



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:50 AM UTC

PDB ID : 9IOZ / pdb_00009ioz
EMDB ID : EMD-60750
Title : Structure of the bacteriophage T5 tail tip complex
Authors : Peng, Y.N.; Liu, H.R.
Deposited on : 2024-07-10
Resolution : 3.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

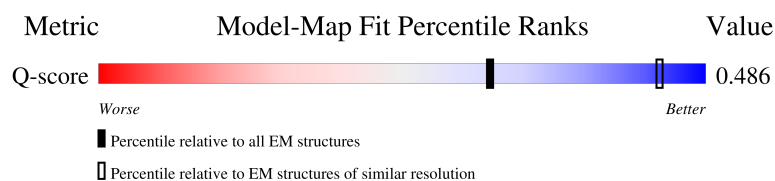
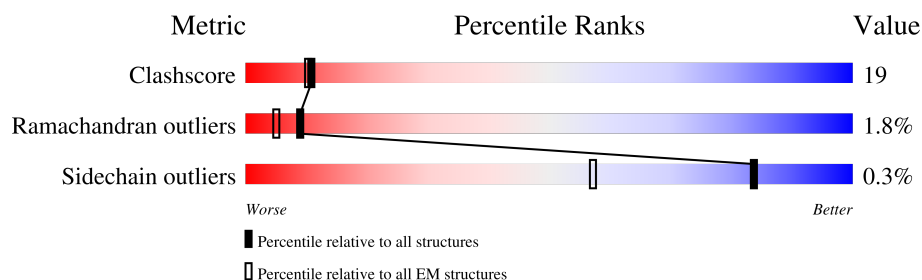
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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.



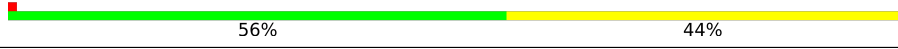
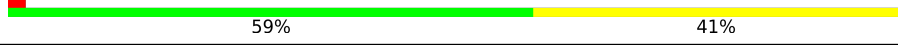
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	298	 5% 67% 31% ..
1	B	298	 5% 64% 34% ..
1	C	298	 5% 69% 28% ..
2	D	204	 58% 42%

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Mol	Chain	Length	Quality of chain
2	E	204	 67%32%
2	F	204	 62%38%
2	G	204	 56%44%
2	H	204	 59%41%
2	I	204	 61%39%
3	J	949	 48%36%•14%
3	K	949	 49%35%•14%
3	L	949	 49%35%•14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 36407 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 Baseplate tube protein p140.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	293	Total	C	N	O	S	0	0
			2379	1526	388	456	9		
1	B	293	Total	C	N	O	S	0	0
			2379	1526	388	456	9		
1	C	293	Total	C	N	O	S	0	0
			2379	1526	388	456	9		

- Molecule 2 is a protein called Distal tail protein pb9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	204	Total	C	N	O	S	0	0
			1609	1030	264	312	3		
2	E	204	Total	C	N	O	S	0	0
			1609	1030	264	312	3		
2	F	204	Total	C	N	O	S	0	0
			1609	1030	264	312	3		
2	G	204	Total	C	N	O	S	0	0
			1609	1030	264	312	3		
2	H	204	Total	C	N	O	S	0	0
			1609	1030	264	312	3		
2	I	204	Total	C	N	O	S	0	0
			1609	1030	264	312	3		

- Molecule 3 is a protein called Baseplate hub protein pb3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	816	Total	C	N	O	S	0	0
			6536	4151	1098	1278	9		
3	K	816	Total	C	N	O	S	0	0
			6536	4151	1098	1278	9		
3	L	817	Total	C	N	O	S	0	0
			6544	4155	1100	1280	9		

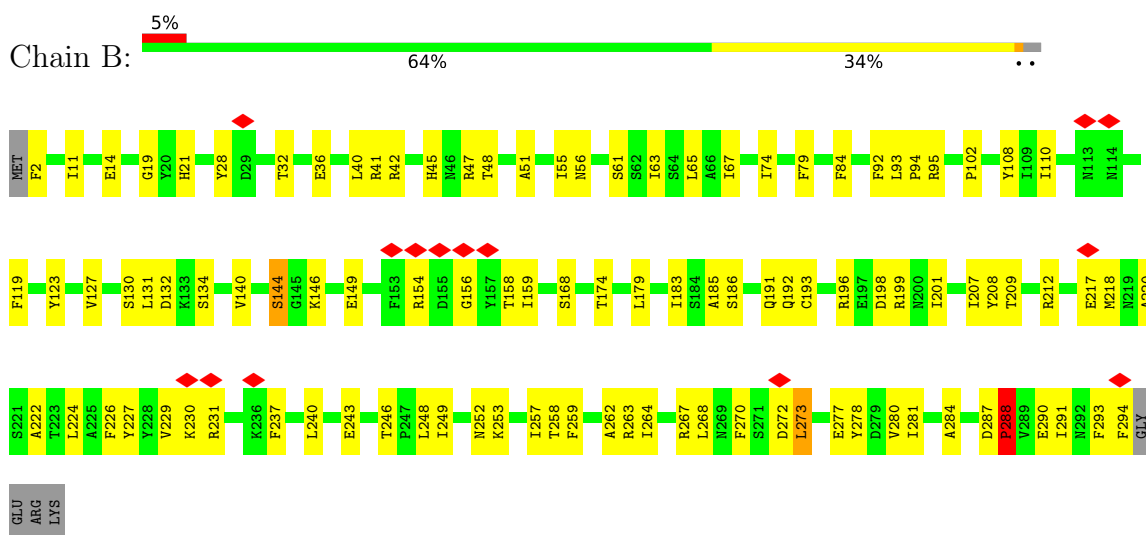
3 Residue-property plots

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: Baseplate tube protein p140

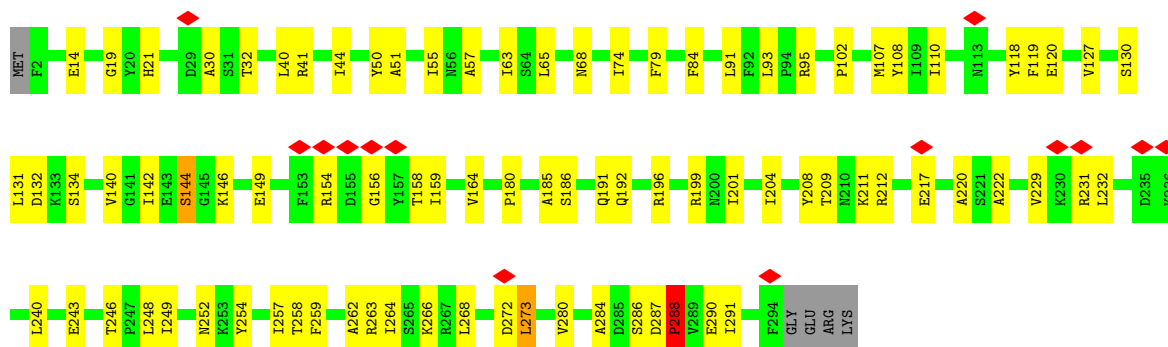


- Molecule 1: Baseplate tube protein p140

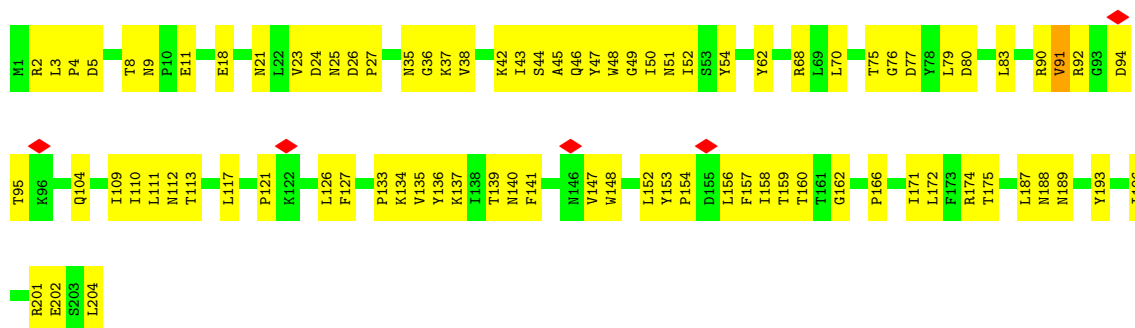


- Molecule 1: Baseplate tube protein p140

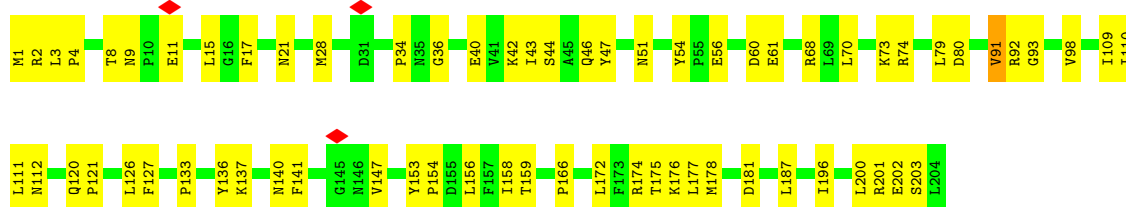




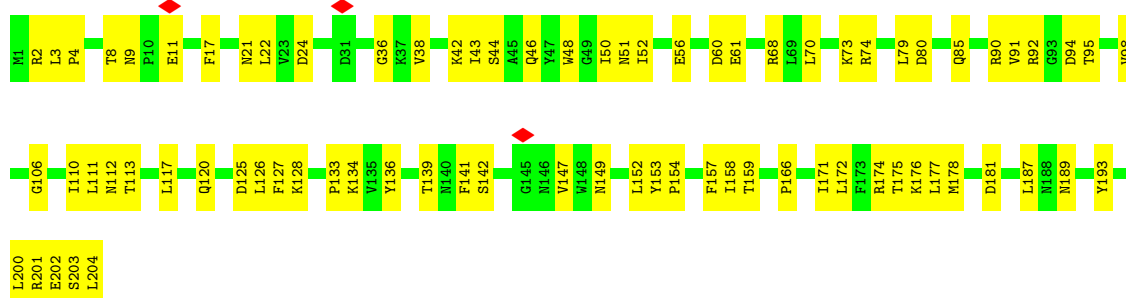
• Molecule 2: Distal tail protein pb9



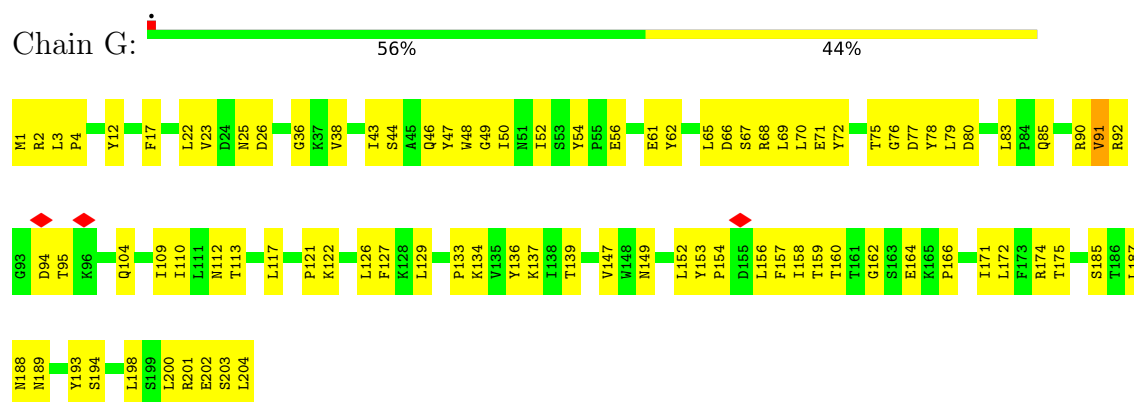
• Molecule 2: Distal tail protein pb9



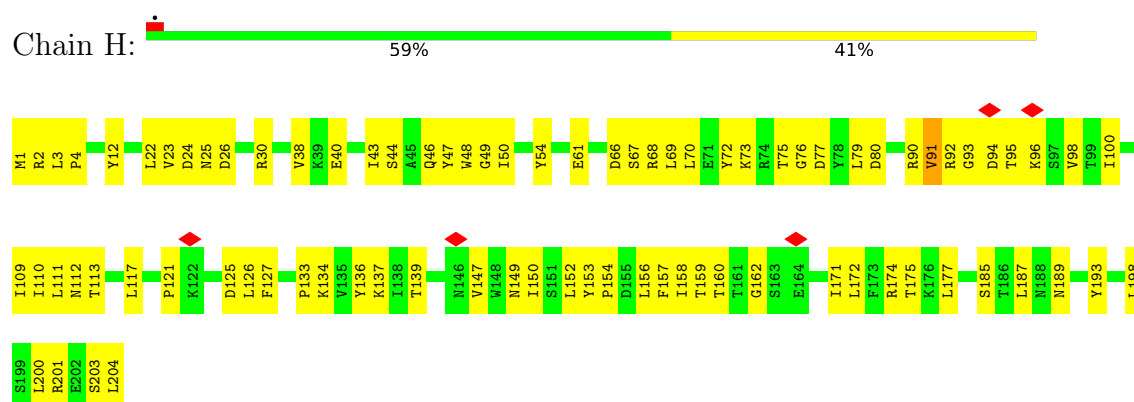
• Molecule 2: Distal tail protein pb9



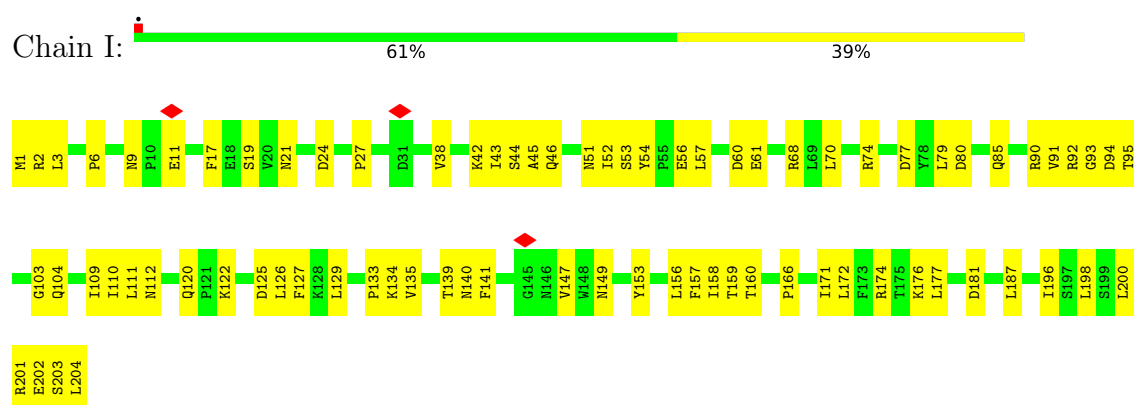
- Molecule 2: Distal tail protein pb9



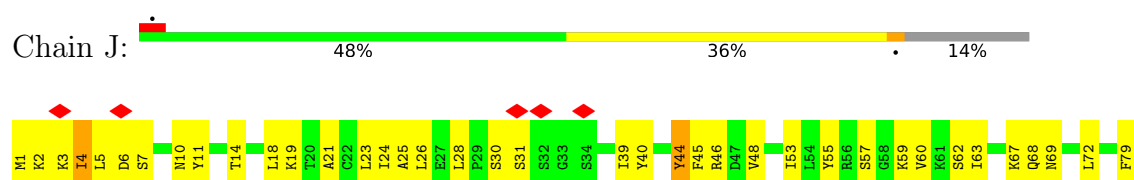
- Molecule 2: Distal tail protein pb9

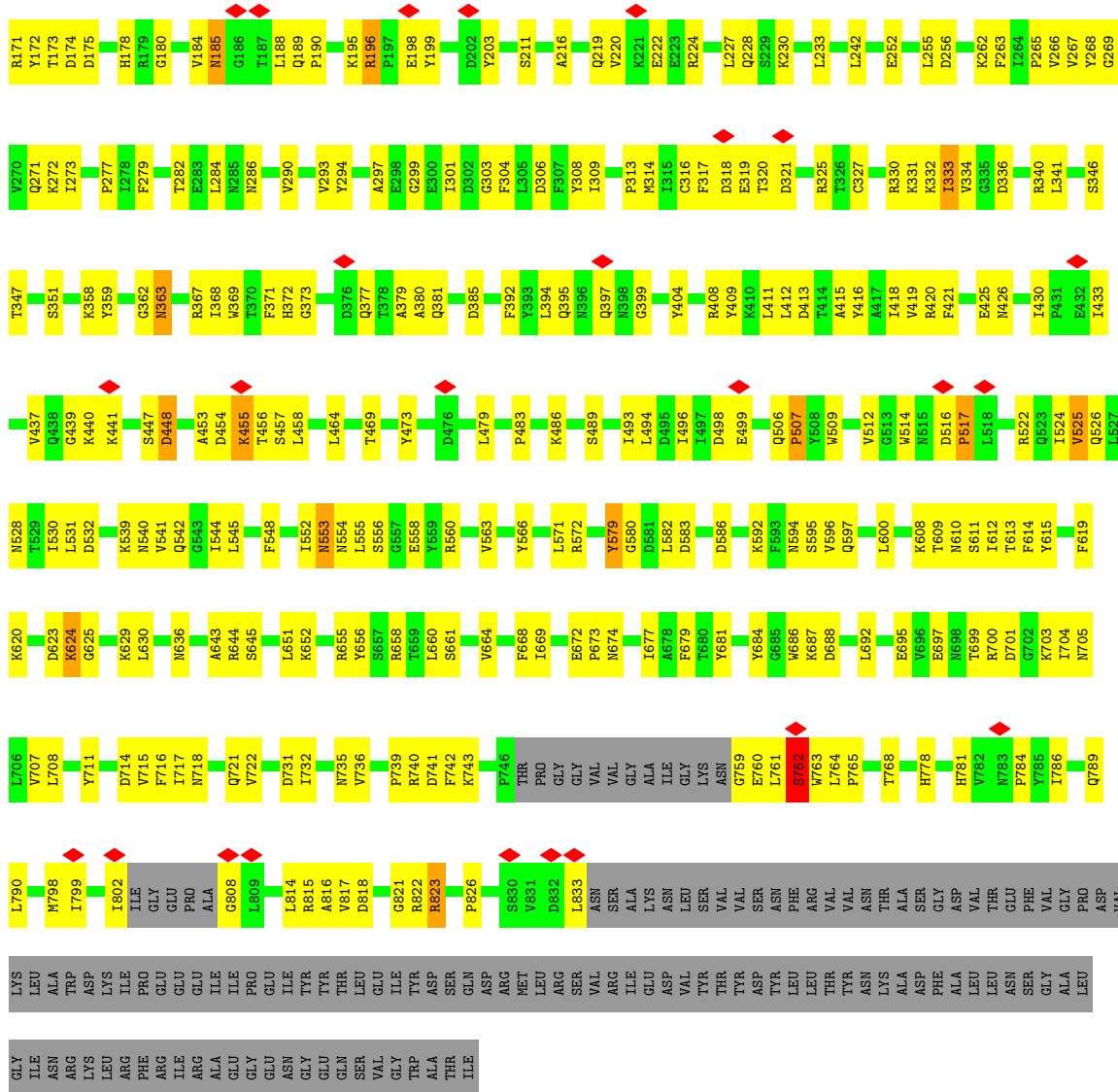


- Molecule 2: Distal tail protein pb9



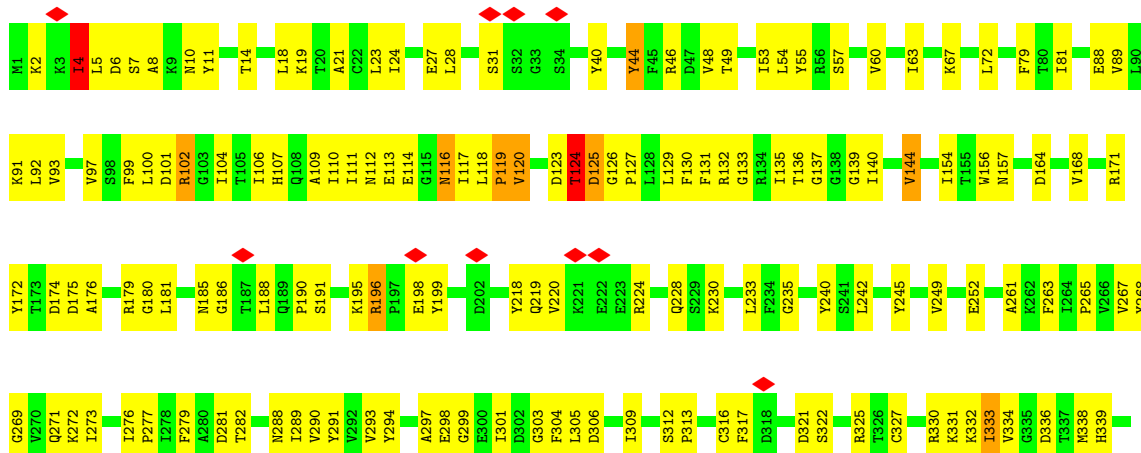
- Molecule 3: Baseplate hub protein pb3





• Molecule 3: Baseplate hub protein pb3

Chain L: 49% 35% 14%



ASN	LYS	ALA	ASP	PHE	ALA	LEU	LEU	ASN	SER	GLY	ALA	ASP	VAL	THR	GLU	PHE	VAL	GLY	ASP	LEU	VAL	LYS	ILE	LEU	ARG	ILE	GLY	PRO	ARG	GLU	ILE	ALA	GLU	ILE	GLY	GLU	GLN	THR	ILE																					
H781	V782	N783	T786	V787	Q788	Q789	L790	E796	R797	N798	I799	Q900	E901	I902	ILE	GLY	PRO	ALA	G808	L809	E813	L814	R815	A816	V817	D818	G821	R822	R823	P826	L829	S830	V831	D832	L833	ASN	SER	ALA	LYS	LEU	VAL	THR	VAL	ASP	VAL	ARG	ILE	GLU	ASP	ARG	LEU	ASN	PHE	THR	TYR	THR	VAL	THR	ASN	THR
T347	S348	Q349	P350	S351	Q355	E356	Y357	K358	Y359	G362	N363	R367	I368	V369	T370	F371	H372	G373	K374	P375	D376	Q377	A380	Q381	D385	F392	Q395	Y404	L411	L412	D413	T414	A415	A416	I418	V419	R420	F421	M426	I430	I433	E436	V437	Q438	G439															
K440	K441	D448	A453	D454	K455	T456	S457	L458	M459	W462	Q463	L464	M465	R472	D476	V487	I488	S489	K492	I493	L494	D498	E499	S500	Y501	W505	Q506	P507	T508	W509	V512	D516	P517	L518	S519	E520	N521	R522	Q523	I524	V525	N528	T529	I530	L531	D532	T533													
S534	K539	N540	V541	Q542	L545	F548	A551	I552	N553	N554	L555	S556	G557	E558	Y559	R560	V563	E564	K565	Y566	F575	T578	Y579	G580	D581	L582	D583	L584	S585	D586	T587	T588	G589	R590	N591	K592	F593	N594	S595	V596	Q597	L600	T609	I612	T613	F614	Y615	K620												
D623	K624	G625	L626	D627	K628	A635	N636	Y640	A643	R644	L651	K652	K653	R654	R655	R658	T659	L660	S661	F662	S663	V664	P665	Y666	K667	F668	E672	P673	P676	I677	A678	F679	T680	Y681	E682	R683	W686	K687	D688	K689	F690	F691	L692	V693	D694	E695	V696	E697	M698	T699										
R700	D701	G702	K703	I704	N705	L706	V707	L708	Q709	E710	Y711	D714	V715	F716	I717	N718	V722	D731	I732	S733	N734	N735	P739	R740	D741	F742	K743	P746	THR	PRO	GLY	VAL	GLY	VAL	ALA	ILE	GLY	GLY	LYS	N758	L761	S762	W763	L767	V771	V772	Y773	H778	S779	G780										
H781	V782	N783	T786	V787	Q788	Q789	L790	E796	R797	N798	I799	Q900	E901	I902	ILE	GLY	PRO	ALA	G808	L809	E813	L814	R815	A816	V817	D818	G821	R822	R823	P826	L829	S830	V831	D832	L833	ASN	SER	ALA	LYS	LEU	VAL	THR	VAL	ASP	VAL	ARG	ILE	GLU	ASP	ARG	LEU	ASN	PHE	THR	TYR	THR	VAL	THR	ASN	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30589	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.124	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	260.0, 260.0, 260.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3, 1.3, 1.3	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	0.31	1/2439 (0.0%)	0.51	2/3314 (0.1%)
1	B	0.31	1/2439 (0.0%)	0.50	2/3314 (0.1%)
1	C	0.30	1/2439 (0.0%)	0.52	3/3314 (0.1%)
2	D	0.24	0/1648	0.48	0/2239
2	E	0.24	0/1648	0.50	0/2239
2	F	0.24	0/1648	0.51	0/2239
2	G	0.31	0/1648	0.50	0/2239
2	H	0.22	0/1648	0.48	0/2239
2	I	0.24	0/1648	0.50	0/2239
3	J	0.33	1/6678 (0.0%)	0.66	6/9054 (0.1%)
3	K	0.36	1/6678 (0.0%)	0.66	4/9054 (0.0%)
3	L	0.35	1/6686 (0.0%)	0.67	10/9065 (0.1%)
All	All	0.32	6/37247 (0.0%)	0.59	27/50549 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	453	ALA	CA-C	-7.98	1.45	1.52
3	L	453	ALA	CA-C	-6.62	1.44	1.52
1	B	144	SER	CA-C	-6.54	1.45	1.52
1	C	144	SER	CA-C	-5.77	1.45	1.52
1	A	144	SER	CA-C	-5.46	1.46	1.52
3	J	453	ALA	CA-C	-5.30	1.45	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	144	SER	N-CA-C	8.45	123.39	112.41
1	A	144	SER	N-CA-C	7.33	122.26	112.30
3	L	454	ASP	N-CA-C	7.26	120.77	109.07
3	J	760	GLU	N-CA-C	-7.25	101.68	111.54
1	B	144	SER	N-CA-C	7.20	122.09	112.30
3	L	312	SER	CA-C-N	-6.88	113.71	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	312	SER	C-N-CA	-6.88	113.71	120.52
3	K	124	THR	N-CA-C	-6.45	101.32	110.35
3	L	507	PRO	N-CA-C	-6.44	101.53	111.13
1	C	144	SER	CB-CA-C	-6.23	100.93	111.02
3	L	506	GLN	CA-C-N	-6.22	114.36	120.52
3	L	506	GLN	C-N-CA	-6.22	114.36	120.52
3	L	453	ALA	N-CA-C	-6.21	104.33	112.41
3	K	123	ASP	N-CA-C	-5.94	102.13	110.50
3	K	762	SER	N-CA-C	5.93	123.44	110.80
1	B	288	PRO	N-CA-C	5.81	124.44	112.47
3	J	824	SER	N-CA-C	5.80	118.41	109.07
1	C	288	PRO	N-CA-C	5.58	123.96	112.47
3	L	124	THR	N-CA-C	-5.52	102.23	110.23
3	J	453	ALA	N-CA-C	-5.47	105.40	113.61
3	L	453	ALA	CA-C-N	-5.34	115.63	123.00
3	L	453	ALA	C-N-CA	-5.34	115.63	123.00
3	K	4	ILE	N-CA-C	5.27	120.30	109.34
3	J	826	PRO	N-CA-C	5.15	123.08	112.47
3	J	717	ILE	CA-C-N	5.07	131.21	121.54
3	J	717	ILE	C-N-CA	5.07	131.21	121.54
1	A	235	ASP	N-CA-C	-5.02	108.42	114.75

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	2379	0	2298	67	0
1	B	2379	0	2298	79	0
1	C	2379	0	2298	69	0
2	D	1609	0	1590	70	0
2	E	1609	0	1590	55	0
2	F	1609	0	1590	65	0
2	G	1609	0	1590	79	0
2	H	1609	0	1590	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	1609	0	1590	69	0
3	J	6536	0	6383	291	0
3	K	6536	0	6383	271	0
3	L	6544	0	6389	271	0
All	All	36407	0	35589	1334	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 19.

All (1334) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:553:ASN:O	3:K:553:ASN:ND2	2.03	0.90
3:J:176:ALA:HA	3:J:181:LEU:HD23	1.55	0.87
3:J:121:ASP:HB3	3:J:122:PRO:HD2	1.58	0.84
3:K:23:LEU:HB2	3:K:107:HIS:HB2	1.59	0.84
2:D:133:PRO:HB3	2:D:174:ARG:HD3	1.58	0.83
3:L:553:ASN:ND2	3:L:673:PRO:HG2	1.96	0.81
3:L:23:LEU:HB2	3:L:107:HIS:HB2	1.62	0.81
3:L:815:ARG:HE	3:L:826:PRO:HG3	1.46	0.79
3:J:369:TRP:HB2	3:J:418:ILE:HB	1.64	0.78
3:J:168:VAL:HG21	3:K:242:LEU:HD12	1.66	0.77
3:L:338:MET:HE1	3:L:370:THR:HG21	1.64	0.77
3:J:815:ARG:HE	3:J:826:PRO:HG3	1.51	0.76
3:K:198:GLU:HB3	3:K:412:LEU:HD13	1.65	0.76
3:K:553:ASN:HD22	3:K:553:ASN:C	1.90	0.76
3:J:776:ILE:HB	3:J:785:TYR:HB2	1.68	0.76
2:F:21:ASN:HB3	2:F:51:ASN:HB2	1.68	0.75
3:J:23:LEU:HB2	3:J:107:HIS:HB2	1.68	0.75
3:K:512:VAL:O	3:K:528:ASN:ND2	2.20	0.74
2:G:36:GLY:O	2:I:201:ARG:NH1	2.20	0.74
2:I:42:LYS:HB3	3:L:19:LYS:HG2	1.67	0.74
1:B:32:THR:HG22	1:C:268:LEU:H	1.53	0.74
3:K:136:THR:HB	3:L:589:GLY:HA3	1.69	0.74
2:D:2:ARG:NH1	2:D:8:THR:OG1	2.21	0.74
3:J:102:ARG:NH1	3:K:623:ASP:O	2.21	0.73
3:J:695:GLU:HB2	3:J:707:VAL:HB	1.70	0.73
1:C:248:LEU:HD11	1:C:264:ILE:HD11	1.71	0.73
2:I:92:ARG:HG2	2:I:93:GLY:H	1.54	0.73
3:K:137:GLY:HA2	3:K:157:ASN:HB2	1.70	0.73
1:A:95:ARG:NH2	1:A:284:ALA:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:695:GLU:HB2	3:K:707:VAL:HB	1.70	0.72
3:K:72:LEU:HD23	3:K:545:LEU:HD12	1.71	0.72
1:C:95:ARG:NH2	1:C:284:ALA:O	2.21	0.72
3:J:377:GLN:NE2	3:J:411:LEU:O	2.23	0.72
3:K:102:ARG:NH1	3:L:623:ASP:O	2.23	0.72
3:K:168:VAL:HG21	3:L:242:LEU:HD12	1.72	0.71
2:E:3:LEU:HD12	2:E:4:PRO:HD2	1.72	0.71
3:J:181:LEU:HD12	3:J:189:GLN:HB3	1.72	0.71
3:K:101:ASP:OD1	3:K:134:ARG:NH1	2.23	0.71
3:L:362:GLY:HA3	3:L:826:PRO:HG2	1.70	0.71
1:B:224:LEU:HB2	1:B:278:TYR:HB2	1.71	0.71
3:J:692:LEU:HD12	3:J:711:TYR:HD2	1.54	0.71
3:K:68:GLN:NE2	3:K:552:ILE:O	2.23	0.71
1:B:248:LEU:HD11	1:B:264:ILE:HD11	1.72	0.71
1:B:257:ILE:HG13	1:B:291:ILE:HG13	1.73	0.71
3:L:228:GLN:HA	3:L:252:GLU:HA	1.73	0.71
3:L:176:ALA:HA	3:L:181:LEU:HG	1.73	0.71
2:E:21:ASN:HB3	2:E:51:ASN:HB2	1.73	0.71
2:I:24:ASP:OD1	2:I:46:GLN:NE2	2.24	0.71
3:J:362:GLY:HA3	3:J:826:PRO:HG2	1.73	0.70
3:K:303:GLY:HA2	3:K:372:HIS:CE1	2.26	0.70
3:J:242:LEU:HD12	3:L:168:VAL:HG21	1.71	0.70
3:L:137:GLY:HA2	3:L:157:ASN:HB2	1.72	0.70
3:J:303:GLY:HA2	3:J:372:HIS:CE1	2.26	0.70
3:L:368:ILE:HG12	3:L:419:VAL:HG22	1.73	0.70
3:L:371:PHE:HE2	3:L:380:ALA:HB2	1.55	0.70
1:A:32:THR:HG22	1:B:268:LEU:H	1.56	0.70
2:E:42:LYS:HB2	3:K:19:LYS:HG2	1.72	0.70
3:J:101:ASP:OD1	3:J:134:ARG:NH1	2.25	0.69
3:J:765:PRO:HG3	3:J:798:MET:HE1	1.74	0.69
2:E:201:ARG:NH1	2:E:202:GLU:O	2.25	0.69
3:K:230:LYS:HD2	3:K:265:PRO:HG3	1.73	0.69
2:G:126:LEU:HB3	2:G:171:ILE:HD11	1.74	0.69
3:J:137:GLY:HA2	3:J:157:ASN:HB2	1.72	0.69
3:L:439:GLY:HA3	3:L:457:SER:HB3	1.75	0.69
1:A:127:VAL:HG22	1:A:140:VAL:HG12	1.73	0.69
2:D:112:ASN:HB3	2:D:147:VAL:HG22	1.75	0.69
3:K:109:ALA:HA	3:K:127:PRO:HB3	1.75	0.69
1:C:257:ILE:HG13	1:C:291:ILE:HG13	1.75	0.69
3:J:506:GLN:HG2	3:J:514:TRP:CZ2	2.28	0.68
3:J:72:LEU:HD23	3:J:545:LEU:HD12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:171:ARG:NH2	3:L:298:GLU:OE1	2.26	0.68
3:L:494:LEU:HD21	3:L:563:VAL:HG21	1.75	0.68
2:E:109:ILE:HD11	2:E:156:LEU:HD21	1.75	0.68
3:J:605:LEU:HG	3:J:729:ILE:HB	1.76	0.68
3:L:369:TRP:HB2	3:L:418:ILE:HB	1.73	0.68
1:B:55:ILE:HD11	1:C:263:ARG:HD3	1.75	0.68
1:A:268:LEU:H	1:C:32:THR:HG22	1.59	0.68
3:K:595:SER:HB2	3:K:629:LYS:HG2	1.74	0.68
3:K:171:ARG:NH1	3:K:413:ASP:O	2.21	0.68
1:B:249:ILE:HG23	1:B:258:THR:HG22	1.76	0.68
2:F:42:LYS:HB3	3:J:19:LYS:HG2	1.75	0.67
2:F:153:TYR:HB2	2:G:70:LEU:HB3	1.76	0.67
3:L:524:ILE:HG22	3:L:525:VAL:HG23	1.77	0.67
3:L:743:LYS:H	3:L:762:SER:HB2	1.58	0.67
2:D:36:GLY:O	2:F:201:ARG:NH1	2.27	0.67
3:K:736:VAL:HA	3:K:768:THR:HG21	1.75	0.67
2:D:24:ASP:OD2	2:F:73:LYS:NZ	2.28	0.67
2:G:4:PRO:HD3	2:G:68:ARG:HD2	1.77	0.67
2:I:52:ILE:HB	2:I:198:LEU:HB2	1.77	0.67
3:K:31:SER:HB3	3:K:97:VAL:HA	1.77	0.67
3:L:109:ALA:HA	3:L:127:PRO:HB3	1.77	0.67
1:A:44:ILE:HD11	2:E:187:LEU:HD23	1.74	0.67
2:G:43:ILE:HG22	2:G:44:SER:H	1.59	0.67
2:G:109:ILE:HD11	2:G:156:LEU:HD21	1.77	0.67
3:J:332:LYS:HG3	3:J:507:PRO:HB3	1.76	0.66
3:L:303:GLY:HA2	3:L:372:HIS:CE1	2.30	0.66
2:I:112:ASN:HB3	2:I:147:VAL:HG22	1.76	0.66
3:J:614:PHE:HZ	3:J:644:ARG:HG3	1.60	0.66
1:A:187:MET:HE3	1:A:257:ILE:HD13	1.76	0.66
3:J:614:PHE:CZ	3:J:644:ARG:HG3	2.30	0.66
3:L:72:LEU:HD23	3:L:545:LEU:HD12	1.78	0.66
3:J:464:LEU:HD11	3:J:541:VAL:HG13	1.77	0.66
3:L:818:ASP:OD1	3:L:821:GLY:N	2.29	0.66
1:C:154:ARG:NH1	1:C:158:THR:OG1	2.29	0.66
3:L:695:GLU:HB3	3:L:707:VAL:HB	1.77	0.66
3:J:267:VAL:HG21	3:J:273:ILE:HD13	1.77	0.66
3:J:305:LEU:HD21	3:J:511:TYR:CE1	2.31	0.66
1:C:249:ILE:HG23	1:C:258:THR:HG22	1.77	0.65
3:K:316:CYS:HB3	3:K:327:CYS:HB2	1.78	0.65
3:K:79:PHE:HB2	3:K:156:TRP:HB2	1.78	0.65
3:K:524:ILE:HG22	3:K:525:VAL:HG23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:113:THR:HG21	2:H:117:LEU:HD12	1.79	0.65
3:K:377:GLN:NE2	3:K:411:LEU:O	2.27	0.65
3:K:528:ASN:N	3:K:636:ASN:O	2.27	0.65
3:K:597:GLN:HG3	3:K:613:THR:HG22	1.79	0.65
3:K:784:PRO:HD2	3:L:790:LEU:HB3	1.78	0.65
3:J:301:ILE:HG22	3:J:303:GLY:H	1.61	0.65
1:B:95:ARG:NH2	1:B:284:ALA:O	2.20	0.65
1:C:44:ILE:HD11	2:I:187:LEU:HD23	1.78	0.65
3:J:459:ASN:HA	3:J:463:GLN:HE21	1.60	0.65
2:F:46:GLN:H	2:F:157:PHE:HZ	1.45	0.64
2:I:176:LYS:HG3	2:I:203:SER:HB3	1.80	0.64
3:J:739:PRO:HB3	3:J:763:TRP:HB2	1.79	0.64
3:L:512:VAL:O	3:L:528:ASN:ND2	2.30	0.64
3:K:301:ILE:HG22	3:K:303:GLY:H	1.62	0.64
2:I:46:GLN:H	2:I:157:PHE:HZ	1.45	0.64
2:D:140:ASN:OD1	2:D:141:PHE:N	2.30	0.64
2:D:109:ILE:HD11	2:D:156:LEU:HD21	1.78	0.64
3:K:743:LYS:H	3:K:762:SER:HB2	1.61	0.64
3:K:358:LYS:HE3	3:K:367:ARG:HH12	1.61	0.64
2:I:80:ASP:HB3	2:I:172:LEU:HD23	1.79	0.64
3:K:104:ILE:HD11	3:K:135:ILE:HD12	1.80	0.64
3:L:92:LEU:HD21	3:L:139:GLY:HA2	1.80	0.64
2:I:46:GLN:HE22	2:I:153:TYR:HE2	1.45	0.64
3:J:368:ILE:HG12	3:J:419:VAL:HG22	1.79	0.64
3:J:681:TYR:HE1	3:J:683:ARG:HB2	1.61	0.63
1:B:222:ALA:HB3	1:B:280:VAL:HB	1.80	0.63
3:K:608:LYS:NZ	3:K:731:ASP:OD2	2.24	0.63
3:K:739:PRO:HB3	3:K:763:TRP:HB2	1.80	0.63
2:H:4:PRO:HD3	2:H:68:ARG:HD2	1.79	0.63
3:L:79:PHE:HB2	3:L:156:TRP:HB2	1.80	0.63
3:L:596:VAL:HB	3:L:651:LEU:HD12	1.79	0.63
3:J:304:PHE:N	3:J:351:SER:OG	2.32	0.63
2:I:57:LEU:HD12	2:I:196:ILE:HD13	1.79	0.62
1:C:120:GLU:OE2	1:C:146:LYS:NZ	2.30	0.62
3:J:628:LYS:HE3	3:L:100:LEU:HD12	1.81	0.62
1:C:199:ARG:HB3	2:G:189:ASN:ND2	2.15	0.62
2:H:43:ILE:HG22	2:H:44:SER:H	1.64	0.62
3:K:571:LEU:HB2	3:K:677:ILE:HG22	1.81	0.62
3:L:23:LEU:HD21	3:L:48:VAL:HG13	1.81	0.62
1:A:55:ILE:HD11	1:B:263:ARG:HD3	1.80	0.62
3:J:808:GLY:HA2	3:J:833:LEU:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:498:ASP:OD1	3:K:718:ASN:ND2	2.32	0.62
3:L:377:GLN:NE2	3:L:411:LEU:O	2.28	0.62
2:D:18:GLU:HG3	2:F:189:ASN:HD21	1.64	0.62
1:B:154:ARG:NH1	1:B:158:THR:OG1	2.33	0.62
2:H:112:ASN:HB3	2:H:147:VAL:HG22	1.82	0.62
3:K:92:LEU:HD21	3:K:139:GLY:HA2	1.82	0.62
3:K:692:LEU:HD12	3:K:711:TYR:HD2	1.62	0.62
3:L:24:ILE:HG12	3:L:106:ILE:HG12	1.81	0.62
2:D:126:LEU:HB3	2:D:171:ILE:HD11	1.80	0.62
3:K:101:ASP:O	3:K:102:ARG:HB2	1.98	0.62
2:E:178:MET:HE3	2:E:201:ARG:HD3	1.81	0.62
3:K:30:SER:O	3:K:102:ARG:NH2	2.32	0.62
3:K:325:ARG:HD3	3:K:735:ASN:HD22	1.65	0.62
1:C:130:SER:HA	1:C:186:SER:HA	1.80	0.62
3:J:498:ASP:OD1	3:J:718:ASN:ND2	2.33	0.62
3:J:524:ILE:HG22	3:J:525:VAL:HG23	1.81	0.62
3:L:294:TYR:HE2	3:L:433:ILE:HD12	1.65	0.62
3:K:325:ARG:NE	3:K:327:CYS:SG	2.73	0.61
3:L:592:LYS:HE2	3:L:655:ARG:NH1	2.15	0.61
2:D:46:GLN:H	2:D:157:PHE:HZ	1.48	0.61
1:C:264:ILE:HG12	1:C:280:VAL:HG22	1.82	0.61
3:K:369:TRP:HB2	3:K:418:ILE:HB	1.81	0.61
1:C:63:ILE:HG21	1:C:107:MET:HE1	1.82	0.61
3:J:790:LEU:HD21	3:L:786:ILE:HD11	1.82	0.61
3:L:741:ASP:O	3:L:763:TRP:HA	2.01	0.61
2:E:73:LYS:NZ	2:H:24:ASP:OD2	2.30	0.61
2:E:110:ILE:HG13	2:E:110:ILE:O	2.00	0.61
3:J:459:ASN:HA	3:J:463:GLN:NE2	2.15	0.61
3:K:124:THR:O	3:K:126:GLY:N	2.34	0.61
3:L:198:GLU:HB3	3:L:412:LEU:HD13	1.83	0.61
3:J:303:GLY:HA2	3:J:372:HIS:HE1	1.66	0.61
1:B:259:PHE:HB3	1:B:262:ALA:HB2	1.82	0.61
3:J:68:GLN:NE2	3:J:554:ASN:OD1	2.21	0.61
3:J:615:TYR:CD1	3:L:180:GLY:HA2	2.36	0.61
3:K:21:ALA:O	3:K:109:ALA:N	2.34	0.61
3:K:306:ASP:OD2	3:K:331:LYS:NZ	2.32	0.61
3:L:304:PHE:N	3:L:351:SER:OG	2.33	0.61
3:K:195:LYS:O	3:K:196:ARG:HG2	2.01	0.60
3:K:294:TYR:HE2	3:K:433:ILE:HD12	1.65	0.60
1:A:259:PHE:HB3	1:A:262:ALA:HB2	1.83	0.60
3:L:363:ASN:HA	3:L:426:ASN:HD22	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:70:LEU:HB3	2:I:153:TYR:HB2	1.82	0.60
1:B:36:GLU:OE1	1:C:263:ARG:NH2	2.33	0.60
3:K:692:LEU:HD12	3:K:711:TYR:CD2	2.37	0.60
3:K:818:ASP:OD1	3:K:821:GLY:N	2.35	0.60
2:H:160:THR:HG22	2:H:162:GLY:H	1.66	0.60
3:K:24:ILE:HG12	3:K:106:ILE:HG12	1.84	0.60
3:K:506:GLN:O	3:K:507:PRO:C	2.43	0.60
1:C:199:ARG:HB3	2:G:189:ASN:HD21	1.67	0.60
2:D:4:PRO:HD3	2:D:68:ARG:HD2	1.82	0.60
2:H:133:PRO:HB3	2:H:174:ARG:HD3	1.83	0.60
3:J:67:LYS:HB2	3:J:697:GLU:HG3	1.83	0.60
3:L:271:GLN:HG2	3:L:530:ILE:HD11	1.84	0.60
1:C:259:PHE:HB3	1:C:262:ALA:HB2	1.82	0.60
2:F:134:LYS:HG3	2:F:202:GLU:OE2	2.00	0.60
3:K:741:ASP:O	3:K:763:TRP:HA	2.02	0.60
3:L:21:ALA:O	3:L:109:ALA:N	2.35	0.60
3:L:297:ALA:HB3	3:L:301:ILE:HD11	1.83	0.60
3:L:458:LEU:HD12	3:L:462:TRP:HD1	1.66	0.60
3:K:27:GLU:OE2	3:L:624:LYS:NZ	2.34	0.60
2:G:80:ASP:HB3	2:G:172:LEU:HB3	1.83	0.60
2:F:85:GLN:HG2	2:G:187:LEU:HD13	1.84	0.59
2:G:160:THR:HG22	2:G:162:GLY:H	1.67	0.59
3:J:21:ALA:O	3:J:109:ALA:N	2.32	0.59
3:J:697:GLU:HB3	3:J:705:ASN:HB2	1.84	0.59
3:K:18:LEU:HD12	3:K:110:ILE:HD12	1.84	0.59
3:L:316:CYS:HB3	3:L:327:CYS:HB2	1.83	0.59
3:J:18:LEU:HD12	3:J:110:ILE:HD12	1.84	0.59
3:J:230:LYS:HD2	3:J:265:PRO:HG3	1.83	0.59
1:A:40:LEU:HD12	1:A:51:ALA:HB2	1.85	0.59
1:B:41:ARG:O	1:B:48:THR:OG1	2.20	0.59
3:J:816:ALA:O	3:J:823:ARG:HA	2.03	0.59
3:L:120:VAL:HG12	3:L:126:GLY:O	2.01	0.59
3:L:269:GLY:H	3:L:457:SER:HB2	1.67	0.59
2:D:43:ILE:HG22	2:D:44:SER:H	1.67	0.59
2:G:112:ASN:HB3	2:G:147:VAL:HG22	1.85	0.59
3:K:540:ASN:O	3:K:544:ILE:HD12	2.03	0.59
1:B:230:LYS:HE2	1:B:237:PHE:HD2	1.65	0.59
2:H:126:LEU:HB3	2:H:171:ILE:HD11	1.83	0.59
3:J:593:PHE:HD1	3:J:628:LYS:HG2	1.68	0.59
3:K:304:PHE:N	3:K:351:SER:OG	2.34	0.59
3:K:367:ARG:HB3	3:K:420:ARG:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:306:ASP:OD2	3:L:331:LYS:NZ	2.28	0.59
1:A:49:ASN:ND2	1:B:218:MET:HB3	2.17	0.59
3:L:597:GLN:HG3	3:L:613:THR:HG22	1.85	0.59
2:G:153:TYR:HB3	2:G:154:PRO:HD3	1.85	0.59
2:I:109:ILE:HD11	2:I:156:LEU:HD21	1.84	0.59
3:L:367:ARG:HB2	3:L:420:ARG:HB3	1.84	0.59
3:J:23:LEU:HD21	3:J:48:VAL:HG13	1.85	0.58
3:L:49:THR:HG22	3:L:54:LEU:HA	1.84	0.58
3:L:459:ASN:HA	3:L:463:GLN:HE21	1.67	0.58
3:L:743:LYS:HA	3:L:829:LEU:HD11	1.85	0.58
3:K:677:ILE:HD11	3:K:708:LEU:HD21	1.85	0.58
1:A:8:GLU:OE1	1:A:113:ASN:ND2	2.36	0.58
2:G:69:LEU:O	2:G:72:TYR:HB3	2.03	0.58
3:J:700:ARG:O	3:J:700:ARG:NH1	2.37	0.58
3:J:815:ARG:HG2	3:J:826:PRO:HD3	1.84	0.58
3:L:371:PHE:CE2	3:L:380:ALA:HB2	2.37	0.58
1:C:127:VAL:HG22	1:C:140:VAL:HG23	1.85	0.58
3:J:316:CYS:HB3	3:J:327:CYS:HB2	1.85	0.58
2:H:67:SER:O	2:I:139:THR:OG1	2.21	0.58
3:J:282:THR:HG22	3:J:290:VAL:HG22	1.84	0.58
3:K:89:VAL:O	3:K:93:VAL:HG22	2.04	0.58
3:K:256:ASP:O	3:L:609:THR:OG1	2.22	0.58
3:L:303:GLY:HA2	3:L:372:HIS:HE1	1.66	0.58
2:E:47:TYR:CD2	2:E:201:ARG:HG3	2.39	0.58
3:J:198:GLU:HB3	3:J:412:LEU:HD13	1.86	0.58
3:J:578:THR:OG1	3:J:579:TYR:N	2.34	0.58
3:K:123:ASP:O	3:K:124:THR:C	2.47	0.58
3:K:164:ASP:OD2	3:L:628:LYS:NZ	2.36	0.58
2:G:187:LEU:HB2	2:G:193:TYR:CE1	2.39	0.57
3:J:89:VAL:O	3:J:93:VAL:HG22	2.04	0.57
3:J:374:LYS:HB2	3:J:377:GLN:HB3	1.84	0.57
3:K:368:ILE:HG12	3:K:419:VAL:HG22	1.84	0.57
2:F:24:ASP:OD1	2:F:46:GLN:NE2	2.37	0.57
2:I:21:ASN:HB3	2:I:51:ASN:HB2	1.85	0.57
3:K:199:TYR:OH	3:K:413:ASP:HB2	2.04	0.57
3:L:219:GLN:O	3:L:224:ARG:NH2	2.36	0.57
3:L:528:ASN:N	3:L:636:ASN:O	2.29	0.57
2:D:70:LEU:HD13	2:E:153:TYR:CD2	2.40	0.57
2:G:133:PRO:HB3	2:G:174:ARG:HD3	1.86	0.57
3:L:104:ILE:HD11	3:L:135:ILE:HD12	1.85	0.57
3:L:301:ILE:HG22	3:L:303:GLY:H	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:31:SER:HB2	3:J:97:VAL:HA	1.86	0.57
3:K:371:PHE:CZ	3:K:380:ALA:HB2	2.40	0.57
3:J:818:ASP:OD1	3:J:821:GLY:N	2.38	0.57
3:K:816:ALA:O	3:K:823:ARG:HA	2.05	0.57
3:K:582:LEU:HD11	3:K:660:LEU:HD23	1.85	0.57
2:H:187:LEU:HB2	2:H:193:TYR:HE1	1.69	0.57
3:J:741:ASP:O	3:J:763:TRP:HA	2.04	0.57
3:J:67:LYS:NZ	3:J:695:GLU:OE1	2.33	0.56
3:L:195:LYS:O	3:L:196:ARG:HG2	2.05	0.56
3:L:297:ALA:H	3:L:415:ALA:HB3	1.69	0.56
2:G:113:THR:HG21	2:G:117:LEU:HD12	1.88	0.56
1:A:149:GLU:OE1	1:B:240:LEU:HG	2.04	0.56
1:A:263:ARG:HD3	1:C:55:ILE:HD11	1.88	0.56
1:C:222:ALA:HB3	1:C:280:VAL:HB	1.86	0.56
2:D:136:TYR:CG	2:D:152:LEU:HD23	2.41	0.56
3:K:40:TYR:CD1	3:K:53:ILE:HG21	2.41	0.56
3:K:697:GLU:HB3	3:K:705:ASN:HB2	1.87	0.56
3:L:2:LYS:NZ	3:L:120:VAL:HG23	2.19	0.56
2:D:26:ASP:OD2	2:D:42:LYS:NZ	2.38	0.56
3:J:439:GLY:HA3	3:J:457:SER:CB	2.36	0.56
3:J:623:ASP:O	3:L:102:ARG:NH1	2.38	0.56
1:C:74:ILE:HD11	1:C:159:ILE:HG22	1.87	0.56
3:J:677:ILE:HD11	3:J:708:LEU:HD21	1.87	0.56
3:L:281:ASP:OD1	3:L:282:THR:N	2.35	0.56
3:L:652:LYS:HE3	3:L:715:VAL:HA	1.87	0.56
2:G:46:GLN:H	2:G:157:PHE:HZ	1.53	0.56
2:G:110:ILE:HG12	2:G:149:ASN:HB3	1.86	0.56
3:J:499:GLU:HA	3:J:522:ARG:HH12	1.71	0.56
1:C:154:ARG:NH1	1:C:156:GLY:O	2.39	0.56
2:E:112:ASN:HB3	2:E:147:VAL:HG22	1.86	0.56
2:E:176:LYS:HG3	2:E:203:SER:HB2	1.87	0.56
3:J:298:GLU:HG2	3:J:472:ARG:HH21	1.71	0.56
1:A:131:LEU:HB3	1:A:170:PRO:HB3	1.88	0.56
1:C:30:ALA:HB2	1:C:63:ILE:HG13	1.88	0.56
2:G:127:PHE:N	2:G:136:TYR:O	2.36	0.56
2:I:104:GLN:NE2	2:I:110:ILE:H	2.03	0.56
3:K:560:ARG:HE	3:K:672:GLU:CD	2.14	0.56
1:A:199:ARG:O	2:H:189:ASN:ND2	2.35	0.56
2:H:109:ILE:HD11	2:H:156:LEU:HD21	1.88	0.56
3:K:233:LEU:HD22	3:K:609:THR:HG22	1.88	0.56
3:L:381:GLN:O	3:L:385:ASP:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:133:PRO:HB3	2:E:174:ARG:HG3	1.88	0.56
3:J:509:TRP:HB2	3:J:514:TRP:HE1	1.69	0.56
1:B:149:GLU:OE1	1:C:240:LEU:HG	2.06	0.55
2:H:47:TYR:CD2	2:H:201:ARG:HG3	2.41	0.55
3:K:303:GLY:HA2	3:K:372:HIS:HE1	1.69	0.55
3:K:620:LYS:HG2	3:K:625:GLY:HA2	1.87	0.55
3:K:297:ALA:H	3:K:415:ALA:HB3	1.71	0.55
3:L:268:TYR:HE2	3:L:531:LEU:HD12	1.71	0.55
3:L:79:PHE:HE1	3:L:106:ILE:HD11	1.69	0.55
3:J:590:ARG:HG3	3:L:164:ASP:HA	1.89	0.55
3:J:761:LEU:HB2	3:J:798:MET:O	2.07	0.55
3:L:113:GLU:HB2	3:L:114:GLU:OE1	2.06	0.55
3:L:374:LYS:HB2	3:L:377:GLN:HB3	1.88	0.55
2:G:43:ILE:O	2:G:44:SER:OG	2.24	0.55
3:J:506:GLN:O	3:J:507:PRO:C	2.49	0.55
3:J:107:HIS:HB3	3:J:127:PRO:HB2	1.88	0.55
3:K:815:ARG:HE	3:K:826:PRO:HG3	1.71	0.55
3:L:89:VAL:O	3:L:93:VAL:HG22	2.06	0.55
3:L:778:HIS:HB2	3:L:781:HIS:HB2	1.88	0.55
1:B:74:ILE:HD11	1:B:159:ILE:HG22	1.89	0.55
2:G:175:THR:HA	2:G:202:GLU:HA	1.89	0.55
2:I:1:MET:HE1	2:I:68:ARG:HB3	1.89	0.55
2:E:43:ILE:HG22	2:E:44:SER:H	1.70	0.55
2:E:127:PHE:HE1	2:E:166:PRO:HB3	1.72	0.55
2:I:127:PHE:HE1	2:I:166:PRO:HB3	1.72	0.55
3:J:439:GLY:HA3	3:J:457:SER:HB2	1.89	0.55
3:K:290:VAL:HG21	3:K:430:ILE:HD11	1.89	0.55
3:K:700:ARG:O	3:K:700:ARG:NH1	2.40	0.55
1:C:79:PHE:HB2	1:C:91:LEU:HD13	1.89	0.55
3:J:528:ASN:N	3:J:636:ASN:O	2.36	0.55
3:K:301:ILE:HG22	3:K:303:GLY:N	2.21	0.55
2:F:3:LEU:HB2	2:F:79:LEU:HD22	1.88	0.55
3:J:30:SER:O	3:J:102:ARG:NH2	2.40	0.55
3:J:371:PHE:CE2	3:J:380:ALA:HB2	2.42	0.55
3:J:619:PHE:HD2	3:J:655:ARG:HE	1.54	0.54
3:K:664:VAL:HB	3:K:668:PHE:HD2	1.72	0.54
2:D:47:TYR:CD2	2:D:201:ARG:HG3	2.42	0.54
2:G:77:ASP:OD1	2:G:78:TYR:N	2.38	0.54
2:G:109:ILE:HG12	2:G:156:LEU:HD11	1.90	0.54
2:H:73:LYS:NZ	2:I:24:ASP:OD2	2.38	0.54
3:J:395:GLN:HE21	3:J:404:TYR:HB3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:652:LYS:HE3	3:K:715:VAL:HA	1.90	0.54
3:L:322:SER:OG	3:L:330:ARG:NH2	2.38	0.54
1:A:117:ILE:HD13	1:B:270:PHE:HZ	1.72	0.54
2:E:178:MET:HE1	2:H:38:VAL:HG11	1.88	0.54
2:F:46:GLN:HE22	2:F:153:TYR:HE2	1.53	0.54
2:I:43:ILE:HG22	2:I:44:SER:H	1.72	0.54
3:J:640:TYR:OH	3:J:644:ARG:NH1	2.40	0.54
3:J:676:PRO:HB3	3:J:690:PHE:CZ	2.42	0.54
3:L:465:MET:HE2	3:L:487:VAL:HG11	1.88	0.54
2:F:110:ILE:HG13	2:F:110:ILE:O	2.07	0.54
2:G:62:TYR:OH	2:G:185:SER:OG	2.24	0.54
3:K:489:SER:O	3:K:493:ILE:HG12	2.07	0.54
2:H:133:PRO:HG3	2:H:174:ARG:NH1	2.23	0.54
2:H:187:LEU:HB2	2:H:193:TYR:CE1	2.42	0.54
3:L:459:ASN:HA	3:L:463:GLN:NE2	2.23	0.54
1:B:154:ARG:NH1	1:B:156:GLY:O	2.40	0.54
2:F:43:ILE:HG22	2:F:44:SER:H	1.72	0.54
3:J:297:ALA:H	3:J:415:ALA:HB3	1.73	0.54
3:K:381:GLN:O	3:K:385:ASP:HB2	2.08	0.54
3:L:67:LYS:HE2	3:L:695:GLU:OE2	2.08	0.54
2:E:28:MET:HE3	2:E:40:GLU:HB2	1.90	0.54
3:J:596:VAL:HB	3:J:651:LEU:HD12	1.89	0.54
3:K:314:MET:HE1	3:K:368:ILE:HD12	1.89	0.54
3:L:31:SER:HB2	3:L:97:VAL:HA	1.89	0.54
3:L:171:ARG:NH1	3:L:413:ASP:O	2.40	0.54
2:D:160:THR:HG22	2:D:162:GLY:H	1.72	0.54
2:H:2:ARG:H	2:H:80:ASP:HB2	1.72	0.54
3:J:486:LYS:HE3	3:J:560:ARG:HH22	1.73	0.54
3:J:440:LYS:NZ	3:J:473:TYR:OH	2.41	0.54
3:J:759:GLY:HA2	3:J:800:GLN:O	2.07	0.54
3:K:808:GLY:HA2	3:K:833:LEU:HB2	1.88	0.54
1:A:132:ASP:O	1:A:134:SER:N	2.41	0.54
2:D:3:LEU:HD21	2:D:54:TYR:OH	2.08	0.54
2:F:134:LYS:HD3	2:F:204:LEU:HD22	1.90	0.54
2:G:136:TYR:CG	2:G:152:LEU:HD23	2.44	0.54
2:I:104:GLN:HE22	2:I:110:ILE:HB	1.73	0.54
1:A:240:LEU:HG	1:C:149:GLU:OE1	2.07	0.53
1:B:130:SER:HA	1:B:186:SER:HA	1.90	0.53
2:E:34:PRO:HG3	3:K:579:TYR:O	2.08	0.53
2:F:126:LEU:HB3	2:F:171:ILE:HD11	1.90	0.53
2:H:109:ILE:HG12	2:H:156:LEU:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:314:MET:HE1	3:J:368:ILE:HD12	1.90	0.53
3:K:592:LYS:HG3	3:K:655:ARG:HA	1.90	0.53
3:L:325:ARG:NE	3:L:327:CYS:SG	2.81	0.53
2:E:70:LEU:HD11	2:H:137:LYS:HE3	1.89	0.53
2:H:187:LEU:HD13	2:I:85:GLN:HG2	1.90	0.53
3:J:506:GLN:O	3:J:508:TYR:N	2.41	0.53
3:K:121:ASP:CB	3:K:122:PRO:HD2	2.38	0.53
3:L:578:THR:HG22	3:L:664:VAL:HG12	1.90	0.53
2:G:134:LYS:HD3	2:G:204:LEU:HD22	1.88	0.53
2:G:137:LYS:HE3	2:I:70:LEU:HD11	1.88	0.53
3:K:765:PRO:HG3	3:K:798:MET:HE1	1.90	0.53
1:A:130:SER:HA	1:A:186:SER:HA	1.91	0.53
3:J:179:ARG:HE	3:J:181:LEU:HD21	1.73	0.53
3:J:358:LYS:HD3	3:J:367:ARG:HH12	1.72	0.53
3:J:560:ARG:HD3	3:J:672:GLU:OE2	2.09	0.53
3:L:339:HIS:ND1	3:L:349:GLN:OE1	2.40	0.53
3:L:421:PHE:HZ	3:L:433:ILE:HD11	1.74	0.53
2:D:94:ASP:OD1	2:D:95:THR:N	2.41	0.53
2:E:3:LEU:HB2	2:E:79:LEU:HD22	1.91	0.53
3:L:681:TYR:HE1	3:L:683:ARG:HB2	1.72	0.53
3:L:739:PRO:HB3	3:L:763:TRP:HB2	1.90	0.53
1:C:146:LYS:HD3	1:C:209:THR:HG21	1.91	0.53
2:E:2:ARG:NH1	2:E:8:THR:OG1	2.41	0.53
2:E:74:ARG:HD3	2:H:139:THR:HG21	1.91	0.53
2:I:2:ARG:O	2:I:68:ARG:NH1	2.40	0.53
2:I:92:ARG:HG2	2:I:93:GLY:N	2.21	0.53
3:J:24:ILE:HG12	3:J:106:ILE:HG12	1.90	0.53
3:J:140:ILE:HD13	3:J:154:ILE:HG12	1.91	0.53
3:J:772:VAL:HG13	3:J:773:TYR:CD1	2.44	0.53
3:J:772:VAL:HG13	3:J:773:TYR:HD1	1.73	0.53
2:F:133:PRO:HB3	2:F:174:ARG:HD2	1.91	0.53
2:H:94:ASP:OD1	2:H:95:THR:N	2.42	0.53
3:J:619:PHE:HB3	3:J:655:ARG:HH21	1.73	0.53
3:L:179:ARG:NH1	3:L:191:SER:OG	2.41	0.53
3:L:317:PHE:O	3:L:321:ASP:HB2	2.09	0.53
1:B:264:ILE:HG12	1:B:280:VAL:HG22	1.91	0.53
2:G:94:ASP:OD1	2:G:95:THR:N	2.42	0.53
3:J:566:TYR:HB2	3:J:716:PHE:CD2	2.44	0.53
1:A:74:ILE:HD11	1:A:159:ILE:HG22	1.91	0.53
2:E:4:PRO:HD3	2:E:68:ARG:HD2	1.91	0.53
2:I:133:PRO:HB3	2:I:174:ARG:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:501:TYR:HB3	3:J:721:GLN:HE21	1.73	0.53
3:K:572:ARG:NH1	3:K:572:ARG:HB2	2.24	0.53
3:L:489:SER:O	3:L:493:ILE:HG12	2.09	0.53
3:J:1:MET:HE3	3:J:1:MET:HA	1.91	0.53
3:K:669:ILE:HD12	3:K:704:ILE:HD11	1.91	0.53
3:L:101:ASP:O	3:L:102:ARG:HB2	2.09	0.53
3:L:299:GLY:HA2	3:L:373:GLY:HA3	1.91	0.53
3:L:677:ILE:HD11	3:L:708:LEU:HD11	1.91	0.53
2:F:79:LEU:O	2:F:175:THR:N	2.42	0.52
2:G:47:TYR:CD2	2:G:201:ARG:HG3	2.44	0.52
3:J:496:ILE:HG13	3:J:524:ILE:HD12	1.91	0.52
1:C:196:ARG:NH1	2:F:61:GLU:OE1	2.41	0.52
2:H:1:MET:N	2:H:80:ASP:OD1	2.42	0.52
3:J:293:VAL:HG22	3:J:418:ILE:HG12	1.91	0.52
1:C:132:ASP:O	1:C:134:SER:N	2.43	0.52
3:J:79:PHE:HE1	3:J:106:ILE:HD11	1.73	0.52
3:J:761:LEU:HB3	3:J:799:ILE:HA	1.92	0.52
3:L:555:LEU:HD11	3:L:696:VAL:HB	1.90	0.52
3:L:566:TYR:HB2	3:L:716:PHE:CD2	2.44	0.52
1:A:133:LYS:N	1:A:167:TYR:OH	2.42	0.52
1:C:131:LEU:HD22	1:C:252:ASN:ND2	2.25	0.52
1:C:180:PRO:HB3	1:C:232:LEU:HD13	1.92	0.52
3:J:395:GLN:O	3:J:399:GLY:N	2.35	0.52
3:J:506:GLN:HE22	3:J:641:TYR:HD2	1.56	0.52
3:K:4:ILE:O	3:K:8:ALA:HB3	2.09	0.52
3:K:54:LEU:HD12	3:K:56:ARG:HH12	1.74	0.52
3:L:40:TYR:CD1	3:L:53:ILE:HG21	2.44	0.52
3:J:68:GLN:OE1	3:J:553:ASN:HA	2.10	0.52
3:J:489:SER:O	3:J:493:ILE:HG12	2.09	0.52
1:A:248:LEU:HD11	1:A:264:ILE:HD11	1.91	0.52
3:J:109:ALA:HA	3:J:127:PRO:HB3	1.91	0.52
3:J:623:ASP:O	3:J:624:LYS:HB2	2.09	0.52
3:J:761:LEU:HD13	3:J:799:ILE:HG12	1.92	0.52
2:F:9:ASN:HB2	2:F:11:GLU:OE2	2.09	0.52
2:G:26:ASP:OD1	2:G:46:GLN:HG3	2.10	0.52
3:J:40:TYR:CD1	3:J:53:ILE:HG21	2.44	0.52
3:L:48:VAL:O	3:L:55:TYR:HB2	2.10	0.52
2:H:127:PHE:N	2:H:136:TYR:O	2.29	0.52
3:J:761:LEU:CB	3:J:799:ILE:HA	2.40	0.52
1:C:131:LEU:N	1:C:185:ALA:O	2.37	0.52
3:J:48:VAL:O	3:J:55:TYR:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:134:LYS:HD3	2:D:204:LEU:HD22	1.90	0.51
3:K:267:VAL:HG21	3:K:273:ILE:HD13	1.92	0.51
1:B:146:LYS:HB2	1:B:209:THR:HB	1.91	0.51
1:B:272:ASP:O	1:B:273:LEU:HB2	2.09	0.51
3:K:269:GLY:O	3:K:439:GLY:N	2.44	0.51
1:A:14:GLU:HG2	1:A:154:ARG:HH21	1.75	0.51
3:J:294:TYR:CE2	3:J:433:ILE:HD13	2.45	0.51
3:J:829:LEU:HB3	3:J:831:VAL:HG13	1.92	0.51
3:K:309:ILE:HD13	3:K:359:TYR:HE2	1.75	0.51
3:K:332:LYS:O	3:K:333:ILE:HB	2.09	0.51
3:L:111:ILE:HG22	3:L:112:ASN:O	2.11	0.51
1:B:11:ILE:HG21	1:B:65:LEU:HD21	1.93	0.51
1:C:118:TYR:CE2	1:C:120:GLU:HG2	2.45	0.51
2:H:92:ARG:HG2	2:H:93:GLY:H	1.75	0.51
3:J:28:LEU:HD22	3:J:91:LYS:HD2	1.93	0.51
3:J:230:LYS:HD2	3:J:265:PRO:CG	2.41	0.51
3:J:736:VAL:HG13	3:J:824:SER:HB3	1.92	0.51
3:L:464:LEU:HD11	3:L:541:VAL:HG13	1.91	0.51
3:L:816:ALA:O	3:L:823:ARG:HA	2.09	0.51
2:F:98:VAL:HG11	2:F:111:LEU:HD12	1.91	0.51
2:I:103:GLY:HA2	2:I:160:THR:HB	1.91	0.51
3:L:124:THR:O	3:L:126:GLY:N	2.42	0.51
1:A:93:LEU:HD22	1:C:50:TYR:HE1	1.76	0.51
1:B:146:LYS:HD3	1:B:209:THR:HG21	1.93	0.51
1:C:287:ASP:O	1:C:288:PRO:C	2.54	0.51
2:G:75:THR:HG22	2:G:77:ASP:H	1.75	0.51
2:H:94:ASP:OD1	2:H:96:LYS:N	2.40	0.51
3:K:614:PHE:CZ	3:K:644:ARG:HG3	2.46	0.51
1:A:10:LYS:HB2	1:A:110:ILE:HG13	1.91	0.51
3:K:49:THR:HG22	3:K:54:LEU:HA	1.91	0.51
3:K:121:ASP:HB3	3:K:122:PRO:HD2	1.92	0.51
3:K:660:LEU:HB2	3:K:708:LEU:HB2	1.93	0.51
3:L:2:LYS:HZ2	3:L:120:VAL:HG23	1.76	0.51
2:D:137:LYS:HE3	2:F:70:LEU:HD11	1.93	0.51
3:K:496:ILE:HG13	3:K:524:ILE:HD12	1.91	0.51
3:L:363:ASN:HA	3:L:426:ASN:ND2	2.25	0.51
3:L:563:VAL:HG22	3:L:564:GLU:H	1.76	0.51
3:L:620:LYS:HG2	3:L:625:GLY:HA2	1.93	0.51
3:L:808:GLY:HA2	3:L:833:LEU:HB2	1.93	0.51
1:A:243:GLU:OE1	1:A:266:LYS:NZ	2.43	0.51
1:B:127:VAL:HG22	1:B:140:VAL:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:VAL:HG11	2:F:178:MET:HE1	1.94	0.51
3:J:300:GLU:HG2	3:J:441:LYS:HG3	1.92	0.51
3:L:267:VAL:HG21	3:L:273:ILE:HD13	1.93	0.51
3:L:746:PRO:HA	3:L:758:ASN:CG	2.36	0.51
1:B:108:TYR:HB3	1:B:110:ILE:HG23	1.92	0.50
1:C:40:LEU:HD12	1:C:51:ALA:HB2	1.93	0.50
2:E:177:LEU:HD23	2:E:200:LEU:HD21	1.93	0.50
3:J:583:ASP:HB2	3:J:661:SER:HB2	1.92	0.50
3:K:28:LEU:HD22	3:K:91:LYS:HD2	1.94	0.50
3:L:332:LYS:HG3	3:L:507:PRO:HB3	1.93	0.50
1:A:287:ASP:OD1	1:A:287:ASP:N	2.44	0.50
2:D:18:GLU:HG3	2:F:189:ASN:ND2	2.27	0.50
2:D:187:LEU:HB2	2:D:193:TYR:HE1	1.75	0.50
2:E:98:VAL:HG21	2:E:111:LEU:HD12	1.93	0.50
3:J:582:LEU:HD12	3:J:662:PHE:HB3	1.94	0.50
3:K:66:HIS:HB2	3:K:77:LEU:HD11	1.93	0.50
2:E:136:TYR:HD1	2:E:154:PRO:HB2	1.75	0.50
2:G:133:PRO:HG3	2:G:174:ARG:NH1	2.26	0.50
3:J:490:GLU:OE2	3:J:563:VAL:HG12	2.12	0.50
3:J:681:TYR:CE1	3:J:683:ARG:HB2	2.44	0.50
3:J:692:LEU:HD12	3:J:711:TYR:CD2	2.40	0.50
3:L:498:ASP:OD1	3:L:718:ASN:ND2	2.44	0.50
1:A:249:ILE:HG23	1:A:258:THR:HG22	1.91	0.50
1:C:93:LEU:HD13	1:C:220:ALA:HB2	1.93	0.50
3:J:555:LEU:HD11	3:J:696:VAL:HB	1.93	0.50
3:K:174:ASP:OD1	3:K:175:ASP:N	2.44	0.50
3:K:595:SER:O	3:K:630:LEU:N	2.44	0.50
3:L:279:PHE:HB3	3:L:293:VAL:HB	1.94	0.50
3:L:309:ILE:HD13	3:L:359:TYR:HE2	1.76	0.50
3:L:612:ILE:HG12	3:L:640:TYR:CE2	2.46	0.50
2:I:94:ASP:OD1	2:I:95:THR:N	2.45	0.50
3:K:555:LEU:HD11	3:K:673:PRO:HD3	1.94	0.50
3:K:594:ASN:OD1	3:K:655:ARG:NH2	2.44	0.50
3:L:421:PHE:CZ	3:L:433:ILE:HD11	2.47	0.50
1:A:240:LEU:HD22	1:A:268:LEU:HD11	1.93	0.50
1:B:192:GLN:HB2	1:B:217:GLU:HB3	1.92	0.50
2:E:9:ASN:HB2	2:E:11:GLU:OE2	2.11	0.50
2:F:3:LEU:HD12	2:F:4:PRO:HD2	1.92	0.50
3:J:138:GLY:HA2	3:K:586:ASP:H	1.77	0.50
3:J:301:ILE:HG22	3:J:303:GLY:N	2.25	0.50
3:J:341:LEU:HD21	3:J:359:TYR:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:778:HIS:HB2	3:J:781:HIS:HB2	1.92	0.50
3:K:216:ALA:O	3:K:224:ARG:NH1	2.45	0.50
3:K:499:GLU:OE2	3:K:522:ARG:NH2	2.35	0.50
3:L:132:ARG:HD2	3:L:557:GLY:O	2.12	0.50
2:E:120:GLN:HG3	2:E:141:PHE:CE1	2.46	0.50
3:K:268:TYR:HE2	3:K:531:LEU:HD12	1.77	0.50
3:K:299:GLY:HA2	3:K:373:GLY:HA3	1.93	0.50
3:K:358:LYS:HE3	3:K:367:ARG:NH1	2.25	0.50
3:L:321:ASP:OD1	3:L:732:ILE:HG22	2.12	0.50
1:B:199:ARG:O	2:D:189:ASN:ND2	2.44	0.50
3:K:363:ASN:HA	3:K:426:ASN:ND2	2.26	0.50
3:L:174:ASP:OD1	3:L:175:ASP:N	2.43	0.50
1:B:240:LEU:HD22	1:B:268:LEU:HD11	1.93	0.50
3:J:321:ASP:OD1	3:J:732:ILE:HG22	2.12	0.50
3:J:669:ILE:HD12	3:J:704:ILE:HD11	1.93	0.50
1:B:131:LEU:N	1:B:185:ALA:O	2.35	0.49
2:H:134:LYS:HD2	2:H:204:LEU:HD22	1.94	0.49
3:J:302:ASP:HB2	3:J:438:GLN:O	2.11	0.49
3:J:332:LYS:O	3:J:333:ILE:HB	2.11	0.49
3:J:558:GLU:O	3:J:560:ARG:HG3	2.12	0.49
3:K:135:ILE:HD11	3:K:156:TRP:CE3	2.46	0.49
3:L:140:ILE:CD1	3:L:154:ILE:HG12	2.42	0.49
3:L:358:LYS:HB3	3:L:367:ARG:HD2	1.94	0.49
1:C:131:LEU:HD22	1:C:252:ASN:HD22	1.77	0.49
1:C:243:GLU:OE2	1:C:266:LYS:NZ	2.43	0.49
3:J:234:PHE:O	3:J:245:TYR:OH	2.20	0.49
3:J:652:LYS:HE3	3:J:715:VAL:HA	1.94	0.49
3:K:23:LEU:HD21	3:K:48:VAL:HG13	1.92	0.49
3:K:600:LEU:HD13	3:K:612:ILE:HD13	1.93	0.49
3:J:195:LYS:O	3:J:196:ARG:HG2	2.12	0.49
3:K:319:GLU:OE2	3:K:330:ARG:NH2	2.40	0.49
3:J:558:GLU:C	3:J:560:ARG:HG3	2.37	0.49
3:K:464:LEU:HD21	3:K:552:ILE:HD11	1.93	0.49
3:L:301:ILE:HG22	3:L:303:GLY:N	2.28	0.49
1:B:224:LEU:HB3	1:B:226:PHE:HE1	1.78	0.49
2:H:43:ILE:O	2:H:44:SER:OG	2.28	0.49
2:I:120:GLN:HG3	2:I:141:PHE:CE2	2.46	0.49
3:J:124:THR:O	3:J:126:GLY:N	2.46	0.49
3:J:555:LEU:HD12	3:J:672:GLU:HA	1.94	0.49
3:J:571:LEU:HB2	3:J:677:ILE:HG22	1.95	0.49
3:K:440:LYS:H	3:K:457:SER:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:619:PHE:HB3	3:K:655:ARG:HH22	1.77	0.49
2:D:111:LEU:HD23	2:D:111:LEU:H	1.77	0.49
2:H:69:LEU:O	2:H:72:TYR:HB3	2.12	0.49
3:J:189:GLN:CD	3:K:722:VAL:HG11	2.38	0.49
3:J:269:GLY:O	3:J:439:GLY:N	2.46	0.49
3:K:24:ILE:HD11	3:K:63:ILE:HD11	1.95	0.49
3:L:294:TYR:O	3:L:416:TYR:HA	2.13	0.49
3:L:301:ILE:HD12	3:L:415:ALA:HB2	1.95	0.49
2:F:2:ARG:NH1	2:F:8:THR:OG1	2.46	0.49
2:F:111:LEU:HD23	2:F:111:LEU:H	1.78	0.49
2:I:126:LEU:HB3	2:I:171:ILE:HD11	1.95	0.49
3:J:363:ASN:HA	3:J:426:ASN:ND2	2.27	0.49
1:A:272:ASP:O	1:A:273:LEU:HB2	2.12	0.49
2:D:174:ARG:HH12	2:D:204:LEU:HA	1.77	0.49
2:G:36:GLY:HA3	2:I:204:LEU:HD21	1.95	0.49
2:G:43:ILE:HG22	2:G:44:SER:N	2.28	0.49
2:I:54:TYR:HB2	2:I:196:ILE:O	2.13	0.49
3:L:623:ASP:O	3:L:624:LYS:HB2	2.13	0.49
3:J:268:TYR:HE2	3:J:531:LEU:HD12	1.77	0.49
3:K:600:LEU:HD21	3:K:643:ALA:HB3	1.95	0.49
1:B:191:GLN:HG2	1:B:193:CYS:SG	2.53	0.49
3:J:560:ARG:NH1	3:J:672:GLU:OE1	2.43	0.49
3:J:743:LYS:H	3:J:762:SER:HB2	1.77	0.49
3:K:454:ASP:O	3:K:455:LYS:HB2	2.11	0.49
3:L:79:PHE:CE1	3:L:106:ILE:HD11	2.48	0.49
3:L:660:LEU:HD13	3:L:691:PHE:CE2	2.48	0.49
1:C:146:LYS:HB2	1:C:209:THR:HB	1.94	0.48
3:K:188:LEU:O	3:K:190:PRO:HD3	2.13	0.48
3:K:271:GLN:HG2	3:K:530:ILE:HD11	1.95	0.48
3:K:623:ASP:O	3:K:624:LYS:HB2	2.13	0.48
3:L:28:LEU:HD22	3:L:91:LYS:HD2	1.95	0.48
3:L:582:LEU:HD12	3:L:662:PHE:HB3	1.95	0.48
1:C:21:HIS:HB2	1:C:158:THR:HG21	1.94	0.48
1:C:102:PRO:HB3	1:C:191:GLN:HE22	1.78	0.48
1:C:287:ASP:OD1	1:C:287:ASP:N	2.46	0.48
2:F:4:PRO:HD3	2:F:68:ARG:HD2	1.94	0.48
3:L:313:PRO:HG2	3:L:317:PHE:CZ	2.48	0.48
2:D:201:ARG:NH1	2:D:202:GLU:O	2.47	0.48
2:E:80:ASP:HB3	2:E:172:LEU:HB3	1.94	0.48
2:G:104:GLN:NE2	2:G:110:ILE:H	2.12	0.48
2:G:153:TYR:HB2	2:I:70:LEU:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:121:ASP:O	3:J:123:ASP:N	2.47	0.48
3:J:589:GLY:HA3	3:L:136:THR:HB	1.94	0.48
3:J:623:ASP:OD1	3:L:100:LEU:HD23	2.12	0.48
3:J:824:SER:O	3:J:825:SER:C	2.55	0.48
3:K:761:LEU:O	3:K:763:TRP:N	2.46	0.48
3:L:664:VAL:HB	3:L:668:PHE:HD2	1.78	0.48
1:A:49:ASN:HD22	1:B:218:MET:HB3	1.75	0.48
3:K:531:LEU:HD21	3:K:544:ILE:HD11	1.95	0.48
3:L:185:ASN:OD1	3:L:186:GLY:N	2.47	0.48
3:L:269:GLY:O	3:L:439:GLY:N	2.47	0.48
2:F:2:ARG:HH11	2:F:2:ARG:HG2	1.77	0.48
2:H:26:ASP:OD1	2:H:46:GLN:HG3	2.14	0.48
2:H:48:TRP:CZ2	2:H:137:LYS:HG3	2.49	0.48
2:I:110:ILE:HD12	2:I:149:ASN:OD1	2.14	0.48
3:J:660:LEU:HB2	3:J:708:LEU:HB2	1.96	0.48
3:K:325:ARG:HD3	3:K:735:ASN:ND2	2.27	0.48
3:L:129:LEU:HB2	3:L:556:SER:O	2.13	0.48
3:J:109:ALA:HB1	3:J:116:ASN:OD1	2.13	0.48
3:J:597:GLN:HG3	3:J:613:THR:HG22	1.95	0.48
3:J:763:TRP:NE1	3:J:798:MET:SD	2.86	0.48
3:K:282:THR:HG22	3:K:290:VAL:HG22	1.95	0.48
3:K:464:LEU:HD11	3:K:541:VAL:HG13	1.94	0.48
1:A:267:ARG:NH1	1:A:277:GLU:OE1	2.46	0.48
2:D:90:ARG:O	2:D:92:ARG:N	2.47	0.48
2:E:111:LEU:H	2:E:111:LEU:HD23	1.78	0.48
2:F:120:GLN:HG3	2:F:141:PHE:CE1	2.49	0.48
2:I:111:LEU:HD23	2:I:111:LEU:H	1.78	0.48
3:J:506:GLN:O	3:J:506:GLN:HG3	2.13	0.48
3:J:595:SER:O	3:J:630:LEU:N	2.46	0.48
3:K:4:ILE:HD12	3:K:4:ILE:HA	1.73	0.48
3:K:341:LEU:HD21	3:K:359:TYR:HB2	1.96	0.48
1:A:56:ASN:O	1:A:207:ILE:HA	2.14	0.48
2:D:158:ILE:HG12	2:D:159:THR:O	2.13	0.48
3:J:660:LEU:HD13	3:J:691:PHE:CE2	2.49	0.48
3:K:272:LYS:HD2	3:K:308:TYR:CE2	2.48	0.48
3:L:120:VAL:HG13	3:L:123:ASP:HB3	1.96	0.48
3:L:679:PHE:CE2	3:L:681:TYR:HB2	2.48	0.48
3:L:697:GLU:HB3	3:L:705:ASN:HB2	1.95	0.48
1:B:132:ASP:O	1:B:134:SER:N	2.47	0.48
3:J:664:VAL:HB	3:J:668:PHE:HD2	1.78	0.48
3:L:426:ASN:HD21	3:L:815:ARG:NE	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:127:PHE:HE1	2:D:166:PRO:HB3	1.78	0.48
2:E:1:MET:HE2	2:E:68:ARG:O	2.13	0.48
2:E:46:GLN:NE2	2:E:153:TYR:CE2	2.78	0.48
2:H:43:ILE:HG22	2:H:44:SER:N	2.29	0.48
3:J:266:VAL:HG21	3:J:473:TYR:CD2	2.48	0.48
3:J:4:ILE:O	3:J:5:LEU:HB2	2.14	0.47
3:K:539:LYS:HA	3:K:542:GLN:HG2	1.96	0.47
3:L:699:THR:HG22	3:L:701:ASP:H	1.79	0.47
1:B:174:THR:HG22	1:B:248:LEU:HG	1.95	0.47
1:C:258:THR:OG1	1:C:290:GLU:HG2	2.14	0.47
2:D:117:LEU:HB2	2:D:148:TRP:HH2	1.80	0.47
3:J:79:PHE:HZ	3:J:104:ILE:HG21	1.79	0.47
3:J:104:ILE:HD11	3:J:135:ILE:HD12	1.96	0.47
3:J:111:ILE:HG22	3:J:112:ASN:O	2.14	0.47
3:J:144:VAL:HG23	3:K:580:GLY:HA2	1.96	0.47
3:J:243:LYS:O	3:J:247:GLU:HG2	2.14	0.47
3:K:5:LEU:HD12	3:K:119:PRO:HA	1.97	0.47
3:K:173:THR:OG1	3:K:262:LYS:HB3	2.14	0.47
3:L:545:LEU:HD13	3:L:551:ALA:HA	1.96	0.47
1:B:92:PHE:CD1	1:B:290:GLU:HB3	2.49	0.47
2:G:48:TRP:CZ2	2:G:137:LYS:HG3	2.49	0.47
2:H:134:LYS:NZ	2:H:154:PRO:HB3	2.30	0.47
3:J:651:LEU:O	3:J:654:SER:OG	2.23	0.47
3:L:48:VAL:HG21	3:L:111:ILE:HD11	1.95	0.47
3:L:545:LEU:HD23	3:L:548:PHE:CZ	2.48	0.47
3:L:600:LEU:O	3:L:609:THR:HA	2.14	0.47
1:A:146:LYS:HD3	1:A:209:THR:HG21	1.95	0.47
1:B:42:ARG:HE	1:B:47:ARG:HB3	1.79	0.47
3:J:326:THR:HG23	3:J:825:SER:HB2	1.95	0.47
3:K:421:PHE:HZ	3:K:433:ILE:HD11	1.80	0.47
3:K:614:PHE:HZ	3:K:644:ARG:HG3	1.79	0.47
3:L:135:ILE:HD11	3:L:156:TRP:CE3	2.49	0.47
2:D:135:VAL:HG13	2:D:171:ILE:HD12	1.97	0.47
2:G:187:LEU:HD23	2:G:188:ASN:O	2.15	0.47
2:H:75:THR:HG22	2:H:76:GLY:N	2.29	0.47
2:H:80:ASP:HB3	2:H:172:LEU:HB3	1.96	0.47
2:H:177:LEU:HD21	2:H:198:LEU:HD22	1.96	0.47
3:J:545:LEU:HD23	3:J:548:PHE:CZ	2.50	0.47
3:L:578:THR:OG1	3:L:579:TYR:N	2.48	0.47
1:A:146:LYS:HB2	1:A:209:THR:HB	1.97	0.47
2:D:48:TRP:CZ2	2:D:137:LYS:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:77:ASP:N	2:D:77:ASP:OD1	2.46	0.47
2:F:127:PHE:HE1	2:F:166:PRO:HB3	1.80	0.47
2:G:201:ARG:NH1	2:G:202:GLU:O	2.47	0.47
3:J:279:PHE:HB3	3:J:293:VAL:HB	1.95	0.47
3:K:111:ILE:HG22	3:K:112:ASN:O	2.14	0.47
3:K:619:PHE:HB3	3:K:655:ARG:NH2	2.29	0.47
3:L:218:TYR:HB2	3:L:430:ILE:HD12	1.96	0.47
1:A:240:LEU:HA	1:A:266:LYS:HD2	1.97	0.47
1:B:267:ARG:NH1	1:B:277:GLU:OE1	2.48	0.47
2:D:25:ASN:HA	2:F:181:ASP:O	2.15	0.47
2:F:176:LYS:HG3	2:F:203:SER:HB2	1.97	0.47
2:G:50:ILE:HG22	2:G:52:ILE:HG13	1.97	0.47
2:G:126:LEU:CB	2:G:171:ILE:HD11	2.45	0.47
2:H:158:ILE:HG12	2:H:159:THR:O	2.14	0.47
3:J:79:PHE:CE1	3:J:106:ILE:HD11	2.50	0.47
3:J:539:LYS:HA	3:J:542:GLN:HG2	1.97	0.47
3:K:2:LYS:NZ	3:K:120:VAL:HG13	2.30	0.47
3:K:48:VAL:O	3:K:55:TYR:HB2	2.15	0.47
3:K:395:GLN:HE21	3:K:404:TYR:HB3	1.79	0.47
3:K:483:PRO:HD3	3:K:558:GLU:HB3	1.96	0.47
1:A:242:PRO:HG2	1:C:55:ILE:HG21	1.96	0.47
2:D:139:THR:HG21	2:F:74:ARG:HD3	1.95	0.47
2:D:204:LEU:HD11	2:E:36:GLY:HA3	1.96	0.47
3:K:66:HIS:CD2	3:K:555:LEU:HD23	2.50	0.47
3:K:69:ASN:HB3	3:K:695:GLU:HG2	1.95	0.47
3:K:100:LEU:HD23	3:L:628:LYS:HD2	1.97	0.47
3:L:558:GLU:O	3:L:560:ARG:HG3	2.14	0.47
3:L:815:ARG:HG2	3:L:826:PRO:HD3	1.97	0.47
1:A:192:GLN:N	1:A:217:GLU:O	2.48	0.47
1:B:168:SER:OG	1:B:252:ASN:OD1	2.25	0.47
1:B:198:ASP:OD1	1:B:208:TYR:OH	2.31	0.47
2:H:1:MET:HE2	2:H:1:MET:HB3	1.69	0.47
2:H:77:ASP:OD1	2:H:77:ASP:N	2.45	0.47
3:J:18:LEU:HD23	3:J:18:LEU:H	1.80	0.47
3:J:46:ARG:O	3:J:57:SER:OG	2.33	0.47
3:J:596:VAL:HG12	3:J:614:PHE:HD2	1.80	0.47
3:K:100:LEU:HD22	3:L:623:ASP:OD2	2.14	0.47
3:L:282:THR:HG22	3:L:290:VAL:HG22	1.96	0.47
1:A:100:ILE:HD12	1:A:100:ILE:H	1.80	0.47
2:D:126:LEU:CB	2:D:171:ILE:HD11	2.44	0.47
3:J:59:LYS:HB3	3:J:81:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:610:ASN:OD1	3:J:611:SER:N	2.47	0.47
3:L:81:ILE:HD12	3:L:156:TRP:HD1	1.80	0.47
1:B:56:ASN:O	1:B:207:ILE:HA	2.15	0.46
2:D:43:ILE:O	2:D:44:SER:OG	2.28	0.46
2:D:104:GLN:HE22	2:D:110:ILE:HB	1.80	0.46
3:K:421:PHE:CZ	3:K:433:ILE:HD11	2.49	0.46
3:L:240:TYR:HB3	3:L:245:TYR:HB2	1.97	0.46
2:I:3:LEU:HB2	2:I:79:LEU:HD22	1.97	0.46
2:I:134:LYS:HG2	2:I:135:VAL:H	1.79	0.46
3:J:313:PRO:HG2	3:J:317:PHE:CE2	2.50	0.46
3:J:549:GLY:O	3:J:563:VAL:HG23	2.15	0.46
1:A:49:ASN:ND2	1:B:218:MET:HE2	2.30	0.46
1:B:287:ASP:O	1:B:288:PRO:C	2.56	0.46
2:G:129:LEU:HD22	2:G:164:GLU:HB3	1.97	0.46
3:J:44:TYR:CG	3:J:45:PHE:N	2.83	0.46
3:K:313:PRO:HG2	3:K:317:PHE:CE2	2.51	0.46
2:D:104:GLN:NE2	2:D:110:ILE:H	2.14	0.46
2:H:111:LEU:HD21	2:H:150:ILE:HD12	1.97	0.46
3:J:798:MET:SD	3:J:798:MET:N	2.87	0.46
3:L:11:TYR:CG	3:L:117:ILE:HD13	2.50	0.46
3:L:411:LEU:HD12	3:L:416:TYR:CG	2.50	0.46
2:F:17:PHE:HE1	2:F:52:ILE:HD13	1.79	0.46
2:G:134:LYS:HG3	2:G:202:GLU:OE1	2.15	0.46
3:J:135:ILE:HD11	3:J:156:TRP:CE3	2.50	0.46
3:J:228:GLN:HA	3:J:252:GLU:HA	1.97	0.46
3:L:188:LEU:O	3:L:190:PRO:HD3	2.16	0.46
3:L:714:ASP:O	3:L:717:ILE:HG22	2.15	0.46
1:A:131:LEU:HD13	1:A:187:MET:HE1	1.98	0.46
2:D:62:TYR:HE1	2:D:196:ILE:HG21	1.80	0.46
2:F:142:SER:OG	2:F:149:ASN:OD1	2.25	0.46
3:K:645:SER:HB3	3:K:721:GLN:NE2	2.31	0.46
3:L:277:PRO:HG3	3:L:294:TYR:HE1	1.80	0.46
3:L:575:PHE:HE1	3:L:582:LEU:HB2	1.80	0.46
2:E:181:ASP:O	2:H:25:ASN:HA	2.15	0.46
2:F:50:ILE:HG22	2:F:52:ILE:HG13	1.96	0.46
2:H:185:SER:N	2:I:21:ASN:OD1	2.48	0.46
3:J:120:VAL:CG1	3:J:123:ASP:HB3	2.45	0.46
3:J:586:ASP:OD1	3:J:658:ARG:HG2	2.16	0.46
3:J:677:ILE:HD11	3:J:708:LEU:HD11	1.97	0.46
3:K:211:SER:OG	3:K:277:PRO:O	2.27	0.46
3:L:301:ILE:HG21	3:L:437:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:652:LYS:NZ	3:L:714:ASP:O	2.42	0.46
3:L:692:LEU:HD22	3:L:711:TYR:CD2	2.51	0.46
1:C:201:ILE:HG12	2:G:187:LEU:HD22	1.98	0.46
2:F:187:LEU:HD13	2:F:193:TYR:CE1	2.50	0.46
2:H:46:GLN:H	2:H:157:PHE:HZ	1.64	0.46
2:I:3:LEU:HD12	2:I:79:LEU:HD13	1.98	0.46
3:J:294:TYR:O	3:J:416:TYR:HA	2.15	0.46
3:K:53:ILE:H	3:K:53:ILE:HD12	1.81	0.46
3:L:660:LEU:HD21	3:L:686:TRP:HZ3	1.79	0.46
1:A:2:PHE:HD2	1:B:231:ARG:HG2	1.81	0.46
1:A:191:GLN:HG2	1:A:193:CYS:SG	2.56	0.46
1:B:179:LEU:HB3	1:B:226:PHE:HE2	1.80	0.46
1:C:201:ILE:O	1:C:204:ILE:HG12	2.16	0.46
2:E:91:VAL:HG22	2:E:121:PRO:HG3	1.98	0.46
3:J:101:ASP:O	3:J:102:ARG:HB2	2.16	0.46
3:J:221:LYS:HA	3:J:224:ARG:HH11	1.80	0.46
3:K:228:GLN:HA	3:K:252:GLU:HA	1.98	0.46
3:K:279:PHE:HD2	3:K:293:VAL:HG23	1.80	0.46
3:K:294:TYR:CE2	3:K:433:ILE:HD12	2.49	0.46
3:L:220:VAL:C	3:L:224:ARG:HH21	2.24	0.46
2:F:48:TRP:HB2	2:F:202:GLU:OE1	2.16	0.46
2:H:90:ARG:O	2:H:92:ARG:N	2.49	0.46
3:J:612:ILE:HG12	3:J:640:TYR:CE2	2.50	0.46
3:J:786:ILE:HD11	3:K:790:LEU:HD22	1.97	0.46
3:L:4:ILE:O	3:L:8:ALA:HB3	2.15	0.46
3:L:88:GLU:HA	3:L:91:LYS:HZ1	1.80	0.46
3:L:539:LYS:HA	3:L:542:GLN:HG2	1.97	0.46
2:E:140:ASN:OD1	2:E:141:PHE:N	2.48	0.45
2:F:17:PHE:HD1	2:F:52:ILE:HG23	1.81	0.45
2:F:112:ASN:HA	2:F:147:VAL:HA	1.98	0.45
2:G:54:TYR:HE2	2:G:65:LEU:HD21	1.80	0.45
2:I:2:ARG:H	2:I:80:ASP:HB2	1.81	0.45
2:I:112:ASN:HA	2:I:147:VAL:HA	1.97	0.45
3:K:28:LEU:HD23	3:K:28:LEU:HA	1.80	0.45
3:K:129:LEU:HB2	3:K:556:SER:O	2.16	0.45
3:L:458:LEU:HD13	3:L:459:ASN:H	1.81	0.45
2:I:140:ASN:OD1	2:I:141:PHE:N	2.49	0.45
3:J:298:GLU:HG2	3:J:472:ARG:NH2	2.31	0.45
3:J:426:ASN:HD21	3:J:815:ARG:NE	2.14	0.45
3:K:220:VAL:HG12	3:K:222:GLU:H	1.82	0.45
3:K:610:ASN:OD1	3:K:611:SER:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:72:LEU:HD12	3:L:72:LEU:O	2.17	0.45
3:L:509:TRP:CZ3	3:L:517:PRO:HD3	2.51	0.45
3:L:673:PRO:HA	3:L:693:VAL:HG23	1.98	0.45
2:D:75:THR:HG22	2:D:76:GLY:N	2.31	0.45
3:J:140:ILE:HG13	3:K:684:TYR:CE1	2.52	0.45
3:J:355:GLN:HA	3:J:357:TYR:CE1	2.52	0.45
3:J:580:GLY:HA2	3:L:144:VAL:HG23	1.98	0.45
3:K:441:LYS:O	3:K:441:LYS:HG3	2.16	0.45
3:L:271:GLN:HG2	3:L:530:ILE:CD1	2.46	0.45
1:C:79:PHE:HB3	1:C:84:PHE:CD2	2.52	0.45
2:H:126:LEU:CB	2:H:171:ILE:HD11	2.46	0.45
3:J:101:ASP:CG	3:J:102:ARG:H	2.24	0.45
3:J:271:GLN:HG3	3:J:272:LYS:N	2.30	0.45
3:J:603:PRO:HG3	3:J:607:TRP:CZ3	2.51	0.45
3:L:6:ASP:OD1	3:L:7:SER:N	2.49	0.45
1:A:92:PHE:CD1	1:A:290:GLU:HG2	2.52	0.45
1:B:196:ARG:HD2	2:E:56:GLU:O	2.16	0.45
2:F:106:GLY:HA3	3:J:114:GLU:HG3	1.99	0.45
2:F:128:LYS:HE2	2:F:171:ILE:HG22	1.97	0.45
3:K:180:GLY:HA2	3:L:615:TYR:CD1	2.51	0.45
3:K:395:GLN:O	3:K:399:GLY:N	2.39	0.45
3:L:110:ILE:HD11	3:L:666:TYR:HE2	1.81	0.45
2:I:158:ILE:HG12	2:I:159:THR:O	2.17	0.45
3:K:46:ARG:O	3:K:57:SER:OG	2.34	0.45
3:K:317:PHE:O	3:K:321:ASP:HB2	2.16	0.45
3:K:494:LEU:HD21	3:K:563:VAL:HG11	1.98	0.45
3:K:566:TYR:HB2	3:K:716:PHE:CD2	2.51	0.45
3:L:412:LEU:HA	3:L:412:LEU:HD23	1.77	0.45
3:L:560:ARG:HE	3:L:672:GLU:CD	2.23	0.45
3:L:586:ASP:OD1	3:L:658:ARG:HG2	2.17	0.45
3:L:771:VAL:HG13	3:L:789:GLN:NE2	2.31	0.45
2:H:90:ARG:NH2	2:H:125:ASP:OD1	2.36	0.45
3:J:268:TYR:HA	3:J:439:GLY:HA2	1.97	0.45
3:K:277:PRO:HG3	3:K:294:TYR:HE1	1.82	0.45
3:L:294:TYR:CE2	3:L:433:ILE:HD12	2.50	0.45
1:A:93:LEU:HD13	1:A:220:ALA:HB2	1.98	0.45
1:B:65:LEU:HD23	1:B:67:ILE:HD11	1.98	0.45
1:C:196:ARG:HD2	2:F:56:GLU:O	2.17	0.45
1:C:201:ILE:HG23	2:G:187:LEU:HD22	1.99	0.45
2:F:36:GLY:HA3	2:G:204:LEU:HD11	1.99	0.45
2:G:22:LEU:HD23	2:G:50:ILE:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:136:TYR:CG	2:H:152:LEU:HD13	2.52	0.45
2:H:175:THR:OG1	2:H:200:LEU:HD23	2.17	0.45
3:J:592:LYS:HG3	3:L:100:LEU:HD21	1.98	0.45
1:A:252:ASN:C	1:A:254:TYR:H	2.24	0.45
1:C:57:ALA:HB2	1:C:208:TYR:HB3	1.99	0.45
2:I:134:LYS:HD3	2:I:204:LEU:HD22	1.99	0.45
3:K:586:ASP:OD1	3:K:658:ARG:HG2	2.17	0.45
3:K:600:LEU:O	3:K:609:THR:HA	2.17	0.45
3:L:588:THR:OG1	3:L:592:LYS:HD2	2.17	0.45
1:B:63:ILE:HD11	1:B:119:PHE:CZ	2.52	0.45
3:J:69:ASN:HB3	3:J:695:GLU:HG2	1.98	0.45
3:J:304:PHE:HB3	3:J:307:PHE:HE1	1.82	0.45
3:J:553:ASN:OD1	3:J:553:ASN:O	2.35	0.45
3:K:140:ILE:CD1	3:K:154:ILE:HG12	2.47	0.45
3:K:655:ARG:O	3:K:655:ARG:HD3	2.17	0.45
3:K:714:ASP:O	3:K:717:ILE:HG22	2.17	0.45
3:L:118:LEU:HA	3:L:125:ASP:O	2.17	0.45
3:L:230:LYS:HD3	3:L:265:PRO:HG3	1.98	0.45
3:L:501:TYR:HB2	3:L:505:TRP:HE1	1.83	0.45
1:C:19:GLY:HA3	1:C:154:ARG:NH2	2.32	0.44
2:G:1:MET:HB3	2:G:1:MET:HE2	1.69	0.44
2:G:158:ILE:HG12	2:G:159:THR:O	2.17	0.44
2:I:2:ARG:HD3	2:I:172:LEU:HD21	1.99	0.44
3:J:271:GLN:HG2	3:J:530:ILE:HD11	1.98	0.44
3:J:578:THR:O	3:J:579:TYR:CD1	2.70	0.44
3:K:672:GLU:O	3:K:674:ASN:N	2.50	0.44
3:L:578:THR:O	3:L:579:TYR:CD1	2.70	0.44
2:D:26:ASP:OD1	2:D:46:GLN:HG3	2.17	0.44
2:D:117:LEU:HD12	2:D:148:TRP:HZ2	1.81	0.44
2:E:126:LEU:HD23	2:E:137:LYS:HG2	1.99	0.44
2:F:158:ILE:HG12	2:F:159:THR:O	2.17	0.44
3:J:24:ILE:HD11	3:J:63:ILE:HD11	1.99	0.44
3:J:28:LEU:HD11	3:J:39:ILE:HG12	1.98	0.44
3:J:183:VAL:HG12	3:J:183:VAL:O	2.17	0.44
3:J:256:ASP:OD2	3:K:608:LYS:HE3	2.17	0.44
3:L:54:LEU:HD23	3:L:54:LEU:H	1.83	0.44
3:L:694:ASP:OD2	3:L:709:GLN:HB2	2.17	0.44
1:B:93:LEU:HD13	1:B:220:ALA:HB2	1.98	0.44
2:G:12:TYR:HB3	2:G:61:GLU:HG2	1.99	0.44
2:G:90:ARG:O	2:G:92:ARG:N	2.51	0.44
2:H:3:LEU:HD21	2:H:54:TYR:OH	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:90:ARG:HH21	2:I:125:ASP:CG	2.25	0.44
2:I:92:ARG:HG3	2:I:92:ARG:HH11	1.82	0.44
3:J:288:ASN:OD1	3:J:289:ILE:N	2.51	0.44
3:K:109:ALA:HB1	3:K:116:ASN:OD1	2.17	0.44
3:L:355:GLN:HA	3:L:357:TYR:CE1	2.52	0.44
1:B:196:ARG:NH1	2:E:61:GLU:OE1	2.50	0.44
2:G:38:VAL:HG23	2:I:201:ARG:NH1	2.32	0.44
2:H:203:SER:OG	2:I:38:VAL:HG22	2.17	0.44
3:K:59:LYS:HB3	3:K:81:ILE:HG23	1.98	0.44
3:K:144:VAL:HG23	3:L:580:GLY:HA2	1.99	0.44
3:K:196:ARG:HG2	3:K:199:TYR:HD2	1.83	0.44
3:K:271:GLN:HG3	3:K:272:LYS:N	2.33	0.44
3:K:421:PHE:CZ	3:K:430:ILE:HG23	2.52	0.44
3:L:304:PHE:CZ	3:L:415:ALA:HB1	2.53	0.44
2:I:27:PRO:HD2	2:I:45:ALA:O	2.18	0.44
3:J:740:ARG:HD3	3:J:767:LEU:HD21	2.00	0.44
3:K:1:MET:SD	3:K:571:LEU:HD11	2.58	0.44
3:K:362:GLY:HA3	3:K:826:PRO:HG2	1.99	0.44
3:L:196:ARG:HD3	3:L:199:TYR:CE1	2.53	0.44
2:D:127:PHE:N	2:D:136:TYR:O	2.35	0.44
2:F:60:ASP:OD1	2:F:61:GLU:N	2.50	0.44
2:F:90:ARG:O	2:F:92:ARG:N	2.50	0.44
2:F:113:THR:HG21	2:F:117:LEU:HD12	2.00	0.44
3:J:595:SER:HB3	3:J:614:PHE:O	2.18	0.44
3:K:66:HIS:NE2	3:K:554:ASN:O	2.48	0.44
3:K:687:LYS:O	3:K:688:ASP:C	2.61	0.44
3:L:120:VAL:CG1	3:L:123:ASP:HB3	2.47	0.44
3:L:600:LEU:HD21	3:L:643:ALA:HB3	1.98	0.44
1:B:40:LEU:HD12	1:B:51:ALA:HB2	1.99	0.44
1:C:243:GLU:OE1	1:C:246:THR:HG21	2.18	0.44
1:C:272:ASP:O	1:C:273:LEU:HB2	2.18	0.44
2:D:43:ILE:HG22	2:D:44:SER:N	2.31	0.44
2:H:3:LEU:HD12	2:H:79:LEU:HD13	1.98	0.44
3:J:92:LEU:HD21	3:J:139:GLY:HA2	2.00	0.44
3:J:309:ILE:HD13	3:J:359:TYR:HE2	1.81	0.44
3:J:494:LEU:HD11	3:J:563:VAL:HG21	1.99	0.44
3:K:592:LYS:HB2	3:K:592:LYS:HE3	1.75	0.44
3:L:325:ARG:HD3	3:L:735:ASN:ND2	2.33	0.44
1:A:13:ILE:HD11	1:A:107:MET:HE2	1.99	0.44
1:A:14:GLU:O	1:A:105:PHE:HB2	2.18	0.44
1:C:95:ARG:NH1	1:C:286:SER:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:300:GLU:H	3:J:373:GLY:CA	2.30	0.44
3:J:381:GLN:O	3:J:385:ASP:HB2	2.17	0.44
3:K:266:VAL:HG21	3:K:473:TYR:CD2	2.53	0.44
3:L:10:ASN:O	3:L:14:THR:HG23	2.18	0.44
3:L:829:LEU:HB3	3:L:831:VAL:HG13	2.00	0.44
1:A:49:ASN:HD21	1:B:218:MET:HE2	1.83	0.44
2:F:139:THR:OG1	2:G:71:GLU:HB2	2.18	0.44
2:I:9:ASN:HB2	2:I:11:GLU:OE1	2.18	0.44
3:J:26:LEU:HD12	3:J:104:ILE:HG12	2.00	0.44
3:J:693:VAL:HA	3:J:708:LEU:HD23	1.99	0.44
3:K:332:LYS:HG2	3:K:507:PRO:HB3	1.99	0.44
3:K:514:TRP:HZ3	3:K:526:GLN:HE22	1.65	0.44
3:K:679:PHE:CE2	3:K:681:TYR:HB2	2.53	0.44
3:L:271:GLN:HG3	3:L:272:LYS:N	2.33	0.44
1:A:43:THR:HG1	1:A:46:ASN:H	1.60	0.43
2:D:121:PRO:HD2	2:D:141:PHE:CE1	2.53	0.43
2:I:90:ARG:O	2:I:92:ARG:N	2.51	0.43
3:J:1:MET:SD	3:J:571:LEU:HD11	2.58	0.43
3:J:173:THR:OG1	3:J:262:LYS:HB3	2.18	0.43
3:J:357:TYR:HB3	3:J:358:LYS:H	1.64	0.43
3:K:195:LYS:O	3:K:199:TYR:HD2	2.00	0.43
3:K:219:GLN:O	3:K:224:ARG:NH2	2.51	0.43
3:L:172:TYR:HA	3:L:263:PHE:HA	2.00	0.43
3:L:771:VAL:HG13	3:L:789:GLN:HE22	1.83	0.43
1:B:45:HIS:NE2	2:D:5:ASP:OD2	2.51	0.43
1:B:243:GLU:OE1	1:B:246:THR:HG21	2.18	0.43
2:D:117:LEU:HD12	2:D:148:TRP:CZ2	2.53	0.43
2:I:109:ILE:HD13	2:I:129:LEU:HD21	2.00	0.43
3:J:290:VAL:HG21	3:J:430:ILE:HD11	1.99	0.43
3:K:439:GLY:HA3	3:K:457:SER:CB	2.48	0.43
3:K:817:VAL:HG22	3:K:823:ARG:HG2	1.99	0.43
3:L:24:ILE:HD11	3:L:63:ILE:HD11	1.99	0.43
3:L:593:PHE:HD1	3:L:628:LYS:HG2	1.82	0.43
1:A:196:ARG:HD2	2:I:56:GLU:O	2.17	0.43
1:C:192:GLN:N	1:C:217:GLU:O	2.50	0.43
2:F:80:ASP:HB3	2:F:172:LEU:HD23	1.99	0.43
2:G:139:THR:HG21	2:I:74:ARG:HD3	1.99	0.43
3:K:760:GLU:CD	3:K:802:ILE:HD11	2.44	0.43
3:L:27:GLU:HG2	3:L:102:ARG:HG2	1.99	0.43
3:L:762:SER:HA	3:L:797:ARG:HE	1.83	0.43
1:A:201:ILE:HD12	2:I:17:PHE:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:HIS:HB2	1:B:158:THR:HG21	2.01	0.43
1:B:119:PHE:HB3	1:B:144:SER:HB2	2.01	0.43
1:B:253:LYS:O	1:B:253:LYS:HG2	2.18	0.43
1:B:263:ARG:HH22	1:B:281:ILE:HD12	1.83	0.43
2:E:54:TYR:HB2	2:E:196:ILE:O	2.17	0.43
2:G:3:LEU:HD12	2:G:79:LEU:HD13	2.00	0.43
3:J:160:ASN:OD1	3:J:161:GLN:N	2.48	0.43
3:J:483:PRO:HD3	3:J:558:GLU:HB3	1.99	0.43
3:K:68:GLN:NE2	3:K:553:ASN:HA	2.33	0.43
3:K:525:VAL:HG11	3:K:548:PHE:HB2	2.00	0.43
3:L:230:LYS:NZ	3:L:261:ALA:O	2.48	0.43
3:L:620:LYS:NZ	3:L:627:ASP:OD1	2.45	0.43
2:D:2:ARG:HA	2:D:80:ASP:O	2.17	0.43
2:D:9:ASN:HB2	2:D:11:GLU:OE1	2.18	0.43
2:D:35:ASN:ND2	2:D:37:LYS:HG3	2.33	0.43
2:D:127:PHE:CE1	2:D:166:PRO:HB3	2.53	0.43
2:H:30:ARG:HG2	2:H:40:GLU:HG2	2.01	0.43
3:K:113:GLU:HB3	3:K:114:GLU:OE1	2.18	0.43
3:L:120:VAL:HG13	3:L:120:VAL:O	2.19	0.43
3:L:492:LYS:HE2	3:L:492:LYS:HB2	1.87	0.43
3:L:563:VAL:HG22	3:L:564:GLU:N	2.33	0.43
1:A:222:ALA:HB3	1:A:280:VAL:HB	2.01	0.43
1:B:11:ILE:HD11	1:B:28:TYR:CG	2.53	0.43
1:B:183:ILE:HD11	1:B:227:TYR:CD1	2.54	0.43
2:D:83:LEU:HD23	2:D:83:LEU:HA	1.85	0.43
2:I:60:ASP:OD1	2:I:61:GLU:N	2.51	0.43
3:J:196:ARG:HE	3:J:198:GLU:HB2	1.84	0.43
3:K:172:TYR:HA	3:K:263:PHE:HA	1.99	0.43
3:K:761:LEU:HB3	3:K:799:ILE:HA	1.99	0.43
3:K:786:ILE:HD11	3:L:790:LEU:HD11	2.01	0.43
3:L:109:ALA:HB1	3:L:116:ASN:OD1	2.19	0.43
3:L:332:LYS:O	3:L:333:ILE:HB	2.18	0.43
1:B:123:TYR:CE1	1:B:193:CYS:HB2	2.54	0.43
2:D:187:LEU:HD23	2:D:188:ASN:O	2.19	0.43
2:G:17:PHE:HD1	2:G:54:TYR:HE1	1.67	0.43
2:H:98:VAL:HG22	2:H:113:THR:HG22	2.00	0.43
3:J:89:VAL:HG23	3:J:140:ILE:HD11	2.01	0.43
3:J:195:LYS:HD3	3:J:472:ARG:HA	2.01	0.43
3:K:160:ASN:OD1	3:K:161:GLN:N	2.47	0.43
3:L:421:PHE:CZ	3:L:430:ILE:HG23	2.53	0.43
1:A:124:VAL:O	1:A:191:GLN:NE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ARG:NH1	1:A:279:ASP:OD2	2.50	0.43
1:B:2:PHE:HD2	1:C:231:ARG:HG2	1.83	0.43
2:D:50:ILE:HG22	2:D:52:ILE:HG13	1.99	0.43
3:J:699:THR:HG22	3:J:701:ASP:H	1.84	0.43
3:J:717:ILE:O	3:J:718:ASN:OD1	2.37	0.43
3:J:761:LEU:C	3:J:763:TRP:H	2.26	0.43
3:K:79:PHE:CE1	3:K:106:ILE:HD11	2.53	0.43
3:K:592:LYS:HD3	3:K:655:ARG:HD3	1.99	0.43
3:L:21:ALA:HB2	3:L:44:TYR:CD1	2.53	0.43
3:L:288:ASN:OD1	3:L:289:ILE:N	2.50	0.43
3:L:465:MET:CE	3:L:487:VAL:HG11	2.49	0.43
1:A:233:VAL:HG12	1:A:237:PHE:HA	2.01	0.43
1:C:211:LYS:HB2	1:C:211:LYS:HE2	1.79	0.43
1:C:252:ASN:C	1:C:254:TYR:H	2.27	0.43
2:E:70:LEU:HD13	2:H:153:TYR:HB2	2.01	0.43
2:G:52:ILE:N	2:G:198:LEU:O	2.51	0.43
2:H:90:ARG:HH21	2:H:125:ASP:CG	2.23	0.43
3:J:3:LYS:O	3:J:4:ILE:HB	2.18	0.43
3:J:602:ASP:HB3	3:J:605:LEU:HD13	2.00	0.43
3:J:687:LYS:O	3:J:688:ASP:C	2.61	0.43
3:L:118:LEU:N	3:L:119:PRO:HD3	2.34	0.43
3:L:336:ASP:HA	3:L:347:THR:O	2.19	0.43
3:L:594:ASN:O	3:L:651:LEU:HD11	2.19	0.43
1:A:183:ILE:HD11	1:A:227:TYR:CE1	2.54	0.43
1:B:192:GLN:N	1:B:217:GLU:O	2.52	0.43
1:C:63:ILE:HG23	1:C:142:ILE:HB	2.01	0.43
1:C:102:PRO:HB3	1:C:191:GLN:NE2	2.34	0.43
2:E:79:LEU:N	2:E:175:THR:O	2.52	0.43
2:G:134:LYS:NZ	2:G:154:PRO:HB3	2.34	0.43
3:J:185:ASN:OD1	3:J:186:GLY:N	2.52	0.43
3:J:779:SER:HG	3:J:811:ILE:H	1.65	0.43
3:K:742:PHE:CZ	3:K:814:LEU:HD11	2.54	0.43
3:L:687:LYS:O	3:L:688:ASP:C	2.61	0.43
1:B:201:ILE:HD13	2:E:17:PHE:HB2	2.00	0.42
1:C:41:ARG:HH12	2:G:61:GLU:CD	2.26	0.42
2:D:21:ASN:HB3	2:D:51:ASN:HB2	2.01	0.42
2:E:2:ARG:O	2:E:68:ARG:NH1	2.52	0.42
2:F:94:ASP:OD1	2:F:95:THR:N	2.52	0.42
3:J:789:GLN:OE1	3:J:798:MET:HE2	2.19	0.42
3:K:486:LYS:HE3	3:K:560:ARG:HH22	1.83	0.42
3:K:516:ASP:HA	3:K:517:PRO:HD2	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:298:GLU:HB3	3:L:472:ARG:NH2	2.34	0.42
3:L:426:ASN:HA	3:L:823:ARG:HD3	2.00	0.42
2:E:11:GLU:H	2:E:11:GLU:CD	2.27	0.42
2:E:112:ASN:HA	2:E:147:VAL:HA	2.01	0.42
2:F:90:ARG:HH21	2:F:125:ASP:CG	2.28	0.42
3:J:11:TYR:CG	3:J:117:ILE:HD13	2.54	0.42
3:J:240:TYR:HB3	3:J:245:TYR:HB2	2.01	0.42
3:J:458:LEU:HD23	3:J:458:LEU:HA	1.85	0.42
3:J:509:TRP:CZ3	3:J:517:PRO:HD3	2.54	0.42
3:J:628:LYS:NZ	3:L:164:ASP:OD2	2.53	0.42
3:J:675:ASP:HA	3:J:676:PRO:HD3	1.88	0.42
2:E:15:LEU:O	2:E:54:TYR:HE1	2.02	0.42
2:E:60:ASP:OD1	2:E:61:GLU:N	2.49	0.42
2:F:21:ASN:OD1	2:G:185:SER:N	2.52	0.42
2:H:75:THR:HG22	2:H:76:GLY:H	1.84	0.42
2:I:109:ILE:HD12	2:I:127:PHE:HE2	1.85	0.42
3:J:10:ASN:O	3:J:14:THR:HG23	2.19	0.42
3:J:532:ASP:OD1	3:J:532:ASP:N	2.53	0.42
3:J:554:ASN:HA	3:J:558:GLU:O	2.19	0.42
3:K:279:PHE:HB3	3:K:293:VAL:HB	2.01	0.42
3:L:106:ILE:O	3:L:130:PHE:N	2.51	0.42
3:L:676:PRO:HB3	3:L:690:PHE:CE1	2.54	0.42
3:L:690:PHE:HD2	3:L:711:TYR:O	2.02	0.42
2:E:92:ARG:HG3	2:E:93:GLY:N	2.35	0.42
2:E:127:PHE:CE1	2:E:166:PRO:HB3	2.53	0.42
2:E:136:TYR:CD1	2:E:154:PRO:HB2	2.53	0.42
3:J:100:LEU:HD22	3:K:623:ASP:OD2	2.19	0.42
3:J:600:LEU:O	3:J:609:THR:HA	2.19	0.42
3:K:583:ASP:HB2	3:K:661:SER:HB2	2.02	0.42
1:A:264:ILE:HG12	1:A:280:VAL:HG22	2.01	0.42
1:B:229:VAL:HG23	1:B:229:VAL:O	2.19	0.42
2:F:85:GLN:OE1	2:G:193:TYR:OH	2.32	0.42
2:G:127:PHE:HE1	2:G:166:PRO:HB3	1.84	0.42
3:J:72:LEU:HD12	3:J:72:LEU:O	2.19	0.42
3:J:588:THR:O	3:J:592:LYS:HG2	2.20	0.42
3:L:230:LYS:HE2	3:L:276:ILE:HD11	2.00	0.42
3:L:772:VAL:HG13	3:L:773:TYR:CD1	2.55	0.42
1:A:243:GLU:OE2	1:A:246:THR:HG21	2.19	0.42
1:B:14:GLU:OE2	1:B:154:ARG:NE	2.38	0.42
1:C:65:LEU:HB2	1:C:140:VAL:HG13	2.01	0.42
2:G:3:LEU:HD21	2:G:54:TYR:OH	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:23:VAL:N	2:H:49:GLY:O	2.46	0.42
3:J:502:GLN:H	3:J:505:TRP:NE1	2.17	0.42
3:K:284:LEU:C	3:K:286:ASN:H	2.26	0.42
3:K:740:ARG:NH2	3:K:764:LEU:HD13	2.34	0.42
3:L:395:GLN:NE2	3:L:404:TYR:HB3	2.34	0.42
3:L:740:ARG:HD3	3:L:767:LEU:HD21	2.00	0.42
1:A:202:PHE:CE2	2:I:6:PRO:HD2	2.55	0.42
2:G:122:LYS:HE2	2:G:122:LYS:HB2	1.84	0.42
2:H:91:VAL:HG22	2:H:121:PRO:HG3	2.02	0.42
3:J:136:THR:HG21	3:J:163:TYR:CD2	2.55	0.42
3:J:230:LYS:NZ	3:J:261:ALA:HA	2.34	0.42
3:K:294:TYR:O	3:K:416:TYR:HA	2.19	0.42
3:K:509:TRP:HB2	3:K:514:TRP:HE1	1.84	0.42
3:L:123:ASP:O	3:L:124:THR:C	2.62	0.42
3:L:763:TRP:HZ2	3:L:787:VAL:HG11	1.83	0.42
1:A:11:ILE:HD11	1:A:28:TYR:CG	2.55	0.42
1:B:61:SER:OG	1:B:144:SER:OG	2.34	0.42
2:F:44:SER:O	3:J:45:PHE:HB3	2.20	0.42
2:G:2:ARG:H	2:G:80:ASP:HB2	1.83	0.42
2:G:91:VAL:HG22	2:G:121:PRO:HG3	2.02	0.42
3:J:2:LYS:NZ	3:J:120:VAL:HG13	2.35	0.42
3:J:6:ASP:OD1	3:J:7:SER:N	2.53	0.42
3:J:531:LEU:HD11	3:J:544:ILE:HD11	2.01	0.42
3:K:822:ARG:O	3:K:823:ARG:HB2	2.19	0.42
3:L:281:ASP:OD2	3:L:392:PHE:HB3	2.19	0.42
3:L:587:THR:OG1	3:L:591:ASN:OD1	2.24	0.42
2:G:104:GLN:HE22	2:G:110:ILE:HB	1.85	0.42
2:G:175:THR:OG1	2:G:200:LEU:HD23	2.20	0.42
3:J:742:PHE:CE2	3:J:814:LEU:HD13	2.55	0.42
3:J:765:PRO:HG2	3:J:793:ASN:O	2.20	0.42
3:J:817:VAL:HG22	3:J:823:ARG:HE	1.85	0.42
3:K:106:ILE:O	3:K:130:PHE:N	2.49	0.42
3:K:184:VAL:O	3:K:185:ASN:OD1	2.38	0.42
2:F:11:GLU:H	2:F:11:GLU:CD	2.27	0.42
2:I:19:SER:OG	2:I:53:SER:OG	2.34	0.42
2:I:177:LEU:HD23	2:I:200:LEU:HD21	2.02	0.42
3:K:273:ILE:HD11	3:K:437:VAL:HG21	2.02	0.42
3:K:318:ASP:OD1	3:K:332:LYS:HD3	2.19	0.42
3:K:458:LEU:HD23	3:K:458:LEU:HA	1.73	0.42
3:K:532:ASP:OD1	3:K:532:ASP:N	2.51	0.42
1:B:168:SER:OG	1:B:252:ASN:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ASN:HB3	1:C:164:VAL:HG13	2.01	0.41
2:D:91:VAL:HG22	2:D:121:PRO:HG3	2.01	0.41
2:E:176:LYS:HG3	2:E:203:SER:CB	2.49	0.41
2:H:110:ILE:HG12	2:H:149:ASN:HB3	2.01	0.41
3:J:433:ILE:HD12	3:J:433:ILE:H	1.85	0.41
3:K:59:LYS:HD3	3:K:88:GLU:HG3	2.01	0.41
3:K:411:LEU:HD12	3:K:416:TYR:CG	2.55	0.41
2:E:127:PHE:N	2:E:136:TYR:O	2.36	0.41
2:F:38:VAL:HG22	2:G:203:SER:OG	2.19	0.41
2:G:164:GLU:HA	2:G:164:GLU:OE2	2.19	0.41
3:K:394:LEU:HA	3:K:397:GLN:HB3	2.02	0.41
3:L:305:LEU:O	3:L:436:GLU:HB2	2.20	0.41
3:L:520:GLU:OE1	3:L:522:ARG:N	2.51	0.41
1:B:79:PHE:HB3	1:B:84:PHE:CD2	2.55	0.41
2:D:27:PRO:HD2	2:D:45:ALA:O	2.21	0.41
2:D:113:THR:HG21	2:D:117:LEU:HG	2.02	0.41
2:H:156:LEU:HD23	2:H:156:LEU:HA	1.93	0.41
3:K:340:ARG:HG3	3:K:346:SER:HA	2.02	0.41
3:K:371:PHE:HZ	3:K:380:ALA:HB2	1.83	0.41
3:L:796:GLU:HG3	3:L:797:ARG:N	2.35	0.41
1:B:102:PRO:HB3	1:B:191:GLN:HE22	1.85	0.41
2:F:126:LEU:CB	2:F:171:ILE:HD11	2.49	0.41
2:H:66:ASP:O	2:H:70:LEU:HG	2.20	0.41
3:J:81:ILE:HG21	3:J:88:GLU:HG3	2.03	0.41
3:J:120:VAL:HG12	3:J:123:ASP:HB3	2.03	0.41
3:J:180:GLY:HA2	3:K:615:TYR:CD1	2.55	0.41
3:K:69:ASN:HB3	3:K:695:GLU:CG	2.50	0.41
3:K:72:LEU:HD12	3:K:72:LEU:O	2.20	0.41
3:K:203:TYR:HB3	3:K:408:ARG:HG2	2.02	0.41
3:K:660:LEU:HD21	3:K:686:TRP:HZ3	1.84	0.41
3:K:778:HIS:HB2	3:K:781:HIS:HB2	2.03	0.41
3:L:242:LEU:HD23	3:L:242:LEU:HA	1.92	0.41
1:A:122:CYS:SG	1:A:144:SER:HB2	2.61	0.41
2:D:2:ARG:NH1	2:D:8:THR:HG1	2.15	0.41
2:D:80:ASP:HB3	2:D:172:LEU:HB3	2.02	0.41
2:I:134:LYS:HG2	2:I:135:VAL:N	2.36	0.41
3:J:317:PHE:O	3:J:321:ASP:HB2	2.20	0.41
3:J:740:ARG:NH2	3:J:764:LEU:HD13	2.35	0.41
3:K:447:SER:O	3:K:448:ASP:HB2	2.20	0.41
3:L:532:ASP:N	3:L:532:ASP:OD1	2.52	0.41
3:L:640:TYR:OH	3:L:644:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:66:ASP:O	2:G:67:SER:C	2.61	0.41
2:H:100:ILE:HG22	2:H:160:THR:HG21	2.03	0.41
3:J:182:GLU:HG3	3:K:615:TYR:O	2.20	0.41
3:J:486:LYS:CE	3:J:560:ARG:HH22	2.32	0.41
3:K:189:GLN:NE2	3:L:722:VAL:HB	2.36	0.41
3:K:271:GLN:HG2	3:K:530:ILE:CD1	2.49	0.41
3:K:516:ASP:O	3:K:517:PRO:C	2.63	0.41
3:K:596:VAL:HG12	3:K:614:PHE:HB2	2.03	0.41
3:L:263:PHE:HB2	3:L:534:SER:HB3	2.02	0.41
1:B:224:LEU:HB3	1:B:226:PHE:CE1	2.56	0.41
1:C:108:TYR:HB3	1:C:110:ILE:HG23	2.01	0.41
1:C:229:VAL:HG23	1:C:229:VAL:O	2.20	0.41
2:I:201:ARG:HD3	2:I:202:GLU:O	2.21	0.41
3:J:660:LEU:HD21	3:J:686:TRP:HZ3	1.86	0.41
3:K:178:HIS:NE2	3:K:199:TYR:HD1	2.18	0.41
3:K:195:LYS:HG2	3:L:627:ASP:OD2	2.20	0.41
3:K:336:ASP:HA	3:K:347:THR:O	2.21	0.41
3:L:279:PHE:HD2	3:L:293:VAL:HG23	1.85	0.41
3:L:813:GLU:OE1	3:L:815:ARG:NH2	2.54	0.41
1:B:84:PHE:HA	1:B:94:PRO:HD3	2.03	0.41
1:B:291:ILE:O	1:B:291:ILE:HG23	2.21	0.41
1:B:293:PHE:HB3	1:B:294:PHE:H	1.68	0.41
2:D:79:LEU:O	2:D:175:THR:N	2.52	0.41
2:D:156:LEU:HD23	2:D:156:LEU:HA	1.91	0.41
2:F:85:GLN:HG2	2:G:187:LEU:CD1	2.51	0.41
3:J:196:ARG:HA	3:J:197:PRO:HD3	1.98	0.41
3:K:379:ALA:HB2	3:K:409:TYR:O	2.21	0.41
3:L:290:VAL:HG21	3:L:430:ILE:HD11	2.02	0.41
3:L:579:TYR:HE2	3:L:703:LYS:HE3	1.85	0.41
1:C:14:GLU:OE2	1:C:154:ARG:NE	2.41	0.41
2:D:187:LEU:HB2	2:D:193:TYR:CE1	2.54	0.41
2:F:2:ARG:O	2:F:68:ARG:NH1	2.54	0.41
2:G:23:VAL:N	2:G:49:GLY:O	2.40	0.41
2:G:25:ASN:HA	2:I:181:ASP:O	2.21	0.41
2:G:83:LEU:HD13	2:G:85:GLN:HE21	1.86	0.41
3:J:62:SER:N	3:J:80:THR:OG1	2.53	0.41
3:J:355:GLN:HA	3:J:357:TYR:HE1	1.86	0.41
3:J:499:GLU:HA	3:J:522:ARG:NH1	2.35	0.41
3:J:575:PHE:HE1	3:J:582:LEU:HB2	1.85	0.41
3:J:684:TYR:HE1	3:L:140:ILE:HG13	1.86	0.41
3:K:320:THR:HB	3:K:732:ILE:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:544:ILE:HG22	3:K:548:PHE:CE2	2.56	0.41
3:K:789:GLN:NE2	3:K:789:GLN:HA	2.36	0.41
3:L:18:LEU:HD23	3:L:18:LEU:H	1.86	0.41
3:L:268:TYR:HA	3:L:439:GLY:HA2	2.02	0.41
3:L:596:VAL:HG12	3:L:614:PHE:HB2	2.03	0.41
1:A:108:TYR:HB3	1:A:110:ILE:HG23	2.02	0.41
1:B:40:LEU:HD23	1:B:42:ARG:HG3	2.03	0.41
2:D:80:ASP:HB3	2:D:172:LEU:HD23	2.03	0.41
2:F:22:LEU:HD23	2:F:50:ILE:HG12	2.03	0.41
2:F:177:LEU:HD23	2:F:200:LEU:HD21	2.03	0.41
2:I:11:GLU:H	2:I:11:GLU:CD	2.28	0.41
3:J:118:LEU:HG	3:J:125:ASP:O	2.21	0.41
3:K:759:GLY:O	3:K:760:GLU:HB2	2.20	0.41
3:L:46:ARG:O	3:L:57:SER:OG	2.39	0.41
3:L:172:TYR:HE2	3:L:174:ASP:HB2	1.86	0.41
3:L:233:LEU:HA	3:L:249:VAL:HG11	2.03	0.41
3:L:235:GLY:N	3:L:635:ALA:HB2	2.35	0.41
1:A:40:LEU:HD23	1:A:42:ARG:HG2	2.03	0.40
1:B:19:GLY:HA3	1:B:154:ARG:NH2	2.35	0.40
2:D:23:VAL:N	2:D:49:GLY:O	2.48	0.40
2:H:22:LEU:HD23	2:H:50:ILE:HG12	2.02	0.40
2:I:77:ASP:OD1	2:I:77:ASP:C	2.64	0.40
3:J:316:CYS:SG	3:J:330:ARG:HD3	2.62	0.40
3:K:594:ASN:O	3:K:651:LEU:HD11	2.20	0.40
3:K:699:THR:HG22	3:K:701:ASP:H	1.87	0.40
3:L:113:GLU:H	3:L:113:GLU:HG2	1.76	0.40
3:L:291:TYR:CE1	3:L:420:ARG:HB2	2.56	0.40
3:L:731:ASP:OD2	3:L:734:ASN:ND2	2.54	0.40
1:C:119:PHE:HB3	1:C:144:SER:HB2	2.03	0.40
1:C:291:ILE:HG23	1:C:291:ILE:O	2.21	0.40
2:G:56:GLU:HG2	2:G:194:SER:HB3	2.02	0.40
2:G:75:THR:HG22	2:G:76:GLY:N	2.36	0.40
2:H:201:ARG:HD3	2:I:38:VAL:HG11	2.03	0.40
3:J:298:GLU:CG	3:J:299:GLY:H	2.35	0.40
3:J:652:LYS:NZ	3:J:714:ASP:O	2.39	0.40
3:J:761:LEU:O	3:J:763:TRP:N	2.54	0.40
3:K:425:GLU:HG3	3:L:790:LEU:O	2.21	0.40
3:K:486:LYS:HG2	3:K:560:ARG:CZ	2.52	0.40
3:K:579:TYR:HE2	3:K:703:LYS:HE3	1.86	0.40
1:A:211:LYS:HE2	1:A:211:LYS:HB2	1.83	0.40
1:A:229:VAL:HG23	1:A:229:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:158:ILE:HG12	2:E:159:THR:O	2.21	0.40
3:J:294:TYR:HE2	3:J:433:ILE:HD13	1.86	0.40
3:J:304:PHE:CE1	3:J:415:ALA:HB1	2.56	0.40
3:J:588:THR:HG21	3:L:99:PHE:CZ	2.57	0.40
3:K:101:ASP:CG	3:K:102:ARG:H	2.29	0.40
3:K:139:GLY:HA3	3:L:584:LEU:HD23	2.02	0.40
3:K:227:LEU:HD12	3:K:255:LEU:HD12	2.03	0.40
3:K:469:THR:HG21	3:K:479:LEU:HD13	2.04	0.40
3:L:651:LEU:O	3:L:654:SER:OG	2.35	0.40
1:A:123:TYR:CE1	1:A:193:CYS:HB2	2.56	0.40
2:D:153:TYR:HB3	2:D:154:PRO:HD3	2.03	0.40
2:F:136:TYR:CE1	2:F:154:PRO:HB2	2.57	0.40
2:F:136:TYR:CG	2:F:152:LEU:HD13	2.57	0.40
2:H:12:TYR:HB3	2:H:61:GLU:HG2	2.02	0.40
2:I:122:LYS:HE2	2:I:122:LYS:HB2	1.93	0.40
3:J:184:VAL:CG2	3:J:190:PRO:HG2	2.52	0.40
3:J:619:PHE:HB3	3:J:655:ARG:NH2	2.36	0.40
3:K:81:ILE:HD12	3:K:156:TRP:HD1	1.86	0.40
3:K:392:PHE:HB2	3:K:395:GLN:CD	2.45	0.40
3:L:579:TYR:HD2	3:L:663:SER:HB2	1.86	0.40
2:H:80:ASP:HB3	2:H:172:LEU:HD23	2.04	0.40
2:H:134:LYS:HZ1	2:H:154:PRO:HB3	1.86	0.40
3:J:25:ALA:HB3	3:J:105:THR:HB	2.04	0.40
3:J:320:THR:O	3:J:324:THR:HG23	2.22	0.40
3:J:563:VAL:HG22	3:J:564:GLU:N	2.36	0.40
3:J:690:PHE:HE1	3:J:692:LEU:HG	1.87	0.40
3:K:18:LEU:H	3:K:18:LEU:HD23	1.86	0.40
3:K:304:PHE:CE1	3:K:415:ALA:HB1	2.56	0.40
3:K:595:SER:HB3	3:K:614:PHE:O	2.22	0.40
3:K:656:TYR:HD1	3:K:656:TYR:HA	1.70	0.40
3:K:798:MET:HE3	3:K:798:MET:HB3	1.94	0.40
3:L:131:PHE:CE2	3:L:133:GLY:HA3	2.56	0.40
3:L:313:PRO:HG2	3:L:317:PHE:CE2	2.57	0.40
3:L:692:LEU:HD22	3:L:711:TYR:HD2	1.86	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	291/298 (98%)	261 (90%)	27 (9%)	3 (1%)	12	45
1	B	291/298 (98%)	258 (89%)	30 (10%)	3 (1%)	12	45
1	C	291/298 (98%)	259 (89%)	29 (10%)	3 (1%)	12	45
2	D	202/204 (99%)	186 (92%)	15 (7%)	1 (0%)	24	59
2	E	202/204 (99%)	180 (89%)	21 (10%)	1 (0%)	24	59
2	F	202/204 (99%)	179 (89%)	22 (11%)	1 (0%)	24	59
2	G	202/204 (99%)	180 (89%)	21 (10%)	1 (0%)	24	59
2	H	202/204 (99%)	185 (92%)	16 (8%)	1 (0%)	24	59
2	I	202/204 (99%)	180 (89%)	21 (10%)	1 (0%)	24	59
3	J	810/949 (85%)	676 (84%)	111 (14%)	23 (3%)	4	27
3	K	810/949 (85%)	673 (83%)	112 (14%)	25 (3%)	3	25
3	L	811/949 (86%)	685 (84%)	107 (13%)	19 (2%)	5	30
All	All	4516/4965 (91%)	3902 (86%)	532 (12%)	82 (2%)	9	34

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	PRO
1	B	288	PRO
1	C	288	PRO
3	J	4	ILE
3	J	44	TYR
3	J	102	ARG
3	J	122	PRO
3	J	448	ASP
3	J	507	PRO
3	J	517	PRO
3	J	624	LYS
3	K	4	ILE

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Mol	Chain	Res	Type
3	K	44	TYR
3	K	102	ARG
3	K	122	PRO
3	K	448	ASP
3	K	455	LYS
3	K	507	PRO
3	K	517	PRO
3	K	579	TYR
3	K	624	LYS
3	K	762	SER
3	L	4	ILE
3	L	44	TYR
3	L	102	ARG
3	L	125	ASP
3	L	448	ASP
3	L	624	LYS
3	J	334	VAL
3	J	363	ASN
3	K	5	LEU
3	K	333	ILE
3	K	334	VAL
3	K	363	ASN
3	L	333	ILE
3	L	334	VAL
3	L	363	ASN
1	B	212	ARG
1	C	212	ARG
2	F	91	VAL
3	J	196	ARG
3	J	333	ILE
3	J	454	ASP
3	J	456	THR
3	J	762	SER
3	K	125	ASP
1	A	212	ARG
2	D	91	VAL
2	G	91	VAL
2	H	91	VAL
2	I	91	VAL
3	J	116	ASN
3	K	116	ASN
3	L	5	LEU

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Mol	Chain	Res	Type
3	L	116	ASN
3	L	196	ARG
1	A	273	LEU
1	C	273	LEU
3	J	120	VAL
3	J	825	SER
3	K	119	PRO
3	K	120	VAL
3	K	823	ARG
3	L	119	PRO
3	L	441	LYS
1	B	273	LEU
2	E	91	VAL
3	J	823	ARG
3	K	185	ASN
3	K	196	ARG
3	L	458	LEU
3	K	60	VAL
3	L	120	VAL
3	L	826	PRO
3	J	60	VAL
3	J	826	PRO
3	L	60	VAL
3	K	525	VAL
3	J	144	VAL
3	J	525	VAL
3	K	144	VAL
3	L	144	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	268/273 (98%)	268 (100%)	0	100	100
1	B	268/273 (98%)	267 (100%)	1 (0%)	84	83
1	C	268/273 (98%)	268 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	181/181 (100%)	181 (100%)	0	100	100
2	E	181/181 (100%)	181 (100%)	0	100	100
2	F	181/181 (100%)	181 (100%)	0	100	100
2	G	181/181 (100%)	181 (100%)	0	100	100
2	H	181/181 (100%)	181 (100%)	0	100	100
2	I	181/181 (100%)	181 (100%)	0	100	100
3	J	723/834 (87%)	721 (100%)	2 (0%)	86	85
3	K	723/834 (87%)	717 (99%)	6 (1%)	73	77
3	L	724/834 (87%)	720 (99%)	4 (1%)	78	80
All	All	4060/4407 (92%)	4047 (100%)	13 (0%)	84	85

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	288	PRO
3	J	456	THR
3	J	761	LEU
3	K	4	ILE
3	K	121	ASP
3	K	122	PRO
3	K	124	THR
3	K	456	THR
3	K	553	ASN
3	L	4	ILE
3	L	124	THR
3	L	441	LYS
3	L	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	112	HIS
1	C	113	ASN
2	D	104	GLN
2	E	46	GLN
2	E	104	GLN
2	F	189	ASN

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Mol	Chain	Res	Type
2	G	46	GLN
2	G	104	GLN
2	I	46	GLN
2	I	51	ASN
2	I	104	GLN
3	J	107	HIS
3	J	207	HIS
3	J	506	GLN
3	J	526	GLN
3	J	540	ASN
3	J	553	ASN
3	J	594	ASN
3	J	721	GLN
3	J	800	GLN
3	K	143	ASN
3	K	157	ASN
3	K	397	GLN
3	K	515	ASN
3	K	540	ASN
3	K	639	ASN
3	L	108	GLN
3	L	143	ASN
3	L	353	HIS
3	L	515	ASN
3	L	521	ASN
3	L	540	ASN
3	L	636	ASN
3	L	788	GLN
3	L	792	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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.

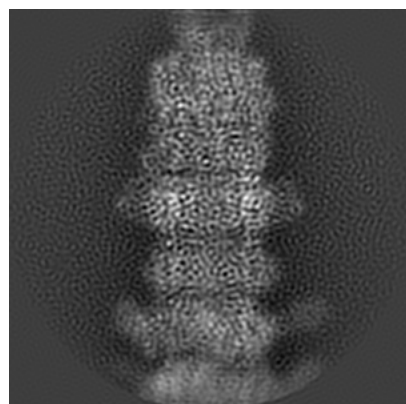
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60750. These allow visual inspection of the internal detail of the map and identification of artifacts.

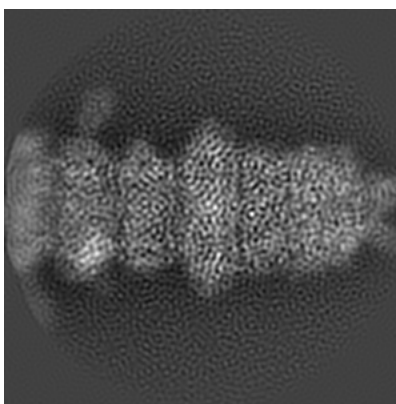
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

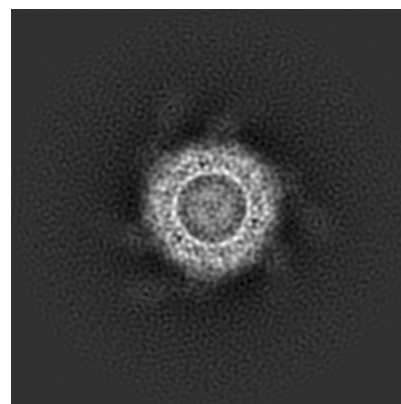
6.1.1 Primary map



X



Y

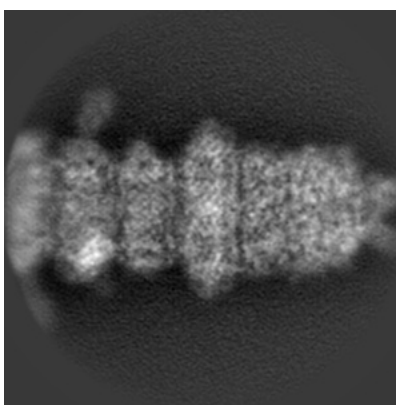


Z

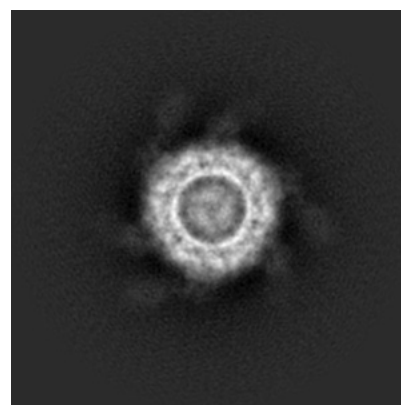
6.1.2 Raw map



X



Y



Z

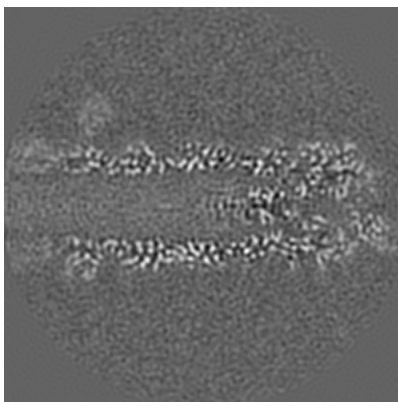
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

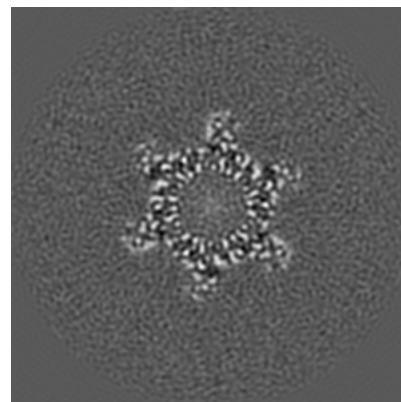
6.2.1 Primary map



X Index: 100

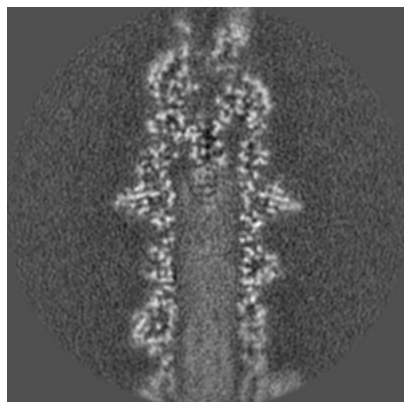


Y Index: 100

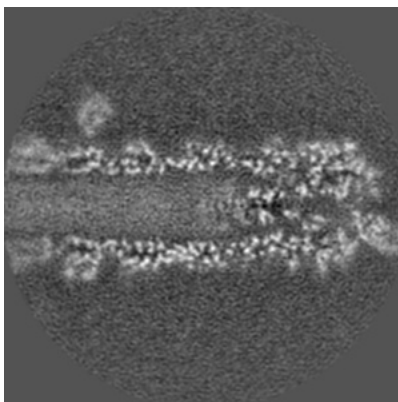


Z Index: 100

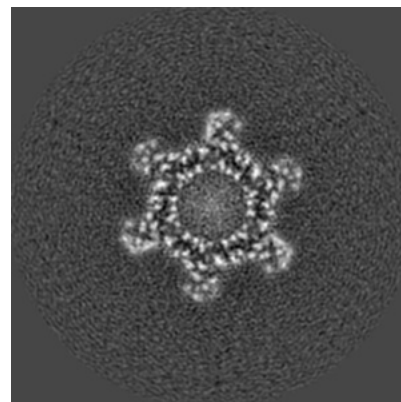
6.2.2 Raw map



X Index: 100



Y Index: 100

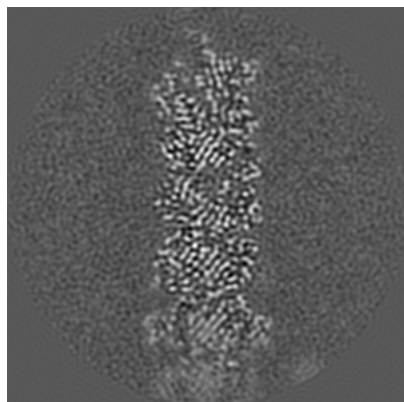


Z Index: 100

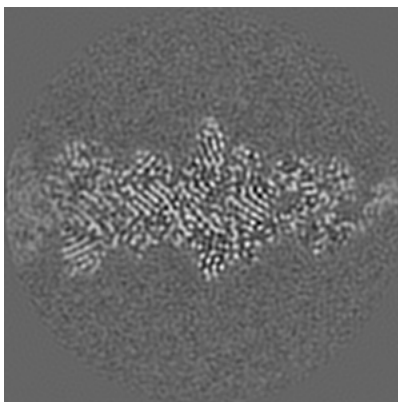
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

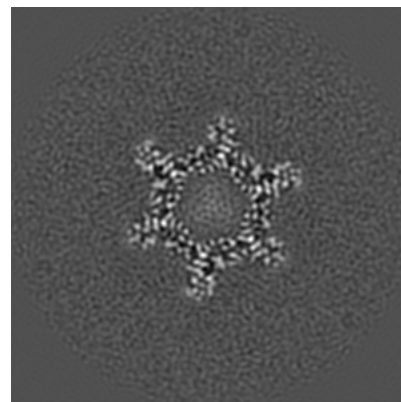
6.3.1 Primary map



X Index: 118

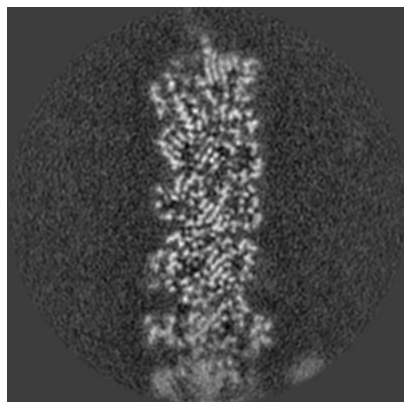


Y Index: 118

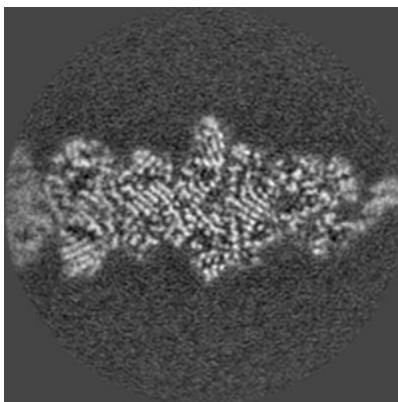


Z Index: 104

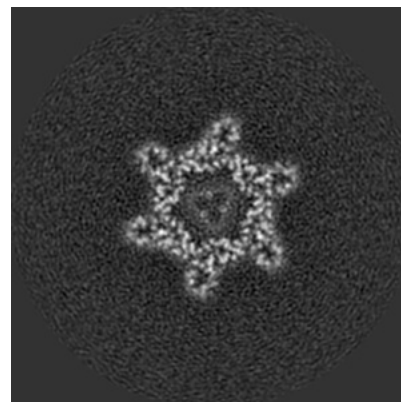
6.3.2 Raw map



X Index: 119



Y Index: 118

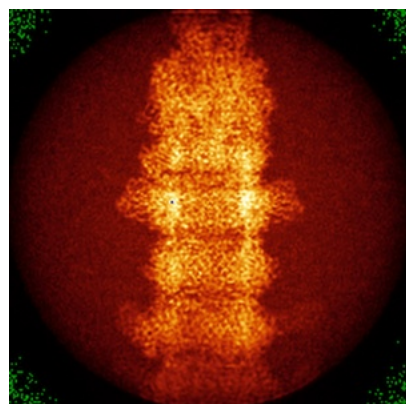


Z Index: 106

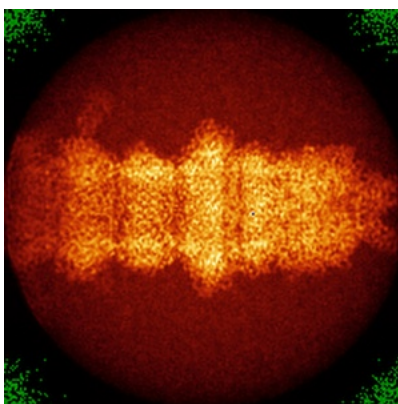
The images above show the largest variance slices of the map in three orthogonal directions.

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

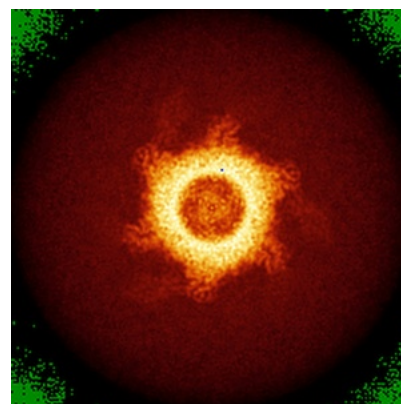
6.4.1 Primary map



X

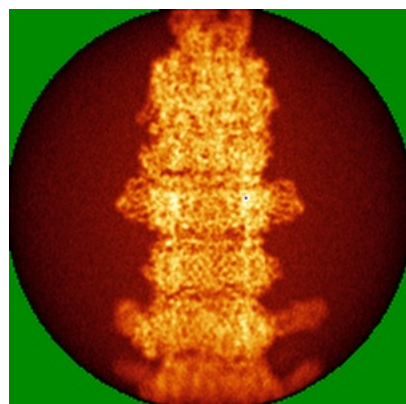


Y

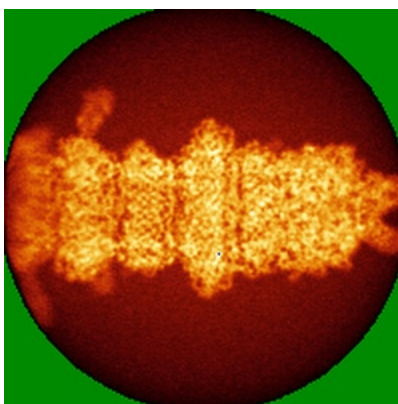


Z

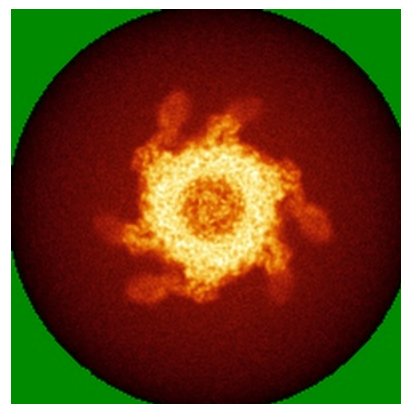
6.4.2 Raw map



X



Y

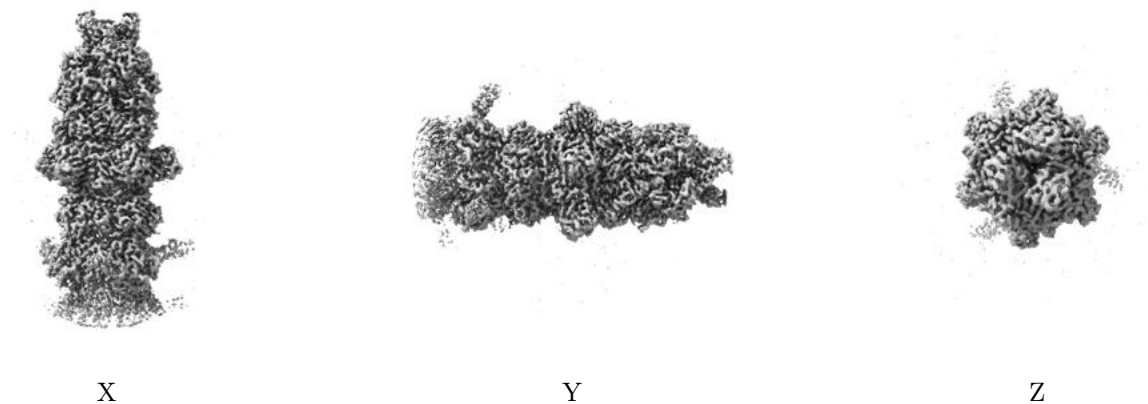


Z

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

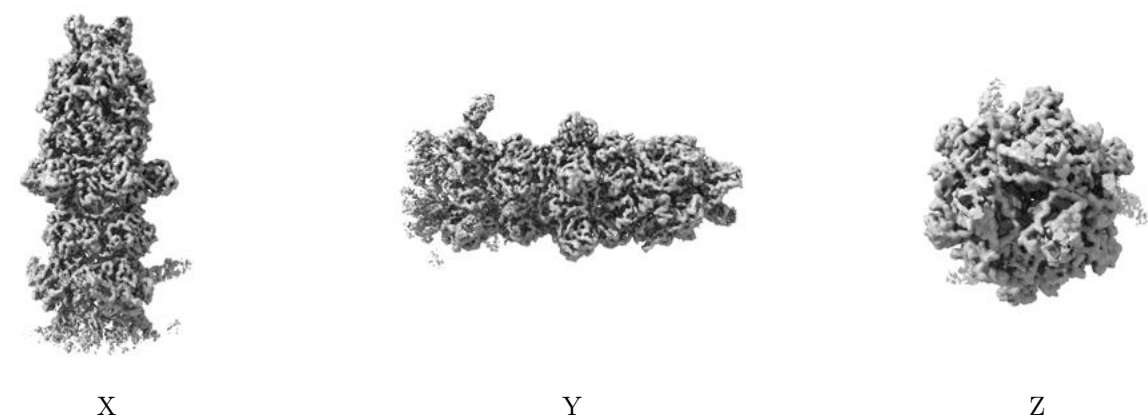
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

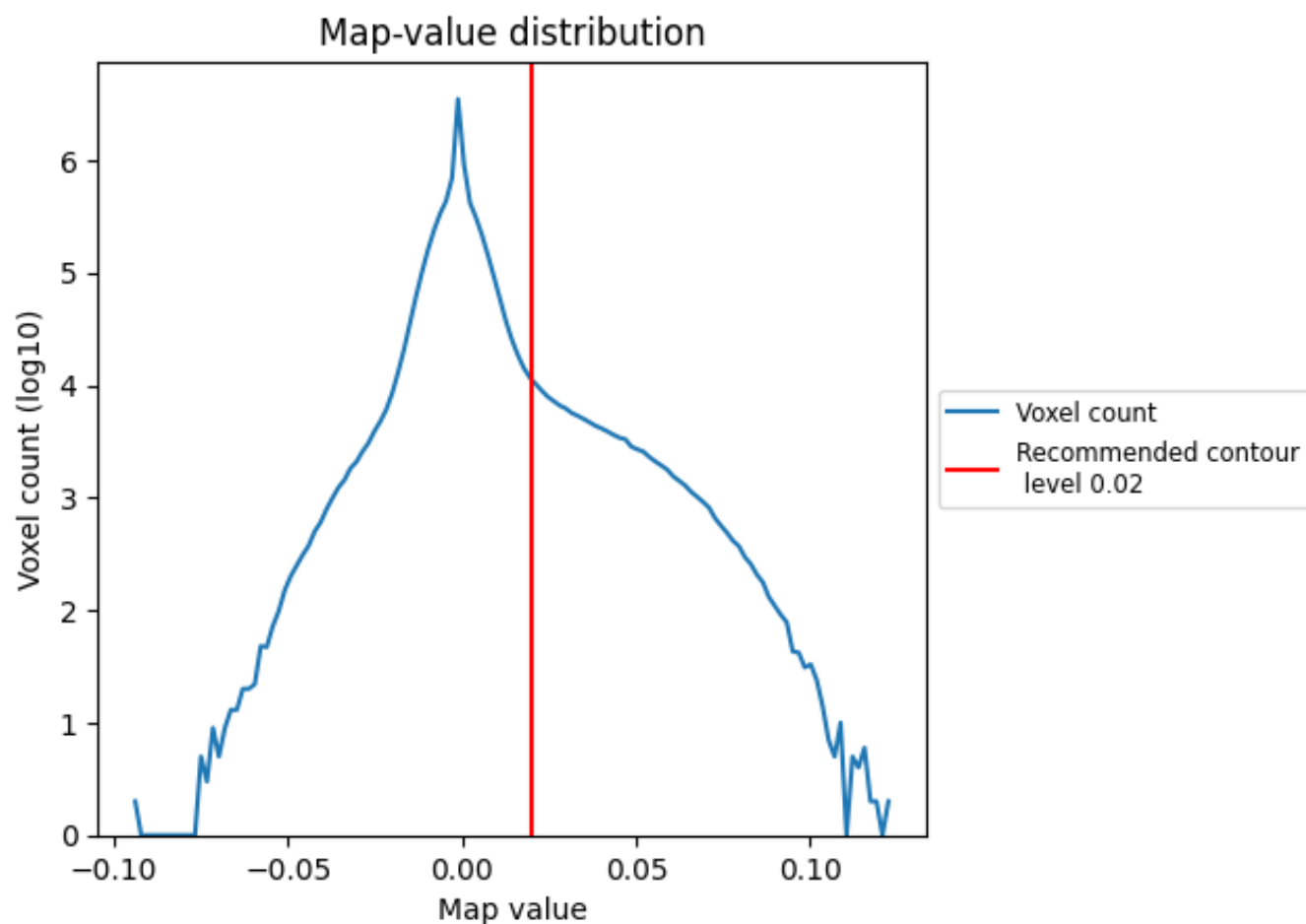
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

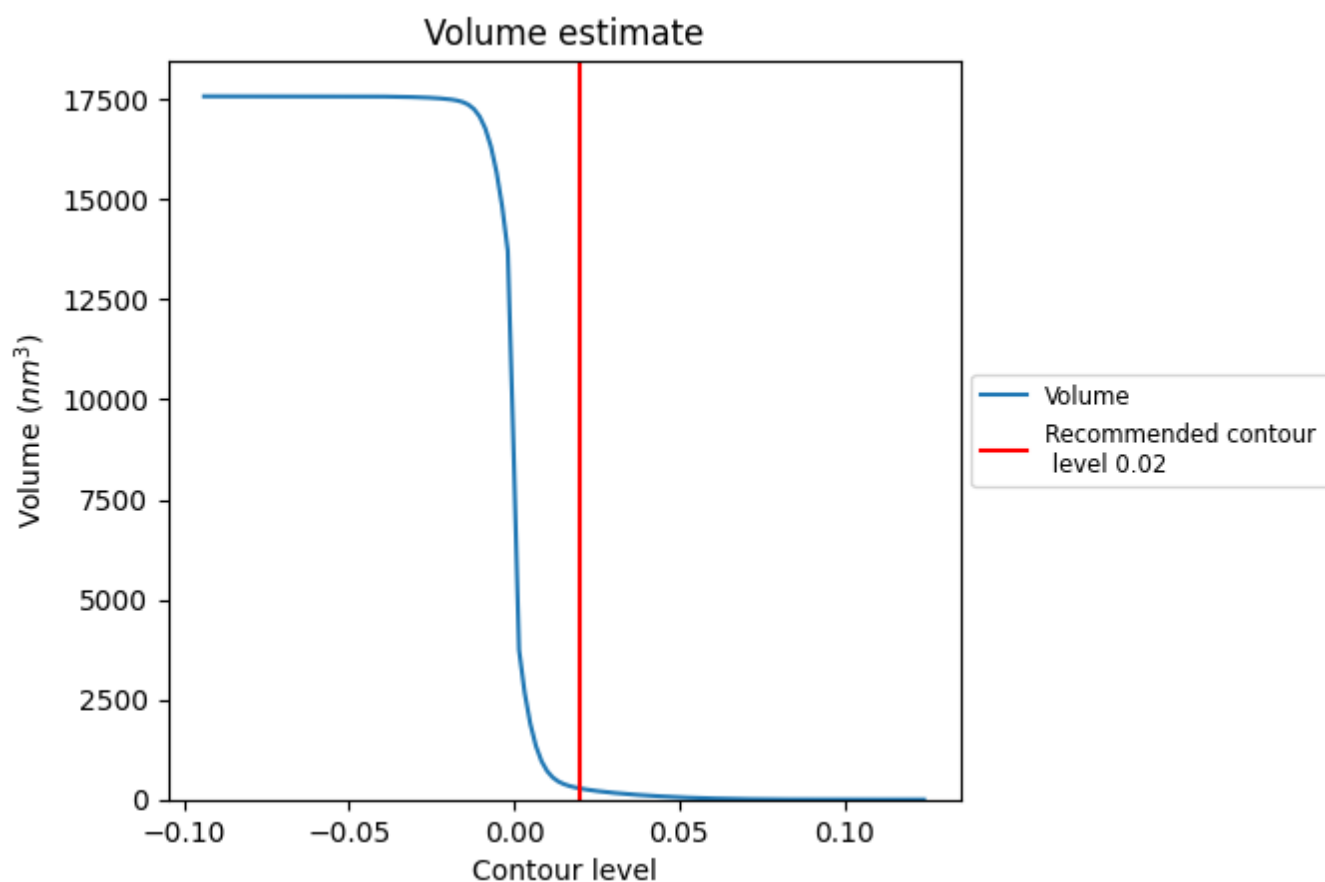
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

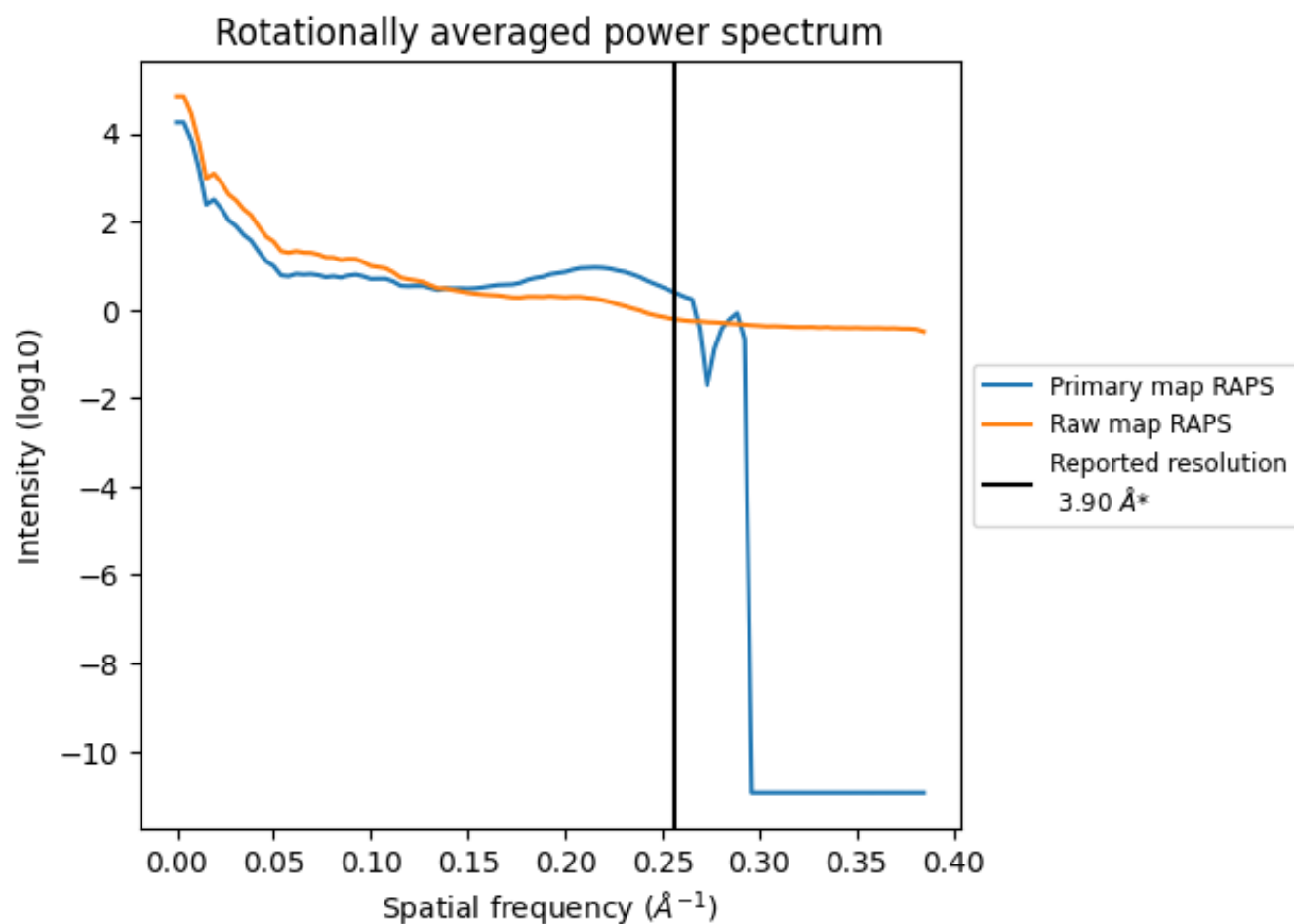
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 279 nm³; this corresponds to an approximate mass of 252 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 ⓘ

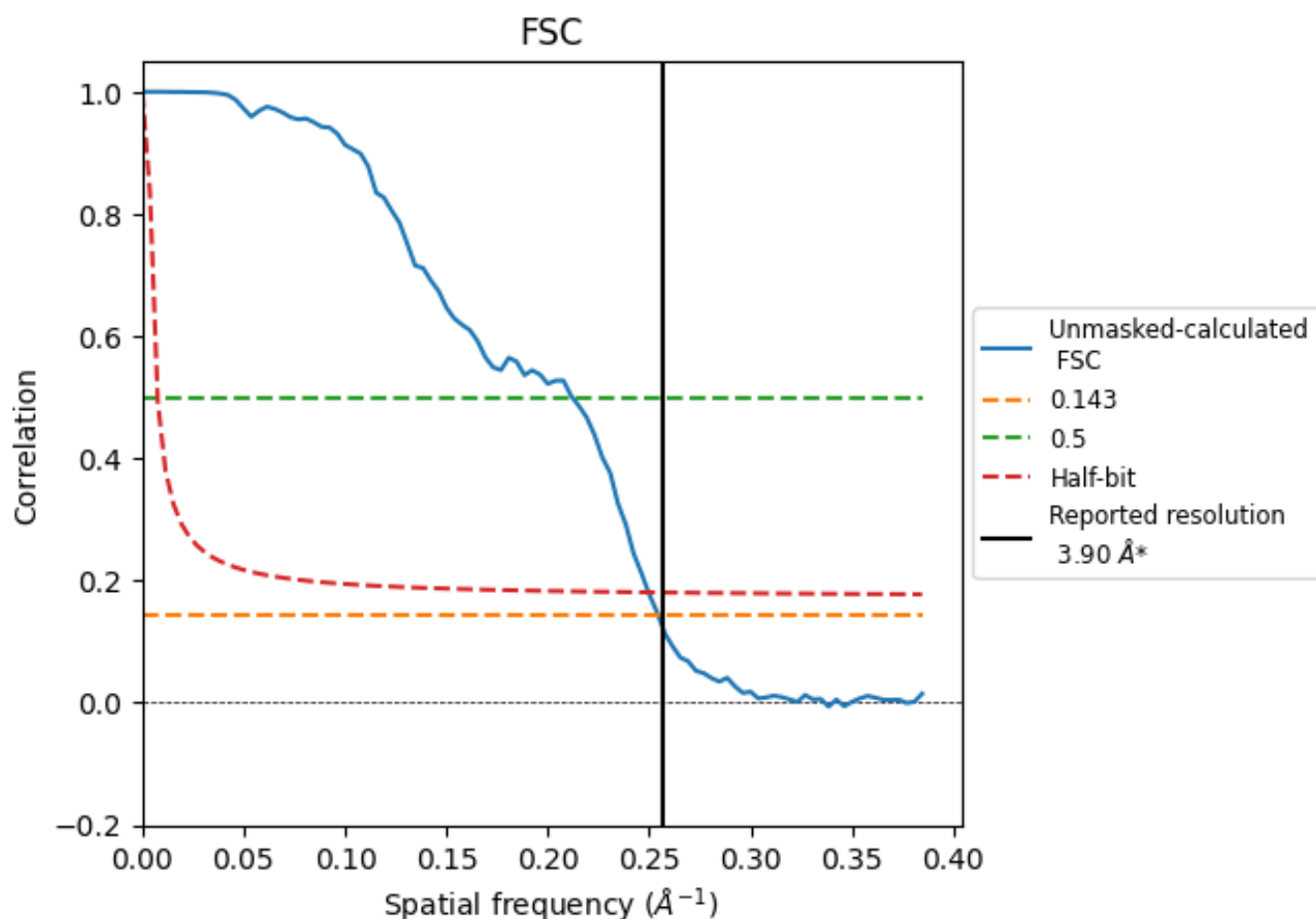


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

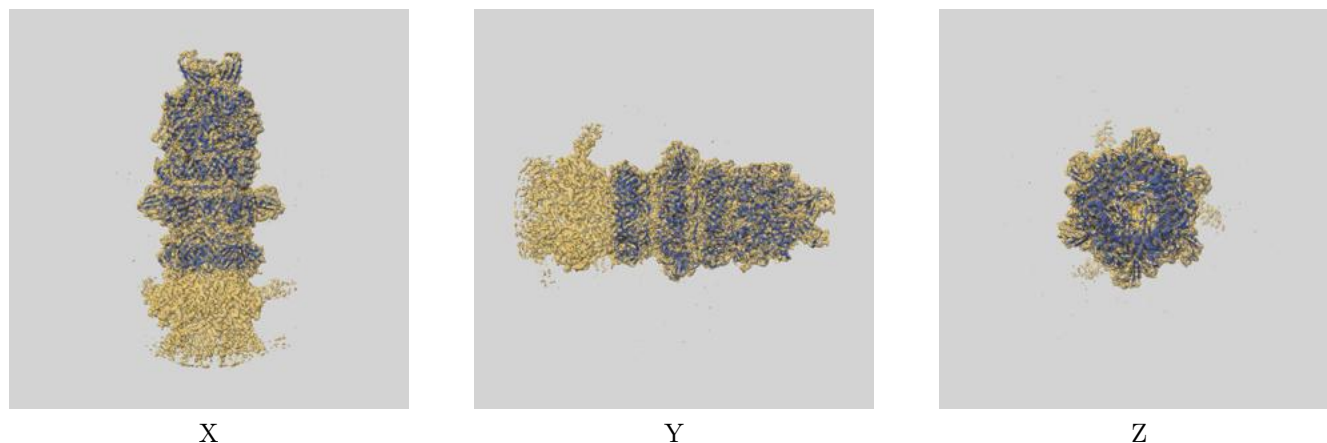
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.93	4.72	4.00

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

9 Map-model fit [i](#)

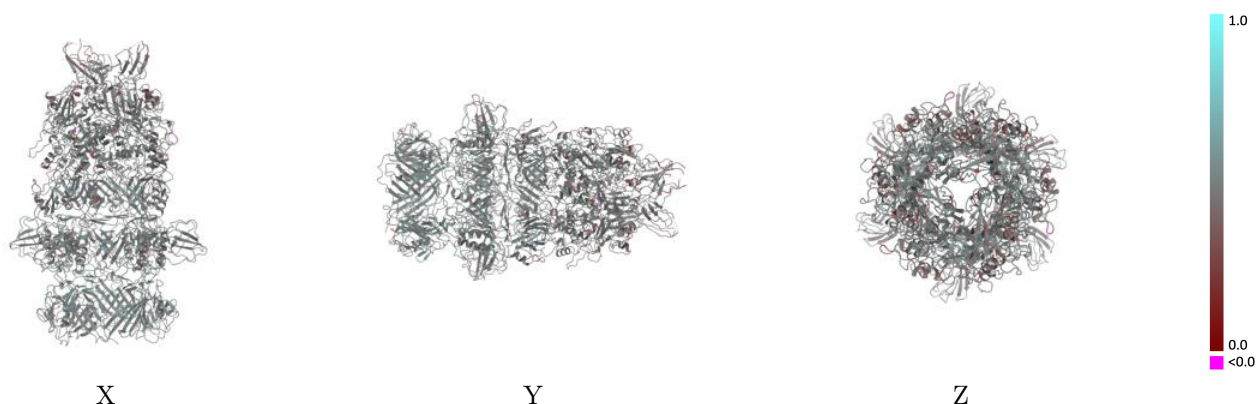
This section contains information regarding the fit between EMDB map EMD-60750 and PDB model 9IOZ. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



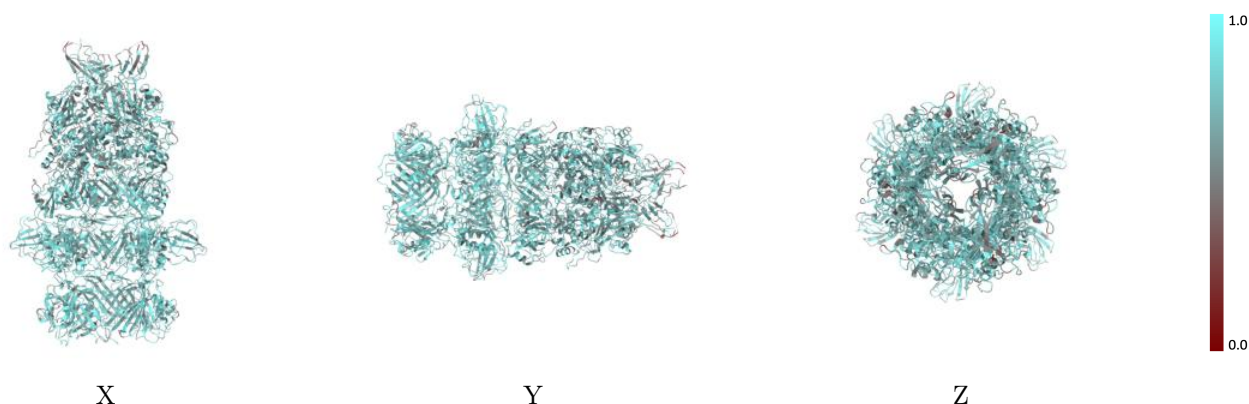
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



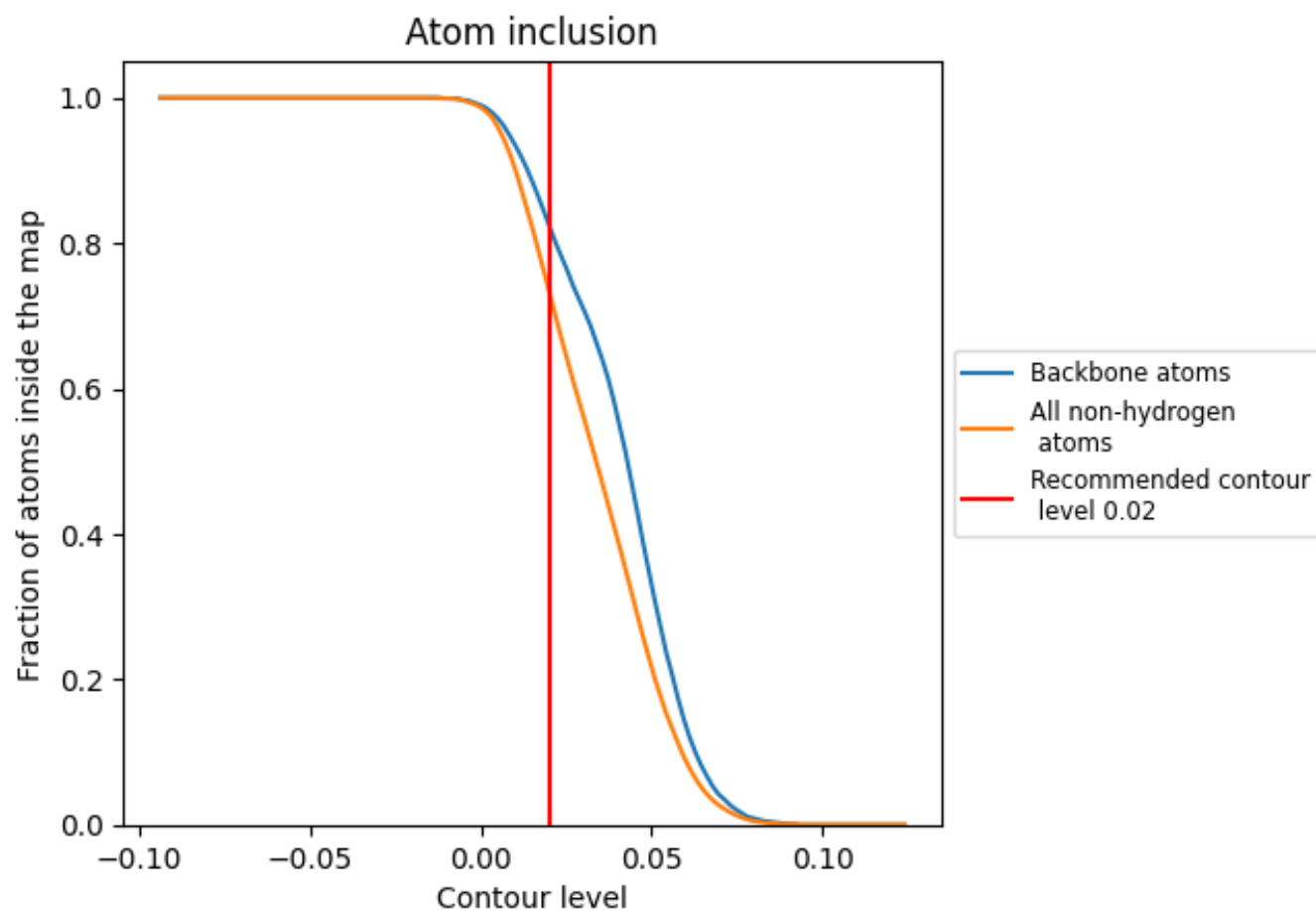
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7330	0.4860
A	0.7440	0.5000
B	0.7390	0.5010
C	0.7400	0.5020
D	0.7600	0.5030
E	0.7580	0.4900
F	0.7610	0.4910
G	0.7650	0.5000
H	0.7650	0.5000
I	0.7670	0.4910
J	0.7210	0.4750
K	0.7130	0.4750
L	0.7140	0.4750

1.0

0.0

<0.0