113 Y114 T118 P119 I120 K121 E126 K127 S128 K129 P54 E55 E56 Q57 T58 R59 R134 L60

Y136 L137 L138 S139

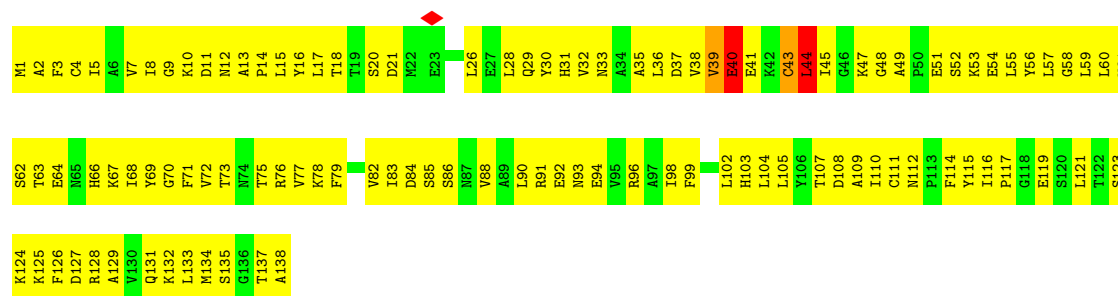
- Molecule 6: Trafficking protein particle complex subunit 5

Chain F:  26% 57% 15%

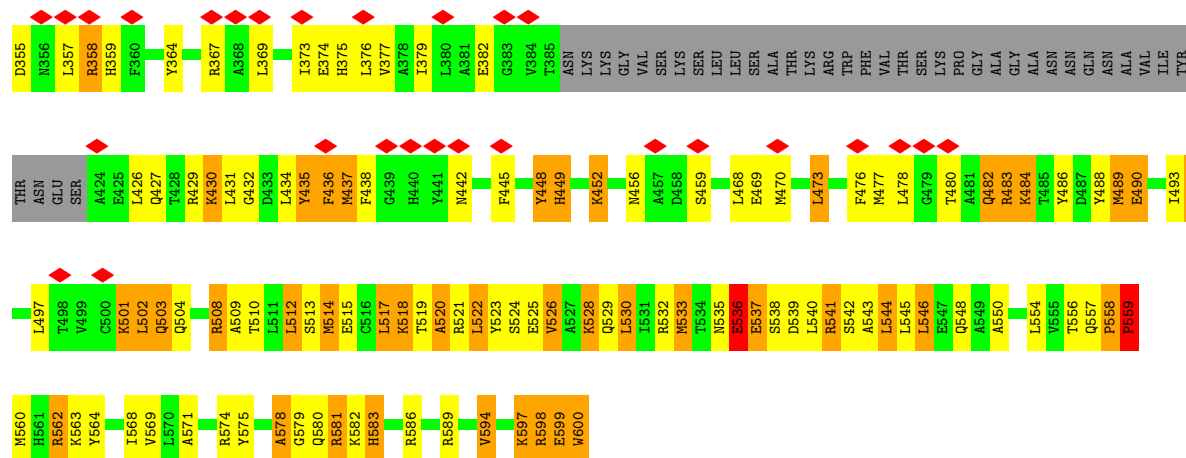
MET GLU LYS LEU GLU ALA LYS ILE SER SER MET ARG PRO ARG SER ASN ILE LEU ASP ARG PRO LEU SER LYS GLY LYS THR GLU VAL S31 Q32 S33 I34 V35 A36 L37 L38 F39 S40 E41 I42 I43 V43 Q44 Y45 S46 Q47 S48 R49 V50 F51 T52 V53 P54 E55 E56 Q57 T58 R59 R134 L60



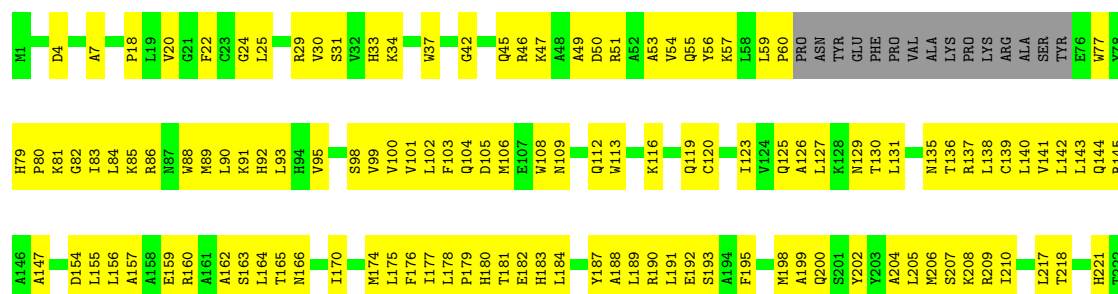
• Molecule 7: TRAPPC2L



• Molecule 8: FI18195p1



• Molecule 9: Trafficking protein particle complex subunit 11



SER	GLN	GLU	PRO	LYS	ASN	PHE	GLU	LYS	ASN	MET	ARG	LEU	GLU	PRO	GLY	S676	L680	F681	G682	S683	T684	E685	A686	Q687	Q688	N692	T693	Q694	L695	V698	R699	L700	E701	A702	H703	M704	G705	T706	D707	Q708	V709	A710	A711	T714	N718										
L596	Q597	L598	Q599	L600	I601	V602	L605	T606	D607	I608	P609	L610	R611	T612	R613	S614	F615	H616	L619	A620	D621	P625	G626	ASN	SER	TYR	LYS	LEU	GLU	ALA	LEU	LYS	TYR	PHE	CYS	PHE	PRO	THR	LEU	THR	GLN	ARG	GLY	GLN	LYS	GLN	PRO	ASP	ASP	GLU	GLN	LEU	GLU	ASN	PRO
H520	Q521	S522	D523	Q524	R527	I528	L529	I530	W535	Q536	V541	P542	P543	M544	P545	K546	P551	Q554	L556	T558	S559	A560	L561	A562	R563	V564	K565	S566	PRO	ILE	GLN	ILE	ASP	LEU	ASP	LEU	LYS	VAL	ASN	VAL	V579	E580	M581	T584	L590	S591	R592	D593	D594	L595					
K440	I441	Y442	K443	C444	L445	R446	F447	R448	K449	I453	D454	M455	A456	E457	Y458	L460	K461	S462	L471	Y472	M475	L476	Y479	K483	W484	T485	I486	I487	F488	T489	L492	R497	C498	A499	L500	L501	V505	A506	B507	Y508	I509	S512	V513	E514	A515	L516	S517	L518	R519						
D364	A365	A366	M367	E368	A369	Y370	M373	S377	GLU	ALA	THR	PRO	THR	PRO	ILE	GLN	ASN	PRO	LEU	SER	LEU	TYR	THR	GLU	PHE	PHE	GLY	ILE	ARG	ALA	VAL	LYS	THR	GLY	ASP	LEU	V406	Q409	M412	L415	C416	D417	Q418	E419	R420	S421	Y422	I428	M436	A437	Q438	F439			
S223	L224	K225	I226	Q229	F230	K231	L232	F234	V235	M238	R239	Q240	S243	T244	G245	Q246	K247	H248	Y249	A252	N255	L256	D257	E258	I259	R260	I261	C266	L269	K270	A273	G274	F275	L276	M277	Y278	K279	I280	L283	M284	F285	K286	L287	K288	T289	P290	R291	D292	A293						
I294	N295	Q296	F297	I298	I299	H300	K303	H304	K305	S306	R307	F310	K311	D312	L313	A314	F315	E316	H317	H318	A319	W320	L321	Q324	H325	L331	F332	C333	E334	A335	I336	G339	L343	Q344	T345	Q346	H347	P348	G349	I350	Y351	Y352	H353	K354	A355	A356	E357	F358	V359	M360	K361	R362	R363		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	486758	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 ($e^-/\text{\AA}^2$)	45.6	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	502.56, 502.56, 502.56	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2564, 1.2564, 1.2564	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	0.38	0/1360	0.67	0/1841
1	G	0.33	0/1386	0.55	0/1876
2	B	0.36	0/1250	0.65	0/1686
3	C	0.34	0/1237	0.58	0/1675
4	D	0.36	0/1776	0.62	0/2406
5	E	0.37	0/1207	0.63	1/1623 (0.1%)
6	F	0.37	0/1359	0.62	0/1833
7	H	0.45	0/1108	0.79	3/1498 (0.2%)
8	I	0.90	0/1749	1.23	3/2360 (0.1%)
9	J	0.31	0/5004	0.62	0/6769
All	All	0.44	0/17436	0.72	7/23567 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
6	F	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	40	GLU	N-CA-C	-7.22	103.73	112.54
7	H	39	VAL	N-CA-C	-6.94	105.30	113.42
8	I	569	VAL	N-CA-C	-6.06	104.39	111.00
7	H	44	LEU	N-CA-C	-5.95	106.07	113.15
5	E	40	ILE	N-CA-C	-5.26	104.39	111.44
8	I	578	ALA	N-CA-C	-5.11	108.31	114.75
8	I	558	PRO	N-CA-C	5.09	116.91	110.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	214	ILE	Peptide
6	F	134	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1337	0	1334	108	0
1	G	1363	0	1352	112	0
2	B	1226	0	1217	163	0
3	C	1204	0	1213	108	0
4	D	1741	0	1768	169	0
5	E	1177	0	1151	106	0
6	F	1333	0	1338	146	0
7	H	1089	0	1099	182	0
8	I	1710	0	1682	196	0
9	J	4904	0	4942	349	0
All	All	17084	0	17096	1481	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 43.

All (1481) 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)
8:I:510:THR:HG21	8:I:533:MET:CE	1.41	1.49
8:I:575:TYR:CA	8:I:579:GLY:HA3	1.38	1.47
8:I:575:TYR:HA	8:I:579:GLY:CA	1.42	1.45
8:I:514:MET:CG	8:I:526:VAL:HG11	1.53	1.38
8:I:537:GLU:OE1	8:I:545:LEU:HD11	1.24	1.35
8:I:537:GLU:HG3	8:I:545:LEU:CD1	1.53	1.35
8:I:518:LYS:O	8:I:523:TYR:CE1	1.81	1.34
8:I:539:ASP:OD1	8:I:578:ALA:HB3	1.21	1.31
8:I:358:ARG:HH21	8:I:359:HIS:N	1.24	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:513:SER:O	8:I:517:LEU:HG	1.17	1.29
8:I:537:GLU:CG	8:I:545:LEU:CD1	2.08	1.29
8:I:598:ARG:HG3	8:I:600:TRP:CZ3	1.70	1.26
8:I:518:LYS:O	8:I:523:TYR:HE1	0.92	1.25
8:I:358:ARG:HD2	8:I:358:ARG:C	1.65	1.21
8:I:358:ARG:NH2	8:I:359:HIS:N	1.91	1.18
8:I:598:ARG:HG3	8:I:600:TRP:CE3	1.83	1.14
8:I:537:GLU:CG	8:I:545:LEU:HD12	1.74	1.13
8:I:514:MET:HG2	8:I:526:VAL:HG11	1.29	1.13
8:I:514:MET:CB	8:I:526:VAL:CG1	2.27	1.12
8:I:537:GLU:CD	8:I:545:LEU:HD11	1.74	1.12
8:I:510:THR:HG21	8:I:533:MET:HE3	1.18	1.12
7:H:31:HIS:CD2	9:J:486:THR:HG22	1.85	1.11
8:I:513:SER:O	8:I:517:LEU:CG	1.99	1.10
8:I:355:ASP:O	8:I:358:ARG:NH2	1.83	1.10
7:H:31:HIS:HB2	9:J:486:THR:HG22	1.33	1.09
8:I:493:ILE:HG22	8:I:509:ALA:CB	1.83	1.08
8:I:493:ILE:HG22	8:I:509:ALA:HB3	1.33	1.08
7:H:31:HIS:CG	9:J:486:THR:HG22	1.88	1.08
8:I:514:MET:HA	8:I:526:VAL:CG1	1.82	1.07
8:I:358:ARG:NH2	8:I:359:HIS:H	1.52	1.07
8:I:514:MET:HA	8:I:526:VAL:HG13	1.18	1.06
8:I:514:MET:CG	8:I:526:VAL:CG1	2.32	1.06
7:H:31:HIS:CB	9:J:486:THR:HG22	1.86	1.06
8:I:510:THR:CG2	8:I:533:MET:CE	2.34	1.06
8:I:539:ASP:OD1	8:I:578:ALA:CB	2.03	1.05
8:I:575:TYR:O	8:I:579:GLY:O	1.73	1.05
8:I:514:MET:CB	8:I:526:VAL:HG11	1.86	1.03
8:I:518:LYS:HA	8:I:523:TYR:HD1	1.24	1.03
8:I:490:GLU:HA	8:I:493:ILE:CD1	1.90	1.02
8:I:510:THR:HG21	8:I:533:MET:HE2	1.36	1.01
8:I:546:LEU:HD12	8:I:574:ARG:HH21	1.23	1.00
7:H:31:HIS:CD2	9:J:486:THR:CG2	2.23	0.99
8:I:518:LYS:HA	8:I:523:TYR:CD1	1.97	0.99
8:I:575:TYR:O	8:I:579:GLY:N	1.96	0.98
8:I:358:ARG:HH21	8:I:359:HIS:H	1.02	0.97
8:I:514:MET:CA	8:I:526:VAL:CG1	2.41	0.97
8:I:598:ARG:CG	8:I:600:TRP:CZ3	2.47	0.96
8:I:514:MET:CA	8:I:526:VAL:HG13	1.95	0.96
8:I:537:GLU:OE1	8:I:545:LEU:CD1	2.14	0.96
8:I:493:ILE:HG13	8:I:494:VAL:H	1.32	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:143:LEU:HA	9:J:178:LEU:HB2	1.48	0.94
9:J:314:ALA:HB1	9:J:365:ALA:HB1	1.51	0.92
8:I:575:TYR:CA	8:I:579:GLY:CA	2.17	0.92
7:H:31:HIS:HB2	9:J:486:THR:CG2	2.00	0.91
4:D:148:GLN:HG3	4:D:150:LEU:H	1.35	0.91
8:I:546:LEU:HD12	8:I:574:ARG:NH2	1.86	0.91
8:I:530:LEU:HD12	8:I:545:LEU:HD22	1.53	0.90
8:I:358:ARG:NH2	8:I:359:HIS:HB2	1.87	0.90
8:I:493:ILE:CG2	8:I:509:ALA:CB	2.50	0.89
8:I:518:LYS:C	8:I:523:TYR:HE1	1.81	0.89
8:I:493:ILE:CG1	8:I:494:VAL:H	1.86	0.88
2:B:56:LEU:HA	2:B:127:LEU:HD12	1.56	0.88
1:A:69:GLU:HG2	4:D:52:ASN:HA	1.56	0.86
6:F:80:ARG:HH22	6:F:99:VAL:HG23	1.40	0.86
8:I:598:ARG:HG3	8:I:600:TRP:HZ3	1.38	0.86
7:H:3:PHE:HE2	7:H:137:THR:HG23	1.38	0.86
8:I:537:GLU:CD	8:I:545:LEU:CD1	2.42	0.86
8:I:575:TYR:CB	8:I:579:GLY:HA3	2.03	0.86
8:I:510:THR:CG2	8:I:533:MET:HE3	1.98	0.85
9:J:90:LEU:HA	9:J:93:LEU:HD13	1.56	0.85
8:I:493:ILE:CG2	8:I:509:ALA:HB3	2.07	0.84
1:G:101:SER:OG	1:G:161:ARG:NH1	2.08	0.84
8:I:448:TYR:OH	8:I:488:TYR:CE2	2.30	0.84
9:J:113:TRP:HE1	9:J:160:ARG:HD3	1.43	0.84
5:E:57:ASN:O	6:F:84:ARG:NH1	2.10	0.84
4:D:103:MET:HE2	4:D:108:LYS:HE2	1.60	0.83
8:I:537:GLU:HG3	8:I:545:LEU:HD12	0.85	0.83
1:G:65:ARG:O	1:G:75:ARG:NH1	2.12	0.82
7:H:29:GLN:O	7:H:33:ASN:N	2.12	0.82
6:F:80:ARG:HH21	6:F:95:VAL:HA	1.45	0.82
4:D:197:LEU:HD12	4:D:198:PHE:H	1.43	0.81
8:I:514:MET:HB2	8:I:526:VAL:CG1	2.08	0.81
2:B:117:CYS:SG	2:B:133:VAL:N	2.53	0.81
7:H:60:LEU:HD21	7:H:68:ILE:HG22	1.63	0.81
8:I:514:MET:HG3	8:I:526:VAL:HG11	1.62	0.81
8:I:490:GLU:HA	8:I:493:ILE:CG1	2.09	0.81
9:J:257:ASP:O	9:J:260:ARG:NH1	2.12	0.81
7:H:91:ARG:NH1	7:H:92:GLU:OE2	2.14	0.81
4:D:32:PHE:N	4:D:94:ILE:O	2.14	0.81
8:I:489:MET:HE1	8:I:509:ALA:HB1	1.60	0.81
8:I:545:LEU:HA	8:I:548:GLN:OE1	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:66:ASP:OD1	6:F:70:ARG:NH1	2.14	0.80
8:I:483:ARG:CZ	8:I:486:TYR:HD1	1.93	0.80
8:I:490:GLU:HA	8:I:493:ILE:HG12	1.62	0.80
7:H:16:TYR:OH	9:J:486:THR:OG1	2.00	0.80
6:F:187:ARG:HG2	6:F:191:MET:HE2	1.62	0.80
7:H:45:ILE:HG13	7:H:49:ALA:HB3	1.64	0.79
9:J:18:PRO:HA	9:J:238:MET:HE1	1.63	0.79
8:I:483:ARG:NH2	8:I:486:TYR:HD1	1.80	0.79
8:I:489:MET:HE1	8:I:509:ALA:CB	2.12	0.79
8:I:514:MET:CA	8:I:526:VAL:HG11	2.12	0.79
7:H:51:GLU:HG3	7:H:53:LYS:H	1.47	0.79
6:F:128:PRO:HB2	6:F:130:VAL:HG12	1.65	0.79
2:B:59:MET:SD	2:B:86:TYR:OH	2.39	0.78
8:I:598:ARG:O	8:I:598:ARG:HG2	1.84	0.78
8:I:575:TYR:HA	8:I:579:GLY:N	1.98	0.78
8:I:514:MET:HG3	8:I:526:VAL:CG1	2.12	0.78
6:F:57:GLN:HB3	6:F:147:ASN:HD22	1.48	0.78
6:F:65:GLN:HA	6:F:155:ALA:HB2	1.64	0.78
8:I:493:ILE:CG2	8:I:509:ALA:HB1	2.14	0.78
8:I:427:GLN:O	8:I:430:LYS:HG3	1.82	0.77
8:I:493:ILE:HG13	8:I:494:VAL:HG22	1.66	0.77
6:F:71:ILE:HA	6:F:74:LEU:HD12	1.66	0.77
3:C:68:ARG:NH2	4:D:129:PRO:O	2.18	0.77
8:I:598:ARG:CB	8:I:600:TRP:CZ3	2.67	0.77
7:H:71:PHE:HB3	7:H:79:PHE:HB2	1.64	0.76
1:G:128:LEU:HB2	1:G:147:PHE:HZ	1.48	0.76
7:H:31:HIS:O	9:J:487:ILE:CG2	2.34	0.76
7:H:1:MET:HE2	7:H:3:PHE:HE1	1.49	0.76
8:I:431:LEU:O	8:I:434:LEU:HB2	1.86	0.76
2:B:59:MET:HE1	2:B:126:ASN:HA	1.67	0.76
3:C:74:LEU:HB3	3:C:82:PHE:HB2	1.67	0.76
7:H:41:GLU:HA	7:H:45:ILE:HB	1.67	0.75
6:F:77:VAL:HA	6:F:82:SER:HA	1.69	0.75
6:F:60:LEU:HA	6:F:63:LEU:HD12	1.68	0.75
6:F:142:SER:O	6:F:170:TRP:NE1	2.19	0.75
2:B:123:ALA:H	7:H:76:ARG:HD2	1.52	0.75
8:I:358:ARG:HH21	8:I:358:ARG:C	1.95	0.75
8:I:482:GLN:OE1	8:I:482:GLN:HA	1.84	0.75
2:B:40:ARG:NE	7:H:107:THR:OG1	2.19	0.75
2:B:110:PRO:HA	2:B:113:VAL:HG12	1.69	0.75
3:C:72:HIS:HB2	3:C:142:ILE:HD11	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:700:LEU:HD12	9:J:709:VAL:HG11	1.69	0.75
4:D:9:VAL:HG12	4:D:15:LEU:HA	1.69	0.74
7:H:31:HIS:CB	9:J:486:THR:CG2	2.58	0.74
9:J:243:SER:OG	9:J:247:LYS:NZ	2.20	0.74
4:D:63:LEU:HG	4:D:71:VAL:HG11	1.68	0.74
8:I:575:TYR:HD2	8:I:579:GLY:CA	2.00	0.74
5:E:96:ASN:HB2	5:E:136:TYR:CE2	2.23	0.74
8:I:448:TYR:HH	8:I:488:TYR:HE2	1.33	0.74
6:F:49:ARG:HH22	6:F:59:ARG:HH21	1.32	0.74
9:J:164:LEU:HD11	9:J:175:LEU:HD12	1.70	0.74
4:D:54:LYS:NZ	4:D:55:ASP:OD2	2.17	0.74
6:F:166:VAL:HG22	6:F:178:VAL:HG12	1.68	0.74
1:A:18:LEU:HD21	2:B:7:PHE:HB2	1.69	0.74
1:G:77:GLN:HG2	1:G:90:ILE:HD11	1.70	0.74
5:E:58:MET:H	6:F:83:LYS:HZ3	1.33	0.74
8:I:530:LEU:HD12	8:I:545:LEU:CD2	2.18	0.74
1:A:115:GLU:OE2	7:H:112:ASN:ND2	2.20	0.73
1:G:66:CYS:HA	1:G:75:ARG:HH22	1.52	0.73
8:I:538:SER:OG	8:I:539:ASP:N	2.20	0.73
1:A:38:ASP:O	1:A:42:GLN:NE2	2.21	0.73
2:B:33:ILE:HG23	7:H:110:ILE:HG22	1.70	0.73
2:B:56:LEU:HD13	2:B:126:ASN:HB3	1.70	0.73
7:H:67:LYS:O	7:H:83:ILE:N	2.21	0.73
3:C:53:SER:O	4:D:25:ARG:NH2	2.22	0.73
9:J:608:ILE:HD12	9:J:609:PRO:HD2	1.69	0.73
1:A:99:ASP:HB3	1:A:164:LYS:HG2	1.69	0.73
8:I:497:LEU:HD21	8:I:503:GLN:HA	1.69	0.73
8:I:537:GLU:CG	8:I:545:LEU:HD13	2.18	0.73
6:F:35:VAL:HG22	1:G:17:LEU:HD13	1.71	0.73
8:I:493:ILE:HG13	8:I:494:VAL:N	2.03	0.73
8:I:537:GLU:HA	8:I:537:GLU:OE2	1.86	0.73
9:J:207:SER:HA	9:J:210:ILE:HD12	1.69	0.73
2:B:119:LEU:N	2:B:131:SER:OG	2.19	0.72
6:F:167:THR:HG1	6:F:169:HIS:HE2	1.37	0.72
8:I:483:ARG:NH2	8:I:486:TYR:CD1	2.57	0.72
5:E:53:TRP:O	6:F:87:LYS:NZ	2.21	0.72
2:B:61:PHE:O	2:B:64:THR:OG1	2.03	0.72
8:I:575:TYR:O	8:I:579:GLY:CA	2.37	0.72
5:E:45:LEU:HA	5:E:48:VAL:HG12	1.71	0.72
8:I:431:LEU:HD22	8:I:435:TYR:HE2	1.55	0.72
8:I:544:LEU:C	8:I:548:GLN:OE1	2.13	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:105:LEU:HD13	7:H:129:ALA:HB1	1.72	0.72
8:I:358:ARG:HD2	8:I:358:ARG:O	1.89	0.72
9:J:33:HIS:HE1	9:J:37:TRP:HE3	1.37	0.72
4:D:42:TYR:HB2	4:D:83:ARG:HH12	1.54	0.72
4:D:197:LEU:HD13	6:F:134:ILE:HG12	1.70	0.71
7:H:93:ASN:OD1	7:H:94:GLU:N	2.22	0.71
8:I:490:GLU:HA	8:I:493:ILE:HD11	1.72	0.71
6:F:184:VAL:HG22	6:F:187:ARG:HH21	1.54	0.71
2:B:87:VAL:HG23	2:B:146:HIS:HA	1.70	0.71
1:G:105:ASP:O	1:G:151:GLN:NE2	2.23	0.71
3:C:30:THR:OG1	3:C:33:GLU:OE1	2.08	0.71
8:I:489:MET:CE	8:I:509:ALA:HB1	2.20	0.71
8:I:533:MET:O	8:I:537:GLU:HG2	1.90	0.71
9:J:104:GLN:NE2	9:J:120:CYS:SG	2.64	0.71
9:J:106:MET:HE3	9:J:177:ILE:HD12	1.73	0.71
3:C:68:ARG:NH1	4:D:130:LYS:O	2.24	0.71
3:C:67:ASN:OD1	4:D:132:SER:OG	2.06	0.71
7:H:21:ASP:HA	7:H:135:SER:HA	1.71	0.71
8:I:489:MET:O	8:I:493:ILE:HG23	1.90	0.71
9:J:84:LEU:HB3	9:J:88:TRP:CZ3	2.26	0.71
2:B:73:LYS:HZ1	2:B:93:PHE:HA	1.54	0.70
9:J:515:ALA:HB3	9:J:519:ARG:HH21	1.55	0.70
1:G:41:GLN:OE1	1:G:44:ARG:NH2	2.24	0.70
1:G:63:ALA:O	1:G:65:ARG:NH2	2.24	0.70
7:H:31:HIS:CG	9:J:486:THR:CG2	2.61	0.70
6:F:130:VAL:HB	6:F:145:CYS:HB3	1.73	0.70
2:B:67:TRP:O	2:B:72:LYS:N	2.16	0.70
8:I:575:TYR:O	8:I:579:GLY:C	2.35	0.70
1:G:149:GLN:O	1:G:159:GLU:N	2.23	0.70
8:I:434:LEU:C	8:I:436:PHE:H	2.00	0.70
9:J:141:VAL:HG11	9:J:191:LEU:HD11	1.72	0.70
7:H:116:ILE:HD12	7:H:117:PRO:HD2	1.73	0.70
4:D:186:PHE:H	6:F:44:GLN:HE22	1.40	0.69
1:A:138:GLU:O	3:C:11:LYS:NZ	2.26	0.69
8:I:575:TYR:C	8:I:579:GLY:CA	2.64	0.69
1:G:69:MET:HE3	1:G:69:MET:HA	1.73	0.69
8:I:431:LEU:HD22	8:I:435:TYR:CE2	2.27	0.69
8:I:513:SER:O	8:I:517:LEU:CD1	2.40	0.69
5:E:93:GLY:O	5:E:97:PHE:HB2	1.93	0.69
6:F:167:THR:OG1	6:F:169:HIS:NE2	2.25	0.69
1:G:43:GLU:OE2	1:G:123:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:108:LYS:HA	4:D:111:LEU:HD12	1.74	0.69
5:E:10:GLY:O	5:E:81:ARG:NH2	2.26	0.69
1:G:133:ARG:HH21	1:G:145:CYS:H	1.39	0.69
9:J:346:GLN:OE1	9:J:347:HIS:ND1	2.21	0.69
2:B:51:ARG:HG3	7:H:48:GLY:HA3	1.74	0.69
9:J:30:VAL:HA	9:J:33:HIS:HB3	1.75	0.69
7:H:3:PHE:CE2	7:H:137:THR:HG23	2.25	0.68
3:C:108:PHE:HD2	3:C:125:LEU:HD13	1.59	0.68
4:D:6:VAL:HG23	4:D:157:ILE:HG22	1.74	0.68
1:G:151:GLN:H	1:G:158:THR:HG22	1.58	0.68
4:D:25:ARG:HD2	4:D:100:ARG:HD2	1.76	0.68
4:D:197:LEU:HD12	4:D:198:PHE:N	2.07	0.68
5:E:39:PHE:HD1	5:E:42:HIS:CE1	2.11	0.68
2:B:58:THR:HG22	2:B:126:ASN:HD21	1.58	0.68
2:B:121:ARG:NH1	2:B:132:THR:OG1	2.26	0.68
4:D:128:GLU:HG2	4:D:129:PRO:HD2	1.76	0.68
5:E:50:GLU:HA	5:E:53:TRP:CD1	2.28	0.68
9:J:266:CYS:HA	9:J:269:ILE:HD12	1.75	0.68
1:A:79:GLN:OE1	1:A:82:ARG:NH1	2.27	0.68
5:E:64:ASP:H	5:E:71:VAL:HB	1.57	0.68
1:G:87:GLN:NE2	1:G:88:PRO:O	2.25	0.68
7:H:55:LEU:HB3	7:H:72:VAL:H	1.57	0.68
2:B:94:ARG:O	2:B:97:THR:OG1	2.11	0.68
1:A:22:TYR:OH	1:A:125:TYR:O	2.10	0.68
3:C:51:LYS:HD2	4:D:111:LEU:HD21	1.74	0.68
2:B:19:LEU:HB2	2:B:25:HIS:HE1	1.59	0.67
9:J:348:PRO:HB2	9:J:438:GLN:HG3	1.75	0.67
9:J:412:ASN:HA	9:J:415:LEU:HD12	1.76	0.67
8:I:358:ARG:NH2	8:I:359:HIS:CB	2.57	0.67
9:J:105:ASP:O	9:J:116:LYS:NZ	2.26	0.67
2:B:11:HIS:O	2:B:15:VAL:HG23	1.94	0.67
8:I:575:TYR:C	8:I:579:GLY:N	2.52	0.67
7:H:57:LEU:HD13	7:H:60:LEU:HD13	1.77	0.67
7:H:8:ILE:HB	7:H:78:LYS:HB2	1.77	0.67
5:E:50:GLU:HA	5:E:53:TRP:HD1	1.60	0.67
8:I:358:ARG:HD2	8:I:359:HIS:N	2.09	0.67
1:A:71:ARG:HD3	1:A:94:TRP:CZ2	2.30	0.67
9:J:517:SER:HA	9:J:579:VAL:HG12	1.76	0.67
9:J:47:LYS:HE2	9:J:49:ALA:HB3	1.76	0.67
9:J:109:ASN:ND2	9:J:112:GLN:OE1	2.18	0.67
5:E:5:TYR:HE2	5:E:34:ARG:HG2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:598:ARG:CG	8:I:600:TRP:HZ3	1.99	0.67
9:J:360:MET:HG2	9:J:428:ILE:HD13	1.77	0.67
6:F:117:ASP:OD2	6:F:179:LYS:NZ	2.28	0.66
8:I:510:THR:HB	8:I:529:GLN:OE1	1.95	0.66
9:J:278:TYR:CE1	9:J:331:LEU:HD21	2.30	0.66
9:J:581:MET:HB2	9:J:602:VAL:HA	1.77	0.66
4:D:71:VAL:HA	4:D:76:LEU:HA	1.77	0.66
8:I:550:ALA:HB1	8:I:564:TYR:HD1	1.59	0.66
6:F:101:LYS:HA	6:F:105:GLY:HA2	1.77	0.66
9:J:359:VAL:HG23	9:J:428:ILE:HG12	1.76	0.66
8:I:537:GLU:HG2	8:I:545:LEU:CD1	2.20	0.66
8:I:599:GLU:OE2	8:I:600:TRP:NE1	2.28	0.66
7:H:1:MET:HE1	7:H:83:ILE:HG23	1.77	0.66
8:I:545:LEU:CA	8:I:548:GLN:OE1	2.44	0.66
9:J:187:TYR:HA	9:J:190:ARG:HG3	1.77	0.66
3:C:65:LYS:NZ	3:C:88:THR:O	2.29	0.66
4:D:32:PHE:HB3	4:D:36:LEU:HD21	1.77	0.66
1:G:144:GLN:HB2	1:G:163:LYS:HB3	1.76	0.66
1:A:87:ILE:HG23	1:A:89:PRO:HD3	1.76	0.66
6:F:182:ASP:OD1	6:F:183:PHE:N	2.27	0.66
1:G:84:LEU:HD12	1:G:108:PRO:HD2	1.78	0.66
2:B:23:LYS:HD3	2:B:24:GLU:N	2.11	0.65
8:I:358:ARG:NH2	8:I:359:HIS:CA	2.59	0.65
5:E:51:HIS:HA	5:E:54:LYS:HD2	1.78	0.65
7:H:35:ALA:HA	7:H:38:VAL:HG22	1.78	0.65
8:I:575:TYR:CD2	8:I:579:GLY:HA3	2.30	0.65
4:D:178:SER:OG	1:G:55:GLU:OE1	2.13	0.65
8:I:483:ARG:CZ	8:I:486:TYR:CD1	2.78	0.65
9:J:99:VAL:HG22	9:J:198:MET:HE3	1.79	0.65
7:H:31:HIS:C	9:J:487:ILE:HG22	2.22	0.65
9:J:113:TRP:HZ2	9:J:160:ARG:HB2	1.60	0.65
9:J:144:GLN:NE2	9:J:147:ALA:O	2.30	0.65
4:D:65:ALA:HB3	4:D:97:LYS:HD3	1.78	0.65
1:G:133:ARG:NH2	1:G:145:CYS:H	1.95	0.65
7:H:28:LEU:HD13	7:H:30:TYR:HE2	1.62	0.65
6:F:145:CYS:O	6:F:148:PHE:N	2.30	0.65
3:C:72:HIS:HB2	3:C:142:ILE:CD1	2.26	0.65
6:F:143:LEU:HD11	6:F:168:ALA:HB3	1.79	0.65
9:J:544:MET:O	9:J:546:LYS:N	2.28	0.64
4:D:58:ASN:HB3	4:D:61:HIS:CD2	2.32	0.64
7:H:16:TYR:HH	9:J:484:TRP:CD1	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:181:THR:HA	9:J:184:LEU:HB3	1.80	0.64
5:E:39:PHE:CD1	5:E:42:HIS:CE1	2.85	0.64
9:J:311:LYS:N	9:J:312:ASP:HB2	2.12	0.64
8:I:514:MET:HB2	8:I:526:VAL:HG12	1.79	0.64
1:G:102:LEU:HB3	1:G:160:LEU:HD13	1.80	0.64
8:I:575:TYR:CD2	8:I:579:GLY:CA	2.80	0.64
8:I:434:LEU:O	8:I:436:PHE:N	2.30	0.64
9:J:200:GLN:HE22	9:J:239:ARG:HA	1.63	0.64
6:F:68:GLY:HA2	6:F:71:ILE:HG12	1.80	0.64
9:J:232:LEU:HD12	9:J:235:VAL:HB	1.79	0.64
9:J:238:MET:O	9:J:240:GLN:NE2	2.31	0.64
1:A:42:GLN:HG3	1:A:45:ARG:HH21	1.63	0.64
1:A:66:ARG:NH1	3:C:77:PRO:O	2.32	0.64
3:C:90:ALA:O	3:C:143:ARG:HG2	1.97	0.63
5:E:111:ASN:OD1	1:G:114:GLU:N	2.29	0.63
7:H:59:LEU:HD11	7:H:67:LYS:HB3	1.80	0.63
9:J:51:ARG:NH2	9:J:55:GLN:OE1	2.31	0.63
2:B:51:ARG:NH1	7:H:45:ILE:O	2.31	0.63
2:B:47:ARG:NE	7:H:51:GLU:HB2	2.13	0.63
7:H:91:ARG:HD2	7:H:92:GLU:HG3	1.81	0.63
9:J:350:ILE:HD12	9:J:350:ILE:H	1.63	0.63
5:E:97:PHE:HD1	5:E:136:TYR:HB2	1.63	0.63
9:J:225:LYS:HD3	9:J:255:ASN:HD22	1.63	0.63
2:B:121:ARG:HH11	2:B:150:ASN:HB3	1.63	0.63
9:J:561:LEU:HA	9:J:564:VAL:HB	1.78	0.63
2:B:98:ARG:NH1	3:C:111:ARG:HB3	2.14	0.63
9:J:137:ARG:HH22	9:J:202:TYR:N	1.97	0.63
9:J:685:GLU:OE2	9:J:687:GLN:NE2	2.28	0.63
5:E:65:ARG:NH1	5:E:71:VAL:O	2.31	0.63
5:E:75:ILE:O	6:F:84:ARG:NH2	2.30	0.63
1:A:56:GLU:OE2	3:C:110:VAL:HG11	1.99	0.63
2:B:121:ARG:NH1	2:B:131:SER:O	2.32	0.63
2:B:121:ARG:NE	2:B:130:ASN:OD1	2.32	0.63
7:H:93:ASN:HA	7:H:96:ARG:HE	1.64	0.63
1:G:10:LYS:HG2	1:G:12:VAL:HG12	1.79	0.62
8:I:575:TYR:HA	8:I:579:GLY:HA3	0.65	0.62
4:D:146:CYS:HB2	4:D:156:ILE:HG22	1.81	0.62
4:D:148:GLN:HG3	4:D:150:LEU:N	2.11	0.62
4:D:29:GLU:OE2	4:D:97:LYS:NZ	2.24	0.62
1:A:95:SER:HB2	1:A:100:GLU:H	1.64	0.62
2:B:32:TYR:HA	2:B:35:PHE:CE2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:LEU:HD23	1:G:152:LEU:HD22	1.82	0.62
3:C:64:TYR:HB2	4:D:134:ILE:CD1	2.30	0.62
9:J:106:MET:N	9:J:143:LEU:O	2.30	0.62
7:H:15:LEU:HD11	7:H:17:LEU:HG	1.81	0.62
7:H:91:ARG:NH1	7:H:93:ASN:HB3	2.14	0.62
2:B:60:LYS:HE2	2:B:78:LEU:HD12	1.81	0.62
3:C:7:TYR:HB2	3:C:83:VAL:HB	1.82	0.62
5:E:5:TYR:HB3	5:E:85:VAL:HG23	1.81	0.62
6:F:80:ARG:NH2	6:F:99:VAL:HG23	2.12	0.62
7:H:112:ASN:OD1	7:H:114:PHE:N	2.33	0.62
2:B:36:THR:O	2:B:40:ARG:HG3	1.99	0.62
6:F:49:ARG:NH2	6:F:59:ARG:HH21	1.98	0.62
3:C:108:PHE:CE2	3:C:129:LYS:HG3	2.34	0.61
6:F:136:VAL:HG22	6:F:137:PRO:HD2	1.82	0.61
7:H:53:LYS:NZ	7:H:56:TYR:H	1.97	0.61
3:C:42:LEU:O	3:C:46:LYS:HG3	2.00	0.61
7:H:55:LEU:HG	7:H:57:LEU:HG	1.82	0.61
3:C:87:ASP:OD1	3:C:88:THR:N	2.28	0.61
9:J:243:SER:O	9:J:246:GLN:HG2	2.00	0.61
9:J:415:LEU:O	9:J:419:GLU:HG2	2.01	0.61
2:B:58:THR:HA	2:B:126:ASN:OD1	2.01	0.61
3:C:2:THR:HG22	3:C:3:ILE:H	1.66	0.61
5:E:2:SER:OG	5:E:88:ASN:ND2	2.34	0.61
9:J:519:ARG:HB3	9:J:527:ARG:HE	1.66	0.61
5:E:57:ASN:HD21	5:E:60:LEU:HG	1.66	0.61
8:I:599:GLU:OE2	8:I:600:TRP:CD1	2.54	0.61
9:J:556:LEU:O	9:J:559:SER:OG	2.18	0.61
1:A:172:VAL:HG12	1:A:173:ILE:H	1.65	0.61
4:D:88:ALA:O	4:D:91:ASN:ND2	2.34	0.61
4:D:117:PRO:O	4:D:121:ILE:N	2.34	0.61
6:F:36:ALA:HB1	6:F:133:PHE:HB3	1.82	0.61
4:D:4:TYR:HD1	4:D:23:VAL:HG21	1.64	0.61
8:I:358:ARG:C	8:I:358:ARG:CD	2.52	0.61
6:F:181:GLU:OE1	6:F:184:VAL:N	2.32	0.61
1:G:94:SER:HB2	1:G:99:GLU:CD	2.25	0.61
6:F:113:HIS:HB2	6:F:121:TYR:CE1	2.36	0.60
4:D:149:THR:HG21	4:D:153:ILE:HB	1.83	0.60
5:E:37:THR:HA	5:E:40:ILE:HB	1.83	0.60
6:F:57:GLN:HB3	6:F:147:ASN:ND2	2.16	0.60
1:G:90:ILE:HD12	1:G:90:ILE:H	1.65	0.60
1:A:130:SER:HB2	1:A:148:PHE:CZ	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:597:GLN:NE2	9:J:683:SER:OG	2.25	0.60
1:A:82:ARG:NH2	1:A:88:GLN:OE1	2.34	0.60
1:A:67:CYS:HB3	1:A:73:THR:HG22	1.82	0.60
3:C:5:ASN:OD1	3:C:85:ASN:ND2	2.34	0.60
5:E:101:MET:HE2	5:E:132:PHE:HD2	1.67	0.60
7:H:21:ASP:HB2	7:H:138:ALA:HB3	1.83	0.60
8:I:575:TYR:C	8:I:579:GLY:O	2.45	0.60
2:B:124:LEU:HB3	2:B:127:LEU:HD13	1.83	0.60
8:I:427:GLN:NE2	8:I:431:LEU:HG	2.17	0.60
8:I:575:TYR:CA	8:I:579:GLY:N	2.59	0.60
2:B:68:MET:HE2	2:B:68:MET:N	2.17	0.60
1:G:84:LEU:HB3	1:G:86:ILE:HG12	1.83	0.60
8:I:518:LYS:C	8:I:523:TYR:CE1	2.67	0.60
9:J:594:ASP:O	9:J:688:GLN:NE2	2.31	0.60
1:A:95:SER:HB3	1:A:99:ASP:N	2.16	0.60
7:H:40:GLU:HA	7:H:44:LEU:HB3	1.84	0.60
8:I:544:LEU:HA	8:I:575:TYR:OH	2.02	0.60
9:J:479:TYR:HB3	9:J:488:PHE:HD1	1.65	0.60
9:J:698:VAL:HG12	9:J:699:ARG:HG3	1.82	0.60
3:C:68:ARG:HH12	4:D:130:LYS:HG3	1.66	0.60
4:D:78:ASP:O	4:D:80:ARG:NH2	2.35	0.60
7:H:94:GLU:O	7:H:98:ILE:HG12	2.02	0.60
8:I:493:ILE:HG13	8:I:494:VAL:CG2	2.32	0.60
9:J:680:LEU:HG	9:J:681:PHE:CD1	2.37	0.59
8:I:598:ARG:HA	8:I:600:TRP:CH2	2.37	0.59
2:B:31:GLU:OE2	2:B:31:GLU:N	2.32	0.59
3:C:53:SER:OG	3:C:55:HIS:O	2.11	0.59
6:F:96:LYS:HD2	6:F:123:ILE:HD11	1.84	0.59
9:J:91:LYS:HG3	9:J:95:VAL:HB	1.84	0.59
2:B:39:TYR:HE2	7:H:73:THR:HG22	1.66	0.59
2:B:60:LYS:HG3	2:B:78:LEU:HD12	1.84	0.59
2:B:130:ASN:ND2	2:B:150:ASN:OD1	2.36	0.59
1:G:128:LEU:HB2	1:G:147:PHE:CZ	2.36	0.59
7:H:10:LYS:O	7:H:78:LYS:NZ	2.35	0.59
9:J:82:GLY:O	9:J:92:HIS:NE2	2.34	0.59
9:J:590:LEU:O	9:J:692:ASN:N	2.34	0.59
8:I:448:TYR:OH	8:I:488:TYR:HE2	1.77	0.59
9:J:33:HIS:HE1	9:J:37:TRP:CE3	2.19	0.59
1:G:66:CYS:HB3	1:G:167:ARG:HH12	1.67	0.59
7:H:8:ILE:HB	7:H:78:LYS:HE2	1.84	0.59
7:H:115:TYR:OH	7:H:119:GLU:O	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:84:LEU:HD23	3:C:97:LEU:HD21	1.83	0.59
9:J:24:GLY:H	9:J:60:PRO:C	2.11	0.59
9:J:125:GLN:NE2	9:J:129:ASN:HD21	1.99	0.59
1:A:95:SER:HB3	1:A:99:ASP:H	1.68	0.59
3:C:99:GLN:HG3	3:C:103:LYS:HE2	1.85	0.59
5:E:59:GLN:HE22	5:E:61:LYS:HA	1.67	0.59
5:E:82:PHE:HB3	5:E:98:PHE:CE1	2.38	0.59
1:G:98:ASP:HB3	1:G:99:GLU:OE1	2.03	0.59
8:I:358:ARG:HH22	8:I:359:HIS:HB2	1.63	0.59
1:A:125:TYR:CD2	1:A:153:LEU:HD22	2.38	0.59
9:J:536:GLN:O	9:J:541:VAL:N	2.36	0.59
1:A:70:MET:HE1	4:D:52:ASN:HD21	1.67	0.58
1:A:152:GLN:HE21	1:A:158:VAL:HA	1.67	0.58
2:B:15:VAL:HG22	2:B:111:LYS:HD3	1.85	0.58
4:D:183:LYS:HD3	4:D:184:ASN:HB2	1.84	0.58
4:D:186:PHE:H	6:F:44:GLN:NE2	2.00	0.58
5:E:49:ASP:OD1	5:E:50:GLU:N	2.36	0.58
5:E:82:PHE:HB3	5:E:98:PHE:HE1	1.68	0.58
9:J:305:LYS:HA	9:J:317:HIS:NE2	2.18	0.58
3:C:64:TYR:HB2	4:D:134:ILE:HD13	1.85	0.58
4:D:11:LYS:HD3	4:D:152:GLY:HA2	1.85	0.58
1:G:72:THR:HA	1:G:75:ARG:HD2	1.85	0.58
9:J:597:GLN:HE21	9:J:683:SER:HG	1.50	0.58
7:H:39:VAL:HG21	9:J:447:PHE:HB2	1.86	0.58
7:H:93:ASN:HA	7:H:96:ARG:NE	2.19	0.58
4:D:183:LYS:HA	6:F:133:PHE:CD1	2.39	0.58
7:H:133:LEU:O	7:H:137:THR:HG22	2.04	0.58
6:F:177:MET:SD	6:F:179:LYS:HE3	2.44	0.58
9:J:205:LEU:HA	9:J:208:LYS:HD2	1.84	0.58
9:J:554:GLN:HA	9:J:557:TRP:CZ2	2.38	0.58
9:J:305:LYS:HA	9:J:317:HIS:CE1	2.39	0.58
9:J:535:TRP:HZ2	9:J:610:LEU:HD12	1.68	0.58
1:G:136:LEU:HA	1:G:139:VAL:HG12	1.85	0.58
1:A:14:ASN:HD21	2:B:72:LYS:NZ	2.01	0.58
2:B:134:THR:O	2:B:146:HIS:N	2.37	0.57
7:H:37:ASP:HA	7:H:40:GLU:HB3	1.86	0.57
8:I:434:LEU:C	8:I:436:PHE:N	2.61	0.57
8:I:530:LEU:CD1	8:I:545:LEU:CD2	2.82	0.57
7:H:63:THR:HG23	7:H:66:HIS:HB2	1.86	0.57
7:H:125:LYS:O	7:H:125:LYS:NZ	2.36	0.57
2:B:107:GLU:CD	2:B:107:GLU:H	2.06	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:ALA:O	2:B:112:PHE:HB2	2.04	0.57
3:C:137:SER:O	3:C:139:ILE:N	2.35	0.57
4:D:42:TYR:HB2	4:D:83:ARG:NH1	2.20	0.57
4:D:185:PRO:HB3	1:G:52:ARG:HD3	1.85	0.57
1:G:42:LEU:HD11	1:G:126:ALA:HB3	1.87	0.57
7:H:51:GLU:O	7:H:76:ARG:NH2	2.34	0.57
7:H:57:LEU:HB2	7:H:70:GLY:H	1.70	0.57
9:J:437:ALA:O	9:J:441:ILE:HG13	2.05	0.57
3:C:56:ASP:O	3:C:58:LYS:NZ	2.23	0.57
6:F:55:GLU:O	6:F:59:ARG:HG2	2.03	0.57
3:C:41:MET:O	3:C:45:ILE:HG13	2.05	0.57
1:G:147:PHE:HA	1:G:160:LEU:HA	1.86	0.57
8:I:543:ALA:HB2	8:I:574:ARG:HB3	1.86	0.57
3:C:32:GLU:OE1	3:C:32:GLU:N	2.27	0.57
4:D:40:LEU:HD22	4:D:86:LEU:HD11	1.86	0.57
4:D:92:TYR:HA	4:D:94:ILE:HG23	1.85	0.57
4:D:186:PHE:CE2	6:F:44:GLN:HB3	2.39	0.57
9:J:137:ARG:HB2	9:J:198:MET:SD	2.44	0.57
9:J:230:PHE:HA	9:J:249:TYR:HE1	1.70	0.57
9:J:446:ARG:HA	9:J:449:LYS:HB2	1.85	0.57
6:F:31:SER:HB2	1:G:83:TYR:HD1	1.70	0.57
9:J:519:ARG:HA	9:J:521:GLN:HE22	1.70	0.57
5:E:95:LYS:HG3	5:E:96:ASN:H	1.70	0.56
6:F:96:LYS:HD2	6:F:108:ALA:HB3	1.86	0.56
1:A:172:VAL:HG12	1:A:173:ILE:N	2.20	0.56
5:E:8:ILE:HD13	5:E:17:TYR:HB3	1.87	0.56
5:E:86:HIS:HE1	5:E:89:LYS:HD2	1.70	0.56
1:G:39:ASN:HD21	1:G:123:ARG:HB2	1.70	0.56
1:A:25:LEU:HD11	2:B:14:ILE:HD11	1.87	0.56
1:A:100:GLU:HG3	1:A:164:LYS:HB2	1.87	0.56
1:A:144:VAL:HG13	1:A:164:LYS:O	2.06	0.56
2:B:22:ASN:HB3	2:B:25:HIS:CD2	2.40	0.56
7:H:12:ASN:OD1	7:H:13:ALA:N	2.35	0.56
5:E:16:ILE:HG23	5:E:119:PRO:HA	1.87	0.56
1:G:93:TRP:CZ3	1:G:100:PHE:HB3	2.40	0.56
8:I:448:TYR:OH	8:I:488:TYR:CD2	2.49	0.56
9:J:286:LYS:O	9:J:288:LYS:NZ	2.38	0.56
3:C:135:ARG:HA	3:C:138:PRO:HG3	1.87	0.56
4:D:131:SER:OG	4:D:132:SER:N	2.38	0.56
3:C:67:ASN:OD1	3:C:68:ARG:HG2	2.06	0.56
4:D:171:ARG:O	4:D:175:GLU:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:94:ILE:HD13	5:E:137:LEU:HD21	1.88	0.56
6:F:31:SER:OG	6:F:33:SER:N	2.38	0.56
1:A:153:LEU:HD12	1:A:153:LEU:H	1.70	0.56
3:C:63:TYR:HE2	3:C:65:LYS:HG3	1.69	0.56
3:C:63:TYR:HB2	3:C:72:HIS:HA	1.88	0.56
3:C:86:THR:HG21	3:C:142:ILE:HB	1.86	0.56
4:D:4:TYR:CD1	4:D:23:VAL:HG21	2.39	0.56
1:A:120:LEU:HD23	1:A:123:LEU:HD22	1.87	0.56
4:D:15:LEU:HD11	4:D:18:ASN:HB3	1.88	0.56
9:J:613:ARG:HA	9:J:613:ARG:NH1	2.21	0.56
2:B:39:TYR:HA	2:B:42:ILE:HB	1.88	0.56
2:B:40:ARG:HG2	7:H:107:THR:HG21	1.88	0.56
5:E:100:GLU:HB2	5:E:132:PHE:CZ	2.40	0.56
8:I:598:ARG:CG	8:I:600:TRP:CE3	2.74	0.56
9:J:300:HIS:O	9:J:304:HIS:ND1	2.39	0.56
9:J:113:TRP:CZ2	9:J:160:ARG:HB2	2.41	0.56
2:B:121:ARG:HG3	2:B:130:ASN:CG	2.32	0.55
7:H:35:ALA:HB1	9:J:446:ARG:HE	1.71	0.55
9:J:370:TYR:HE1	9:J:420:ARG:HE	1.53	0.55
7:H:15:LEU:HB2	7:H:121:LEU:HB2	1.88	0.55
5:E:21:PHE:HE2	5:E:130:GLU:HA	1.72	0.55
5:E:86:HIS:ND1	5:E:88:ASN:O	2.39	0.55
7:H:1:MET:HG3	7:H:3:PHE:CE1	2.42	0.55
9:J:273:ALA:O	9:J:277:ASN:HB2	2.06	0.55
2:B:47:ARG:NH1	2:B:50:SER:O	2.40	0.55
7:H:88:VAL:HG23	7:H:90:LEU:HG	1.88	0.55
4:D:8:ILE:HG22	4:D:17:PHE:HB3	1.88	0.55
8:I:490:GLU:O	8:I:493:ILE:HG12	2.06	0.55
8:I:575:TYR:HD2	8:I:579:GLY:HA2	1.70	0.55
9:J:135:ASN:HB2	9:J:202:TYR:HE1	1.71	0.55
9:J:519:ARG:HH11	9:J:527:ARG:HA	1.71	0.55
9:J:611:ARG:HH21	9:J:613:ARG:HG3	1.72	0.55
2:B:60:LYS:O	2:B:64:THR:HG23	2.06	0.55
2:B:137:VAL:HG22	2:B:143:CYS:HA	1.89	0.55
9:J:155:LEU:HD12	9:J:156:LEU:HD12	1.88	0.55
7:H:31:HIS:C	9:J:487:ILE:CG2	2.79	0.55
8:I:510:THR:HG21	8:I:533:MET:HE1	1.72	0.55
8:I:518:LYS:HA	8:I:523:TYR:CE1	2.41	0.55
9:J:126:ALA:O	9:J:130:THR:HG23	2.07	0.55
9:J:57:LYS:NZ	9:J:95:VAL:HA	2.21	0.55
5:E:6:PHE:CE2	5:E:101:MET:HG3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:104:PHE:HZ	6:F:129:LEU:HG	1.73	0.55
1:G:41:GLN:HA	1:G:44:ARG:CZ	2.37	0.55
9:J:515:ALA:HB1	9:J:519:ARG:HE	1.72	0.55
4:D:178:SER:O	4:D:182:LEU:HG	2.07	0.54
7:H:67:LYS:HE2	7:H:83:ILE:O	2.07	0.54
9:J:137:ARG:NH2	9:J:198:MET:O	2.40	0.54
9:J:280:ILE:O	9:J:284:MET:HG2	2.08	0.54
1:A:92:SER:HG	1:A:102:SER:HG	1.55	0.54
2:B:10:LEU:O	2:B:13:GLU:HG3	2.08	0.54
2:B:47:ARG:NH1	2:B:48:GLU:O	2.39	0.54
2:B:138:GLN:HB2	2:B:144:LYS:HZ1	1.71	0.54
3:C:10:ASP:OD2	3:C:16:LEU:HD21	2.06	0.54
5:E:79:GLN:NE2	6:F:159:ASN:O	2.37	0.54
9:J:25:LEU:HD13	9:J:29:ARG:HD2	1.89	0.54
5:E:49:ASP:O	5:E:52:LYS:HG2	2.07	0.54
6:F:113:HIS:HB2	6:F:121:TYR:CZ	2.43	0.54
8:I:510:THR:HG22	8:I:529:GLN:OE1	2.07	0.54
1:A:37:GLU:HG2	1:A:122:ASN:HD21	1.73	0.54
3:C:56:ASP:OD1	4:D:100:ARG:NH2	2.41	0.54
5:E:84:ILE:HG22	5:E:86:HIS:HD2	1.72	0.54
1:A:80:ALA:HA	1:A:83:ILE:HG22	1.89	0.54
6:F:144:ASN:HB2	6:F:170:TRP:CH2	2.42	0.54
1:G:93:TRP:CE3	1:G:100:PHE:HB3	2.42	0.54
7:H:26:LEU:O	7:H:28:LEU:HD22	2.07	0.54
7:H:69:TYR:HD1	7:H:99:PHE:CE1	2.25	0.54
6:F:49:ARG:HH12	6:F:59:ARG:NE	2.05	0.54
6:F:61:HIS:O	6:F:65:GLN:HG2	2.07	0.54
8:I:545:LEU:N	8:I:548:GLN:OE1	2.41	0.54
8:I:580:GLN:HB3	8:I:583:HIS:HB2	1.90	0.54
9:J:145:ARG:HH12	9:J:180:HIS:HA	1.73	0.54
9:J:454:ASP:O	9:J:457:GLU:HG2	2.07	0.54
6:F:38:LEU:O	6:F:42:ILE:HG12	2.08	0.54
8:I:510:THR:CG2	8:I:529:GLN:OE1	2.56	0.54
7:H:12:ASN:HD22	9:J:483:LYS:HB3	1.73	0.54
9:J:100:VAL:HG23	9:J:136:THR:HG21	1.90	0.54
2:B:29:THR:HA	2:B:32:TYR:HD2	1.73	0.54
2:B:103:THR:HG22	2:B:139:SER:HA	1.90	0.54
3:C:137:SER:O	3:C:139:ILE:HG12	2.08	0.54
1:G:72:THR:HG22	1:G:75:ARG:NH1	2.23	0.54
7:H:33:ASN:HA	7:H:36:LEU:HG	1.89	0.54
7:H:56:TYR:OH	7:H:92:GLU:OE1	2.17	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:343:LEU:O	9:J:346:GLN:HG3	2.08	0.54
2:B:37:THR:HA	2:B:40:ARG:CD	2.38	0.53
1:G:119:LEU:HD23	1:G:122:LEU:HD22	1.90	0.53
7:H:31:HIS:O	9:J:487:ILE:HG21	2.08	0.53
8:I:514:MET:HG3	8:I:526:VAL:HG12	1.91	0.53
1:A:114:VAL:O	1:A:115:GLU:HG2	2.08	0.53
1:A:165:PHE:HZ	1:A:168:ARG:HB2	1.73	0.53
5:E:102:TYR:OH	6:F:73:ASP:OD1	2.24	0.53
9:J:561:LEU:HD12	9:J:564:VAL:HB	1.89	0.53
4:D:47:VAL:HG11	4:D:82:VAL:HG21	1.90	0.53
8:I:358:ARG:CZ	8:I:359:HIS:HB2	2.39	0.53
9:J:154:ASP:CG	9:J:157:ALA:H	2.15	0.53
7:H:129:ALA:HA	7:H:132:LYS:NZ	2.23	0.53
2:B:40:ARG:O	2:B:43:GLU:HG2	2.08	0.53
2:B:49:VAL:HA	7:H:53:LYS:HE3	1.90	0.53
2:B:54:ASP:HB2	2:B:124:LEU:HD22	1.90	0.53
1:G:18:THR:HG21	1:G:112:PHE:HB2	1.90	0.53
1:G:166:ARG:HG2	1:G:167:ARG:H	1.73	0.53
9:J:141:VAL:HG13	9:J:176:PHE:HB2	1.90	0.53
9:J:141:VAL:HG22	9:J:176:PHE:HD2	1.73	0.53
9:J:362:ARG:HH22	9:J:419:GLU:HB3	1.73	0.53
1:A:130:SER:HB2	1:A:148:PHE:CE2	2.44	0.53
2:B:68:MET:HE1	2:B:74:GLN:HA	1.91	0.53
2:B:130:ASN:OD1	2:B:131:SER:N	2.41	0.53
3:C:10:ASP:HA	3:C:80:LEU:HD12	1.90	0.53
5:E:110:MET:HE1	6:F:70:ARG:O	2.09	0.53
7:H:2:ALA:HA	7:H:20:SER:OG	2.09	0.53
9:J:47:LYS:HG3	9:J:50:ASP:H	1.74	0.53
2:B:23:LYS:HD3	2:B:23:LYS:C	2.33	0.53
4:D:3:ILE:O	4:D:21:ASN:HB2	2.08	0.53
4:D:106:ASN:OD1	4:D:107:GLU:N	2.40	0.53
9:J:351:TYR:HA	9:J:354:LYS:HE2	1.89	0.53
3:C:65:LYS:O	4:D:134:ILE:HD12	2.09	0.53
4:D:62:VAL:N	4:D:99:SER:O	2.42	0.53
6:F:80:ARG:HH21	6:F:95:VAL:CA	2.19	0.53
1:G:150:ASP:N	1:G:155:ASP:OD2	2.39	0.53
7:H:53:LYS:HZ1	7:H:56:TYR:H	1.56	0.53
8:I:537:GLU:HG2	8:I:545:LEU:HD13	1.86	0.53
9:J:99:VAL:HG11	9:J:195:PHE:CD1	2.44	0.53
9:J:229:GLN:HB3	9:J:248:HIS:HB3	1.91	0.53
9:J:439:PHE:O	9:J:444:CYS:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:516:LEU:HD23	9:J:519:ARG:NH1	2.24	0.53
9:J:700:LEU:HG	9:J:714:THR:OG1	2.08	0.53
7:H:45:ILE:HA	7:H:49:ALA:HB2	1.90	0.53
9:J:162:ALA:O	9:J:166:ASN:ND2	2.42	0.53
9:J:175:LEU:HD23	9:J:176:PHE:N	2.24	0.53
9:J:225:LYS:HD3	9:J:255:ASN:ND2	2.24	0.53
1:A:53:ARG:HD2	3:C:110:VAL:HG23	1.90	0.53
4:D:151:THR:HG21	1:G:139:VAL:CG2	2.39	0.53
7:H:11:ASP:OD1	7:H:12:ASN:N	2.41	0.53
8:I:546:LEU:CD1	8:I:574:ARG:NH2	2.66	0.53
9:J:316:GLU:OE1	9:J:317:HIS:HB2	2.08	0.53
5:E:9:VAL:HB	5:E:81:ARG:HB2	1.91	0.52
1:G:104:PHE:HB2	1:G:158:THR:OG1	2.10	0.52
9:J:18:PRO:O	9:J:55:GLN:N	2.41	0.52
2:B:138:GLN:H	2:B:144:LYS:CE	2.22	0.52
9:J:519:ARG:HD2	9:J:527:ARG:HG2	1.91	0.52
2:B:140:ILE:HB	2:B:141:PRO:HD3	1.92	0.52
4:D:95:ASN:OD1	4:D:96:LEU:N	2.42	0.52
7:H:12:ASN:ND2	9:J:483:LYS:CB	2.73	0.52
7:H:90:LEU:HD13	7:H:94:GLU:OE2	2.07	0.52
9:J:24:GLY:N	9:J:59:LEU:O	2.42	0.52
2:B:68:MET:HE1	2:B:73:LYS:C	2.34	0.52
2:B:108:HIS:HA	2:B:111:LYS:NZ	2.24	0.52
2:B:123:ALA:N	7:H:76:ARG:HD2	2.24	0.52
3:C:27:SER:HA	4:D:125:LEU:HD12	1.91	0.52
8:I:598:ARG:HB2	8:I:600:TRP:CZ3	2.42	0.52
9:J:292:ASP:OD1	9:J:296:GLN:NE2	2.41	0.52
2:B:64:THR:HG22	2:B:75:VAL:CG2	2.40	0.52
9:J:127:LEU:O	9:J:130:THR:OG1	2.18	0.52
2:B:33:ILE:HD12	7:H:110:ILE:HG23	1.91	0.52
2:B:47:ARG:HB3	7:H:53:LYS:HB2	1.92	0.52
4:D:91:ASN:OD1	4:D:92:TYR:N	2.43	0.52
6:F:70:ARG:HD2	1:G:19:LEU:HD11	1.91	0.52
9:J:116:LYS:HG3	9:J:119:GLN:HE21	1.73	0.52
2:B:77:ASN:HB2	2:B:89:GLN:HB2	1.91	0.52
3:C:92:ASN:ND2	3:C:95:GLU:OE1	2.43	0.52
4:D:16:ILE:HG23	4:D:192:PRO:HA	1.91	0.52
1:G:149:GLN:HB2	1:G:159:GLU:HB3	1.92	0.52
2:B:40:ARG:HA	7:H:103:HIS:HE1	1.74	0.52
4:D:21:ASN:O	4:D:23:VAL:HG23	2.10	0.52
4:D:188:SER:N	4:D:191:MET:SD	2.83	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:172:ILE:HG13	1:G:173:PRO:HD2	1.92	0.52
3:C:59:GLU:N	4:D:140:ASP:OD2	2.41	0.52
1:G:129:SER:OG	1:G:145:CYS:O	2.28	0.52
8:I:490:GLU:CA	8:I:493:ILE:HG12	2.37	0.52
5:E:100:GLU:HB2	5:E:132:PHE:CE2	2.45	0.51
6:F:104:PHE:HE2	6:F:129:LEU:HD12	1.75	0.51
9:J:42:GLY:HA2	9:J:45:GLN:CD	2.34	0.51
9:J:596:LEU:O	9:J:685:GLU:HB3	2.10	0.51
6:F:120:THR:OG1	6:F:179:LYS:NZ	2.27	0.51
1:G:77:GLN:OE1	1:G:87:GLN:NE2	2.43	0.51
9:J:318:HIS:CE1	9:J:361:LYS:HD2	2.45	0.51
1:A:14:ASN:HD21	2:B:72:LYS:HZ1	1.56	0.51
1:A:68:LEU:HD12	4:D:53:ARG:HE	1.75	0.51
2:B:47:ARG:NH2	2:B:53:LYS:O	2.44	0.51
2:B:58:THR:HG22	2:B:126:ASN:ND2	2.24	0.51
2:B:105:GLN:HB3	2:B:108:HIS:CE1	2.45	0.51
4:D:41:ASP:N	4:D:41:ASP:OD1	2.42	0.51
9:J:104:GLN:NE2	9:J:123:ILE:HD11	2.25	0.51
9:J:180:HIS:O	9:J:184:LEU:N	2.30	0.51
9:J:243:SER:O	9:J:247:LYS:HG2	2.11	0.51
9:J:581:MET:SD	9:J:581:MET:N	2.83	0.51
8:I:598:ARG:HA	8:I:600:TRP:CZ3	2.45	0.51
9:J:436:MET:HG2	9:J:448:ARG:HB2	1.91	0.51
9:J:614:SER:OG	9:J:703:HIS:HB3	2.10	0.51
2:B:59:MET:CE	2:B:126:ASN:HA	2.39	0.51
2:B:78:LEU:H	2:B:79:ARG:NH2	2.08	0.51
7:H:67:LYS:HZ1	7:H:86:SER:HA	1.75	0.51
8:I:575:TYR:CG	8:I:579:GLY:HA3	2.45	0.51
2:B:37:THR:HA	2:B:40:ARG:NE	2.26	0.51
3:C:56:ASP:N	4:D:100:ARG:HH22	2.08	0.51
7:H:91:ARG:NH2	7:H:93:ASN:HD22	2.09	0.51
9:J:348:PRO:HG3	9:J:442:TYR:HB2	1.92	0.51
2:B:57:GLU:OE1	2:B:57:GLU:N	2.43	0.51
6:F:188:ASP:HA	6:F:191:MET:HE3	1.92	0.51
7:H:31:HIS:O	9:J:484:TRP:CZ2	2.64	0.51
9:J:204:ALA:HB2	9:J:239:ARG:NH2	2.25	0.51
9:J:204:ALA:HB2	9:J:239:ARG:HH22	1.74	0.51
3:C:101:TYR:O	3:C:106:VAL:HG23	2.10	0.51
4:D:58:ASN:OD1	4:D:59:VAL:N	2.44	0.51
6:F:52:THR:HG23	6:F:54:PRO:HD2	1.91	0.51
6:F:107:GLU:OE1	6:F:107:GLU:N	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:182:ASP:O	6:F:185:ILE:HG22	2.11	0.51
7:H:1:MET:SD	7:H:85:SER:HB3	2.50	0.51
7:H:51:GLU:CD	7:H:55:LEU:HD13	2.36	0.51
7:H:55:LEU:HB3	7:H:72:VAL:N	2.23	0.51
1:A:168:ARG:NE	1:A:170:GLU:OE1	2.43	0.51
3:C:2:THR:HG22	3:C:3:ILE:N	2.26	0.51
3:C:3:ILE:HG23	3:C:85:ASN:O	2.10	0.51
4:D:177:TYR:O	4:D:181:VAL:HG22	2.11	0.51
6:F:49:ARG:HH22	6:F:59:ARG:NH2	2.05	0.51
7:H:56:TYR:CE2	7:H:96:ARG:HG2	2.46	0.51
2:B:67:TRP:O	2:B:71:TYR:N	2.44	0.51
3:C:80:LEU:HD23	3:C:82:PHE:CE2	2.46	0.51
6:F:80:ARG:NH2	6:F:95:VAL:HA	2.21	0.51
9:J:83:ILE:HG12	9:J:231:LYS:HZ1	1.76	0.51
1:A:171:GLU:OE2	1:A:171:GLU:N	2.44	0.50
2:B:113:VAL:HG21	2:B:134:THR:C	2.36	0.50
1:G:147:PHE:CD1	1:G:160:LEU:HG	2.46	0.50
7:H:12:ASN:ND2	9:J:483:LYS:HB3	2.26	0.50
1:A:87:ILE:HD13	1:A:109:PRO:HG3	1.93	0.50
2:B:57:GLU:H	2:B:127:LEU:HA	1.76	0.50
8:I:510:THR:CB	8:I:529:GLN:OE1	2.59	0.50
2:B:105:GLN:HB3	2:B:108:HIS:HE1	1.76	0.50
7:H:31:HIS:CE1	9:J:488:PHE:N	2.44	0.50
4:D:30:LYS:HE3	4:D:32:PHE:HE1	1.75	0.50
4:D:192:PRO:HD2	4:D:194:ARG:NH2	2.25	0.50
5:E:60:LEU:HB2	5:E:73:ALA:HB3	1.94	0.50
8:I:493:ILE:HG21	8:I:509:ALA:HB1	1.91	0.50
9:J:179:PRO:HG2	9:J:187:TYR:CD2	2.47	0.50
9:J:304:HIS:HA	9:J:307:ARG:HG2	1.93	0.50
9:J:438:GLN:HA	9:J:441:ILE:HD12	1.93	0.50
2:B:120:VAL:O	2:B:129:ILE:HG12	2.11	0.50
7:H:58:GLY:HA2	7:H:69:TYR:CD2	2.46	0.50
7:H:61:TYR:HB3	7:H:68:ILE:HB	1.92	0.50
1:A:66:ARG:HB3	3:C:77:PRO:HB3	1.93	0.50
2:B:109:ALA:O	2:B:112:PHE:N	2.43	0.50
4:D:200:ASN:HA	4:D:203:GLN:HG2	1.94	0.50
6:F:164:CYS:C	6:F:165:LYS:HD2	2.36	0.50
9:J:621:ASP:HA	9:J:625:PRO:HA	1.93	0.50
1:A:130:SER:O	1:A:133:ILE:HG22	2.10	0.50
3:C:4:PHE:HB2	3:C:85:ASN:HB2	1.92	0.50
6:F:80:ARG:HA	6:F:94:PHE:HZ	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:121:TYR:CG	6:F:180:PHE:HZ	2.29	0.50
3:C:18:TYR:CE2	3:C:20:GLU:HB2	2.46	0.50
2:B:51:ARG:HB2	7:H:48:GLY:O	2.11	0.50
4:D:32:PHE:CD2	4:D:36:LEU:HG	2.46	0.50
1:G:107:ASN:HB2	1:G:110:THR:HB	1.94	0.50
9:J:255:ASN:HA	9:J:258:GLU:HG2	1.94	0.50
2:B:96:LEU:HD22	2:B:140:ILE:HG23	1.93	0.49
3:C:7:TYR:N	3:C:83:VAL:O	2.36	0.49
5:E:91:ASP:O	5:E:95:LYS:HG2	2.12	0.49
9:J:297:PHE:CE1	9:J:324:GLN:HG3	2.47	0.49
1:A:70:MET:CE	4:D:52:ASN:HD21	2.26	0.49
2:B:29:THR:O	2:B:33:ILE:HG12	2.12	0.49
9:J:225:LYS:HE3	9:J:229:GLN:HE22	1.76	0.49
4:D:167:ASP:OD1	4:D:168:LEU:N	2.46	0.49
5:E:29:ARG:HG2	5:E:33:HIS:CE1	2.46	0.49
5:E:93:GLY:HA2	5:E:136:TYR:HD2	1.78	0.49
1:G:145:CYS:HA	1:G:161:ARG:O	2.12	0.49
9:J:409:GLN:OE1	9:J:409:GLN:N	2.39	0.49
9:J:524:GLN:CD	9:J:607:ASP:HB3	2.38	0.49
1:A:78:GLN:NE2	1:A:82:ARG:HH22	2.11	0.49
1:A:148:PHE:HE1	1:A:161:LEU:HD12	1.76	0.49
3:C:25:LYS:HB2	4:D:129:PRO:HA	1.95	0.49
4:D:132:SER:HA	1:G:172:ILE:HG13	1.95	0.49
6:F:119:ARG:NH1	6:F:180:PHE:O	2.44	0.49
9:J:489:THR:HA	9:J:492:LEU:HB2	1.95	0.49
2:B:51:ARG:HH11	7:H:49:ALA:N	2.10	0.49
6:F:50:VAL:HG13	6:F:55:GLU:OE2	2.12	0.49
1:G:107:ASN:HB2	1:G:110:THR:CB	2.41	0.49
8:I:510:THR:CG2	8:I:533:MET:HE2	2.24	0.49
8:I:562:ARG:HB2	8:I:598:ARG:HH11	1.76	0.49
9:J:298:ILE:O	9:J:299:ILE:C	2.56	0.49
1:A:145:GLN:HE22	1:A:147:TRP:CD1	2.30	0.49
7:H:2:ALA:H	7:H:84:ASP:HB2	1.76	0.49
9:J:365:ALA:HA	9:J:368:GLU:OE2	2.12	0.49
9:J:611:ARG:HE	9:J:613:ARG:CG	2.26	0.49
2:B:8:ASP:OD2	2:B:98:ARG:NH1	2.45	0.49
3:C:11:LYS:HB3	3:C:79:GLY:HA3	1.93	0.49
5:E:5:TYR:O	5:E:84:ILE:HD13	2.13	0.49
5:E:8:ILE:O	5:E:16:ILE:N	2.46	0.49
7:H:53:LYS:NZ	7:H:54:GLU:O	2.32	0.49
9:J:108:TRP:HB2	9:J:160:ARG:HH22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:515:ALA:O	9:J:519:ARG:HB2	2.12	0.49
2:B:93:PHE:N	2:B:141:PRO:O	2.45	0.49
2:B:121:ARG:HE	2:B:150:ASN:CG	2.20	0.49
4:D:25:ARG:HH11	4:D:100:ARG:CB	2.26	0.49
3:C:71:LEU:HD21	3:C:83:VAL:HG13	1.95	0.49
4:D:146:CYS:SG	4:D:147:PHE:N	2.85	0.49
6:F:181:GLU:OE2	6:F:183:PHE:HB3	2.13	0.49
1:A:100:GLU:HA	1:A:163:VAL:O	2.12	0.49
2:B:88:VAL:CG1	2:B:145:PHE:HB2	2.43	0.49
3:C:1:MET:HB2	3:C:140:PHE:CE1	2.48	0.49
4:D:169:LEU:HD11	4:D:209:VAL:HG11	1.94	0.49
4:D:188:SER:HA	1:G:52:ARG:HH12	1.78	0.49
5:E:30:LYS:HA	5:E:33:HIS:CD2	2.48	0.49
6:F:48:SER:OG	6:F:49:ARG:N	2.44	0.49
1:G:10:LYS:HD3	1:G:85:ASN:HD21	1.78	0.49
1:G:42:LEU:O	1:G:45:ILE:HG12	2.12	0.49
7:H:105:LEU:HD22	7:H:129:ALA:HB1	1.94	0.49
8:I:518:LYS:CA	8:I:523:TYR:CE1	2.96	0.49
9:J:278:TYR:HE1	9:J:331:LEU:HD21	1.73	0.49
2:B:60:LYS:HZ3	2:B:78:LEU:HB3	1.78	0.48
4:D:121:ILE:HG22	4:D:121:ILE:O	2.12	0.48
1:G:78:GLN:O	1:G:82:ILE:HG13	2.13	0.48
7:H:16:TYR:OH	9:J:484:TRP:NE1	2.46	0.48
7:H:31:HIS:O	9:J:484:TRP:CH2	2.66	0.48
9:J:348:PRO:CG	9:J:442:TYR:HB2	2.43	0.48
9:J:590:LEU:HD12	9:J:591:SER:H	1.77	0.48
1:A:121:THR:HG22	1:A:122:ASN:H	1.78	0.48
1:A:141:GLN:HE22	3:C:11:LYS:HB2	1.78	0.48
2:B:33:ILE:HG23	7:H:110:ILE:CG2	2.42	0.48
4:D:135:GLU:HG3	4:D:136:ILE:HG12	1.95	0.48
6:F:125:GLU:HG2	6:F:127:GLU:H	1.77	0.48
7:H:107:THR:HA	7:H:110:ILE:HB	1.94	0.48
9:J:524:GLN:NE2	9:J:607:ASP:HB3	2.28	0.48
1:G:28:MET:HB3	1:G:38:VAL:HB	1.94	0.48
8:I:430:LYS:HD3	8:I:430:LYS:C	2.38	0.48
9:J:141:VAL:HG22	9:J:176:PHE:HB2	1.96	0.48
7:H:93:ASN:HB2	7:H:96:ARG:HH21	1.79	0.48
9:J:4:ASP:OD2	9:J:7:ALA:HB2	2.13	0.48
4:D:176:LEU:HB3	4:D:198:PHE:HE1	1.77	0.48
7:H:66:HIS:HA	7:H:84:ASP:OD1	2.13	0.48
9:J:620:ALA:HB3	9:J:695:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:ASP:CA	4:D:100:ARG:HH22	2.27	0.48
7:H:129:ALA:O	7:H:132:LYS:HG2	2.14	0.48
9:J:226:ILE:HG23	9:J:252:ALA:HB1	1.94	0.48
9:J:449:LYS:HA	9:J:475:MET:HE3	1.95	0.48
1:A:10:ALA:HA	2:B:41:LEU:HD22	1.94	0.48
1:A:84:TYR:HE1	2:B:5:ILE:HG21	1.78	0.48
3:C:25:LYS:HB3	4:D:126:SER:O	2.14	0.48
4:D:4:TYR:HA	4:D:23:VAL:HG21	1.96	0.48
6:F:144:ASN:HB2	6:F:170:TRP:HH2	1.79	0.48
1:G:150:ASP:OD1	1:G:151:GLN:N	2.47	0.48
8:I:449:HIS:HA	8:I:452:LYS:HE3	1.96	0.48
9:J:612:ILE:O	9:J:613:ARG:HD2	2.14	0.48
4:D:15:LEU:HD21	4:D:18:ASN:HB3	1.96	0.48
4:D:182:LEU:HD22	6:F:37:LEU:HG	1.96	0.48
6:F:129:LEU:HD22	6:F:145:CYS:SG	2.53	0.48
6:F:136:VAL:CG2	6:F:137:PRO:HD2	2.43	0.48
1:G:74:ASP:O	1:G:77:GLN:HG3	2.14	0.48
1:G:81:ARG:HD3	1:G:87:GLN:OE1	2.14	0.48
7:H:108:ASP:HA	7:H:111:CYS:SG	2.53	0.48
9:J:90:LEU:HD12	9:J:93:LEU:HD22	1.95	0.48
2:B:40:ARG:HA	7:H:103:HIS:CE1	2.48	0.48
2:B:52:PHE:O	7:H:47:LYS:HE2	2.14	0.48
3:C:95:GLU:HG2	3:C:96:LEU:N	2.28	0.48
5:E:112:ALA:HA	6:F:70:ARG:CZ	2.44	0.48
6:F:31:SER:OG	6:F:32:GLN:N	2.46	0.48
4:D:185:PRO:HB2	1:G:48:ASN:OD1	2.14	0.48
4:D:187:TYR:HE2	4:D:193:ILE:HG12	1.78	0.48
5:E:110:MET:SD	6:F:74:LEU:HG	2.54	0.48
9:J:189:LEU:O	9:J:192:GLU:HB2	2.14	0.48
9:J:333:CYS:HA	9:J:336:ILE:HD12	1.96	0.48
9:J:535:TRP:CZ2	9:J:705:GLY:HA3	2.49	0.48
4:D:143:THR:HG22	4:D:161:THR:HA	1.96	0.47
4:D:197:LEU:HD13	6:F:134:ILE:HG23	1.96	0.47
6:F:31:SER:CB	1:G:83:TYR:HD1	2.27	0.47
8:I:575:TYR:C	8:I:579:GLY:H	2.20	0.47
9:J:33:HIS:CE1	9:J:37:TRP:HE3	2.22	0.47
9:J:187:TYR:HA	9:J:190:ARG:CG	2.41	0.47
9:J:298:ILE:HG13	9:J:299:ILE:N	2.29	0.47
9:J:303:LYS:O	9:J:307:ARG:HG2	2.13	0.47
1:A:52:MET:HE1	3:C:117:PRO:HG3	1.96	0.47
3:C:63:TYR:CE2	3:C:65:LYS:HG3	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:GLN:HB2	1:G:169:GLU:HB2	1.96	0.47
7:H:7:VAL:HG12	7:H:15:LEU:O	2.14	0.47
7:H:67:LYS:HB2	7:H:83:ILE:HB	1.96	0.47
8:I:518:LYS:CA	8:I:523:TYR:CD1	2.85	0.47
9:J:77:TRP:HE3	9:J:218:THR:HG23	1.79	0.47
7:H:5:ILE:CD1	7:H:102:LEU:HD11	2.43	0.47
7:H:7:VAL:CG1	7:H:15:LEU:H	2.27	0.47
7:H:54:GLU:H	7:H:54:GLU:CD	2.22	0.47
7:H:75:THR:HG23	7:H:77:VAL:HG23	1.96	0.47
8:I:427:GLN:HE22	8:I:431:LEU:HG	1.79	0.47
9:J:449:LYS:O	9:J:453:ILE:HG12	2.15	0.47
1:A:78:GLN:HB2	1:A:89:PRO:HG2	1.96	0.47
3:C:63:TYR:HB3	3:C:72:HIS:ND1	2.30	0.47
4:D:1:MET:HA	4:D:163:LEU:HD22	1.96	0.47
7:H:38:VAL:HG23	9:J:446:ARG:HG2	1.96	0.47
7:H:109:ALA:HB2	7:H:126:PHE:HB2	1.94	0.47
9:J:225:LYS:HG2	9:J:229:GLN:HE22	1.79	0.47
9:J:256:LEU:HD11	9:J:269:ILE:HG23	1.96	0.47
9:J:304:HIS:HA	9:J:307:ARG:CG	2.44	0.47
2:B:81:ASN:HD22	2:B:85:MET:HE3	1.79	0.47
3:C:144:ASN:ND2	3:C:145:ILE:O	2.47	0.47
1:G:101:SER:HG	1:G:161:ARG:HH11	1.59	0.47
9:J:191:LEU:HD22	9:J:195:PHE:CZ	2.49	0.47
2:B:113:VAL:HG23	2:B:145:PHE:HD1	1.78	0.47
3:C:125:LEU:HD12	3:C:126:PHE:N	2.29	0.47
4:D:28:HIS:CE1	4:D:30:LYS:HB2	2.50	0.47
4:D:62:VAL:O	4:D:64:VAL:HG13	2.15	0.47
4:D:180:TYR:HB2	4:D:198:PHE:CD1	2.50	0.47
6:F:160:CYS:HG	6:F:162:PHE:HE2	1.62	0.47
8:I:437:MET:HB2	8:I:437:MET:HE2	1.69	0.47
9:J:79:HIS:HB3	9:J:84:LEU:HD13	1.96	0.47
1:A:38:ASP:C	1:A:42:GLN:HE22	2.23	0.47
1:A:106:ASP:O	1:A:152:GLN:NE2	2.25	0.47
1:A:161:LEU:HD21	1:A:163:VAL:HG13	1.95	0.47
4:D:1:MET:SD	4:D:163:LEU:HD21	2.55	0.47
4:D:92:TYR:CD1	4:D:94:ILE:HG12	2.48	0.47
4:D:176:LEU:HB3	4:D:198:PHE:CE1	2.50	0.47
4:D:183:LYS:O	6:F:40:SER:OG	2.32	0.47
4:D:183:LYS:NZ	4:D:184:ASN:HD22	2.12	0.47
5:E:19:LYS:HD2	5:E:20:GLU:H	1.80	0.47
7:H:91:ARG:CZ	7:H:93:ASN:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:568:ILE:HA	8:I:571:ALA:HB3	1.96	0.47
8:I:598:ARG:CA	8:I:600:TRP:CZ3	2.98	0.47
9:J:80:PRO:HB2	9:J:83:ILE:HB	1.97	0.47
9:J:99:VAL:HA	9:J:198:MET:HE1	1.96	0.47
9:J:106:MET:HB3	9:J:142:LEU:HB3	1.97	0.47
9:J:518:LEU:HD12	9:J:520:HIS:CE1	2.50	0.47
9:J:616:HIS:O	9:J:701:GLU:HB3	2.15	0.47
1:A:47:GLY:O	1:A:132:CYS:HA	2.14	0.47
2:B:80:THR:HG22	2:B:81:ASN:O	2.14	0.47
4:D:104:THR:OG1	4:D:106:ASN:OD1	2.30	0.47
4:D:200:ASN:O	4:D:203:GLN:HG2	2.15	0.47
5:E:119:PRO:HB2	5:E:121:LYS:NZ	2.29	0.47
1:G:47:TYR:O	1:G:134:GLY:HA3	2.14	0.47
7:H:59:LEU:HD11	7:H:67:LYS:CB	2.42	0.47
8:I:598:ARG:HG3	8:I:600:TRP:HE3	1.64	0.47
9:J:101:VAL:HA	9:J:139:CYS:O	2.15	0.47
9:J:275:PHE:O	9:J:279:LYS:HG2	2.14	0.47
2:B:93:PHE:O	2:B:97:THR:HG23	2.15	0.47
4:D:25:ARG:HH11	4:D:100:ARG:HB2	1.79	0.47
4:D:153:ILE:H	4:D:153:ILE:HD12	1.79	0.47
6:F:167:THR:HG1	6:F:169:HIS:CD2	2.31	0.47
9:J:284:MET:HG3	9:J:296:GLN:HE22	1.80	0.47
9:J:449:LYS:HA	9:J:475:MET:CE	2.45	0.47
2:B:13:GLU:O	2:B:16:ASN:HB2	2.15	0.47
5:E:93:GLY:O	5:E:97:PHE:CB	2.63	0.47
5:E:114:TYR:HE1	5:E:118:THR:O	1.98	0.47
1:G:46:GLY:O	1:G:49:MET:HB2	2.14	0.47
8:I:581:ARG:H	8:I:581:ARG:HG2	1.43	0.47
9:J:206:MET:O	9:J:209:ARG:HB3	2.14	0.47
2:B:148:GLU:O	2:B:148:GLU:HG2	2.14	0.46
5:E:65:ARG:HH21	5:E:89:LYS:NZ	2.13	0.46
7:H:43:CYS:H	7:H:45:ILE:HG22	1.80	0.46
7:H:71:PHE:HD1	7:H:79:PHE:CD1	2.33	0.46
7:H:125:LYS:HA	7:H:128:ARG:NH1	2.29	0.46
8:I:530:LEU:CD1	8:I:545:LEU:HD23	2.45	0.46
9:J:20:VAL:HG23	9:J:99:VAL:HB	1.96	0.46
9:J:156:LEU:HA	9:J:159:GLU:OE1	2.15	0.46
9:J:255:ASN:O	9:J:258:GLU:HG2	2.15	0.46
9:J:521:GLN:CD	9:J:521:GLN:H	2.23	0.46
9:J:523:ASP:O	9:J:527:ARG:HG3	2.15	0.46
5:E:4:TYR:CD2	5:E:21:PHE:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:85:GLU:HB3	6:F:90:GLN:HE22	1.81	0.46
5:E:86:HIS:CE1	5:E:89:LYS:HD2	2.50	0.46
6:F:166:VAL:HA	6:F:177:MET:O	2.15	0.46
7:H:129:ALA:HA	7:H:132:LYS:HZ2	1.80	0.46
8:I:508:ARG:HA	8:I:508:ARG:HD3	1.69	0.46
9:J:479:TYR:HB3	9:J:488:PHE:CD1	2.48	0.46
9:J:699:ARG:C	9:J:714:THR:HG21	2.41	0.46
9:J:701:GLU:HA	9:J:708:GLN:HG2	1.97	0.46
2:B:139:SER:HB3	2:B:142:ALA:HB3	1.98	0.46
5:E:64:ASP:O	5:E:65:ARG:NH1	2.41	0.46
1:G:66:CYS:HB3	1:G:167:ARG:NH1	2.30	0.46
1:G:120:THR:O	1:G:153:LYS:NZ	2.48	0.46
7:H:127:ASP:O	7:H:131:GLN:HG2	2.15	0.46
9:J:204:ALA:O	9:J:208:LYS:HG3	2.16	0.46
9:J:455:MET:HG2	9:J:459:TYR:CE2	2.50	0.46
1:A:104:VAL:HA	1:A:160:GLU:OE1	2.16	0.46
5:E:21:PHE:HD2	5:E:134:ARG:NH1	2.14	0.46
5:E:65:ARG:NH1	5:E:71:VAL:H	2.14	0.46
7:H:57:LEU:HD23	7:H:57:LEU:HA	1.75	0.46
8:I:490:GLU:HA	8:I:493:ILE:HD13	1.85	0.46
9:J:102:LEU:HD21	9:J:123:ILE:HG13	1.97	0.46
9:J:332:PHE:CE2	9:J:350:ILE:HD13	2.51	0.46
9:J:438:GLN:CD	9:J:441:ILE:HD12	2.41	0.46
1:A:168:ARG:HH11	4:D:51:PHE:HD1	1.62	0.46
3:C:32:GLU:H	3:C:32:GLU:CD	2.19	0.46
7:H:67:LYS:N	7:H:83:ILE:O	2.49	0.46
9:J:113:TRP:CH2	9:J:156:LEU:HB3	2.51	0.46
9:J:703:HIS:HA	9:J:706:THR:O	2.16	0.46
1:A:148:PHE:CE1	1:A:161:LEU:HD12	2.50	0.46
6:F:42:ILE:HD13	1:G:24:LEU:HD21	1.97	0.46
6:F:64:GLY:HA2	6:F:152:ILE:HG12	1.96	0.46
7:H:8:ILE:HA	7:H:13:ALA:HA	1.97	0.46
7:H:28:LEU:HD13	7:H:30:TYR:CE2	2.47	0.46
9:J:506:ALA:O	9:J:509:ILE:HG12	2.15	0.46
1:A:12:LYS:HG3	1:A:13:VAL:N	2.30	0.46
1:A:144:VAL:HG22	1:A:165:PHE:HA	1.97	0.46
3:C:93:VAL:HG22	3:C:142:ILE:HG13	1.97	0.46
8:I:493:ILE:CG1	8:I:494:VAL:N	2.54	0.46
8:I:501:LYS:HA	8:I:501:LYS:HD3	1.72	0.46
9:J:244:THR:HG22	9:J:248:HIS:CD2	2.51	0.46
1:A:16:GLU:O	1:A:19:THR:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:PHE:HE1	7:H:75:THR:HB	1.81	0.46
2:B:40:ARG:NH1	7:H:111:CYS:SG	2.86	0.46
3:C:80:LEU:HG	3:C:81:LYS:N	2.31	0.46
4:D:105:THR:O	4:D:109:ILE:HG12	2.15	0.46
9:J:590:LEU:HB3	9:J:693:THR:HB	1.96	0.46
2:B:15:VAL:HG22	2:B:111:LYS:CD	2.45	0.46
3:C:123:SER:OG	3:C:125:LEU:HG	2.16	0.46
4:D:58:ASN:H	4:D:61:HIS:CE1	2.33	0.46
4:D:96:LEU:HB3	4:D:98:PHE:CE2	2.51	0.46
6:F:49:ARG:HH12	6:F:59:ARG:CZ	2.29	0.46
1:G:133:ARG:HH21	1:G:145:CYS:N	2.10	0.46
7:H:26:LEU:O	7:H:30:TYR:OH	2.34	0.46
9:J:34:LYS:O	9:J:37:TRP:N	2.48	0.46
1:A:69:GLU:OE1	1:A:71:ARG:HB2	2.16	0.45
2:B:27:LEU:HA	2:B:27:LEU:HD12	1.79	0.45
2:B:47:ARG:HG3	7:H:52:SER:HB3	1.98	0.45
3:C:48:PHE:O	3:C:52:ILE:HG12	2.16	0.45
4:D:57:ILE:HA	4:D:61:HIS:ND1	2.31	0.45
6:F:80:ARG:NE	6:F:95:VAL:HG22	2.31	0.45
6:F:81:SER:C	6:F:83:LYS:H	2.24	0.45
1:G:104:PHE:O	1:G:157:VAL:HB	2.16	0.45
7:H:55:LEU:HD21	7:H:57:LEU:HD11	1.97	0.45
9:J:116:LYS:HA	9:J:119:GLN:HG3	1.97	0.45
9:J:313:LEU:HD23	9:J:313:LEU:O	2.16	0.45
9:J:460:LEU:HD21	9:J:498:CYS:SG	2.56	0.45
2:B:109:ALA:HA	2:B:112:PHE:CD2	2.52	0.45
4:D:216:ASN:O	4:D:218:ASP:N	2.49	0.45
7:H:123:SER:OG	7:H:126:PHE:N	2.26	0.45
9:J:164:LEU:HD12	9:J:165:THR:N	2.31	0.45
4:D:172:LYS:HD2	4:D:219:LYS:CE	2.46	0.45
5:E:7:VAL:HG23	5:E:18:GLU:HG3	1.97	0.45
5:E:57:ASN:HA	6:F:83:LYS:HZ2	1.81	0.45
5:E:88:ASN:OD1	5:E:89:LYS:N	2.49	0.45
6:F:31:SER:C	1:G:10:LYS:HG3	2.41	0.45
6:F:136:VAL:HG13	6:F:137:PRO:O	2.17	0.45
8:I:522:LEU:HD13	8:I:522:LEU:HA	1.77	0.45
9:J:83:ILE:HG12	9:J:231:LYS:NZ	2.31	0.45
9:J:83:ILE:HD11	9:J:209:ARG:NE	2.30	0.45
9:J:99:VAL:HG22	9:J:198:MET:CE	2.46	0.45
9:J:163:SER:HA	9:J:166:ASN:HD21	1.81	0.45
9:J:318:HIS:HB2	9:J:362:ARG:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:THR:HA	2:B:32:TYR:CD2	2.51	0.45
6:F:45:TYR:CD1	1:G:28:MET:HE1	2.52	0.45
6:F:60:LEU:HD23	6:F:145:CYS:HA	1.98	0.45
1:G:77:GLN:OE1	1:G:88:PRO:HD2	2.16	0.45
9:J:120:CYS:HA	9:J:123:ILE:HG12	1.97	0.45
1:A:17:PHE:HE2	2:B:7:PHE:CZ	2.35	0.45
2:B:102:GLY:O	2:B:104:LYS:N	2.50	0.45
3:C:65:LYS:N	4:D:136:ILE:O	2.48	0.45
5:E:84:ILE:HG22	5:E:86:HIS:CD2	2.50	0.45
5:E:101:MET:CE	5:E:132:PHE:HD2	2.30	0.45
7:H:12:ASN:HD22	9:J:483:LYS:CB	2.29	0.45
7:H:16:TYR:HH	9:J:484:TRP:NE1	2.15	0.45
9:J:536:GLN:HB3	9:J:541:VAL:O	2.17	0.45
9:J:584:THR:HB	9:J:600:LEU:HA	1.97	0.45
2:B:124:LEU:O	2:B:127:LEU:HB2	2.17	0.45
3:C:68:ARG:HD3	4:D:132:SER:N	2.32	0.45
6:F:100:TRP:HB3	6:F:106:LYS:O	2.16	0.45
9:J:513:VAL:HA	9:J:516:LEU:HD12	1.98	0.45
1:A:46:ILE:HD12	1:A:46:ILE:HA	1.76	0.45
1:A:102:SER:HB3	1:A:162:ARG:HH11	1.82	0.45
2:B:23:LYS:HZ2	2:B:110:PRO:HB2	1.82	0.45
3:C:24:THR:OG1	4:D:129:PRO:HD3	2.17	0.45
9:J:102:LEU:HD12	9:J:103:PHE:H	1.81	0.45
1:A:167:ARG:HD2	1:A:168:ARG:C	2.41	0.45
2:B:88:VAL:HG12	2:B:145:PHE:HB2	1.99	0.45
5:E:62:SER:HA	5:E:65:ARG:HH22	1.81	0.45
6:F:67:VAL:HG11	6:F:152:ILE:HD13	1.99	0.45
6:F:104:PHE:CZ	6:F:129:LEU:HG	2.51	0.45
7:H:60:LEU:H	7:H:60:LEU:HD23	1.81	0.45
9:J:290:PRO:O	9:J:294:ILE:HG12	2.16	0.45
9:J:554:GLN:HA	9:J:557:TRP:CE2	2.52	0.45
2:B:127:LEU:HD11	7:H:52:SER:HB2	1.99	0.45
6:F:68:GLY:HA3	6:F:155:ALA:HB3	1.99	0.45
1:G:21:TYR:HE2	1:G:124:TYR:CE2	2.34	0.45
7:H:112:ASN:ND2	7:H:115:TYR:H	2.15	0.45
9:J:279:LYS:O	9:J:283:LEU:HG	2.16	0.45
9:J:500:LEU:HB3	9:J:508:TYR:HE2	1.81	0.45
1:A:64:ALA:HB2	1:A:76:ARG:HE	1.82	0.45
2:B:121:ARG:NH1	2:B:150:ASN:HB3	2.29	0.45
5:E:12:ASN:HB2	5:E:14:ASN:OD1	2.17	0.45
5:E:25:ASN:O	5:E:30:LYS:HE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:7:VAL:HG13	7:H:14:PRO:HD2	1.99	0.45
7:H:64:GLU:O	7:H:66:HIS:ND1	2.37	0.45
9:J:109:ASN:H	9:J:113:TRP:HB2	1.82	0.45
9:J:126:ALA:HA	9:J:129:ASN:HD22	1.82	0.45
2:B:60:LYS:NZ	2:B:78:LEU:HB3	2.32	0.44
4:D:25:ARG:HD2	4:D:100:ARG:HB2	1.98	0.44
4:D:172:LYS:HD2	4:D:219:LYS:HE2	1.99	0.44
6:F:39:PHE:O	6:F:42:ILE:HB	2.17	0.44
8:I:432:GLY:C	8:I:434:LEU:N	2.74	0.44
9:J:261:ILE:HG22	9:J:269:ILE:HD13	1.98	0.44
9:J:364:ASP:O	9:J:367:MET:HB2	2.17	0.44
9:J:365:ALA:HA	9:J:368:GLU:CD	2.42	0.44
9:J:620:ALA:HB3	9:J:695:LEU:CD1	2.46	0.44
6:F:136:VAL:HG22	6:F:137:PRO:CD	2.47	0.44
1:G:40:LYS:HG2	1:G:44:ARG:HH11	1.82	0.44
9:J:190:ARG:O	9:J:193:SER:OG	2.27	0.44
9:J:528:ILE:HG23	9:J:608:ILE:HG12	1.99	0.44
1:A:37:GLU:OE2	1:A:122:ASN:ND2	2.50	0.44
1:A:141:GLN:NE2	3:C:11:LYS:HD2	2.32	0.44
2:B:136:GLU:O	2:B:136:GLU:HG2	2.17	0.44
3:C:71:LEU:HG	3:C:84:LEU:O	2.17	0.44
5:E:6:PHE:HD2	5:E:84:ILE:HD11	1.83	0.44
6:F:129:LEU:HD13	6:F:149:THR:HG22	1.98	0.44
8:I:503:GLN:HE21	8:I:503:GLN:HB3	1.55	0.44
9:J:106:MET:SD	9:J:144:GLN:HB2	2.57	0.44
9:J:229:GLN:CB	9:J:248:HIS:HB3	2.47	0.44
9:J:579:VAL:N	9:J:605:LEU:HB2	2.32	0.44
9:J:611:ARG:CZ	9:J:705:GLY:HA2	2.48	0.44
1:A:89:PRO:HB3	1:A:105:PHE:CE1	2.52	0.44
1:A:174:PRO:HB3	3:C:43:PHE:CD2	2.52	0.44
3:C:68:ARG:NE	4:D:131:SER:HA	2.33	0.44
5:E:11:GLN:HA	5:E:81:ARG:HH12	1.83	0.44
9:J:98:SER:OG	9:J:199:ALA:HA	2.17	0.44
9:J:356:ALA:O	9:J:360:MET:HG3	2.18	0.44
9:J:517:SER:HB2	9:J:580:GLU:CG	2.47	0.44
1:A:142:LEU:HD21	4:D:51:PHE:CE1	2.53	0.44
1:A:142:LEU:HD21	4:D:51:PHE:CZ	2.53	0.44
3:C:142:ILE:HG12	3:C:144:ASN:HB2	1.99	0.44
6:F:113:HIS:HB2	6:F:121:TYR:CD1	2.53	0.44
6:F:187:ARG:HH11	6:F:191:MET:HE1	1.81	0.44
1:G:36:GLU:OE1	1:G:36:GLU:N	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:5:ILE:HB	7:H:134:MET:CE	2.48	0.44
9:J:108:TRP:CZ2	9:J:156:LEU:HD22	2.53	0.44
9:J:311:LYS:HA	9:J:312:ASP:C	2.42	0.44
4:D:138:GLU:OE1	4:D:139:ALA:N	2.51	0.44
4:D:151:THR:HG21	1:G:139:VAL:HG23	1.98	0.44
5:E:5:TYR:CE2	5:E:34:ARG:HG2	2.46	0.44
6:F:121:TYR:CD2	6:F:180:PHE:HZ	2.35	0.44
6:F:169:HIS:O	6:F:175:THR:HG22	2.18	0.44
6:F:188:ASP:O	6:F:192:GLU:HG3	2.17	0.44
7:H:56:TYR:HE2	7:H:96:ARG:HD3	1.82	0.44
7:H:66:HIS:C	7:H:67:LYS:HD3	2.42	0.44
9:J:362:ARG:HG2	9:J:422:TYR:HE2	1.83	0.44
9:J:542:PRO:HB3	9:J:557:TRP:CH2	2.52	0.44
1:A:11:LYS:HZ1	2:B:72:LYS:HE2	1.83	0.44
1:A:114:VAL:HG13	1:A:115:GLU:N	2.32	0.44
3:C:45:ILE:HG12	4:D:118:LEU:HD13	1.99	0.44
4:D:61:HIS:HD2	4:D:100:ARG:HG2	1.82	0.44
4:D:149:THR:C	4:D:151:THR:H	2.24	0.44
6:F:39:PHE:HA	6:F:42:ILE:HG12	1.99	0.44
6:F:57:GLN:HG2	6:F:143:LEU:HD23	1.99	0.44
6:F:164:CYS:HA	6:F:179:LYS:O	2.17	0.44
7:H:108:ASP:O	7:H:111:CYS:HB2	2.17	0.44
9:J:188:ALA:O	9:J:192:GLU:HG3	2.17	0.44
1:A:22:TYR:O	1:A:26:VAL:HG13	2.18	0.44
2:B:33:ILE:HD12	7:H:110:ILE:O	2.18	0.44
4:D:172:LYS:HA	4:D:175:GLU:HG2	1.99	0.44
6:F:72:ILE:HB	6:F:156:VAL:HG12	1.99	0.44
7:H:57:LEU:HB2	7:H:70:GLY:N	2.33	0.44
9:J:297:PHE:CZ	9:J:324:GLN:HG3	2.52	0.44
9:J:347:HIS:O	9:J:350:ILE:HD11	2.18	0.44
9:J:703:HIS:ND1	9:J:707:ASP:O	2.51	0.44
2:B:51:ARG:HH12	7:H:45:ILE:C	2.24	0.44
2:B:101:PRO:HA	2:B:140:ILE:HB	2.00	0.44
5:E:8:ILE:HG22	5:E:16:ILE:HB	1.99	0.44
6:F:31:SER:N	1:G:83:TYR:O	2.51	0.44
6:F:80:ARG:HA	6:F:94:PHE:CZ	2.53	0.44
1:G:21:TYR:O	1:G:25:VAL:HG23	2.18	0.44
9:J:170:ILE:HG23	9:J:174:MET:SD	2.58	0.44
2:B:22:ASN:OD1	2:B:23:LYS:N	2.51	0.43
2:B:72:LYS:HZ2	2:B:72:LYS:HG3	1.43	0.43
3:C:5:ASN:HB2	3:C:18:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:50:VAL:HG13	6:F:55:GLU:HG3	2.00	0.43
1:G:106:SER:HB2	1:G:111:GLU:HG3	2.00	0.43
9:J:321:LEU:HG	9:J:358:PHE:CD2	2.53	0.43
2:B:84:GLY:O	2:B:149:VAL:HG13	2.19	0.43
2:B:119:LEU:H	2:B:131:SER:HG	1.53	0.43
3:C:56:ASP:CG	4:D:100:ARG:HH22	2.26	0.43
4:D:209:VAL:HG12	4:D:214:ILE:HG13	1.99	0.43
5:E:19:LYS:HE3	5:E:20:GLU:O	2.18	0.43
1:G:52:ARG:O	1:G:55:GLU:HG3	2.18	0.43
1:G:71:GLU:CD	1:G:75:ARG:HH21	2.26	0.43
8:I:541:ARG:HH12	8:I:544:LEU:HD22	1.82	0.43
9:J:81:LYS:O	9:J:209:ARG:NH1	2.51	0.43
9:J:225:LYS:CG	9:J:229:GLN:HE22	2.31	0.43
1:A:12:LYS:HZ3	1:A:13:VAL:HB	1.83	0.43
4:D:121:ILE:O	4:D:123:SER:N	2.50	0.43
5:E:11:GLN:C	5:E:81:ARG:HH22	2.26	0.43
1:G:35:ALA:HA	1:G:38:VAL:HG22	2.00	0.43
9:J:593:ASP:HA	9:J:688:GLN:OE1	2.19	0.43
2:B:117:CYS:O	2:B:119:LEU:HG	2.19	0.43
4:D:103:MET:HB2	4:D:108:LYS:CE	2.48	0.43
4:D:146:CYS:HA	4:D:155:PHE:O	2.19	0.43
5:E:97:PHE:O	5:E:101:MET:HG2	2.17	0.43
1:G:65:ARG:HH11	1:G:65:ARG:HG2	1.83	0.43
8:I:435:TYR:HA	8:I:438:PHE:HB2	1.99	0.43
8:I:514:MET:CG	8:I:526:VAL:HG12	2.39	0.43
8:I:528:LYS:HE3	8:I:528:LYS:HB3	1.45	0.43
8:I:599:GLU:H	8:I:599:GLU:HG3	1.44	0.43
1:A:172:VAL:CG1	1:A:173:ILE:H	2.32	0.43
2:B:80:THR:HG23	2:B:86:TYR:HB3	1.99	0.43
2:B:99:ILE:HD13	3:C:112:ASP:OD1	2.19	0.43
3:C:107:GLU:HB3	3:C:108:PHE:CD1	2.53	0.43
4:D:41:ASP:OD2	4:D:50:SER:HB3	2.19	0.43
5:E:70:PHE:O	5:E:85:VAL:HA	2.19	0.43
6:F:80:ARG:O	6:F:81:SER:OG	2.31	0.43
6:F:85:GLU:HB3	6:F:90:GLN:NE2	2.33	0.43
7:H:2:ALA:N	7:H:84:ASP:HB2	2.34	0.43
7:H:59:LEU:HA	7:H:59:LEU:HD13	1.66	0.43
9:J:373:MET:HA	9:J:377:SER:O	2.19	0.43
3:C:87:ASP:C	3:C:141:GLY:HA2	2.43	0.43
6:F:77:VAL:HG23	6:F:78:ARG:N	2.34	0.43
7:H:49:ALA:O	7:H:72:VAL:HG21	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:519:THR:O	8:I:520:ALA:O	2.37	0.43
9:J:47:LYS:HG2	9:J:50:ASP:HB2	2.00	0.43
9:J:310:PHE:CD1	9:J:311:LYS:HB2	2.53	0.43
1:A:53:ARG:HD2	3:C:110:VAL:CG2	2.49	0.43
1:A:58:PHE:HB2	1:A:84:TYR:HE2	1.84	0.43
2:B:136:GLU:OE2	2:B:146:HIS:HB2	2.18	0.43
5:E:65:ARG:HH21	5:E:89:LYS:HZ3	1.66	0.43
6:F:181:GLU:HB3	6:F:184:VAL:HB	2.00	0.43
6:F:189:LYS:HD3	6:F:192:GLU:CD	2.44	0.43
9:J:18:PRO:HD2	9:J:53:ALA:C	2.43	0.43
9:J:182:GLU:HG2	9:J:183:HIS:ND1	2.34	0.43
9:J:270:LYS:HD2	9:J:320:TRP:CE3	2.53	0.43
1:A:81:PHE:CE2	1:A:105:PHE:HZ	2.36	0.43
4:D:212:THR:O	4:D:214:ILE:HD12	2.19	0.43
7:H:90:LEU:HD12	7:H:90:LEU:O	2.18	0.43
8:I:469:GLU:HG2	8:I:512:LEU:HD21	2.01	0.43
9:J:126:ALA:HA	9:J:129:ASN:ND2	2.32	0.43
9:J:305:LYS:HE2	9:J:305:LYS:HB2	1.75	0.43
1:A:35:ASN:OD1	1:A:36:ALA:N	2.52	0.43
1:A:42:GLN:HG3	1:A:45:ARG:NH2	2.31	0.43
1:A:60:ALA:HA	3:C:101:TYR:HE2	1.83	0.43
3:C:87:ASP:HB3	3:C:140:PHE:C	2.44	0.43
4:D:82:VAL:O	4:D:85:THR:OG1	2.35	0.43
4:D:171:ARG:O	4:D:174:TYR:HB3	2.18	0.43
6:F:121:TYR:HB2	6:F:178:VAL:CG2	2.49	0.43
7:H:103:HIS:ND1	7:H:104:LEU:HD23	2.33	0.43
9:J:29:ARG:NH2	9:J:103:PHE:HB3	2.33	0.43
9:J:140:LEU:HD23	9:J:170:ILE:HG21	1.99	0.43
9:J:231:LYS:O	9:J:235:VAL:HG23	2.19	0.43
9:J:512:SER:O	9:J:519:ARG:NH2	2.52	0.43
1:A:102:SER:HB3	1:A:162:ARG:NH1	2.34	0.43
2:B:25:HIS:CD2	2:B:25:HIS:N	2.87	0.43
2:B:109:ALA:N	2:B:110:PRO:HD2	2.33	0.43
2:B:120:VAL:O	2:B:129:ILE:HG23	2.18	0.43
3:C:59:GLU:HG3	4:D:140:ASP:OD2	2.19	0.43
5:E:56:ALA:O	6:F:83:LYS:HD2	2.19	0.43
5:E:58:MET:N	6:F:83:LYS:HZ3	2.09	0.43
6:F:128:PRO:HG2	6:F:131:ASN:HB2	2.01	0.43
6:F:165:LYS:HD2	6:F:165:LYS:N	2.34	0.43
1:G:148:VAL:HG13	1:G:149:GLN:OE1	2.19	0.43
7:H:12:ASN:ND2	9:J:483:LYS:O	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:124:LYS:O	7:H:127:ASP:HB3	2.18	0.43
9:J:33:HIS:O	9:J:33:HIS:ND1	2.52	0.43
9:J:139:CYS:HA	9:J:174:MET:HE2	2.01	0.43
9:J:333:CYS:SG	9:J:352:TYR:OH	2.76	0.43
9:J:459:TYR:HA	9:J:462:SER:HB3	2.00	0.43
4:D:28:HIS:HE1	4:D:30:LYS:HB2	1.84	0.42
1:G:167:ARG:HG3	1:G:168:LEU:N	2.34	0.42
7:H:1:MET:HA	7:H:1:MET:HE3	2.00	0.42
7:H:61:TYR:CD1	7:H:68:ILE:HD12	2.53	0.42
9:J:505:VAL:HG23	9:J:564:VAL:HG11	2.00	0.42
9:J:520:HIS:CE1	9:J:605:LEU:HB3	2.54	0.42
9:J:584:THR:H	9:J:600:LEU:HA	1.84	0.42
3:C:107:GLU:O	3:C:111:ARG:HB2	2.18	0.42
4:D:146:CYS:CB	4:D:156:ILE:HG22	2.48	0.42
4:D:187:TYR:CE2	4:D:193:ILE:HA	2.55	0.42
8:I:484:LYS:H	8:I:484:LYS:HG2	1.42	0.42
9:J:31:SER:HA	9:J:34:LYS:HG2	2.01	0.42
9:J:154:ASP:OD2	9:J:157:ALA:N	2.52	0.42
1:A:38:ASP:C	1:A:42:GLN:NE2	2.77	0.42
2:B:39:TYR:CE2	7:H:73:THR:HG22	2.51	0.42
2:B:51:ARG:O	7:H:48:GLY:HA2	2.19	0.42
2:B:107:GLU:O	2:B:110:PRO:HD2	2.19	0.42
2:B:139:SER:H	2:B:144:LYS:NZ	2.17	0.42
3:C:11:LYS:HE3	3:C:12:PHE:CE1	2.54	0.42
3:C:72:HIS:CG	3:C:73:TYR:N	2.86	0.42
5:E:96:ASN:HB2	5:E:136:TYR:CZ	2.54	0.42
1:G:18:THR:OG1	1:G:108:PRO:O	2.25	0.42
7:H:103:HIS:O	7:H:107:THR:HG22	2.19	0.42
9:J:18:PRO:HD2	9:J:53:ALA:O	2.19	0.42
9:J:191:LEU:HD23	9:J:191:LEU:HA	1.83	0.42
9:J:221:HIS:C	9:J:223:SER:H	2.27	0.42
9:J:235:VAL:O	9:J:239:ARG:HG3	2.20	0.42
4:D:6:VAL:HG23	4:D:157:ILE:CG2	2.46	0.42
6:F:187:ARG:NH1	6:F:191:MET:HE1	2.33	0.42
1:G:13:ASN:HB3	1:G:15:GLU:OE1	2.19	0.42
7:H:43:CYS:N	7:H:45:ILE:HG22	2.34	0.42
8:I:493:ILE:HG21	8:I:509:ALA:CB	2.41	0.42
8:I:514:MET:HE3	8:I:514:MET:HB3	1.86	0.42
8:I:594:VAL:HG12	8:I:597:LYS:HD3	2.02	0.42
9:J:89:MET:O	9:J:92:HIS:HB2	2.18	0.42
5:E:31:GLU:OE1	5:E:34:ARG:NE	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:119:PRO:HB2	5:E:121:LYS:HE3	2.01	0.42
6:F:117:ASP:OD2	6:F:120:THR:OG1	2.37	0.42
1:G:133:ARG:NH2	1:G:144:GLN:HA	2.34	0.42
7:H:32:VAL:HA	7:H:35:ALA:HB3	2.01	0.42
7:H:85:SER:HB2	7:H:88:VAL:HG13	2.02	0.42
8:I:379:ILE:HG22	8:I:434:LEU:HD21	2.00	0.42
8:I:486:TYR:CD1	8:I:517:LEU:HD23	2.54	0.42
9:J:89:MET:HE1	9:J:231:LYS:HE3	2.01	0.42
9:J:116:LYS:HG3	9:J:119:GLN:NE2	2.33	0.42
9:J:497:ARG:O	9:J:500:LEU:HG	2.19	0.42
9:J:562:ALA:O	9:J:565:LYS:NZ	2.52	0.42
3:C:10:ASP:OD1	3:C:16:LEU:HD11	2.19	0.42
5:E:8:ILE:HD13	5:E:17:TYR:CD2	2.55	0.42
5:E:72:SER:O	5:E:83:ILE:HA	2.19	0.42
7:H:4:CYS:H	7:H:82:VAL:HG12	1.84	0.42
9:J:332:PHE:O	9:J:336:ILE:HG13	2.20	0.42
9:J:551:PRO:O	9:J:554:GLN:HB2	2.19	0.42
1:A:77:ILE:HD11	1:A:101:PHE:HE1	1.84	0.42
2:B:2:SER:O	2:B:5:ILE:HG22	2.19	0.42
4:D:25:ARG:HG2	4:D:102:LYS:HE2	2.01	0.42
4:D:53:ARG:O	4:D:53:ARG:HG3	2.20	0.42
4:D:188:SER:OG	4:D:190:GLU:OE1	2.29	0.42
7:H:59:LEU:HD12	7:H:62:SER:HB2	2.02	0.42
9:J:516:LEU:HD23	9:J:519:ARG:HH12	1.85	0.42
1:A:114:VAL:HG13	1:A:115:GLU:H	1.84	0.42
3:C:62:LEU:HA	3:C:62:LEU:HD23	1.76	0.42
3:C:105:TRP:CD1	3:C:109:VAL:HG21	2.55	0.42
6:F:179:LYS:HE2	6:F:179:LYS:HA	2.01	0.42
1:G:94:SER:OG	1:G:96:ALA:N	2.49	0.42
1:G:105:ASP:HA	1:G:157:VAL:CG1	2.50	0.42
7:H:91:ARG:CD	7:H:92:GLU:HG3	2.48	0.42
8:I:575:TYR:CA	8:I:579:GLY:H	2.28	0.42
9:J:7:ALA:HB3	9:J:86:ARG:HD2	2.02	0.42
9:J:217:LEU:HD12	9:J:218:THR:H	1.83	0.42
9:J:565:LYS:HA	9:J:565:LYS:HD3	1.88	0.42
1:A:115:GLU:HB3	1:A:118:PRO:HG3	2.01	0.42
5:E:47:LEU:HB3	5:E:51:HIS:NE2	2.35	0.42
8:I:517:LEU:HB2	8:I:526:VAL:HG22	2.01	0.42
9:J:165:THR:HG22	9:J:170:ILE:O	2.18	0.42
9:J:232:LEU:HD23	9:J:248:HIS:NE2	2.34	0.42
1:A:56:GLU:CD	3:C:110:VAL:HG11	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:MET:HA	2:B:128:GLY:HA2	2.02	0.42
3:C:3:ILE:O	3:C:21:TRP:HB2	2.19	0.42
5:E:77:ALA:HB2	6:F:76:PHE:HB2	2.02	0.42
6:F:87:LYS:O	6:F:90:GLN:NE2	2.53	0.42
1:G:29:LEU:HD11	1:G:119:LEU:HD21	2.02	0.42
7:H:18:THR:HG21	7:H:30:TYR:CD1	2.55	0.42
9:J:284:MET:CG	9:J:296:GLN:HE22	2.33	0.42
9:J:584:THR:HB	9:J:599:GLN:O	2.19	0.42
1:A:145:GLN:HE22	1:A:147:TRP:NE1	2.17	0.41
2:B:51:ARG:NH1	7:H:49:ALA:N	2.68	0.41
4:D:28:HIS:ND1	4:D:57:ILE:HD11	2.35	0.41
4:D:37:ASP:OD1	4:D:37:ASP:N	2.52	0.41
4:D:188:SER:HA	1:G:52:ARG:NH1	2.35	0.41
5:E:93:GLY:HA2	5:E:136:TYR:CD2	2.55	0.41
6:F:32:GLN:HE21	6:F:32:GLN:HB2	1.58	0.41
8:I:536:GLU:H	8:I:536:GLU:HG2	1.41	0.41
9:J:364:ASP:O	9:J:368:GLU:OE1	2.38	0.41
2:B:58:THR:O	2:B:61:PHE:N	2.54	0.41
2:B:93:PHE:O	2:B:97:THR:N	2.53	0.41
3:C:32:GLU:HG2	3:C:33:GLU:N	2.35	0.41
3:C:41:MET:HG3	4:D:118:LEU:HD22	2.02	0.41
3:C:48:PHE:CE1	4:D:115:PHE:HB2	2.55	0.41
4:D:183:LYS:HD3	4:D:183:LYS:C	2.45	0.41
5:E:57:ASN:ND2	5:E:59:GLN:O	2.53	0.41
5:E:60:LEU:N	5:E:73:ALA:O	2.52	0.41
6:F:53:VAL:HG22	6:F:57:GLN:OE1	2.20	0.41
1:G:122:LEU:O	1:G:153:LYS:NZ	2.27	0.41
8:I:448:TYR:CZ	8:I:488:TYR:CD2	3.08	0.41
9:J:86:ARG:O	9:J:89:MET:HB3	2.20	0.41
9:J:471:LEU:HD23	9:J:471:LEU:HA	1.84	0.41
1:A:61:ARG:NH2	2:B:2:SER:HB3	2.35	0.41
2:B:7:PHE:CE2	2:B:95:PHE:HZ	2.37	0.41
2:B:117:CYS:HA	2:B:131:SER:HB2	2.01	0.41
5:E:127:LYS:HE3	5:E:127:LYS:HB3	1.84	0.41
6:F:46:SER:O	6:F:50:VAL:HB	2.19	0.41
6:F:87:LYS:N	6:F:90:GLN:HE21	2.17	0.41
6:F:97:THR:O	6:F:101:LYS:HG2	2.20	0.41
6:F:113:HIS:O	6:F:113:HIS:ND1	2.53	0.41
1:G:40:LYS:HA	1:G:43:GLU:OE1	2.20	0.41
1:G:68:GLU:CD	1:G:70:ARG:HG2	2.45	0.41
9:J:88:TRP:O	9:J:92:HIS:CD2	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:260:ARG:HH21	9:J:307:ARG:NH1	2.19	0.41
9:J:417:ASP:O	9:J:420:ARG:HB3	2.21	0.41
9:J:519:ARG:NH2	9:J:530:ILE:HG21	2.36	0.41
1:A:12:LYS:HG3	1:A:13:VAL:HG12	2.01	0.41
2:B:43:GLU:OE1	7:H:103:HIS:CE1	2.74	0.41
2:B:113:VAL:CG2	2:B:133:VAL:HG12	2.50	0.41
4:D:95:ASN:O	4:D:96:LEU:HD22	2.21	0.41
4:D:119:PHE:HA	4:D:134:ILE:HG21	2.03	0.41
4:D:151:THR:HG21	1:G:139:VAL:HG22	2.01	0.41
5:E:11:GLN:C	5:E:13:ASP:H	2.29	0.41
5:E:110:MET:CE	6:F:70:ARG:HB2	2.51	0.41
6:F:49:ARG:HD2	6:F:49:ARG:O	2.20	0.41
1:G:24:LEU:O	1:G:28:MET:HG2	2.20	0.41
1:G:40:LYS:O	1:G:44:ARG:HG3	2.19	0.41
9:J:29:ARG:HH21	9:J:103:PHE:HB3	1.86	0.41
1:A:11:LYS:HE3	1:A:14:ASN:HB2	2.02	0.41
2:B:28:ALA:O	2:B:31:GLU:N	2.53	0.41
2:B:93:PHE:HE2	2:B:95:PHE:HB2	1.84	0.41
2:B:98:ARG:HH22	3:C:111:ARG:HH21	1.68	0.41
4:D:11:LYS:HE3	1:G:177:ASP:OD2	2.20	0.41
4:D:66:VAL:HG23	4:D:71:VAL:HB	2.02	0.41
5:E:5:TYR:OH	5:E:18:GLU:HG2	2.20	0.41
7:H:38:VAL:HA	7:H:41:GLU:HG2	2.03	0.41
9:J:131:LEU:HD12	9:J:138:LEU:HD22	2.02	0.41
9:J:344:GLN:OE1	9:J:438:GLN:NE2	2.54	0.41
9:J:500:LEU:HD12	9:J:501:LEU:N	2.36	0.41
1:A:37:GLU:HB3	1:A:41:LYS:NZ	2.36	0.41
2:B:31:GLU:HB3	2:B:119:LEU:CD2	2.50	0.41
4:D:216:ASN:C	4:D:218:ASP:N	2.78	0.41
5:E:6:PHE:HE1	5:E:8:ILE:HG13	1.84	0.41
5:E:45:LEU:HD11	5:E:81:ARG:HE	1.86	0.41
5:E:58:MET:HG2	5:E:59:GLN:N	2.34	0.41
5:E:134:ARG:NE	5:E:138:LEU:HD23	2.35	0.41
7:H:9:GLY:N	7:H:14:PRO:HD3	2.36	0.41
9:J:370:TYR:O	9:J:373:MET:N	2.54	0.41
5:E:126:GLU:O	5:E:129:SER:OG	2.30	0.41
5:E:127:LYS:O	5:E:131:ILE:HG12	2.20	0.41
6:F:77:VAL:HG23	6:F:78:ARG:H	1.85	0.41
7:H:59:LEU:HA	7:H:68:ILE:O	2.20	0.41
8:I:558:PRO:O	8:I:559:PRO:C	2.64	0.41
8:I:562:ARG:HG3	8:I:598:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:106:MET:HG3	9:J:143:LEU:O	2.20	0.41
9:J:497:ARG:CZ	9:J:497:ARG:HB3	2.50	0.41
9:J:704:MET:N	9:J:704:MET:SD	2.94	0.41
1:A:12:LYS:HE2	1:A:12:LYS:HB2	1.89	0.41
3:C:65:LYS:HE3	3:C:143:ARG:HA	2.02	0.41
5:E:114:TYR:CE1	5:E:118:THR:HB	2.56	0.41
6:F:93:LEU:O	6:F:96:LYS:HB3	2.20	0.41
1:A:20:LEU:HA	1:A:20:LEU:HD13	1.85	0.41
1:A:67:CYS:HA	1:A:72:GLU:CD	2.46	0.41
1:A:140:VAL:HG13	1:A:142:LEU:HD12	2.03	0.41
2:B:4:GLU:OE2	3:C:111:ARG:NH2	2.54	0.41
2:B:77:ASN:HB3	2:B:79:ARG:NH1	2.36	0.41
4:D:92:TYR:HD1	4:D:94:ILE:HG12	1.85	0.41
4:D:95:ASN:C	4:D:96:LEU:HD22	2.46	0.41
4:D:180:TYR:CE2	4:D:193:ILE:HG23	2.55	0.41
5:E:93:GLY:O	5:E:136:TYR:HD2	2.03	0.41
5:E:113:PHE:CZ	1:G:115:LEU:HD13	2.55	0.41
6:F:31:SER:HB3	6:F:34:ILE:HG22	2.02	0.41
6:F:100:TRP:O	6:F:105:GLY:N	2.54	0.41
1:G:54:ILE:HB	1:G:135:ALA:HB1	2.02	0.41
1:G:69:MET:HA	1:G:69:MET:CE	2.47	0.41
8:I:490:GLU:HB2	8:I:493:ILE:HD11	2.03	0.41
9:J:22:PHE:HZ	9:J:37:TRP:HZ3	1.69	0.41
9:J:42:GLY:O	9:J:46:ARG:HG3	2.21	0.41
9:J:179:PRO:O	9:J:184:LEU:HB2	2.19	0.41
9:J:305:LYS:HG3	9:J:317:HIS:NE2	2.35	0.41
9:J:325:HIS:HB2	9:J:355:ALA:HB2	2.03	0.41
9:J:367:MET:O	9:J:370:TYR:HB2	2.21	0.41
2:B:77:ASN:HB2	2:B:89:GLN:O	2.21	0.41
2:B:108:HIS:HA	2:B:111:LYS:HZ2	1.84	0.41
3:C:4:PHE:HE2	3:C:86:THR:C	2.28	0.41
4:D:104:THR:O	4:D:105:THR:C	2.64	0.41
6:F:145:CYS:O	6:F:146:ALA:C	2.63	0.41
7:H:43:CYS:SG	9:J:444:CYS:HB2	2.61	0.41
9:J:418:GLN:O	9:J:421:SER:HB2	2.21	0.41
1:A:41:LYS:O	1:A:45:ARG:HG2	2.20	0.40
3:C:58:LYS:HE2	3:C:58:LYS:HB2	1.85	0.40
4:D:75:THR:HG22	4:D:81:ASP:OD1	2.21	0.40
4:D:183:LYS:HD3	4:D:184:ASN:N	2.35	0.40
5:E:68:GLN:HE21	5:E:69:TRP:NE1	2.19	0.40
1:G:54:ILE:HD12	1:G:54:ILE:HA	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:ASP:OD1	1:G:118:ASP:N	2.51	0.40
8:I:497:LEU:CD2	8:I:503:GLN:HA	2.47	0.40
8:I:502:LEU:HD13	8:I:502:LEU:HA	1.75	0.40
9:J:18:PRO:HB2	9:J:54:VAL:HA	2.03	0.40
9:J:42:GLY:O	9:J:46:ARG:N	2.36	0.40
9:J:140:LEU:O	9:J:175:LEU:HA	2.21	0.40
1:A:55:ILE:HG21	1:A:139:MET:HB2	2.03	0.40
1:A:95:SER:CB	1:A:100:GLU:H	2.33	0.40
2:B:38:GLY:O	2:B:42:ILE:HG13	2.21	0.40
3:C:142:ILE:HG23	3:C:143:ARG:N	2.36	0.40
1:G:68:GLU:HG3	1:G:71:GLU:H	1.86	0.40
7:H:85:SER:O	7:H:86:SER:C	2.64	0.40
8:I:473:LEU:HA	8:I:473:LEU:HD22	1.80	0.40
9:J:335:ALA:O	9:J:339:GLY:N	2.48	0.40
9:J:590:LEU:HD12	9:J:591:SER:N	2.36	0.40
9:J:615:PHE:HA	9:J:703:HIS:HB2	2.03	0.40
9:J:709:VAL:C	9:J:711:ALA:H	2.29	0.40
1:A:25:LEU:HD23	1:A:25:LEU:HA	1.84	0.40
5:E:70:PHE:HD2	5:E:86:HIS:HD1	1.69	0.40
6:F:80:ARG:NH2	6:F:98:THR:HB	2.36	0.40
7:H:44:LEU:HD21	7:H:60:LEU:O	2.21	0.40
9:J:20:VAL:O	9:J:56:TYR:HA	2.21	0.40
9:J:619:LEU:HD23	9:J:619:LEU:HA	1.87	0.40
4:D:172:LYS:HA	4:D:172:LYS:HD3	1.88	0.40
7:H:31:HIS:HB2	9:J:486:THR:HG21	1.99	0.40
8:I:510:THR:CG2	8:I:533:MET:HE1	2.43	0.40
9:J:85:LYS:HE2	9:J:85:LYS:HB3	1.82	0.40
9:J:156:LEU:HA	9:J:159:GLU:CD	2.47	0.40
9:J:362:ARG:HH22	9:J:419:GLU:CB	2.34	0.40
1:A:28:GLN:NE2	1:A:32:ASP:OD2	2.54	0.40
2:B:106:LEU:HD22	2:B:137:VAL:O	2.21	0.40
4:D:24:PRO:HA	4:D:102:LYS:NZ	2.37	0.40
4:D:148:GLN:C	4:D:150:LEU:H	2.30	0.40
4:D:197:LEU:HD13	6:F:134:ILE:CG1	2.44	0.40
1:G:34:ASN:OD1	1:G:37:ASP:HB3	2.22	0.40
9:J:89:MET:SD	9:J:234:PHE:CE2	3.15	0.40
9:J:472:TYR:O	9:J:476:LEU:HD23	2.21	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	163/178 (92%)	145 (89%)	18 (11%)	0	100	100
1	G	167/178 (94%)	150 (90%)	17 (10%)	0	100	100
2	B	149/152 (98%)	124 (83%)	25 (17%)	0	100	100
3	C	143/145 (99%)	125 (87%)	18 (13%)	0	100	100
4	D	217/219 (99%)	177 (82%)	40 (18%)	0	100	100
5	E	137/139 (99%)	122 (89%)	15 (11%)	0	100	100
6	F	162/194 (84%)	145 (90%)	17 (10%)	0	100	100
7	H	136/138 (99%)	114 (84%)	21 (15%)	1 (1%)	18	54
8	I	204/246 (83%)	183 (90%)	17 (8%)	4 (2%)	6	33
9	J	604/718 (84%)	544 (90%)	60 (10%)	0	100	100
All	All	2082/2307 (90%)	1829 (88%)	248 (12%)	5 (0%)	44	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	I	435	TYR
8	I	520	ALA
8	I	559	PRO
7	H	43	CYS
8	I	536	GLU

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	149/159 (94%)	149 (100%)	0	100	100
1	G	151/159 (95%)	151 (100%)	0	100	100
2	B	136/137 (99%)	136 (100%)	0	100	100
3	C	133/133 (100%)	133 (100%)	0	100	100
4	D	199/199 (100%)	199 (100%)	0	100	100
5	E	129/129 (100%)	128 (99%)	1 (1%)	73	77
6	F	149/177 (84%)	148 (99%)	1 (1%)	76	79
7	H	120/120 (100%)	118 (98%)	2 (2%)	53	68
8	I	173/204 (85%)	93 (54%)	80 (46%)	0	0
9	J	526/621 (85%)	523 (99%)	3 (1%)	78	81
All	All	1865/2038 (92%)	1778 (95%)	87 (5%)	25	46

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	40	ILE
6	F	32	GLN
7	H	40	GLU
7	H	44	LEU
8	I	357	LEU
8	I	358	ARG
8	I	364	TYR
8	I	367	ARG
8	I	369	LEU
8	I	373	ILE
8	I	374	GLU
8	I	375	HIS
8	I	376	LEU
8	I	377	VAL
8	I	382	GLU
8	I	426	LEU
8	I	429	ARG
8	I	430	LYS
8	I	436	PHE
8	I	437	MET
8	I	442	ASN
8	I	445	PHE
8	I	448	TYR
8	I	449	HIS

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Mol	Chain	Res	Type
8	I	452	LYS
8	I	456	ASN
8	I	459	SER
8	I	468	LEU
8	I	470	MET
8	I	473	LEU
8	I	476	PHE
8	I	477	MET
8	I	478	LEU
8	I	480	THR
8	I	482	GLN
8	I	483	ARG
8	I	484	LYS
8	I	489	MET
8	I	490	GLU
8	I	494	VAL
8	I	501	LYS
8	I	502	LEU
8	I	503	GLN
8	I	504	GLN
8	I	508	ARG
8	I	512	LEU
8	I	514	MET
8	I	515	GLU
8	I	517	LEU
8	I	518	LYS
8	I	521	ARG
8	I	522	LEU
8	I	524	SER
8	I	525	GLU
8	I	526	VAL
8	I	528	LYS
8	I	530	LEU
8	I	532	ARG
8	I	533	MET
8	I	535	ASN
8	I	536	GLU
8	I	537	GLU
8	I	540	LEU
8	I	541	ARG
8	I	542	SER
8	I	544	LEU

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Mol	Chain	Res	Type
8	I	546	LEU
8	I	554	LEU
8	I	556	THR
8	I	557	GLN
8	I	559	PRO
8	I	560	MET
8	I	562	ARG
8	I	563	LYS
8	I	581	ARG
8	I	582	LYS
8	I	583	HIS
8	I	586	ARG
8	I	589	ARG
8	I	594	VAL
8	I	597	LYS
8	I	598	ARG
8	I	599	GLU
8	I	600	TRP
9	J	445	LEU
9	J	447	PHE
9	J	448	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	28	GLN
1	A	42	GLN
1	A	122	ASN
2	B	83	HIS
2	B	146	HIS
3	C	144	ASN
4	D	52	ASN
4	D	184	ASN
5	E	33	HIS
5	E	38	GLN
5	E	51	HIS
5	E	59	GLN
5	E	108	ASN
6	F	44	GLN
6	F	47	GLN
6	F	147	ASN

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Mol	Chain	Res	Type
1	G	48	ASN
1	G	85	ASN
1	G	144	GLN
8	I	375	HIS
8	I	446	GLN
8	I	449	HIS
8	I	503	GLN
8	I	504	GLN
8	I	535	ASN
8	I	557	GLN
8	I	561	HIS
8	I	573	ASN
8	I	583	HIS
9	J	33	HIS
9	J	45	GLN
9	J	87	ASN
9	J	119	GLN
9	J	129	ASN
9	J	166	ASN
9	J	318	HIS
9	J	418	GLN
9	J	539	GLN
9	J	597	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.

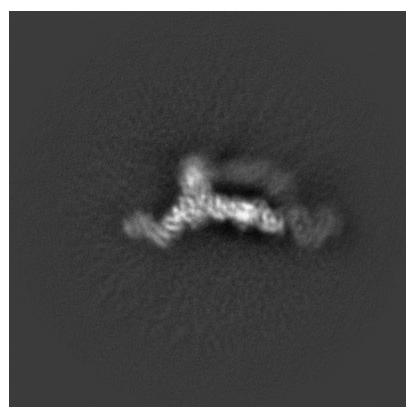
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12063. These allow visual inspection of the internal detail of the map and identification of artifacts.

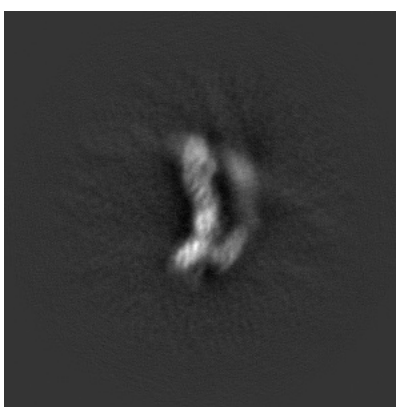
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

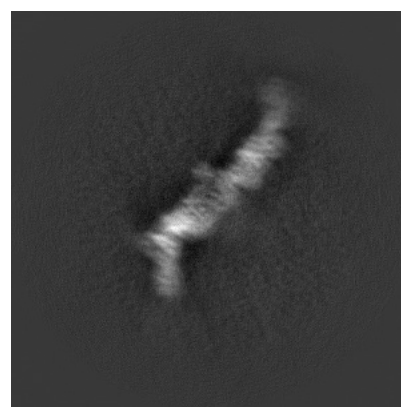
6.1.1 Primary map



X



Y

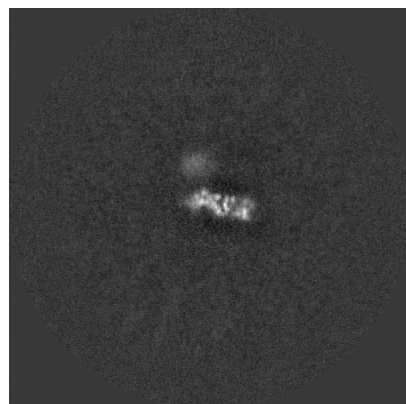


Z

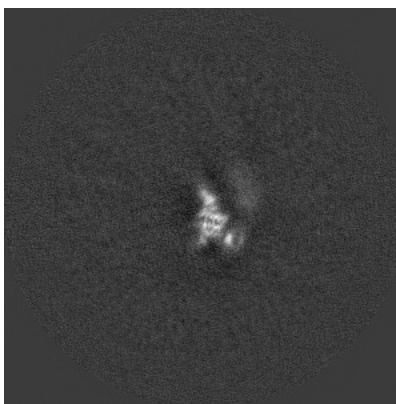
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

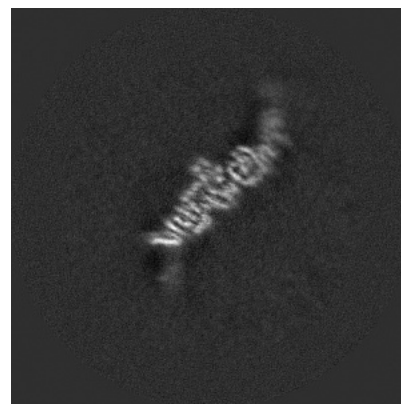
6.2.1 Primary map



X Index: 200



Y Index: 200

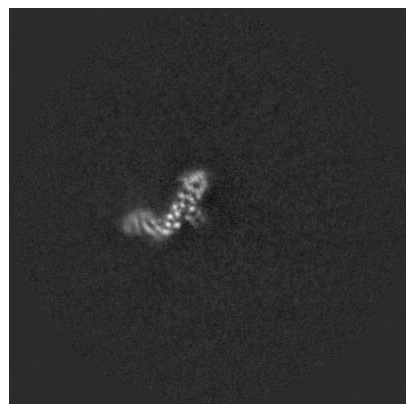


Z Index: 200

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

6.3 Largest variance slices [i](#)

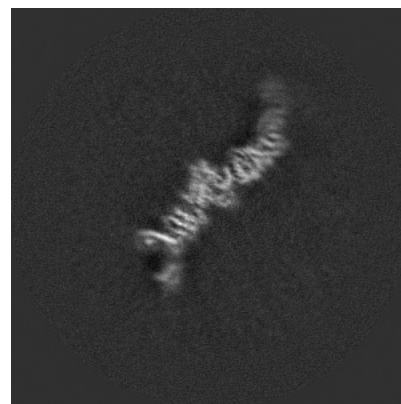
6.3.1 Primary map



X Index: 158



Y Index: 182

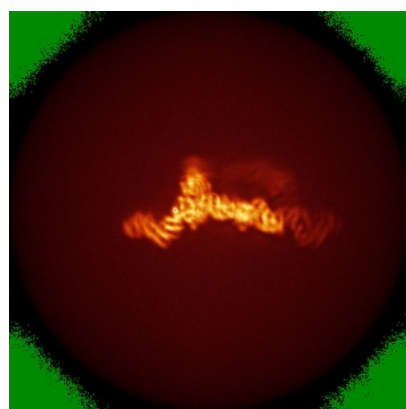


Z Index: 195

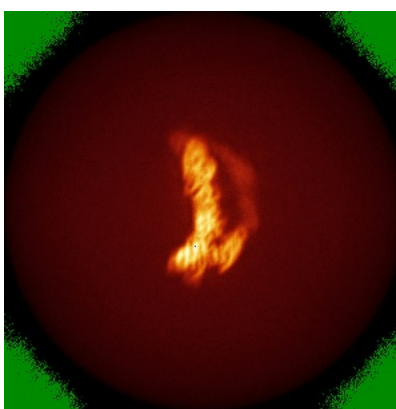
The images above show the largest variance slices of the map in three orthogonal directions.

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

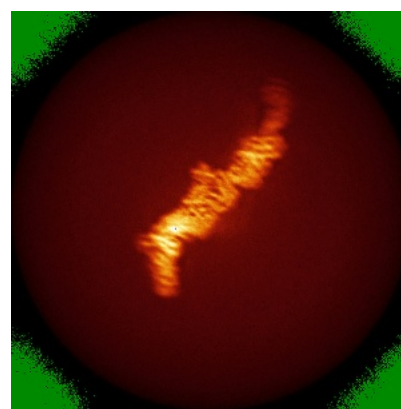
6.4.1 Primary map



X



Y

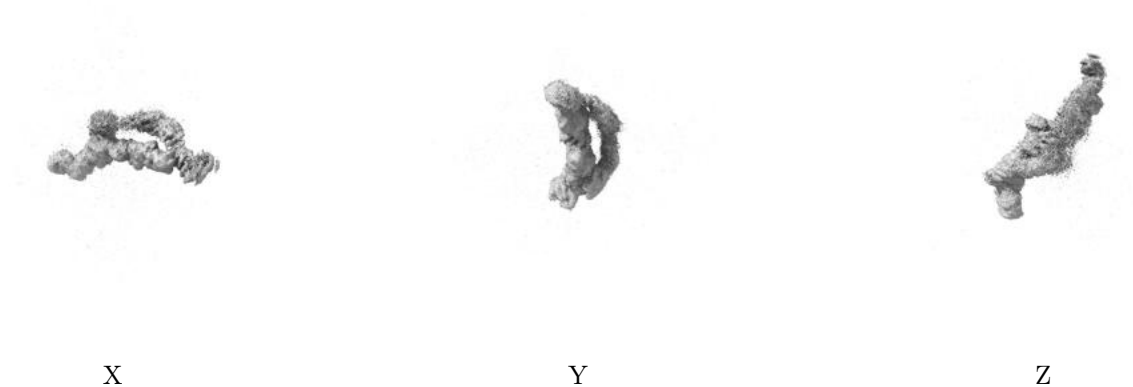


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation [i](#)

This section 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_12063_msk_1.map [i](#)



X



Y

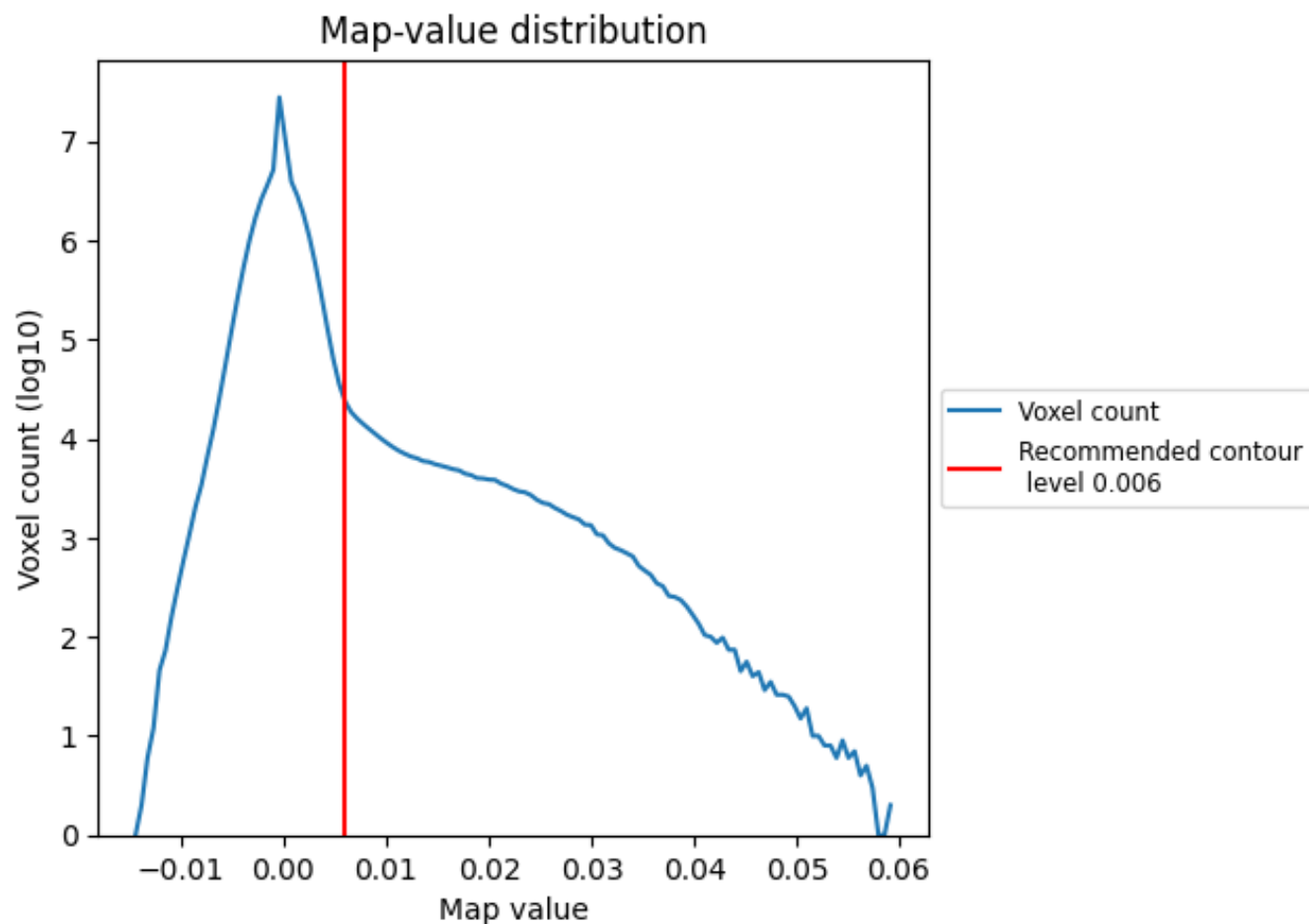


Z

7 Map analysis [i](#)

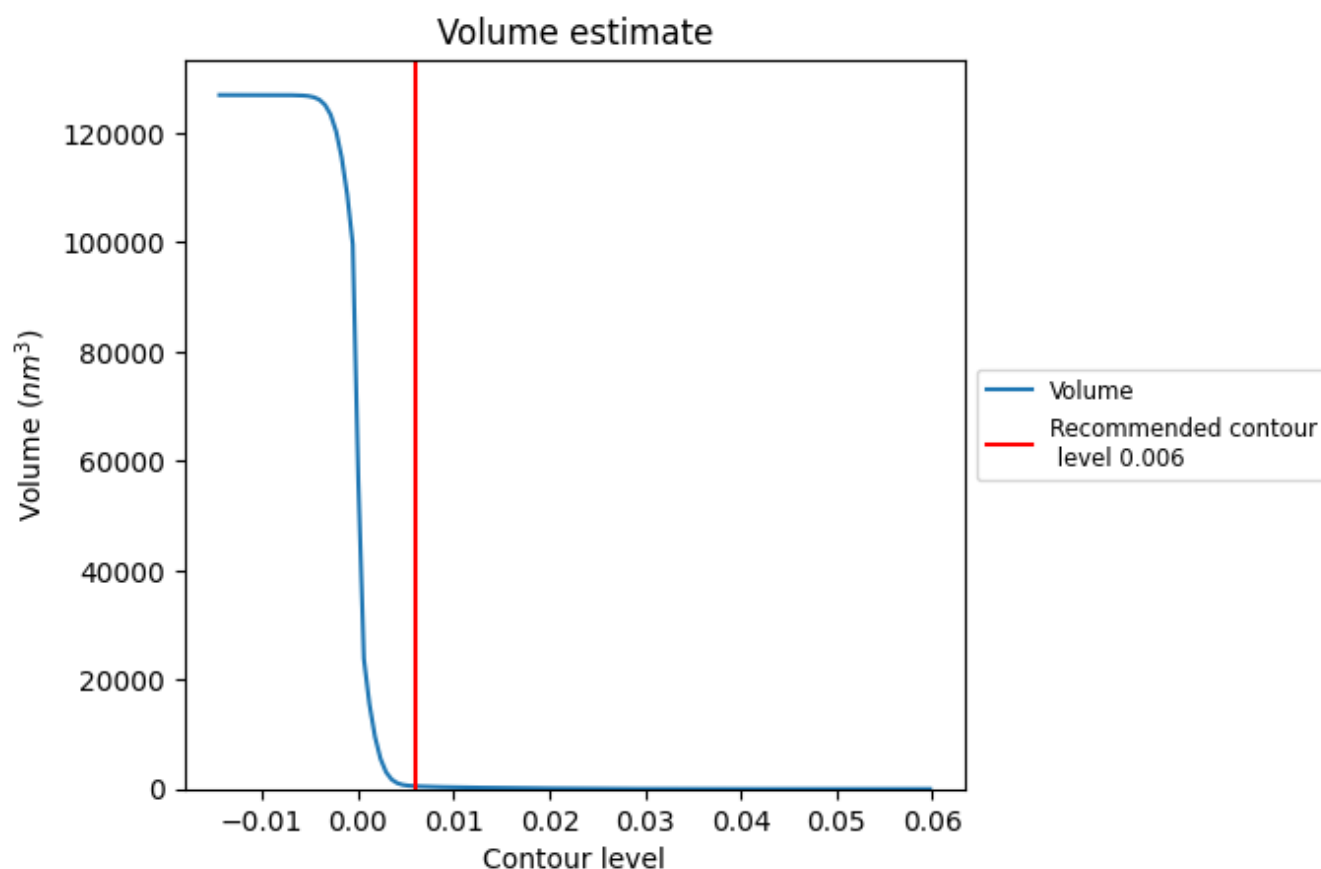
This section contains the results of statistical analysis of the map.

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.

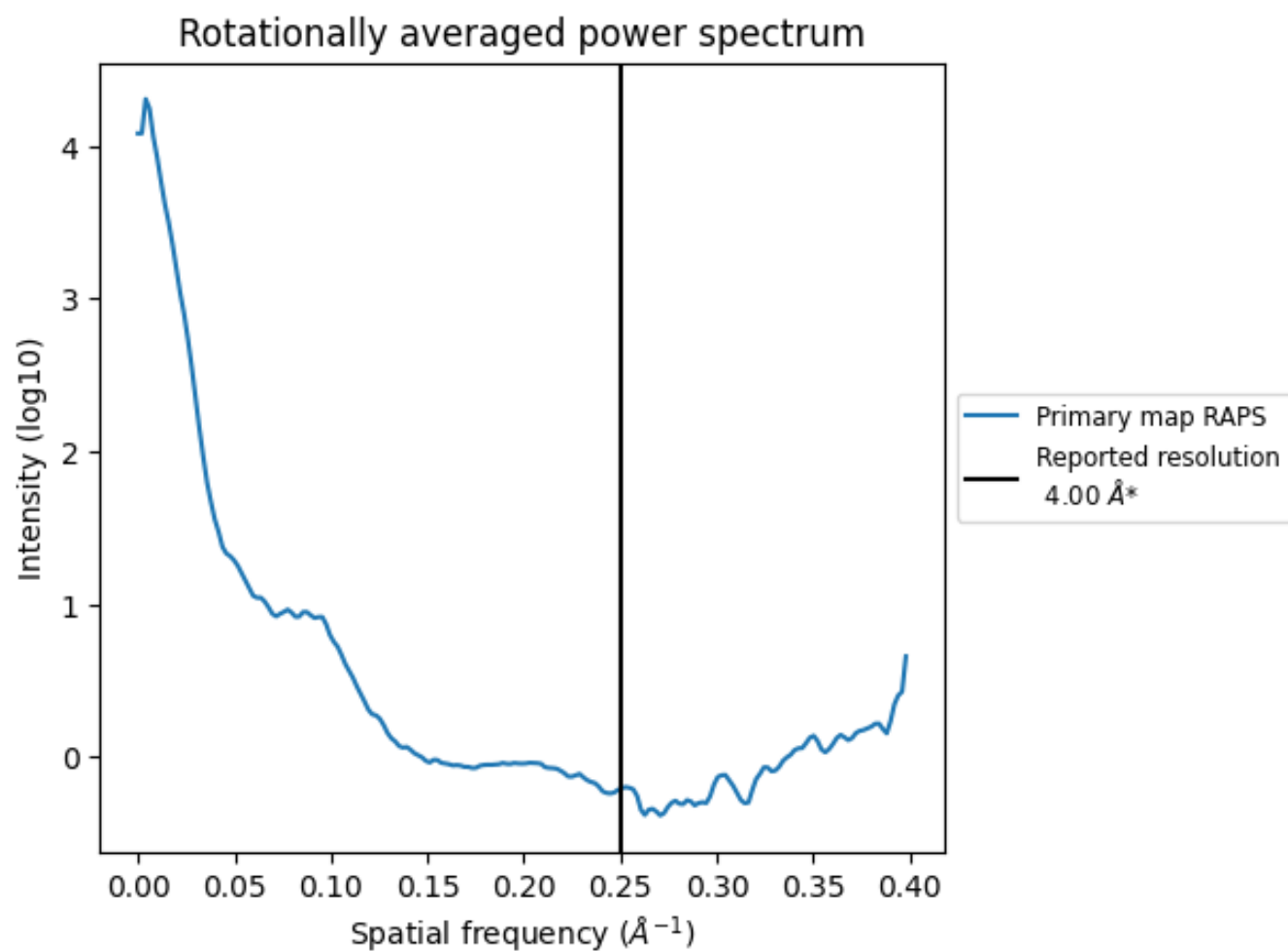
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 515 nm^3 ; this corresponds to an approximate mass of 465 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 ⓘ

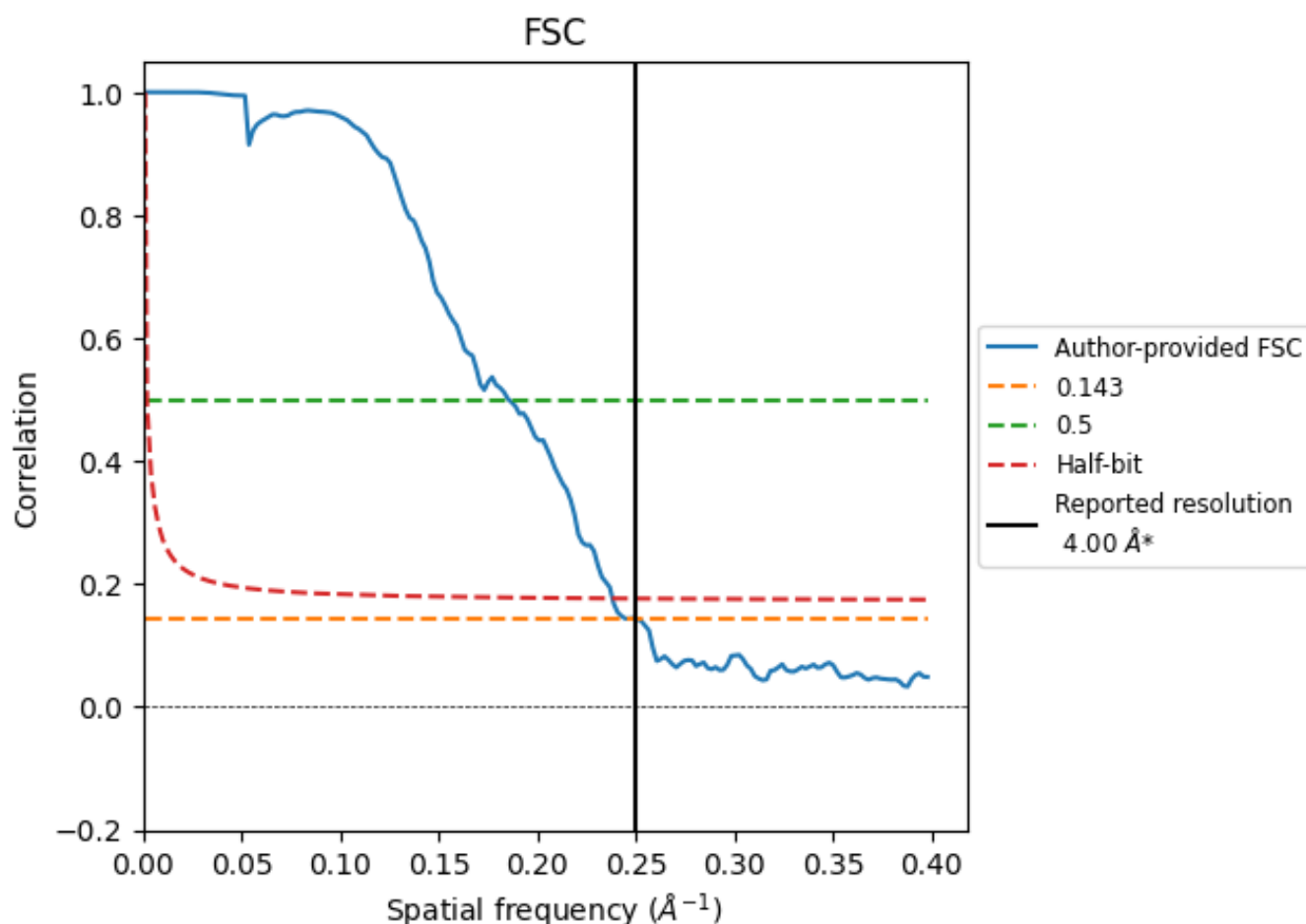


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

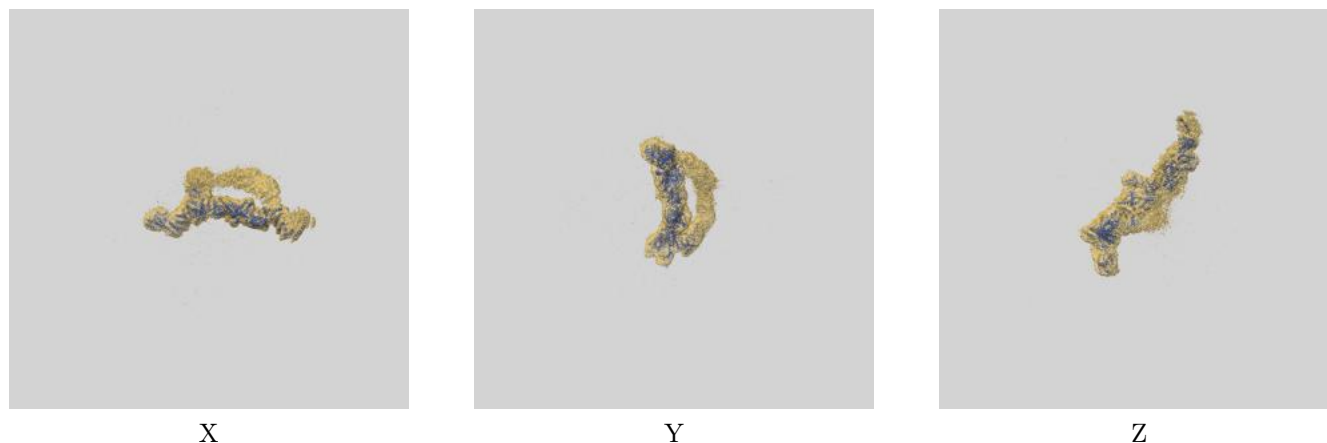
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.99	5.39	4.20
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

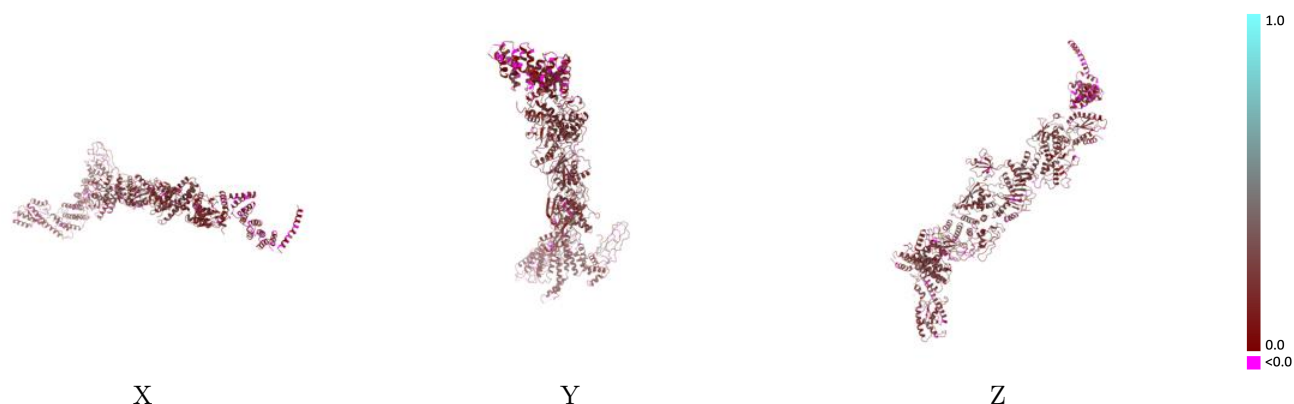
This section contains information regarding the fit between EMDB map EMD-12063 and PDB model 7B70. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



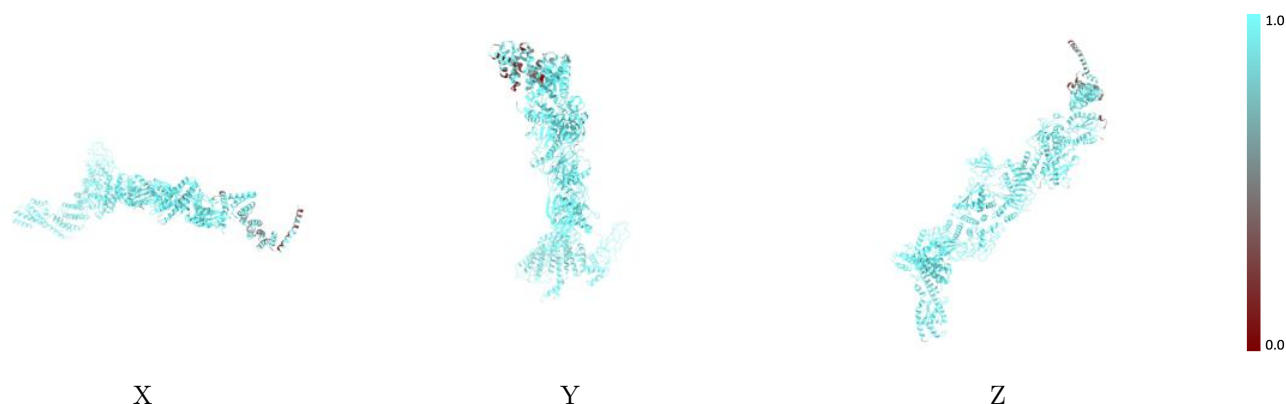
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



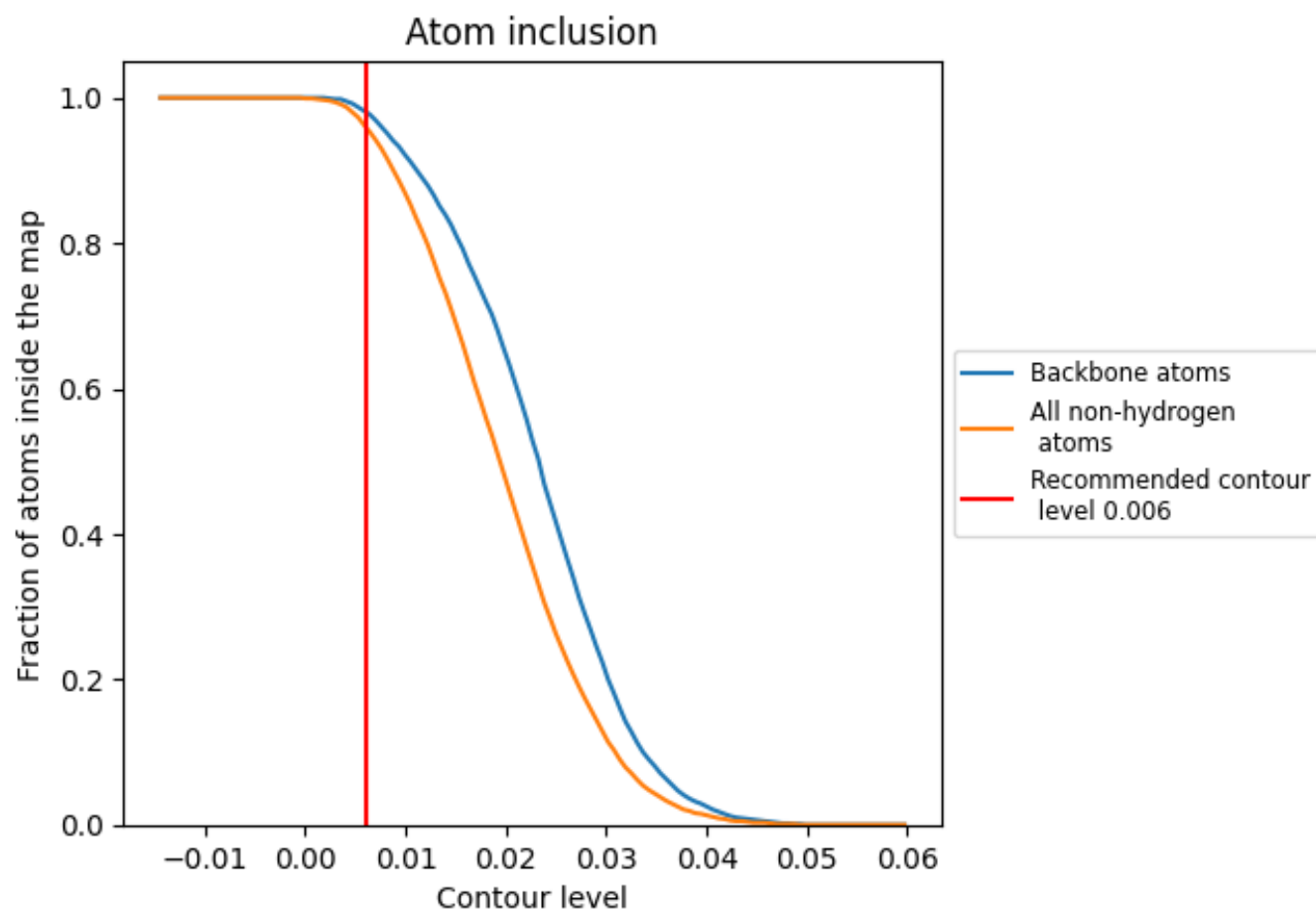
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9600	0.1920
A	0.9940	0.2610
B	0.9910	0.1860
C	0.9720	0.2220
D	0.9830	0.2260
E	0.9540	0.1620
F	0.9770	0.2210
G	0.9720	0.1840
H	0.9700	0.2110
I	0.7760	0.0990
J	0.9880	0.1850

1.0

0.0

<0.0