



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:06 PM UTC

PDB ID : 8WW8 / pdb_00008ww8
EMDB ID : EMD-37884
Title : Structure of Apo-Form AsfvPrimPol Hexamer
Authors : Shi, T.H.; Guo, Y.Y.; Yan, R.H.
Deposited on : 2023-10-25
Resolution : 3.99 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

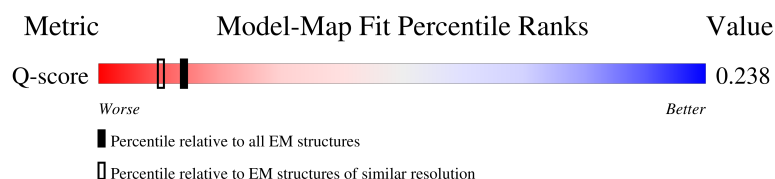
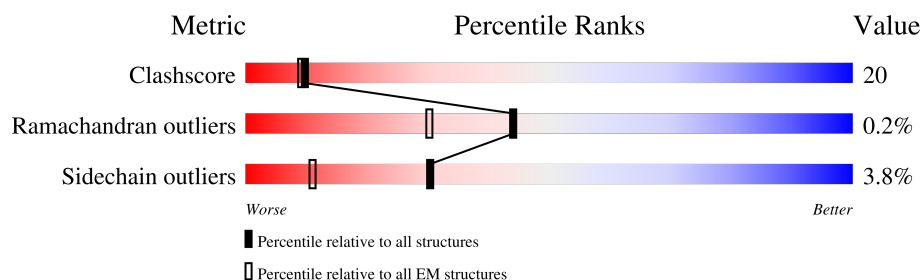
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.99 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	7463 (3.49 - 4.49)

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	972	6% 58% 30% 12%
1	B	972	8% 58% 29% • 12%
1	C	972	12% 58% 29% • 12%
1	D	972	6% 56% 32% • 12%

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Mol	Chain	Length	Quality of chain
1	E	972	
1	F	972	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 40886 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 Putative primase C962R.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	854	Total	C	N	O	S	0	0
			6806	4389	1152	1239	26		
1	B	853	Total	C	N	O	S	0	0
			6796	4383	1149	1238	26		
1	C	854	Total	C	N	O	S	0	0
			6806	4389	1152	1239	26		
1	D	856	Total	C	N	O	S	0	0
			6824	4400	1155	1243	26		
1	E	856	Total	C	N	O	S	0	0
			6824	4400	1155	1243	26		
1	F	856	Total	C	N	O	S	0	0
			6830	4403	1158	1243	26		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	963	LEU	-	expression tag	UNP A0A2X0TKI6
A	964	GLU	-	expression tag	UNP A0A2X0TKI6
A	965	ASP	-	expression tag	UNP A0A2X0TKI6
A	966	TYR	-	expression tag	UNP A0A2X0TKI6
A	967	LYS	-	expression tag	UNP A0A2X0TKI6
A	968	ASP	-	expression tag	UNP A0A2X0TKI6
A	969	ASP	-	expression tag	UNP A0A2X0TKI6
A	970	ASP	-	expression tag	UNP A0A2X0TKI6
A	971	ASP	-	expression tag	UNP A0A2X0TKI6
A	972	LYS	-	expression tag	UNP A0A2X0TKI6
B	963	LEU	-	expression tag	UNP A0A2X0TKI6
B	964	GLU	-	expression tag	UNP A0A2X0TKI6
B	965	ASP	-	expression tag	UNP A0A2X0TKI6
B	966	TYR	-	expression tag	UNP A0A2X0TKI6
B	967	LYS	-	expression tag	UNP A0A2X0TKI6
B	968	ASP	-	expression tag	UNP A0A2X0TKI6
B	969	ASP	-	expression tag	UNP A0A2X0TKI6
B	970	ASP	-	expression tag	UNP A0A2X0TKI6

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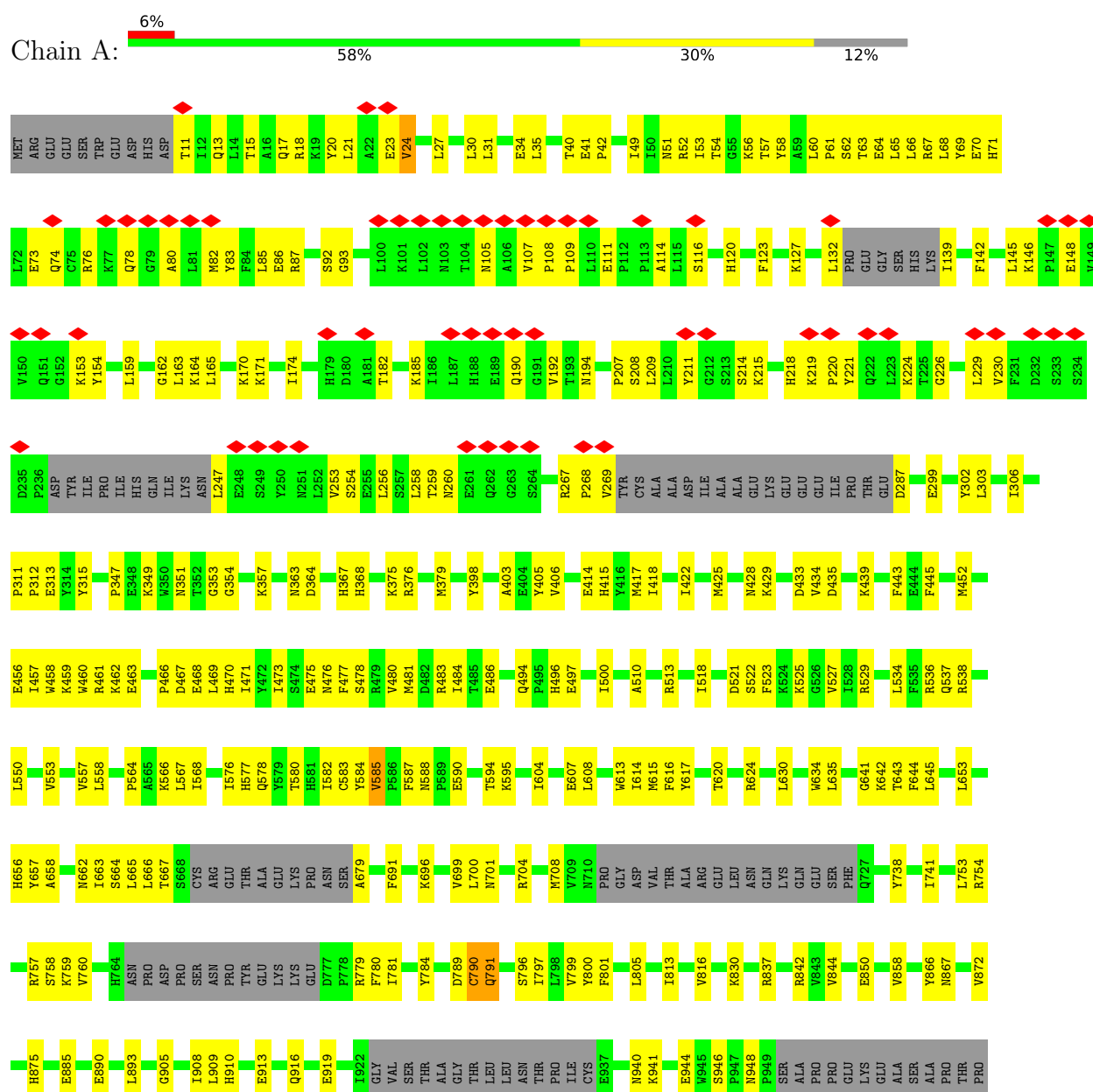
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Chain	Residue	Modelled	Actual	Comment	Reference
B	971	ASP	-	expression tag	UNP A0A2X0TKI6
B	972	LYS	-	expression tag	UNP A0A2X0TKI6
C	963	LEU	-	expression tag	UNP A0A2X0TKI6
C	964	GLU	-	expression tag	UNP A0A2X0TKI6
C	965	ASP	-	expression tag	UNP A0A2X0TKI6
C	966	TYR	-	expression tag	UNP A0A2X0TKI6
C	967	LYS	-	expression tag	UNP A0A2X0TKI6
C	968	ASP	-	expression tag	UNP A0A2X0TKI6
C	969	ASP	-	expression tag	UNP A0A2X0TKI6
C	970	ASP	-	expression tag	UNP A0A2X0TKI6
C	971	ASP	-	expression tag	UNP A0A2X0TKI6
C	972	LYS	-	expression tag	UNP A0A2X0TKI6
D	963	LEU	-	expression tag	UNP A0A2X0TKI6
D	964	GLU	-	expression tag	UNP A0A2X0TKI6
D	965	ASP	-	expression tag	UNP A0A2X0TKI6
D	966	TYR	-	expression tag	UNP A0A2X0TKI6
D	967	LYS	-	expression tag	UNP A0A2X0TKI6
D	968	ASP	-	expression tag	UNP A0A2X0TKI6
D	969	ASP	-	expression tag	UNP A0A2X0TKI6
D	970	ASP	-	expression tag	UNP A0A2X0TKI6
D	971	ASP	-	expression tag	UNP A0A2X0TKI6
D	972	LYS	-	expression tag	UNP A0A2X0TKI6
E	963	LEU	-	expression tag	UNP A0A2X0TKI6
E	964	GLU	-	expression tag	UNP A0A2X0TKI6
E	965	ASP	-	expression tag	UNP A0A2X0TKI6
E	966	TYR	-	expression tag	UNP A0A2X0TKI6
E	967	LYS	-	expression tag	UNP A0A2X0TKI6
E	968	ASP	-	expression tag	UNP A0A2X0TKI6
E	969	ASP	-	expression tag	UNP A0A2X0TKI6
E	970	ASP	-	expression tag	UNP A0A2X0TKI6
E	971	ASP	-	expression tag	UNP A0A2X0TKI6
E	972	LYS	-	expression tag	UNP A0A2X0TKI6
F	963	LEU	-	expression tag	UNP A0A2X0TKI6
F	964	GLU	-	expression tag	UNP A0A2X0TKI6
F	965	ASP	-	expression tag	UNP A0A2X0TKI6
F	966	TYR	-	expression tag	UNP A0A2X0TKI6
F	967	LYS	-	expression tag	UNP A0A2X0TKI6
F	968	ASP	-	expression tag	UNP A0A2X0TKI6
F	969	ASP	-	expression tag	UNP A0A2X0TKI6
F	970	ASP	-	expression tag	UNP A0A2X0TKI6
F	971	ASP	-	expression tag	UNP A0A2X0TKI6
F	972	LYS	-	expression tag	UNP A0A2X0TKI6

3 Residue-property plots

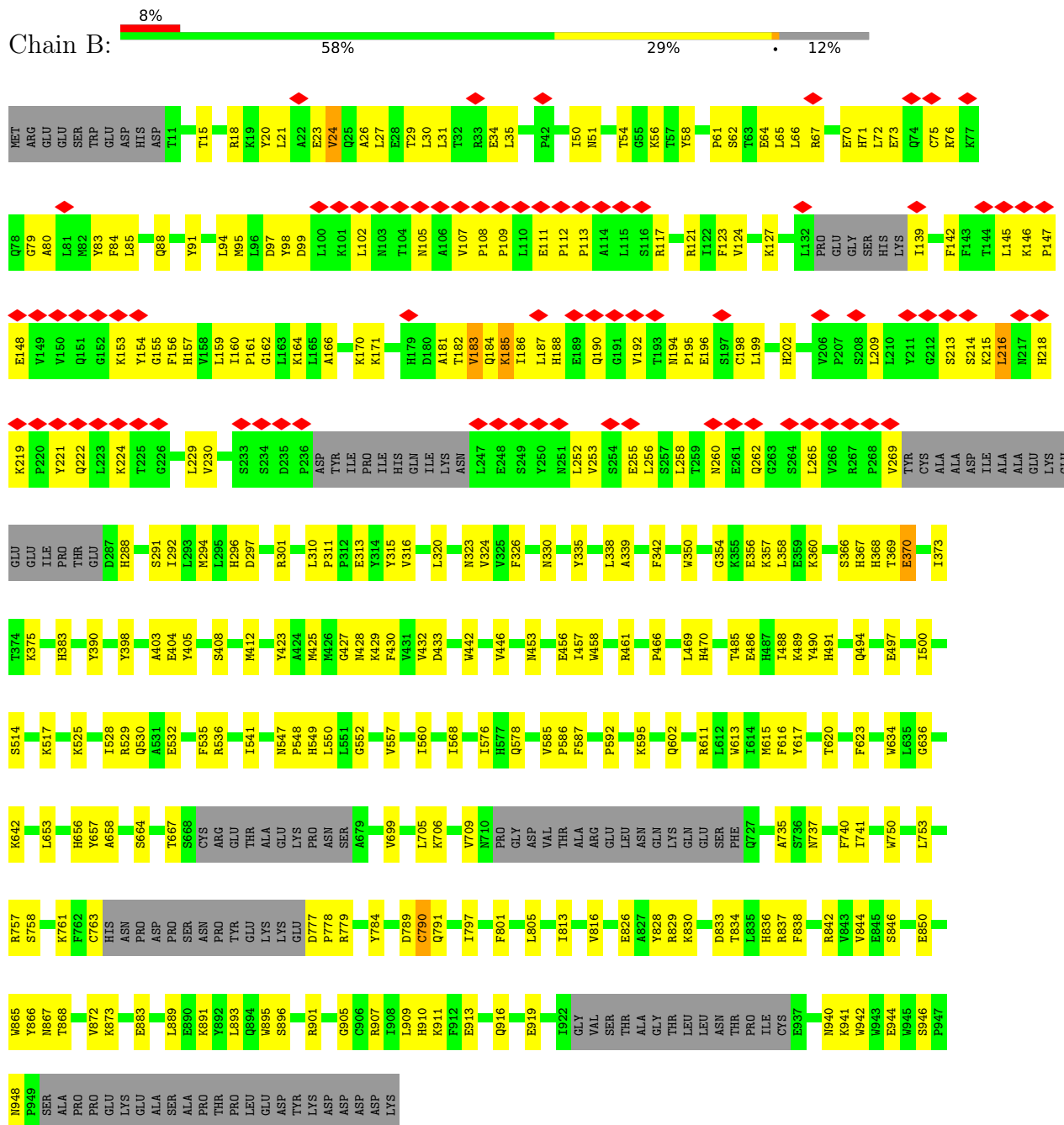
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Putative primase C962R

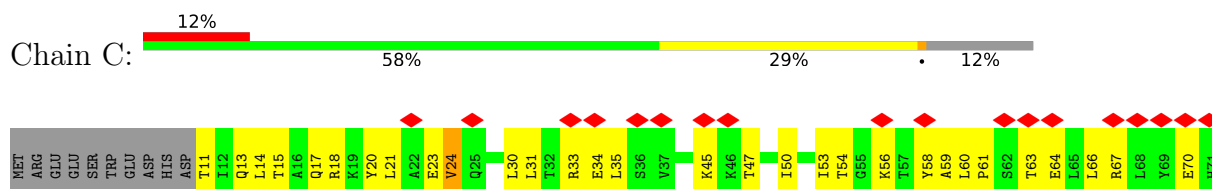


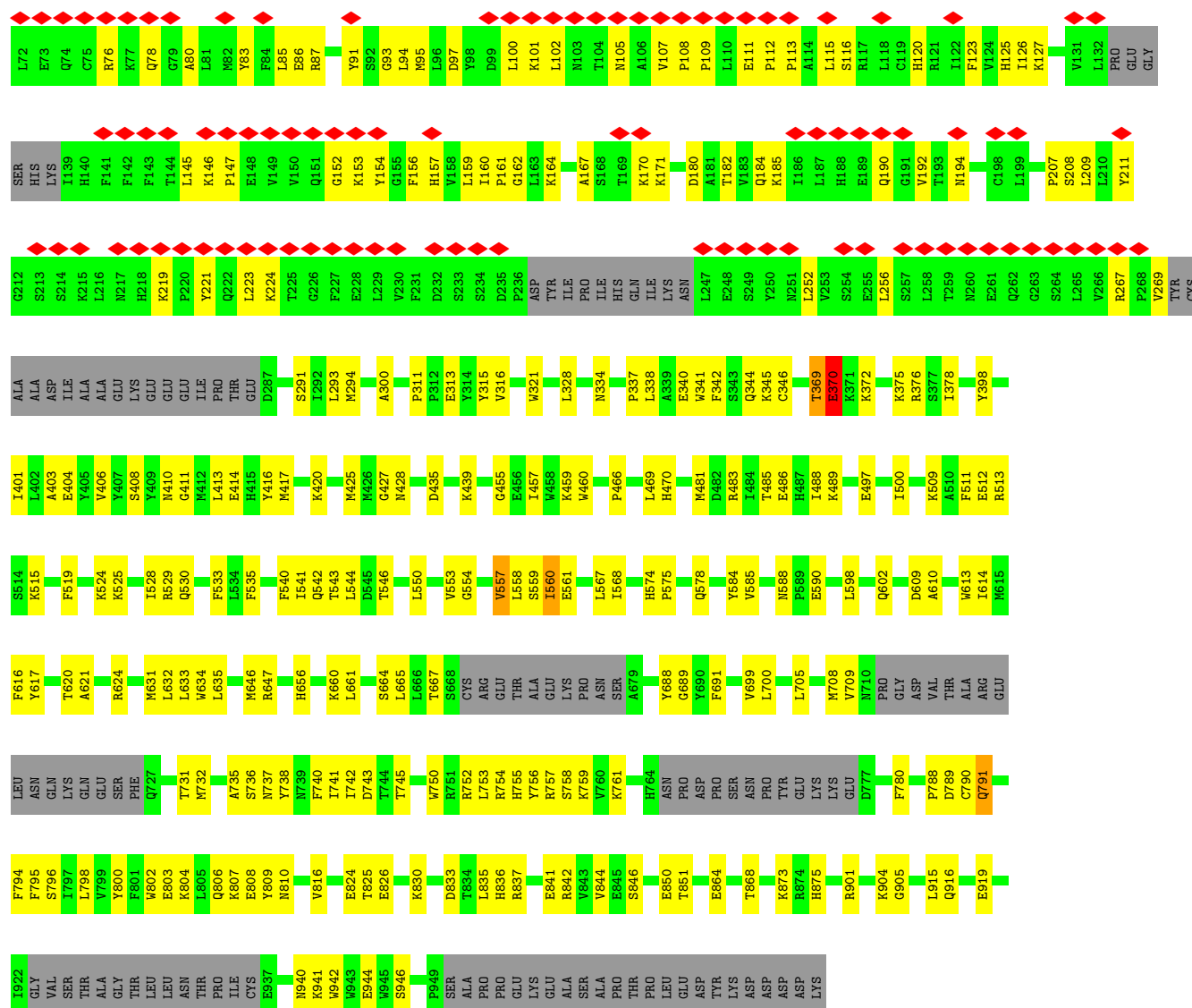
LEU
GLU
ASP
TYR
LYS
ASP
ASP
ASP
LYS

• Molecule 1: Putative primase C962R

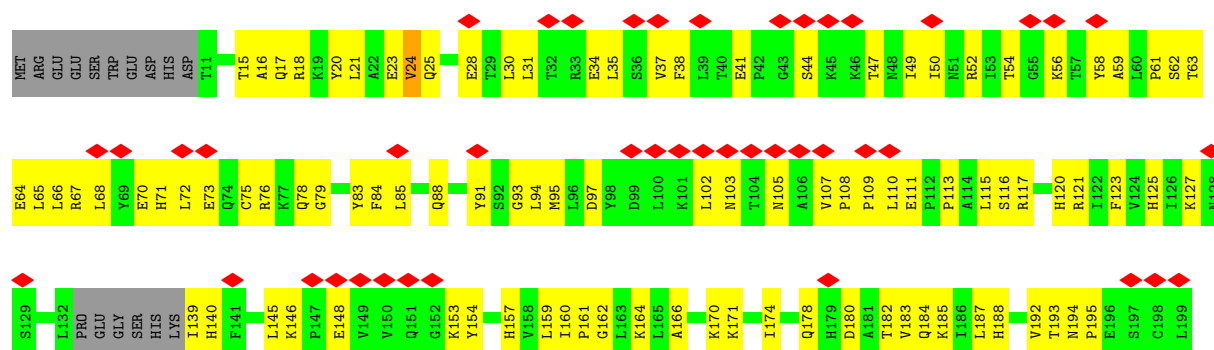


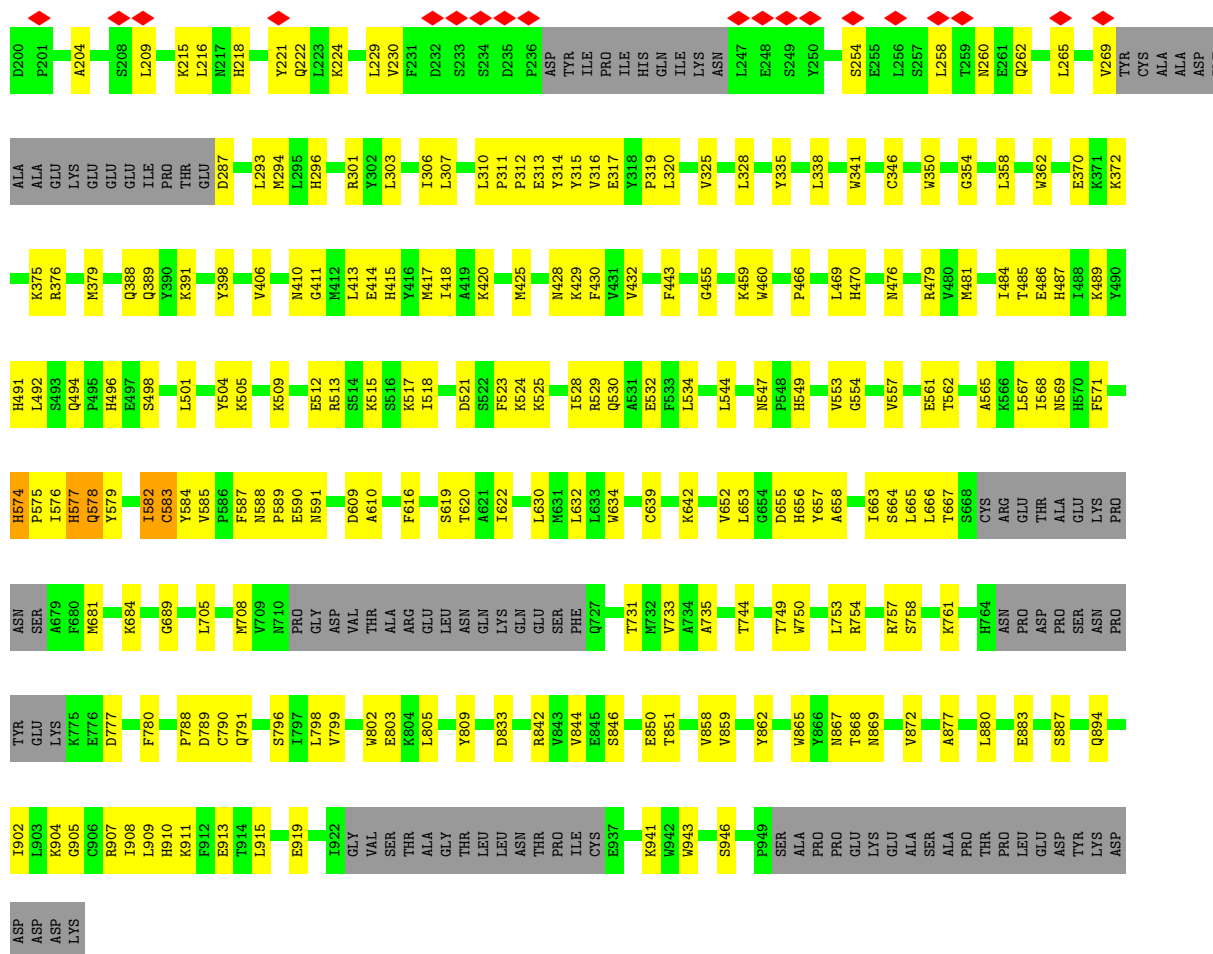
• Molecule 1: Putative primase C962R



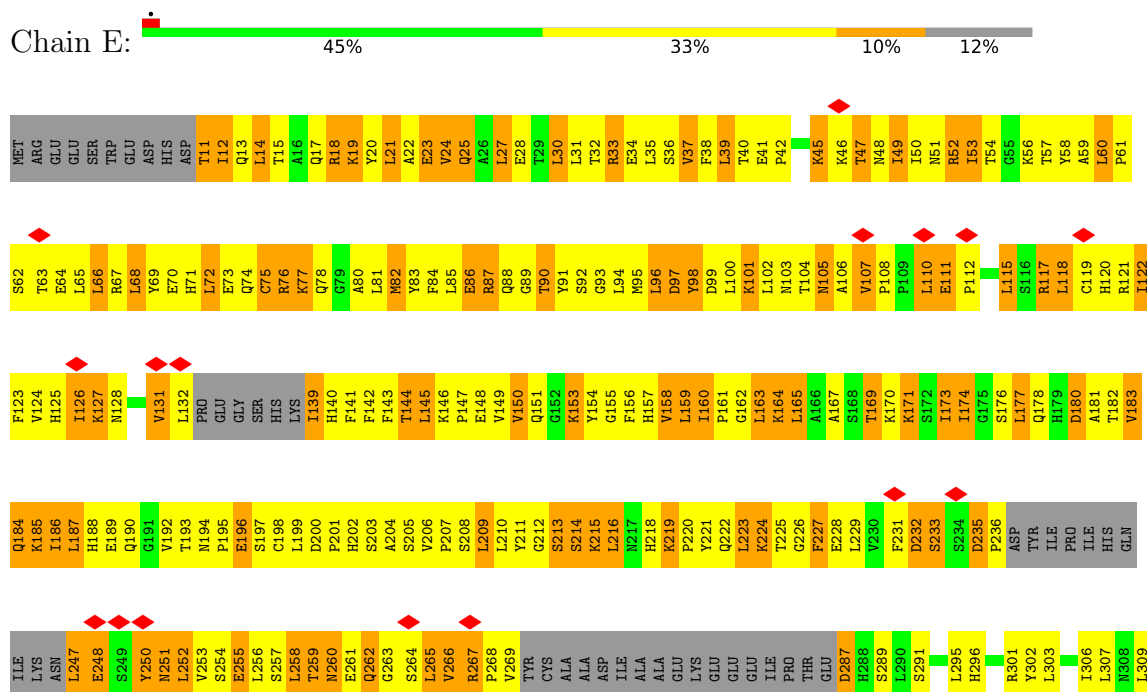


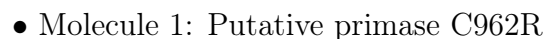
• Molecule 1: Putative primase C962R





• Molecule 1: Putative primase C962R





Frequency	Percentage
Daily	56%
Weekly	31%
Monthly	12%
Other	3%



L618	S619	T620	A621	R624	L630	G641	F644	L645	M646	R647	L653	H656	Y657	A658	S659	K660	L661	S664	L665	L666	T667	S668	CYS	ARG	GLU	THR	ALA	GLU	LYS	PRO	ASN	SER	A679	Y688	K696	S697	E698	V699	L700	N701	T702	S703	N710	PRO	GLY	ASP	VAL	THR	ALA				
ARG	GLU	LEU	ASN	GLN	LYS	GLN	GLU	SER	PHE	Q727	M728	M732	S736	N737	Y738	I742	D743	T744	T745	T749	W750	R751	R752	L753	R754	R757	S758	K759	V760	K761	F762	C763	H764	ASN	PRO	ASP	PRO	SER	ASN	PRD	TYR	GLU	LYS	K775	E776	D777	P778	R779	D787	F788	D789	C790	Q791
F801	E826	K830	R837	T840	E841	R842	W843	V844	E845	S846	T851	N854	V858	E864	N867	T868	N869	I870	N871	V872	E883	S887	V888	L889	E890	K891	Y892	W895	S896	P897	N898	K899	T900	K904	G905	C906	R907	I908	L909	H910	K911	E919	I922										
GLY	VAL	SER	THR	ALA	GLY	THR	LEU	LEU	ASN	THR	PRO	PRO	ILE	CYS	E937	W942	P949	SER	ALA	PRO	PRO	PRO	GLU	LYS	GLU	ALA	SER	ALA	PRO	THR	PRO	LEU	GLU	ASP	TYR	LYS	ASP	ASP	ASP	ASP	ASP	LYS											

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33986	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.023	Depositor
Minimum map value	-0.389	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	420.48, 420.48, 420.48	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.095, 1.095, 1.095	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.13	0/6985	0.37	0/9482
1	B	0.14	0/6974	0.35	0/9467
1	C	0.13	0/6985	0.35	0/9482
1	D	0.13	0/7003	0.35	0/9505
1	E	0.23	0/7003	0.46	0/9505
1	F	0.13	0/7009	0.35	0/9512
All	All	0.15	0/41959	0.38	0/56953

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6806	0	6546	202	0
1	B	6796	0	6539	211	0
1	C	6806	0	6546	206	0
1	D	6824	0	6565	208	0
1	E	6824	0	6565	548	0
1	F	6830	0	6576	221	0
All	All	40886	0	39337	1580	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 20.

All (1580) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:GLY:CA	1:E:161:PRO:HA	1.57	1.34
1:B:412:MET:SD	1:B:514:SER:HB2	1.78	1.22
1:E:93:GLY:HA3	1:E:161:PRO:CA	1.69	1.21
1:E:100:LEU:HG	1:E:156:PHE:H	1.19	1.08
1:A:699:VAL:HG22	1:A:741:ILE:HD12	1.30	1.07
1:E:73:GLU:HG3	1:E:253:VAL:HG23	1.35	1.07
1:E:102:LEU:HA	1:E:192:VAL:HA	1.35	1.05
1:E:174:ILE:HG23	1:E:199:LEU:HG	1.46	0.97
1:E:48:ASN:HA	1:E:87:ARG:HB3	1.48	0.94
1:E:161:PRO:HG2	1:E:266:VAL:HG11	1.48	0.92
1:E:52:ARG:HG2	1:E:83:TYR:HB3	1.49	0.92
1:E:73:GLU:HA	1:E:76:ARG:HD3	1.53	0.91
1:E:224:LYS:HG2	1:E:225:THR:HG22	1.52	0.90
1:B:485:THR:HG22	1:B:489:LYS:HZ3	1.39	0.87
1:B:215:LYS:HB2	1:B:218:HIS:HB2	1.54	0.87
1:E:159:LEU:HD11	1:E:258:LEU:HD23	1.54	0.87
1:E:85:LEU:HA	1:E:209:LEU:HA	1.57	0.86
1:E:146:LYS:HB2	1:E:155:GLY:H	1.40	0.86
1:D:481:MET:HE2	1:D:515:LYS:HD3	1.56	0.86
1:A:699:VAL:CG2	1:A:741:ILE:HD12	2.06	0.84
1:F:749:THR:HA	1:F:752:ARG:HE	1.40	0.84
1:E:143:PHE:HD2	1:E:225:THR:HG23	1.43	0.83
1:E:51:ASN:HD22	1:E:56:LYS:HG3	1.44	0.82
1:A:536:ARG:NH1	1:A:537:GLN:O	2.13	0.81
1:E:91:TYR:HB3	1:E:164:LYS:HD2	1.62	0.81
1:A:538:ARG:HH12	1:B:461:ARG:HH22	1.29	0.80
1:E:21:LEU:HD12	1:E:24:VAL:HG23	1.63	0.80
1:E:94:LEU:HB2	1:E:170:LYS:HE3	1.63	0.80
1:E:40:THR:HG21	1:E:47:THR:HG22	1.63	0.80
1:E:100:LEU:HD13	1:E:192:VAL:HG21	1.64	0.80
1:E:127:LYS:HG2	1:E:236:PRO:HA	1.62	0.79
1:E:142:PHE:HA	1:E:226:GLY:HA2	1.64	0.79
1:E:69:TYR:HB3	1:E:253:VAL:HB	1.63	0.79
1:E:211:TYR:HB3	1:E:253:VAL:HA	1.63	0.79
1:E:51:ASN:HA	1:E:84:PHE:HA	1.65	0.79
1:E:163:LEU:HA	1:E:269:VAL:HB	1.66	0.77
1:E:208:SER:HB3	1:E:258:LEU:HD21	1.67	0.77
1:E:181:ALA:HA	1:E:184:GLN:HG3	1.65	0.77
1:F:466:PRO:HB2	1:F:469:LEU:HB2	1.67	0.76
1:C:806:GLN:HA	1:C:810:ASN:HA	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:VAL:HG23	1:B:184:GLN:HE21	1.51	0.75
1:E:146:LYS:HG2	1:E:221:TYR:CE1	2.21	0.75
1:E:161:PRO:HB3	1:E:258:LEU:HA	1.68	0.75
1:F:73:GLU:HG2	1:F:252:LEU:HG	1.68	0.75
1:A:699:VAL:HG12	1:A:700:LEU:N	2.01	0.75
1:E:102:LEU:HD13	1:E:153:LYS:HB3	1.68	0.75
1:E:127:LYS:HA	1:E:131:VAL:HG21	1.68	0.74
1:C:21:LEU:HD11	1:C:80:ALA:HB2	1.67	0.74
1:D:376:ARG:HE	1:D:428:ASN:HA	1.52	0.74
1:C:111:GLU:HG2	1:C:113:PRO:HD2	1.69	0.74
1:D:567:LEU:HD22	1:D:584:TYR:HD2	1.52	0.74
1:D:64:GLU:HA	1:D:67:ARG:HG2	1.68	0.74
1:E:141:PHE:CE1	1:E:229:LEU:HB3	2.22	0.74
1:F:145:LEU:HD22	1:F:224:LYS:HE3	1.70	0.73
1:C:342:PHE:HA	1:C:345:LYS:HD3	1.69	0.73
1:D:653:LEU:HD23	1:D:658:ALA:HB2	1.70	0.73
1:E:23:GLU:HB3	1:E:78:GLN:HE22	1.52	0.73
1:E:100:LEU:HG	1:E:156:PHE:N	2.00	0.73
1:A:699:VAL:HG22	1:A:741:ILE:CD1	2.16	0.73
1:F:159:LEU:HD11	1:F:258:LEU:HD21	1.71	0.73
1:B:313:GLU:HA	1:B:316:VAL:HG22	1.70	0.73
1:D:513:ARG:O	1:D:517:LYS:NZ	2.20	0.73
1:E:107:VAL:HA	1:E:153:LYS:HZ2	1.53	0.72
1:C:406:VAL:HG23	1:C:411:GLY:HA2	1.70	0.72
1:E:87:ARG:HA	1:E:207:PRO:HB3	1.70	0.72
1:E:470:HIS:HA	1:E:473:ILE:HG12	1.71	0.72
1:F:174:ILE:HD12	1:F:199:LEU:HD21	1.70	0.72
1:C:525:LYS:HE2	1:C:529:ARG:HE	1.52	0.72
1:E:262:GLN:HA	1:E:268:PRO:HD3	1.72	0.72
1:C:108:PRO:HB2	1:C:190:GLN:HB3	1.72	0.71
1:E:93:GLY:HA3	1:E:161:PRO:HA	0.77	0.71
1:B:95:MET:HE3	1:B:258:LEU:HD21	1.72	0.71
1:D:459:LYS:NZ	1:D:553:VAL:O	2.23	0.71
1:E:11:THR:HG23	1:E:14:LEU:HB2	1.72	0.71
1:E:127:LYS:HD2	1:E:233:SER:HA	1.73	0.71
1:E:82:MET:HG2	1:E:213:SER:HA	1.72	0.71
1:E:94:LEU:HD23	1:E:160:ILE:HG13	1.73	0.71
1:D:139:ILE:N	1:D:229:LEU:O	2.24	0.71
1:D:145:LEU:HD22	1:D:224:LYS:HE3	1.73	0.71
1:A:67:ARG:O	1:A:71:HIS:ND1	2.23	0.70
1:D:529:ARG:NH2	1:D:530:GLN:OE1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:CYS:SG	1:E:141:PHE:HB3	2.30	0.70
1:A:701:ASN:HD21	1:A:704:ARG:HD2	1.55	0.70
1:F:621:ALA:HB1	1:F:688:TYR:HB2	1.74	0.70
1:F:111:GLU:HG2	1:F:114:ALA:H	1.56	0.70
1:A:594:THR:HG23	1:A:797:ILE:HD11	1.72	0.70
1:B:485:THR:HA	1:B:488:ILE:HD12	1.74	0.70
1:C:755:HIS:HB3	1:C:825:THR:HA	1.71	0.70
1:B:636:GLY:O	1:B:737:ASN:ND2	2.24	0.70
1:C:91:TYR:HB3	1:C:164:LYS:HB2	1.73	0.70
1:F:550:LEU:O	1:F:624:ARG:NH2	2.25	0.70
1:C:567:LEU:HD22	1:C:584:TYR:HD2	1.56	0.69
1:E:45:LYS:HZ2	1:E:47:THR:HG23	1.56	0.69
1:B:412:MET:SD	1:B:514:SER:CB	2.72	0.69
1:F:153:LYS:HG3	1:F:154:TYR:H	1.58	0.69
1:D:877:ALA:HB3	1:D:880:LEU:HD23	1.73	0.69
1:E:45:LYS:NZ	1:E:47:THR:HG23	2.07	0.69
1:E:140:HIS:CD2	1:E:266:VAL:HA	2.27	0.69
1:E:144:THR:HA	1:E:223:LEU:HA	1.74	0.69
1:E:303:LEU:HA	1:E:306:ILE:HG12	1.74	0.69
1:F:31:LEU:HA	1:F:35:LEU:HB3	1.73	0.69
1:E:710:ASN:OD1	1:F:647:ARG:NH2	2.27	0.68
1:A:376:ARG:NH1	1:A:428:ASN:O	2.27	0.68
1:E:51:ASN:HB3	1:E:56:LYS:HB2	1.74	0.68
1:E:125:HIS:CD2	1:E:177:LEU:HD22	2.28	0.68
1:E:593:TRP:CD1	1:E:789:ASP:HB2	2.29	0.68
1:A:466:PRO:HB2	1:A:469:LEU:HB2	1.75	0.68
1:E:140:HIS:HA	1:E:228:GLU:HG3	1.76	0.68
1:B:552:GLY:HA2	1:B:557:VAL:HG22	1.75	0.68
1:E:143:PHE:HB2	1:E:224:LYS:HD2	1.74	0.68
1:D:642:LYS:HE2	1:D:735:ALA:HB1	1.74	0.68
1:E:414:GLU:CD	1:E:415:HIS:H	2.02	0.68
1:E:72:LEU:HD22	1:E:210:LEU:HB3	1.76	0.68
1:E:49:ILE:HD12	1:E:210:LEU:HD11	1.77	0.67
1:E:589:PRO:O	1:E:595:LYS:NZ	2.25	0.67
1:B:550:LEU:HB3	1:B:576:ILE:HD11	1.76	0.67
1:C:466:PRO:HB2	1:C:469:LEU:HB2	1.76	0.67
1:C:550:LEU:O	1:C:624:ARG:NH2	2.28	0.67
1:E:41:GLU:HB2	1:E:42:PRO:HD2	1.75	0.67
1:F:76:ARG:HD2	1:F:212:GLY:HA3	1.75	0.67
1:A:139:ILE:N	1:A:229:LEU:O	2.27	0.67
1:F:585:VAL:HG13	1:F:586:PRO:HD2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:LEU:HD22	1:E:215:LYS:HZ2	1.60	0.67
1:C:841:GLU:HG3	1:C:842:ARG:HG2	1.76	0.67
1:B:585:VAL:HG13	1:B:586:PRO:HD2	1.77	0.66
1:C:621:ALA:HB1	1:C:688:TYR:HB2	1.76	0.66
1:E:512:GLU:HA	1:E:515:LYS:HZ3	1.59	0.66
1:D:153:LYS:HG3	1:D:154:TYR:H	1.60	0.66
1:E:124:VAL:HG13	1:E:236:PRO:HB2	1.75	0.66
1:C:485:THR:HG22	1:C:489:LYS:HZ2	1.59	0.66
1:F:497:GLU:O	1:F:501:LEU:N	2.29	0.66
1:F:757:ARG:NH1	1:F:758:SER:O	2.29	0.66
1:A:375:LYS:HD2	1:A:379:MET:HE1	1.77	0.66
1:D:358:LEU:O	1:D:362:TRP:N	2.27	0.66
1:E:486:GLU:HA	1:E:489:LYS:HG2	1.77	0.66
1:C:372:LYS:HE2	1:C:574:HIS:HA	1.78	0.66
1:E:119:CYS:HA	1:E:122:ILE:HG23	1.77	0.66
1:A:64:GLU:HA	1:A:67:ARG:HG3	1.77	0.66
1:C:584:TYR:HA	1:C:795:PHE:HE2	1.60	0.66
1:E:35:LEU:HB3	1:E:58:TYR:CE1	2.31	0.66
1:F:219:LYS:HG2	1:F:220:PRO:HD2	1.77	0.66
1:B:466:PRO:HB2	1:B:469:LEU:HB2	1.79	0.65
1:D:466:PRO:HB2	1:D:469:LEU:HB2	1.78	0.65
1:C:632:LEU:HD13	1:C:754:ARG:HB2	1.77	0.65
1:B:188:HIS:HE1	1:B:195:PRO:HB3	1.60	0.65
1:D:62:SER:HB3	1:D:262:GLN:HE22	1.62	0.65
1:E:36:SER:HA	1:E:39:LEU:HB2	1.78	0.65
1:A:699:VAL:HG12	1:A:700:LEU:H	1.61	0.65
1:B:105:ASN:HA	1:B:153:LYS:HD3	1.77	0.65
1:E:143:PHE:CD2	1:E:225:THR:HG23	2.30	0.65
1:D:350:TRP:HA	1:D:354:GLY:HA3	1.79	0.65
1:C:145:LEU:HD22	1:C:224:LYS:HE3	1.79	0.65
1:F:555:ASN:ND2	1:F:584:TYR:O	2.29	0.65
1:C:413:LEU:HA	1:C:417:MET:SD	2.37	0.65
1:E:119:CYS:HG	1:E:143:PHE:HE1	1.45	0.65
1:E:15:THR:O	1:E:18:ARG:HG2	1.97	0.64
1:F:139:ILE:N	1:F:229:LEU:O	2.30	0.64
1:A:941:LYS:NZ	1:A:946:SER:OG	2.30	0.64
1:B:153:LYS:HG3	1:B:154:TYR:H	1.62	0.64
1:E:46:LYS:HD3	1:E:59:ALA:HB2	1.79	0.64
1:D:639:CYS:HB2	1:D:761:LYS:HE2	1.79	0.64
1:E:15:THR:HA	1:E:18:ARG:HD2	1.79	0.64
1:B:147:PRO:HG2	1:B:219:LYS:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:LEU:HD22	1:E:78:GLN:HG3	1.80	0.64
1:A:254:SER:OG	1:A:260:ASN:ND2	2.30	0.64
1:E:66:LEU:HD12	1:E:67:ARG:HE	1.63	0.64
1:F:851:THR:H	1:F:904:LYS:HA	1.61	0.64
1:A:867:ASN:HB3	1:A:872:VAL:HG22	1.80	0.64
1:B:145:LEU:HD22	1:B:224:LYS:HE3	1.79	0.64
1:B:255:GLU:HG3	1:B:265:LEU:HB3	1.80	0.64
1:C:30:LEU:HD11	1:C:67:ARG:HH21	1.63	0.64
1:D:31:LEU:HD23	1:D:35:LEU:HD22	1.78	0.64
1:E:58:TYR:HB3	1:E:60:LEU:HD21	1.80	0.64
1:E:95:MET:HB3	1:E:204:ALA:HA	1.80	0.64
1:D:460:TRP:HD1	1:D:575:PRO:HA	1.62	0.64
1:B:761:LYS:HD2	1:B:763:CYS:H	1.63	0.64
1:B:844:VAL:HB	1:B:919:GLU:HB3	1.79	0.64
1:D:547:ASN:OD1	1:D:549:HIS:CD2	2.51	0.64
1:E:141:PHE:HA	1:E:160:ILE:HD13	1.80	0.64
1:A:481:MET:HA	1:A:484:ILE:HD12	1.80	0.63
1:D:844:VAL:HB	1:D:919:GLU:HB3	1.80	0.63
1:E:250:TYR:HB3	1:E:264:SER:HB3	1.79	0.63
1:F:653:LEU:HD23	1:F:658:ALA:HB2	1.80	0.63
1:B:30:LEU:HD11	1:B:67:ARG:HH21	1.64	0.63
1:C:31:LEU:HD23	1:C:35:LEU:HD22	1.80	0.63
1:C:94:LEU:HB2	1:C:160:ILE:HB	1.80	0.63
1:D:460:TRP:CD1	1:D:575:PRO:HA	2.33	0.63
1:F:215:LYS:HB2	1:F:218:HIS:HB2	1.80	0.63
1:C:486:GLU:HA	1:C:489:LYS:HE2	1.79	0.63
1:C:850:GLU:HA	1:C:905:GLY:H	1.63	0.63
1:E:52:ARG:HD3	1:E:85:LEU:HD11	1.80	0.63
1:E:202:HIS:HB2	1:E:206:VAL:HG13	1.81	0.63
1:F:578:GLN:OE1	1:F:656:HIS:ND1	2.32	0.63
1:D:868:THR:HG21	1:D:911:LYS:CE	2.29	0.63
1:E:69:TYR:CE2	1:E:260:ASN:HB2	2.34	0.63
1:E:459:LYS:NZ	1:E:556:GLY:O	2.32	0.63
1:E:117:ARG:HA	1:E:120:HIS:CD2	2.32	0.63
1:A:363:ASN:O	1:A:367:HIS:CD2	2.51	0.63
1:D:95:MET:HE3	1:D:258:LEU:HD21	1.79	0.63
1:E:223:LEU:HD13	1:E:256:LEU:HD21	1.80	0.63
1:B:139:ILE:N	1:B:229:LEU:O	2.32	0.63
1:B:549:HIS:HD2	1:B:560:ILE:HG13	1.63	0.63
1:D:481:MET:HA	1:D:484:ILE:HD12	1.81	0.63
1:E:20:TYR:CD1	1:E:21:LEU:HD23	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:630:LEU:HA	1:F:752:ARG:HB3	1.81	0.63
1:B:525:LYS:HB3	1:B:529:ARG:HH12	1.65	0.62
1:A:145:LEU:HD22	1:A:224:LYS:HE3	1.81	0.62
1:D:31:LEU:HA	1:D:35:LEU:HB3	1.81	0.62
1:D:859:VAL:HA	1:D:862:TYR:CE2	2.34	0.62
1:D:16:ALA:O	1:D:20:TYR:HB2	1.99	0.62
1:E:22:ALA:C	1:E:24:VAL:N	2.54	0.62
1:E:72:LEU:O	1:E:76:ARG:HG3	1.99	0.62
1:E:83:TYR:CE2	1:E:216:LEU:HA	2.34	0.62
1:C:376:ARG:NH2	1:C:428:ASN:O	2.32	0.62
1:E:31:LEU:HA	1:E:35:LEU:HB2	1.80	0.62
1:E:350:TRP:HA	1:E:354:GLY:HA3	1.82	0.62
1:B:98:TYR:HD2	1:B:156:PHE:HB3	1.64	0.62
1:B:83:TYR:HE1	1:B:214:SER:HB3	1.64	0.62
1:E:187:LEU:HB3	1:E:192:VAL:HB	1.82	0.62
1:F:700:LEU:HD21	1:F:742:ILE:HG12	1.80	0.62
1:E:550:LEU:O	1:E:624:ARG:NH2	2.33	0.62
1:B:578:GLN:OE1	1:B:656:HIS:ND1	2.33	0.62
1:A:757:ARG:NH1	1:A:758:SER:O	2.33	0.61
1:B:159:LEU:HG	1:B:161:PRO:HD3	1.81	0.61
1:C:105:ASN:HA	1:C:153:LYS:HD3	1.81	0.61
1:F:864:GLU:OE2	1:F:868:THR:HG21	2.00	0.61
1:C:315:TYR:HB2	1:C:346:CYS:HB2	1.80	0.61
1:B:653:LEU:HD23	1:B:658:ALA:HB2	1.82	0.61
1:E:73:GLU:HG2	1:E:252:LEU:HG	1.81	0.61
1:E:142:PHE:HD1	1:E:226:GLY:HA3	1.65	0.61
1:D:574:HIS:HB3	1:D:576:ILE:HD11	1.83	0.61
1:F:85:LEU:HD23	1:F:209:LEU:HB3	1.81	0.61
1:B:142:PHE:HB2	1:B:159:LEU:HB3	1.82	0.61
1:E:53:ILE:HG13	1:E:83:TYR:CD2	2.35	0.61
1:E:416:TYR:H	1:E:530:GLN:NE2	1.99	0.61
1:A:699:VAL:CG1	1:A:700:LEU:H	2.13	0.61
1:E:142:PHE:HB3	1:E:223:LEU:CD1	2.30	0.61
1:F:94:LEU:HB2	1:F:160:ILE:HB	1.82	0.61
1:A:699:VAL:CG1	1:A:700:LEU:N	2.63	0.61
1:D:376:ARG:HG2	1:D:571:PHE:CZ	2.35	0.61
1:D:578:GLN:HG3	1:D:656:HIS:HB3	1.82	0.61
1:E:87:ARG:HB2	1:E:87:ARG:CZ	2.30	0.61
1:C:481:MET:HE1	1:C:515:LYS:HE3	1.81	0.61
1:F:28:GLU:HA	1:F:31:LEU:HD12	1.82	0.61
1:F:255:GLU:HG3	1:F:265:LEU:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:LEU:HG	1:E:58:TYR:CE1	2.36	0.61
1:E:174:ILE:HG21	1:E:201:PRO:HA	1.83	0.61
1:F:842:ARG:HA	1:F:909:LEU:HB2	1.82	0.61
1:B:350:TRP:HA	1:B:354:GLY:HA3	1.82	0.60
1:B:907:ARG:HH21	1:B:919:GLU:HG3	1.66	0.60
1:C:830:LYS:O	1:C:837:ARG:NH1	2.32	0.60
1:E:143:PHE:HB3	1:E:156:PHE:CE1	2.36	0.60
1:A:21:LEU:HD11	1:A:80:ALA:HB2	1.83	0.60
1:C:50:ILE:HG23	1:C:85:LEU:HB2	1.83	0.60
1:A:470:HIS:HA	1:A:473:ILE:HG22	1.84	0.60
1:F:481:MET:HE1	1:F:518:ILE:HG21	1.83	0.60
1:E:188:HIS:HE1	1:E:195:PRO:HB3	1.66	0.60
1:A:940:ASN:O	1:A:944:GLU:N	2.27	0.60
1:B:548:PRO:HG2	1:B:549:HIS:CE1	2.37	0.60
1:F:105:ASN:HA	1:F:153:LYS:HD3	1.82	0.60
1:F:187:LEU:HB3	1:F:192:VAL:HB	1.83	0.60
1:B:54:THR:OG1	1:B:56:LYS:NZ	2.24	0.60
1:D:757:ARG:NH1	1:D:758:SER:O	2.34	0.60
1:F:47:THR:O	1:F:87:ARG:NH1	2.35	0.60
1:B:253:VAL:HA	1:B:256:LEU:HB2	1.84	0.60
1:C:14:LEU:HB3	1:C:18:ARG:HH21	1.66	0.60
1:D:146:LYS:NZ	1:D:221:TYR:OH	2.32	0.60
1:E:19:LYS:HZ3	1:E:407:TYR:HB3	1.67	0.60
1:E:53:ILE:H	1:E:83:TYR:HB2	1.67	0.60
1:E:72:LEU:HD13	1:E:210:LEU:HD22	1.84	0.60
1:E:122:ILE:HG22	1:E:177:LEU:HD21	1.83	0.60
1:E:513:ARG:O	1:E:517:LYS:NZ	2.24	0.60
1:B:330:ASN:ND2	1:B:373:ILE:O	2.35	0.60
1:C:750:TRP:HA	1:C:753:LEU:HD12	1.83	0.60
1:D:105:ASN:HA	1:D:153:LYS:HD3	1.84	0.60
1:D:557:VAL:HG21	1:D:576:ILE:HD13	1.84	0.60
1:E:38:PHE:HB3	1:E:59:ALA:O	2.02	0.60
1:B:72:LEU:O	1:B:76:ARG:HG2	2.02	0.59
1:E:182:THR:HA	1:E:185:LYS:HD3	1.83	0.59
1:E:45:LYS:NZ	1:E:87:ARG:HH12	2.00	0.59
1:B:123:PHE:O	1:B:127:LYS:HG2	2.02	0.59
1:B:335:TYR:HB3	1:B:338:LEU:HD12	1.84	0.59
1:D:94:LEU:HD23	1:D:160:ILE:HB	1.83	0.59
1:E:147:PRO:HA	1:E:222:GLN:HE22	1.67	0.59
1:F:414:GLU:HG3	1:F:415:HIS:H	1.66	0.59
1:B:866:TYR:HE2	1:B:873:LYS:HZ3	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:PHE:O	1:C:157:HIS:ND1	2.35	0.59
1:B:30:LEU:HD12	1:B:34:GLU:HB2	1.85	0.59
1:B:294:MET:HB2	1:B:301:ARG:HG3	1.85	0.59
1:D:616:PHE:O	1:D:620:THR:HG23	2.02	0.59
1:F:47:THR:HA	1:F:59:ALA:HB2	1.85	0.59
1:F:515:LYS:O	1:F:518:ILE:HG12	2.02	0.59
1:B:185:LYS:HE3	1:B:186:ILE:HG13	1.84	0.59
1:E:126:ILE:HG22	1:E:173:ILE:HG13	1.85	0.59
1:F:489:LYS:HA	1:F:492:LEU:HD12	1.83	0.59
1:D:162:GLY:O	1:D:269:VAL:N	2.35	0.59
1:E:536:ARG:NH1	1:F:467:ASP:OD2	2.35	0.59
1:B:525:LYS:HB3	1:B:529:ARG:NH1	2.17	0.59
1:C:31:LEU:HA	1:C:35:LEU:HB3	1.84	0.59
1:D:846:SER:N	1:D:905:GLY:O	2.36	0.59
1:E:51:ASN:ND2	1:E:56:LYS:HG3	2.16	0.59
1:E:81:LEU:HG	1:E:83:TYR:CE1	2.38	0.59
1:E:211:TYR:CZ	1:E:223:LEU:HB3	2.38	0.59
1:E:127:LYS:HD3	1:E:131:VAL:HG11	1.85	0.58
1:E:142:PHE:HA	1:E:226:GLY:CA	2.33	0.58
1:E:146:LYS:CB	1:E:155:GLY:H	2.16	0.58
1:C:159:LEU:HG	1:C:161:PRO:HD3	1.86	0.58
1:C:584:TYR:HA	1:C:795:PHE:CE2	2.37	0.58
1:E:565:ALA:N	1:E:803:GLU:OE2	2.36	0.58
1:B:182:THR:O	1:B:185:LYS:HG3	2.04	0.58
1:C:100:LEU:HD11	1:C:192:VAL:HG11	1.85	0.58
1:C:567:LEU:HD22	1:C:584:TYR:CD2	2.37	0.58
1:D:67:ARG:O	1:D:71:HIS:ND1	2.35	0.58
1:D:184:GLN:O	1:D:188:HIS:ND1	2.36	0.58
1:E:20:TYR:CZ	1:E:500:ILE:HG13	2.37	0.58
1:E:20:TYR:HE2	1:E:496:HIS:ND1	1.99	0.58
1:E:215:LYS:HB2	1:E:218:HIS:HB2	1.85	0.58
1:D:15:THR:HG22	1:D:18:ARG:HH22	1.69	0.58
1:E:211:TYR:O	1:E:253:VAL:HG22	2.03	0.58
1:E:859:VAL:HG13	1:E:880:LEU:HD11	1.85	0.58
1:D:28:GLU:HA	1:D:31:LEU:HD12	1.86	0.58
1:D:494:GLN:HB2	1:D:496:HIS:NE2	2.19	0.58
1:E:200:ASP:HB3	1:E:202:HIS:CE1	2.39	0.58
1:E:776:GLU:HG3	1:E:778:PRO:HD3	1.84	0.58
1:B:592:PRO:HA	1:B:595:LYS:HE3	1.85	0.58
1:C:398:TYR:CZ	1:C:425:MET:HA	2.38	0.58
1:D:634:TRP:NE1	1:D:758:SER:OG	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:GLY:O	1:D:459:LYS:NZ	2.35	0.58
1:E:145:LEU:HB2	1:E:154:TYR:CD2	2.39	0.58
1:E:251:ASN:HB2	1:E:254:SER:HB2	1.85	0.58
1:F:615:MET:HA	1:F:618:LEU:HG	1.86	0.58
1:B:184:GLN:O	1:B:187:LEU:HG	2.03	0.58
1:B:188:HIS:CE1	1:B:195:PRO:HB3	2.38	0.58
1:C:826:GLU:OE2	1:C:836:HIS:NE2	2.31	0.58
1:E:585:VAL:HG13	1:E:586:PRO:HD2	1.85	0.58
1:F:422:ILE:HG12	1:F:473:ILE:HG22	1.84	0.58
1:D:91:TYR:HB3	1:D:164:LYS:HB2	1.85	0.57
1:D:111:GLU:HB3	1:D:113:PRO:HD2	1.85	0.57
1:E:112:PRO:HA	1:E:115:LEU:HD12	1.84	0.57
1:E:455:GLY:HA2	1:E:554:GLY:HA2	1.86	0.57
1:F:175:GLY:O	1:F:179:HIS:ND1	2.33	0.57
1:A:653:LEU:HD23	1:A:658:ALA:HB2	1.86	0.57
1:E:49:ILE:HB	1:E:58:TYR:HB2	1.85	0.57
1:F:557:VAL:O	1:F:568:ILE:N	2.35	0.57
1:F:567:LEU:HD22	1:F:584:TYR:HD2	1.69	0.57
1:C:661:LEU:HD23	1:C:691:PHE:HE1	1.69	0.57
1:C:757:ARG:NH1	1:C:758:SER:O	2.37	0.57
1:D:85:LEU:HD23	1:D:209:LEU:HB3	1.86	0.57
1:D:410:ASN:ND2	1:E:512:GLU:OE2	2.37	0.57
1:E:142:PHE:HD2	1:E:159:LEU:HB3	1.68	0.57
1:E:562:THR:OG1	1:E:566:LYS:NZ	2.35	0.57
1:A:590:GLU:O	1:A:595:LYS:NZ	2.37	0.57
1:D:123:PHE:O	1:D:127:LYS:HG2	2.05	0.57
1:E:76:ARG:HH11	1:E:253:VAL:HG22	1.68	0.57
1:F:339:ALA:HB1	1:F:358:LEU:HD11	1.87	0.57
1:A:31:LEU:HA	1:A:35:LEU:HB3	1.86	0.57
1:C:661:LEU:HD11	1:C:665:LEU:HD12	1.85	0.57
1:E:74:GLN:HA	1:E:77:LYS:HE2	1.85	0.57
1:E:110:LEU:HD13	1:E:224:LYS:HE2	1.85	0.57
1:E:143:PHE:CE2	1:E:227:PHE:HB3	2.40	0.57
1:F:75:CYS:HA	1:F:78:GLN:HE21	1.69	0.57
1:F:889:LEU:O	1:F:891:LYS:N	2.38	0.57
1:A:584:TYR:HE1	1:A:799:VAL:HG21	1.68	0.57
1:C:252:LEU:HD23	1:C:256:LEU:HD23	1.87	0.57
1:D:851:THR:H	1:D:904:LYS:HA	1.68	0.57
1:E:20:TYR:CE1	1:E:500:ILE:HG13	2.39	0.57
1:E:121:ARG:NH1	1:E:124:VAL:HB	2.20	0.57
1:F:498:SER:HA	1:F:501:LEU:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:TYR:CZ	1:A:425:MET:HA	2.39	0.57
1:E:22:ALA:O	1:E:23:GLU:C	2.45	0.57
1:E:69:TYR:HE2	1:E:260:ASN:HB2	1.69	0.57
1:E:555:ASN:ND2	1:E:584:TYR:O	2.37	0.57
1:A:219:LYS:HG2	1:A:220:PRO:HD2	1.86	0.57
1:A:584:TYR:CE1	1:A:799:VAL:HG21	2.40	0.57
1:B:291:SER:HA	1:B:294:MET:HE2	1.86	0.57
1:B:490:TYR:O	1:B:494:GLN:NE2	2.27	0.57
1:C:340:GLU:O	1:C:344:GLN:NE2	2.37	0.57
1:D:432:VAL:HG21	1:D:532:GLU:HA	1.86	0.57
1:E:97:ASP:H	1:E:203:SER:HB3	1.68	0.57
1:E:568:ILE:HG21	1:E:572:HIS:HB3	1.85	0.57
1:E:15:THR:O	1:E:19:LYS:HG2	2.04	0.57
1:E:842:ARG:HA	1:E:909:LEU:HB2	1.87	0.57
1:A:49:ILE:HG23	1:A:58:TYR:HB2	1.87	0.57
1:C:293:LEU:HD22	1:C:337:PRO:HB2	1.87	0.57
1:E:894:GLN:H	1:E:903:LEU:HA	1.69	0.57
1:C:459:LYS:NZ	1:C:553:VAL:O	2.27	0.56
1:E:40:THR:HB	1:E:47:THR:HB	1.86	0.56
1:E:164:LYS:HG2	1:E:261:GLU:HG3	1.87	0.56
1:E:515:LYS:O	1:E:518:ILE:HG12	2.05	0.56
1:B:940:ASN:O	1:B:944:GLU:N	2.31	0.56
1:C:375:LYS:HA	1:C:378:ILE:HD13	1.88	0.56
1:E:75:CYS:O	1:E:78:GLN:HG2	2.05	0.56
1:E:121:ARG:HG2	1:E:180:ASP:CG	2.30	0.56
1:E:184:GLN:HB3	1:E:195:PRO:HB2	1.87	0.56
1:B:842:ARG:HA	1:B:909:LEU:HB2	1.86	0.56
1:E:18:ARG:HB2	1:E:25:GLN:HE22	1.70	0.56
1:E:48:ASN:ND2	1:E:59:ALA:HA	2.20	0.56
1:E:208:SER:CB	1:E:258:LEU:HD21	2.34	0.56
1:E:850:GLU:HA	1:E:905:GLY:H	1.70	0.56
1:F:185:LYS:HA	1:F:188:HIS:HB2	1.86	0.56
1:A:753:LEU:O	1:A:754:ARG:NH1	2.32	0.56
1:B:375:LYS:NZ	1:B:428:ASN:OD1	2.39	0.56
1:B:585:VAL:CG1	1:B:586:PRO:HD2	2.35	0.56
1:B:615:MET:HE1	1:B:801:PHE:HB3	1.88	0.56
1:A:142:PHE:HB2	1:A:159:LEU:HB2	1.87	0.56
1:A:153:LYS:HG3	1:A:154:TYR:H	1.71	0.56
1:D:588:ASN:HD22	1:D:591:ASN:HB2	1.70	0.56
1:E:65:LEU:HB3	1:E:69:TYR:CE2	2.41	0.56
1:F:161:PRO:HB3	1:F:258:LEU:HD23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:550:LEU:HD13	1:F:576:ILE:HD11	1.85	0.56
1:A:521:ASP:OD2	1:F:529:ARG:NH1	2.37	0.56
1:B:75:CYS:O	1:B:79:GLY:N	2.38	0.56
1:B:826:GLU:HG3	1:B:830:LYS:HE3	1.88	0.56
1:D:489:LYS:HA	1:D:492:LEU:HD12	1.88	0.56
1:E:45:LYS:C	1:E:47:THR:H	2.14	0.56
1:E:321:TRP:HE1	1:E:358:LEU:HD13	1.70	0.56
1:F:842:ARG:HH12	1:F:911:LYS:HD3	1.69	0.56
1:B:432:VAL:HG22	1:B:442:TRP:CD1	2.41	0.56
1:D:907:ARG:NH1	1:D:913:GLU:OE2	2.39	0.56
1:E:87:ARG:HA	1:E:207:PRO:CB	2.35	0.56
1:F:858:VAL:HG22	1:F:908:ILE:HD11	1.88	0.56
1:F:896:SER:HB2	1:F:900:THR:H	1.70	0.56
1:B:850:GLU:HA	1:B:905:GLY:H	1.70	0.56
1:E:102:LEU:HD21	1:E:108:PRO:HG3	1.88	0.56
1:E:398:TYR:CZ	1:E:425:MET:HA	2.41	0.56
1:F:74:GLN:HA	1:F:77:LYS:HE2	1.86	0.56
1:F:481:MET:HA	1:F:484:ILE:HD12	1.87	0.56
1:D:307:LEU:HD13	1:D:341:TRP:HZ3	1.71	0.56
1:E:250:TYR:HB3	1:E:264:SER:CB	2.36	0.56
1:F:585:VAL:CG1	1:F:586:PRO:HD2	2.35	0.56
1:A:630:LEU:HD11	1:A:754:ARG:HG2	1.88	0.55
1:C:851:THR:H	1:C:904:LYS:HA	1.69	0.55
1:E:98:TYR:CD1	1:E:199:LEU:HD13	2.42	0.55
1:E:578:GLN:OE1	1:E:656:HIS:ND1	2.39	0.55
1:F:312:PRO:HA	1:F:315:TYR:CZ	2.42	0.55
1:F:497:GLU:HB3	1:F:500:ILE:HG22	1.88	0.55
1:C:85:LEU:HD23	1:C:209:LEU:HB3	1.87	0.55
1:C:519:PHE:HA	1:C:524:LYS:HZ1	1.71	0.55
1:D:254:SER:OG	1:D:260:ASN:ND2	2.39	0.55
1:A:422:ILE:HG13	1:A:473:ILE:HD12	1.86	0.55
1:B:187:LEU:HD21	1:B:195:PRO:HA	1.87	0.55
1:C:497:GLU:HB3	1:C:500:ILE:HG12	1.88	0.55
1:C:617:TYR:OH	1:C:732:MET:O	2.24	0.55
1:E:915:LEU:HD12	1:E:919:GLU:HB2	1.87	0.55
1:F:870:ILE:HG22	1:F:871:ASN:H	1.71	0.55
1:F:896:SER:HB2	1:F:900:THR:HG23	1.88	0.55
1:E:465:ASN:C	1:E:465:ASN:HD22	2.09	0.55
1:F:170:LYS:HE3	1:F:204:ALA:HB1	1.88	0.55
1:A:162:GLY:O	1:A:269:VAL:N	2.39	0.55
1:C:192:VAL:HG12	1:C:194:ASN:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:ALA:O	1:E:25:GLN:HG2	2.06	0.55
1:F:31:LEU:HD23	1:F:35:LEU:HD22	1.87	0.55
1:A:107:VAL:O	1:A:109:PRO:HD3	2.07	0.55
1:E:153:LYS:HZ3	1:E:154:TYR:HB3	1.72	0.55
1:E:210:LEU:O	1:E:213:SER:HB2	2.07	0.55
1:E:916:GLN:HG3	1:E:919:GLU:HG2	1.89	0.55
1:E:51:ASN:CA	1:E:84:PHE:HA	2.35	0.55
1:E:120:HIS:CE1	1:E:227:PHE:CZ	2.95	0.55
1:E:307:LEU:HD23	1:E:310:LEU:HD12	1.88	0.55
1:E:757:ARG:NH1	1:E:758:SER:O	2.40	0.55
1:E:844:VAL:HB	1:E:919:GLU:HB3	1.89	0.55
1:D:56:LYS:HD3	1:D:58:TYR:HE2	1.71	0.55
1:E:154:TYR:HH	1:E:190:GLN:HG3	1.72	0.55
1:B:486:GLU:HA	1:B:489:LYS:HE2	1.87	0.55
1:E:855:LEU:O	1:E:858:VAL:HG22	2.07	0.55
1:F:521:ASP:OD2	1:F:525:LYS:NZ	2.40	0.55
1:F:615:MET:HE1	1:F:801:PHE:CG	2.42	0.55
1:A:31:LEU:HD23	1:A:35:LEU:HD22	1.89	0.55
1:A:107:VAL:HG12	1:A:148:GLU:HG2	1.90	0.55
1:A:403:ALA:HA	1:A:406:VAL:HG12	1.88	0.55
1:A:461:ARG:NE	1:A:463:GLU:OE2	2.40	0.55
1:C:153:LYS:HG3	1:C:154:TYR:H	1.71	0.55
1:D:557:VAL:O	1:D:568:ILE:N	2.40	0.55
1:D:565:ALA:N	1:D:803:GLU:OE2	2.37	0.55
1:E:143:PHE:HB3	1:E:156:PHE:HE1	1.71	0.55
1:F:123:PHE:O	1:F:127:LYS:HG2	2.07	0.55
1:B:497:GLU:HB3	1:B:500:ILE:HG12	1.87	0.54
1:B:740:PHE:O	1:B:828:TYR:OH	2.23	0.54
1:C:485:THR:HG22	1:C:489:LYS:NZ	2.22	0.54
1:E:215:LYS:HE2	1:E:219:LYS:O	2.07	0.54
1:E:867:ASN:HB3	1:E:872:VAL:HG22	1.88	0.54
1:E:262:GLN:CD	1:E:262:GLN:H	2.14	0.54
1:F:82:MET:O	1:F:214:SER:N	2.41	0.54
1:B:896:SER:H	1:B:901:ARG:HA	1.71	0.54
1:D:215:LYS:HB2	1:D:218:HIS:HB2	1.89	0.54
1:E:19:LYS:HG3	1:E:407:TYR:HD1	1.72	0.54
1:E:52:ARG:CZ	1:E:215:LYS:HA	2.38	0.54
1:E:111:GLU:O	1:E:115:LEU:HG	2.06	0.54
1:E:159:LEU:HG	1:E:256:LEU:O	2.07	0.54
1:F:106:ALA:C	1:F:153:LYS:HZ3	2.15	0.54
1:A:52:ARG:HH22	1:A:215:LYS:HA	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:547:ASN:OD1	1:D:549:HIS:HD2	1.90	0.54
1:E:50:ILE:O	1:E:85:LEU:HD12	2.07	0.54
1:E:51:ASN:HA	1:E:84:PHE:CA	2.37	0.54
1:E:92:SER:HB2	1:E:258:LEU:HB2	1.90	0.54
1:E:100:LEU:HA	1:E:198:CYS:SG	2.47	0.54
1:F:369:THR:O	1:F:370:GLU:C	2.50	0.54
1:D:744:THR:HG21	1:D:749:THR:HG21	1.90	0.54
1:E:141:PHE:HB2	1:E:227:PHE:CD1	2.42	0.54
1:C:588:ASN:ND2	1:C:590:GLU:OE2	2.40	0.54
1:C:634:TRP:NE1	1:C:758:SER:OG	2.41	0.54
1:C:837:ARG:O	1:C:841:GLU:HG2	2.06	0.54
1:E:86:GLU:OE1	1:E:210:LEU:HA	2.08	0.54
1:E:145:LEU:HB3	1:E:224:LYS:NZ	2.21	0.54
1:E:466:PRO:HB2	1:E:469:LEU:HB2	1.89	0.54
1:B:294:MET:O	1:B:301:ARG:NE	2.29	0.54
1:D:398:TYR:CZ	1:D:425:MET:HA	2.42	0.54
1:E:185:LYS:HG2	1:E:186:ILE:N	2.23	0.54
1:E:214:SER:HA	1:E:220:PRO:N	2.23	0.54
1:A:86:GLU:O	1:A:208:SER:N	2.37	0.54
1:A:108:PRO:HB2	1:A:190:GLN:HB3	1.90	0.54
1:A:456:GLU:HA	1:A:459:LYS:HD2	1.90	0.54
1:A:553:VAL:HA	1:A:580:THR:HG22	1.90	0.54
1:A:616:PHE:O	1:A:620:THR:HG23	2.07	0.54
1:E:60:LEU:HD12	1:E:68:LEU:HD22	1.88	0.54
1:E:497:GLU:HB3	1:E:500:ILE:HG12	1.88	0.54
1:F:21:LEU:HD22	1:F:78:GLN:OE1	2.07	0.54
1:F:146:LYS:HB2	1:F:154:TYR:HB2	1.90	0.54
1:E:48:ASN:HA	1:E:87:ARG:CB	2.31	0.54
1:E:125:HIS:HD2	1:E:177:LEU:HD22	1.70	0.54
1:F:826:GLU:O	1:F:830:LYS:HG2	2.08	0.53
1:A:23:GLU:O	1:A:24:VAL:HB	2.09	0.53
1:B:51:ASN:HD22	1:B:84:PHE:HD1	1.56	0.53
1:B:403:ALA:O	1:B:404:GLU:HG3	2.07	0.53
1:B:830:LYS:O	1:B:837:ARG:NH1	2.36	0.53
1:D:589:PRO:HB3	1:D:943:TRP:NE1	2.22	0.53
1:E:254:SER:O	1:E:260:ASN:HB3	2.08	0.53
1:E:91:TYR:HA	1:E:165:LEU:HA	1.90	0.53
1:E:118:LEU:HD21	1:E:158:VAL:HG21	1.91	0.53
1:C:647:ARG:NH2	1:C:780:PHE:O	2.40	0.53
1:D:941:LYS:HZ3	1:D:946:SER:H	1.54	0.53
1:A:842:ARG:HA	1:A:909:LEU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:GLU:HB3	1:B:360:LYS:NZ	2.23	0.53
1:C:759:LYS:NZ	1:C:824:GLU:OE2	2.41	0.53
1:D:705:LEU:HA	1:D:708:MET:HB2	1.90	0.53
1:E:512:GLU:HA	1:E:515:LYS:NZ	2.23	0.53
1:E:830:LYS:O	1:E:837:ARG:NH1	2.35	0.53
1:C:20:TYR:CZ	1:C:500:ILE:HG13	2.43	0.53
1:E:18:ARG:HB2	1:E:25:GLN:NE2	2.24	0.53
1:E:72:LEU:HD13	1:E:210:LEU:CD2	2.39	0.53
1:E:119:CYS:SG	1:E:143:PHE:HE1	2.31	0.53
1:E:260:ASN:HA	1:E:262:GLN:HE22	1.73	0.53
1:F:665:LEU:HD21	1:F:679:ALA:HB3	1.90	0.53
1:A:866:TYR:HB3	1:A:875:HIS:HE1	1.73	0.53
1:B:216:LEU:O	1:B:218:HIS:ND1	2.41	0.53
1:E:699:VAL:HG12	1:E:700:LEU:N	2.24	0.53
1:F:73:GLU:HB3	1:F:77:LYS:NZ	2.24	0.53
1:F:398:TYR:CZ	1:F:425:MET:HA	2.44	0.53
1:A:850:GLU:HA	1:A:905:GLY:H	1.73	0.53
1:B:31:LEU:HA	1:B:35:LEU:HB3	1.91	0.53
1:C:745:THR:HG21	1:C:835:LEU:HD12	1.91	0.53
1:D:159:LEU:HG	1:D:161:PRO:HD3	1.90	0.53
1:E:12:ILE:HD11	1:E:400:SER:O	2.09	0.53
1:E:143:PHE:CZ	1:E:227:PHE:HB3	2.44	0.53
1:E:153:LYS:NZ	1:E:154:TYR:HB3	2.23	0.53
1:F:561:GLU:HG3	1:F:562:THR:HG23	1.91	0.53
1:E:20:TYR:HA	1:E:500:ILE:HD12	1.91	0.53
1:E:45:LYS:HZ1	1:E:87:ARG:HH12	1.57	0.53
1:E:653:LEU:HD23	1:E:658:ALA:HB2	1.90	0.53
1:F:435:ASP:OD1	1:F:439:LYS:N	2.30	0.53
1:B:525:LYS:HA	1:B:528:ILE:HG12	1.90	0.53
1:B:557:VAL:O	1:B:568:ILE:N	2.42	0.53
1:E:68:LEU:HA	1:E:71:HIS:ND1	2.24	0.53
1:A:61:PRO:HD2	1:A:64:GLU:OE2	2.10	0.52
1:B:826:GLU:OE2	1:B:836:HIS:NE2	2.36	0.52
1:B:111:GLU:HB3	1:B:113:PRO:HD2	1.91	0.52
1:B:260:ASN:HD21	1:B:262:GLN:HE21	1.55	0.52
1:E:22:ALA:O	1:E:24:VAL:N	2.41	0.52
1:E:125:HIS:HA	1:E:128:ASN:ND2	2.25	0.52
1:E:313:GLU:HA	1:E:316:VAL:HG22	1.91	0.52
1:F:53:ILE:HG13	1:F:83:TYR:HB2	1.91	0.52
1:F:369:THR:HG22	1:F:370:GLU:HG3	1.90	0.52
1:A:63:THR:O	1:A:66:LEU:HG	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LYS:HB2	1:B:154:TYR:HB2	1.90	0.52
1:B:432:VAL:HB	1:B:536:ARG:HA	1.91	0.52
1:F:163:LEU:HD13	1:F:165:LEU:HD23	1.91	0.52
1:F:226:GLY:H	1:F:247:LEU:HD11	1.75	0.52
1:B:107:VAL:O	1:B:109:PRO:HD3	2.09	0.52
1:E:51:ASN:HB3	1:E:56:LYS:CB	2.39	0.52
1:E:119:CYS:HA	1:E:122:ILE:HD13	1.91	0.52
1:F:313:GLU:HA	1:F:316:VAL:HG22	1.91	0.52
1:F:864:GLU:O	1:F:868:THR:HG23	2.09	0.52
1:A:111:GLU:HG2	1:A:114:ALA:H	1.74	0.52
1:C:617:TYR:O	1:C:620:THR:OG1	2.23	0.52
1:E:143:PHE:HZ	1:E:227:PHE:CD1	2.27	0.52
1:A:146:LYS:HG3	1:A:154:TYR:HA	1.92	0.52
1:C:300:ALA:HB1	1:C:338:LEU:HD11	1.92	0.52
1:D:107:VAL:O	1:D:109:PRO:HD3	2.10	0.52
1:D:588:ASN:OD1	1:D:590:GLU:HG3	2.10	0.52
1:E:20:TYR:CE2	1:E:500:ILE:HG21	2.45	0.52
1:E:41:GLU:CB	1:E:42:PRO:HD2	2.38	0.52
1:E:93:GLY:CA	1:E:161:PRO:CA	2.52	0.52
1:E:145:LEU:HB2	1:E:154:TYR:CE2	2.45	0.52
1:E:668:SER:O	1:E:701:ASN:ND2	2.42	0.52
1:F:604:ILE:HA	1:F:760:VAL:HG11	1.92	0.52
1:E:52:ARG:HE	1:E:83:TYR:HB3	1.74	0.52
1:E:82:MET:O	1:E:214:SER:N	2.42	0.52
1:E:139:ILE:HG22	1:E:141:PHE:CZ	2.44	0.52
1:B:369:THR:O	1:B:370:GLU:C	2.52	0.52
1:C:864:GLU:O	1:C:868:THR:HG23	2.09	0.52
1:D:587:PHE:HA	1:D:796:SER:HB3	1.91	0.52
1:E:202:HIS:O	1:E:206:VAL:HG22	2.10	0.52
1:A:30:LEU:HD12	1:A:34:GLU:HB2	1.90	0.52
1:A:70:GLU:O	1:A:74:GLN:OE1	2.28	0.52
1:C:153:LYS:HG3	1:C:154:TYR:CD1	2.44	0.52
1:E:196:GLU:C	1:E:198:CYS:H	2.17	0.52
1:E:267:ARG:O	1:E:267:ARG:HG2	2.09	0.52
1:A:347:PRO:O	1:A:351:ASN:ND2	2.43	0.52
1:D:376:ARG:HG2	1:D:571:PHE:HZ	1.74	0.52
1:E:81:LEU:HG	1:E:83:TYR:HE1	1.75	0.52
1:E:115:LEU:HB3	1:E:156:PHE:CZ	2.45	0.52
1:E:120:HIS:HE1	1:E:227:PHE:CZ	2.28	0.52
1:E:528:ILE:HA	1:E:531:ALA:HB3	1.91	0.52
1:C:435:ASP:OD1	1:C:439:LYS:N	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:660:LYS:HE2	1:C:691:PHE:HA	1.91	0.51
1:C:873:LYS:HZ2	1:C:875:HIS:HA	1.75	0.51
1:E:144:THR:HG23	1:E:157:HIS:HB2	1.92	0.51
1:F:108:PRO:HG2	1:F:154:TYR:HE1	1.75	0.51
1:A:830:LYS:O	1:A:837:ARG:NH1	2.42	0.51
1:D:192:VAL:HG12	1:D:194:ASN:H	1.74	0.51
1:D:753:LEU:O	1:D:754:ARG:NH1	2.34	0.51
1:D:850:GLU:HA	1:D:905:GLY:H	1.76	0.51
1:E:66:LEU:HA	1:E:69:TYR:CD2	2.46	0.51
1:E:123:PHE:O	1:E:126:ILE:HG12	2.10	0.51
1:E:209:LEU:HD11	1:E:221:TYR:HB2	1.93	0.51
1:E:533:PHE:HE2	1:F:470:HIS:HD1	1.58	0.51
1:A:123:PHE:O	1:A:127:LYS:HG2	2.09	0.51
1:B:891:LYS:HA	1:C:761:LYS:HZ1	1.76	0.51
1:E:51:ASN:HA	1:E:83:TYR:C	2.35	0.51
1:F:141:PHE:HE2	1:F:229:LEU:HB3	1.76	0.51
1:A:146:LYS:HD3	1:A:221:TYR:CE1	2.45	0.51
1:B:142:PHE:HD2	1:B:159:LEU:HD23	1.75	0.51
1:D:303:LEU:HA	1:D:306:ILE:HG12	1.92	0.51
1:E:444:GLU:OE2	1:E:461:ARG:NE	2.44	0.51
1:F:294:MET:O	1:F:301:ARG:NH2	2.44	0.51
1:F:456:GLU:OE2	1:F:579:TYR:OH	2.25	0.51
1:F:660:LYS:NZ	1:F:661:LEU:O	2.39	0.51
1:B:181:ALA:HA	1:B:184:GLN:HG2	1.92	0.51
1:C:123:PHE:O	1:C:127:LYS:HG2	2.11	0.51
1:C:560:ILE:O	1:C:561:GLU:C	2.53	0.51
1:C:585:VAL:HB	1:C:796:SER:OG	2.10	0.51
1:F:617:TYR:OH	1:F:732:MET:O	2.28	0.51
1:C:808:GLU:HG2	1:C:809:TYR:N	2.25	0.51
1:A:587:PHE:HA	1:A:796:SER:HB3	1.92	0.51
1:B:829:ARG:O	1:B:833:ASP:N	2.42	0.51
1:D:317:GLU:HG3	1:D:319:PRO:HD2	1.93	0.51
1:D:655:ASP:OD1	1:D:656:HIS:N	2.44	0.51
1:D:858:VAL:HG22	1:D:908:ILE:HD11	1.93	0.51
1:E:89:GLY:C	1:E:91:TYR:N	2.69	0.51
1:E:787:ASP:CG	1:E:790:CYS:HB3	2.35	0.51
1:E:146:LYS:HB2	1:E:155:GLY:N	2.19	0.51
1:F:664:SER:HA	1:F:667:THR:HG22	1.93	0.51
1:A:405:TYR:CD2	1:A:417:MET:HB2	2.45	0.51
1:A:588:ASN:OD1	1:A:590:GLU:HG3	2.10	0.51
1:B:548:PRO:HB2	1:B:623:PHE:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:GLN:OE1	1:C:656:HIS:ND1	2.44	0.51
1:D:182:THR:O	1:D:185:LYS:HG3	2.11	0.51
1:E:453:ASN:N	1:E:456:GLU:OE2	2.44	0.51
1:A:303:LEU:HA	1:A:306:ILE:HG12	1.93	0.51
1:A:481:MET:HE3	1:A:518:ILE:HG21	1.93	0.51
1:B:102:LEU:HD21	1:B:108:PRO:HG3	1.92	0.51
1:C:616:PHE:O	1:C:620:THR:HG23	2.11	0.51
1:E:180:ASP:CG	1:E:182:THR:H	2.19	0.51
1:E:909:LEU:HA	1:E:913:GLU:HG2	1.93	0.51
1:F:78:GLN:HE22	1:F:80:ALA:HB2	1.76	0.51
1:B:797:ILE:HG23	1:B:801:PHE:CE2	2.47	0.50
1:C:341:TRP:CE2	1:C:345:LYS:HD2	2.46	0.50
1:D:146:LYS:HB2	1:D:154:TYR:HB2	1.93	0.50
1:E:419:ALA:HB2	1:E:530:GLN:HE21	1.75	0.50
1:F:146:LYS:HG3	1:F:155:GLY:H	1.75	0.50
1:A:64:GLU:HA	1:A:67:ARG:CG	2.40	0.50
1:A:349:LYS:HE3	1:A:353:GLY:HA3	1.93	0.50
1:A:585:VAL:HG23	1:A:796:SER:OG	2.11	0.50
1:B:88:GLN:NE2	1:B:95:MET:HB2	2.26	0.50
1:B:616:PHE:O	1:B:620:THR:HG23	2.11	0.50
1:C:512:GLU:O	1:C:515:LYS:HG2	2.11	0.50
1:C:633:LEU:O	1:C:756:TYR:N	2.43	0.50
1:D:307:LEU:HD23	1:D:310:LEU:HD12	1.92	0.50
1:E:209:LEU:HD21	1:E:221:TYR:CD2	2.46	0.50
1:D:293:LEU:HD21	1:D:335:TYR:HA	1.91	0.50
1:E:82:MET:HE2	1:E:82:MET:H	1.77	0.50
1:E:148:GLU:O	1:E:150:VAL:HG12	2.12	0.50
1:E:779:ARG:HB3	1:E:783:GLU:HB3	1.93	0.50
1:F:518:ILE:HG13	1:F:519:PHE:N	2.27	0.50
1:B:457:ILE:HG13	1:B:458:TRP:CD1	2.47	0.50
1:B:941:LYS:NZ	1:B:948:ASN:O	2.45	0.50
1:E:303:LEU:HD11	1:E:375:LYS:HE3	1.92	0.50
1:F:889:LEU:HA	1:F:892:TYR:CZ	2.47	0.50
1:C:940:ASN:O	1:C:944:GLU:N	2.36	0.50
1:D:443:PHE:HD1	1:D:577:HIS:HE1	1.60	0.50
1:E:19:LYS:NZ	1:E:407:TYR:HB3	2.27	0.50
1:E:65:LEU:O	1:E:68:LEU:HD23	2.12	0.50
1:E:115:LEU:HD13	1:E:224:LYS:HD3	1.93	0.50
1:E:476:ASN:HD22	1:E:479:ARG:NH2	2.09	0.50
1:A:17:GLN:HA	1:A:20:TYR:HB3	1.93	0.50
1:A:363:ASN:O	1:A:367:HIS:HD2	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:LEU:HA	1:A:567:LEU:HA	1.94	0.50
1:B:162:GLY:O	1:B:269:VAL:N	2.45	0.50
1:D:188:HIS:CE1	1:D:195:PRO:HB3	2.46	0.50
1:E:100:LEU:H	1:E:155:GLY:HA2	1.76	0.50
1:F:75:CYS:O	1:F:79:GLY:N	2.44	0.50
1:A:608:LEU:HD21	1:A:941:LYS:HG2	1.94	0.50
1:E:30:LEU:O	1:E:34:GLU:HB2	2.12	0.50
1:E:93:GLY:O	1:E:258:LEU:HB3	2.11	0.50
1:E:40:THR:HG21	1:E:47:THR:CG2	2.37	0.50
1:E:92:SER:C	1:E:164:LYS:HA	2.37	0.50
1:F:30:LEU:HD12	1:F:34:GLU:HB3	1.94	0.50
1:F:415:HIS:HB3	1:F:527:VAL:HA	1.94	0.50
1:B:750:TRP:HA	1:B:753:LEU:HD12	1.94	0.49
1:E:120:HIS:O	1:E:123:PHE:HB3	2.12	0.49
1:E:153:LYS:HZ3	1:E:154:TYR:H	1.60	0.49
1:E:165:LEU:O	1:E:170:LYS:HG3	2.12	0.49
1:E:186:ILE:HG22	1:E:187:LEU:HD23	1.94	0.49
1:A:69:TYR:OH	1:A:259:THR:OG1	2.29	0.49
1:B:146:LYS:HD3	1:B:221:TYR:CE1	2.47	0.49
1:C:635:LEU:HB2	1:C:757:ARG:HG2	1.94	0.49
1:C:664:SER:HA	1:C:667:THR:HG22	1.94	0.49
1:C:689:GLY:N	1:C:731:THR:O	2.42	0.49
1:C:708:MET:HA	1:C:708:MET:HE3	1.92	0.49
1:C:915:LEU:HD13	1:C:919:GLU:HB2	1.92	0.49
1:E:315:TYR:CD1	1:E:346:CYS:HB2	2.47	0.49
1:E:582:ILE:HG23	1:E:792:ASN:OD1	2.13	0.49
1:F:540:PHE:CZ	1:F:544:LEU:HD21	2.47	0.49
1:A:82:MET:SD	1:A:83:TYR:N	2.83	0.49
1:B:192:VAL:HG12	1:B:194:ASN:H	1.76	0.49
1:B:883:GLU:OE1	1:C:738:TYR:OH	2.27	0.49
1:C:53:ILE:HG13	1:C:83:TYR:HB2	1.93	0.49
1:C:87:ARG:HA	1:C:207:PRO:HA	1.95	0.49
1:D:894:GLN:NE2	1:D:902:ILE:O	2.45	0.49
1:A:53:ILE:HG22	1:A:54:THR:HG23	1.94	0.49
1:B:23:GLU:O	1:B:24:VAL:HB	2.13	0.49
1:B:288:HIS:O	1:B:292:ILE:HD12	2.11	0.49
1:C:530:GLN:HA	1:C:533:PHE:HD2	1.77	0.49
1:C:598:LEU:HD11	1:C:942:TRP:HB3	1.93	0.49
1:D:619:SER:O	1:D:622:ILE:HG12	2.12	0.49
1:E:49:ILE:C	1:E:50:ILE:HG13	2.38	0.49
1:E:84:PHE:H	1:E:84:PHE:HD1	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:LEU:HD22	1:E:187:LEU:HD13	1.94	0.49
1:E:185:LYS:HA	1:E:188:HIS:CD2	2.46	0.49
1:F:896:SER:HB3	1:F:897:PRO:HD2	1.94	0.49
1:A:15:THR:O	1:A:18:ARG:HG3	2.12	0.49
1:A:844:VAL:HB	1:A:919:GLU:HB3	1.93	0.49
1:B:159:LEU:HD23	1:B:256:LEU:HG	1.94	0.49
1:B:642:LYS:HE2	1:B:735:ALA:HB1	1.95	0.49
1:D:75:CYS:O	1:D:79:GLY:N	2.43	0.49
1:D:842:ARG:HA	1:D:909:LEU:HB2	1.95	0.49
1:E:25:GLN:HA	1:E:28:GLU:OE2	2.12	0.49
1:E:96:LEU:HD11	1:E:177:LEU:HD23	1.93	0.49
1:E:139:ILE:N	1:E:231:PHE:HB2	2.28	0.49
1:E:527:VAL:HA	1:E:530:GLN:HE22	1.76	0.49
1:F:72:LEU:HD22	1:F:253:VAL:HG21	1.95	0.49
1:E:52:ARG:NH1	1:E:215:LYS:HG3	2.28	0.49
1:E:91:TYR:O	1:E:164:LYS:HB2	2.12	0.49
1:E:123:PHE:HD1	1:E:141:PHE:HZ	1.60	0.49
1:E:403:ALA:HA	1:E:406:VAL:HG12	1.95	0.49
1:C:916:GLN:HG3	1:C:919:GLU:HG2	1.94	0.49
1:E:174:ILE:HG21	1:E:201:PRO:CA	2.42	0.49
1:F:72:LEU:HG	1:F:82:MET:HE3	1.95	0.49
1:F:209:LEU:HD21	1:F:215:LYS:HE3	1.94	0.49
1:F:416:TYR:CZ	1:F:420:LYS:HE3	2.48	0.49
1:A:163:LEU:HD13	1:A:165:LEU:HB2	1.95	0.49
1:A:497:GLU:HB3	1:A:500:ILE:HG12	1.95	0.49
1:A:910:HIS:H	1:A:913:GLU:HG3	1.77	0.49
1:C:542:GLN:O	1:C:546:THR:OG1	2.31	0.49
1:D:664:SER:HA	1:D:667:THR:HG22	1.95	0.49
1:E:65:LEU:HD13	1:E:259:THR:HB	1.95	0.49
1:E:154:TYR:OH	1:E:190:GLN:HG3	2.11	0.49
1:E:214:SER:HB2	1:E:220:PRO:HD3	1.94	0.49
1:F:156:PHE:O	1:F:157:HIS:ND1	2.45	0.49
1:A:696:LYS:HA	1:A:738:TYR:HD2	1.78	0.49
1:B:446:VAL:HG12	1:B:457:ILE:HD12	1.95	0.49
1:D:501:LEU:HB3	1:D:505:LYS:NZ	2.28	0.49
1:F:415:HIS:HA	1:F:527:VAL:HG22	1.93	0.49
1:F:762:PHE:HD2	1:F:776:GLU:HA	1.78	0.49
1:C:33:ARG:NH2	1:D:486:GLU:OE2	2.45	0.48
1:E:60:LEU:CD1	1:E:68:LEU:HD22	2.42	0.48
1:F:616:PHE:O	1:F:620:THR:HG23	2.13	0.48
1:A:470:HIS:O	1:A:473:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:PRO:HA	1:B:222:GLN:HE22	1.78	0.48
1:C:404:GLU:O	1:C:408:SER:OG	2.27	0.48
1:E:679:ALA:N	1:E:681:MET:SD	2.86	0.48
1:F:86:GLU:O	1:F:208:SER:N	2.46	0.48
1:F:750:TRP:CE3	1:F:753:LEU:HD12	2.48	0.48
1:A:662:ASN:OD1	1:A:665:LEU:N	2.45	0.48
1:B:383:HIS:HB2	1:B:390:TYR:CZ	2.48	0.48
1:C:146:LYS:NZ	1:C:221:TYR:OH	2.35	0.48
1:D:313:GLU:HA	1:D:316:VAL:HG22	1.95	0.48
1:E:82:MET:C	1:E:83:TYR:HD1	2.21	0.48
1:E:184:GLN:OE1	1:E:195:PRO:HB2	2.13	0.48
1:E:432:VAL:HG21	1:E:532:GLU:HA	1.96	0.48
1:E:598:LEU:HD13	1:E:943:TRP:CZ3	2.48	0.48
1:F:17:GLN:O	1:F:21:LEU:HG	2.13	0.48
1:A:76:ARG:NH1	1:A:211:TYR:HB3	2.28	0.48
1:B:699:VAL:CG2	1:B:741:ILE:HD12	2.43	0.48
1:E:213:SER:C	1:E:220:PRO:HB3	2.38	0.48
1:F:110:LEU:HD13	1:F:224:LYS:HE2	1.95	0.48
1:F:854:ASN:HA	1:F:858:VAL:HG21	1.96	0.48
1:A:414:GLU:HG3	1:A:415:HIS:ND1	2.29	0.48
1:A:557:VAL:O	1:A:568:ILE:N	2.36	0.48
1:D:117:ARG:NH2	1:D:182:THR:HG21	2.29	0.48
1:E:39:LEU:HA	1:E:58:TYR:CD1	2.49	0.48
1:E:184:GLN:HA	1:E:195:PRO:O	2.13	0.48
1:E:372:LYS:HE3	1:E:574:HIS:CG	2.49	0.48
1:F:66:LEU:O	1:F:70:GLU:HG2	2.14	0.48
1:A:522:SER:HA	1:A:525:LYS:HE2	1.96	0.48
1:A:890:GLU:HA	1:A:893:LEU:HD12	1.95	0.48
1:B:61:PRO:HD2	1:B:64:GLU:OE2	2.13	0.48
1:B:442:TRP:CZ3	1:B:466:PRO:HD3	2.48	0.48
1:D:23:GLU:O	1:D:24:VAL:HB	2.13	0.48
1:D:95:MET:HE2	1:D:159:LEU:HD13	1.96	0.48
1:D:116:SER:O	1:D:120:HIS:ND1	2.44	0.48
1:D:314:TYR:HA	1:D:320:LEU:HB2	1.96	0.48
1:E:20:TYR:HD1	1:E:21:LEU:HD23	1.76	0.48
1:E:98:TYR:HD1	1:E:199:LEU:HB2	1.77	0.48
1:E:110:LEU:HD21	1:E:154:TYR:OH	2.14	0.48
1:E:415:HIS:HE1	1:E:523:PHE:HA	1.78	0.48
1:F:696:LYS:HA	1:F:738:TYR:CD1	2.49	0.48
1:F:701:ASN:OD1	1:F:703:SER:OG	2.24	0.48
1:B:15:THR:HG21	1:B:404:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:HIS:HE1	1:D:523:PHE:HA	1.78	0.48
1:D:561:GLU:HG3	1:D:562:THR:HG23	1.95	0.48
1:E:52:ARG:HG2	1:E:83:TYR:CB	2.32	0.48
1:E:91:TYR:C	1:E:164:LYS:HB2	2.39	0.48
1:E:164:LYS:HG3	1:E:269:VAL:O	2.14	0.48
1:E:295:LEU:O	1:E:301:ARG:NH2	2.46	0.48
1:F:146:LYS:HD3	1:F:221:TYR:CE1	2.49	0.48
1:C:60:LEU:HD13	1:C:64:GLU:HG3	1.96	0.48
1:E:525:LYS:O	1:E:529:ARG:HG2	2.13	0.48
1:F:93:GLY:HA3	1:F:258:LEU:HD22	1.94	0.48
1:F:433:ASP:OD1	1:F:434:VAL:N	2.46	0.48
1:F:520:ASN:OD1	1:F:523:PHE:N	2.35	0.48
1:B:94:LEU:HB2	1:B:160:ILE:H	1.79	0.48
1:B:97:ASP:HA	1:B:157:HIS:CE1	2.49	0.48
1:D:632:LEU:HB2	1:D:733:VAL:HG22	1.96	0.48
1:E:174:ILE:HG12	1:E:199:LEU:HD11	1.95	0.48
1:B:83:TYR:CE1	1:B:214:SER:HB3	2.47	0.48
1:B:423:TYR:HA	1:B:535:PHE:CZ	2.49	0.48
1:E:184:GLN:H	1:E:184:GLN:HG2	1.39	0.48
1:E:187:LEU:HD23	1:E:187:LEU:N	2.28	0.48
1:E:664:SER:HA	1:E:667:THR:HG22	1.95	0.48
1:B:634:TRP:HE1	1:B:758:SER:HB3	1.78	0.47
1:B:699:VAL:HG22	1:B:741:ILE:HB	1.96	0.47
1:C:116:SER:O	1:C:120:HIS:ND1	2.47	0.47
1:C:369:THR:O	1:C:370:GLU:C	2.57	0.47
1:D:67:ARG:O	1:D:70:GLU:HG2	2.14	0.47
1:D:93:GLY:H	1:D:258:LEU:HD22	1.78	0.47
1:E:21:LEU:HD12	1:E:24:VAL:CG2	2.41	0.47
1:E:98:TYR:HB2	1:E:100:LEU:CD2	2.44	0.47
1:E:223:LEU:HD21	1:E:247:LEU:HD12	1.96	0.47
1:A:65:LEU:O	1:A:68:LEU:HG	2.14	0.47
1:C:20:TYR:CE2	1:C:500:ILE:HG21	2.48	0.47
1:C:86:GLU:O	1:C:208:SER:N	2.41	0.47
1:D:73:GLU:HG2	1:D:76:ARG:HH21	1.78	0.47
1:D:544:LEU:HD11	1:D:577:HIS:HB2	1.96	0.47
1:D:883:GLU:O	1:D:887:SER:N	2.47	0.47
1:E:167:ALA:HB3	1:E:169:THR:HG22	1.96	0.47
1:E:598:LEU:HD21	1:E:942:TRP:HB3	1.96	0.47
1:F:895:TRP:HE3	1:F:899:LYS:HA	1.78	0.47
1:A:665:LEU:HD21	1:A:679:ALA:HB3	1.97	0.47
1:B:867:ASN:HB3	1:B:872:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:GLY:O	1:C:459:LYS:NZ	2.35	0.47
1:C:800:TYR:O	1:C:803:GLU:HG3	2.14	0.47
1:E:662:ASN:OD1	1:E:665:LEU:N	2.46	0.47
1:E:668:SER:OG	1:E:704:ARG:NH1	2.47	0.47
1:B:297:ASP:OD2	1:B:335:TYR:OH	2.28	0.47
1:D:868:THR:HG21	1:D:911:LYS:NZ	2.29	0.47
1:E:21:LEU:HD13	1:E:78:GLN:HG3	1.94	0.47
1:E:115:LEU:HB3	1:E:156:PHE:HZ	1.80	0.47
1:E:122:ILE:HG12	1:E:123:PHE:N	2.29	0.47
1:A:663:ILE:O	1:A:666:LEU:HG	2.14	0.47
1:B:252:LEU:HD12	1:B:253:VAL:HG23	1.95	0.47
1:B:398:TYR:CZ	1:B:425:MET:HA	2.50	0.47
1:B:653:LEU:HG	1:B:657:TYR:HB2	1.96	0.47
1:B:907:ARG:HH22	1:B:909:LEU:HD21	1.80	0.47
1:E:53:ILE:HG13	1:E:83:TYR:CG	2.49	0.47
1:E:174:ILE:HG21	1:E:200:ASP:C	2.39	0.47
1:E:231:PHE:CE2	1:E:269:VAL:HG11	2.49	0.47
1:A:615:MET:SD	1:A:801:PHE:HD2	2.37	0.47
1:C:470:HIS:CE1	1:C:524:LYS:HD3	2.50	0.47
1:D:174:ILE:O	1:D:178:GLN:HG2	2.15	0.47
1:E:52:ARG:HG2	1:E:83:TYR:CD2	2.50	0.47
1:E:146:LYS:HD2	1:E:150:VAL:HG11	1.97	0.47
1:A:116:SER:O	1:A:120:HIS:ND1	2.48	0.47
1:A:364:ASP:O	1:A:368:HIS:N	2.47	0.47
1:A:615:MET:HE1	1:A:616:PHE:CE1	2.50	0.47
1:A:624:ARG:HD3	1:A:657:TYR:CE1	2.49	0.47
1:A:800:TYR:OH	1:A:944:GLU:OE2	2.23	0.47
1:B:66:LEU:O	1:B:70:GLU:HG2	2.15	0.47
1:B:777:ASP:HB3	1:B:778:PRO:HD3	1.96	0.47
1:B:846:SER:OG	1:B:907:ARG:HB2	2.15	0.47
1:C:107:VAL:O	1:C:109:PRO:HD3	2.14	0.47
1:C:313:GLU:HA	1:C:316:VAL:HG22	1.97	0.47
1:C:466:PRO:O	1:C:470:HIS:N	2.42	0.47
1:C:634:TRP:HZ3	1:C:646:MET:HE3	1.80	0.47
1:C:699:VAL:CG2	1:C:741:ILE:HD12	2.45	0.47
1:C:846:SER:N	1:C:905:GLY:O	2.44	0.47
1:D:63:THR:O	1:D:66:LEU:HG	2.14	0.47
1:D:187:LEU:HB3	1:D:192:VAL:HB	1.97	0.47
1:E:61:PRO:HD2	1:E:64:GLU:CG	2.45	0.47
1:E:96:LEU:HD22	1:E:174:ILE:HG13	1.96	0.47
1:E:101:LYS:HG3	1:E:194:ASN:HD22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:CYS:HB3	1:E:141:PHE:CD2	2.50	0.47
1:E:548:PRO:HA	1:E:624:ARG:NH1	2.29	0.47
1:F:376:ARG:HA	1:F:379:MET:HE2	1.97	0.47
1:F:405:TYR:OH	1:F:420:LYS:HD2	2.15	0.47
1:F:452:MET:HE1	1:F:456:GLU:H	1.80	0.47
1:A:56:LYS:HD3	1:A:58:TYR:CZ	2.50	0.47
1:C:557:VAL:HB	1:C:568:ILE:HB	1.96	0.47
1:C:808:GLU:HG2	1:C:809:TYR:H	1.80	0.47
1:D:61:PRO:HD2	1:D:64:GLU:OE2	2.15	0.47
1:E:11:THR:O	1:E:15:THR:HG23	2.14	0.47
1:E:101:LYS:C	1:E:192:VAL:HG13	2.40	0.47
1:F:93:GLY:H	1:F:258:LEU:HB3	1.80	0.47
1:F:101:LYS:HA	1:F:152:GLY:O	2.14	0.47
1:A:182:THR:O	1:A:185:LYS:HG3	2.15	0.47
1:A:578:GLN:OE1	1:A:656:HIS:ND1	2.47	0.47
1:B:616:PHE:CG	1:B:805:LEU:HD12	2.50	0.47
1:E:142:PHE:HB2	1:E:159:LEU:HB3	1.97	0.47
1:E:251:ASN:HB2	1:E:254:SER:CB	2.45	0.47
1:D:188:HIS:HE1	1:D:195:PRO:HB3	1.80	0.47
1:E:141:PHE:HE1	1:E:229:LEU:HB3	1.77	0.47
1:E:444:GLU:HG3	1:E:463:GLU:OE2	2.14	0.47
1:A:418:ILE:HG12	1:A:477:PHE:HE2	1.80	0.46
1:B:85:LEU:HD23	1:B:209:LEU:HB3	1.98	0.46
1:B:403:ALA:C	1:B:405:TYR:H	2.24	0.46
1:C:45:LYS:O	1:C:87:ARG:NH1	2.48	0.46
1:D:312:PRO:HA	1:D:315:TYR:CZ	2.50	0.46
1:D:584:TYR:HE1	1:D:799:VAL:HG11	1.80	0.46
1:D:865:TRP:O	1:D:869:ASN:N	2.48	0.46
1:E:86:GLU:HB2	1:E:259:THR:OG1	2.15	0.46
1:E:139:ILE:HD11	1:E:162:GLY:C	2.40	0.46
1:F:745:THR:HA	1:F:750:TRP:HE1	1.80	0.46
1:A:704:ARG:O	1:A:708:MET:HG2	2.16	0.46
1:A:842:ARG:HB3	1:A:909:LEU:O	2.16	0.46
1:B:121:ARG:HH11	1:B:124:VAL:HG23	1.80	0.46
1:B:557:VAL:HG11	1:B:576:ILE:HD13	1.97	0.46
1:D:103:ASN:HB3	1:D:193:THR:HB	1.97	0.46
1:D:487:HIS:CD2	1:D:491:HIS:HE1	2.34	0.46
1:D:867:ASN:HA	1:D:872:VAL:HA	1.97	0.46
1:E:28:GLU:O	1:E:32:THR:HG23	2.16	0.46
1:E:800:TYR:OH	1:E:944:GLU:OE1	2.23	0.46
1:B:117:ARG:HD2	1:B:117:ARG:HA	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:GLN:HE22	1:D:204:ALA:HA	1.80	0.46
1:D:414:GLU:HG3	1:D:415:HIS:H	1.79	0.46
1:D:415:HIS:HD2	1:E:521:ASP:HB2	1.80	0.46
1:F:433:ASP:HB3	1:F:541:ILE:HG13	1.96	0.46
1:A:214:SER:HB2	1:A:218:HIS:O	2.16	0.46
1:B:187:LEU:HA	1:B:190:GLN:NE2	2.30	0.46
1:B:585:VAL:CG1	1:B:586:PRO:CD	2.93	0.46
1:B:889:LEU:O	1:B:893:LEU:N	2.39	0.46
1:C:30:LEU:HD12	1:C:34:GLU:HB2	1.98	0.46
1:C:403:ALA:HA	1:C:406:VAL:HG12	1.97	0.46
1:C:844:VAL:HB	1:C:919:GLU:HB3	1.98	0.46
1:D:216:LEU:O	1:D:218:HIS:ND1	2.43	0.46
1:D:529:ARG:NH2	1:E:521:ASP:OD1	2.45	0.46
1:E:21:LEU:HD22	1:E:78:GLN:HB2	1.97	0.46
1:E:23:GLU:HB3	1:E:78:GLN:NE2	2.27	0.46
1:F:364:ASP:HA	1:F:367:HIS:CD2	2.50	0.46
1:F:728:MET:SD	1:F:728:MET:N	2.88	0.46
1:A:460:TRP:O	1:A:577:HIS:ND1	2.42	0.46
1:C:455:GLY:HA2	1:C:554:GLY:HA2	1.97	0.46
1:F:102:LEU:HG	1:F:192:VAL:HA	1.98	0.46
1:F:311:PRO:HG3	1:F:385:HIS:CE1	2.51	0.46
1:F:646:MET:SD	1:F:647:ARG:HG3	2.56	0.46
1:A:73:GLU:HG3	1:A:253:VAL:HB	1.98	0.46
1:A:634:TRP:CE3	1:A:642:LYS:HB2	2.51	0.46
1:A:635:LEU:HB2	1:A:757:ARG:HG2	1.96	0.46
1:B:323:ASN:OD1	1:B:324:VAL:N	2.48	0.46
1:B:405:TYR:HA	1:B:408:SER:HB3	1.97	0.46
1:C:102:LEU:HD22	1:C:153:LYS:HG2	1.98	0.46
1:D:50:ILE:O	1:D:85:LEU:N	2.40	0.46
1:E:36:SER:C	1:E:38:PHE:N	2.71	0.46
1:E:143:PHE:CZ	1:E:227:PHE:HD1	2.34	0.46
1:E:224:LYS:HE3	1:E:224:LYS:H	1.81	0.46
1:E:260:ASN:HA	1:E:262:GLN:NE2	2.30	0.46
1:F:62:SER:HB3	1:F:262:GLN:NE2	2.30	0.46
1:F:558:LEU:HA	1:F:567:LEU:HA	1.98	0.46
1:D:121:ARG:HG2	1:D:183:VAL:HG13	1.96	0.46
1:D:554:GLY:H	1:D:583:CYS:HA	1.80	0.46
1:A:27:LEU:HD11	1:A:71:HIS:HB3	1.98	0.46
1:A:299:GLU:HA	1:A:302:TYR:CD2	2.50	0.46
1:B:31:LEU:HD23	1:B:35:LEU:HD22	1.96	0.46
1:B:215:LYS:CB	1:B:218:HIS:HB2	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:PHE:HZ	1:B:368:HIS:NE2	2.14	0.46
1:C:171:LYS:HD3	1:C:171:LYS:HA	1.73	0.46
1:C:311:PRO:HB2	1:C:313:GLU:CD	2.41	0.46
1:C:427:GLY:HA2	1:C:535:PHE:HE2	1.81	0.46
1:D:389:GLN:H	1:D:389:GLN:CD	2.24	0.46
1:E:48:ASN:N	1:E:58:TYR:O	2.49	0.46
1:E:118:LEU:CD2	1:E:158:VAL:HG21	2.46	0.46
1:E:415:HIS:HB3	1:E:530:GLN:HE22	1.80	0.46
1:E:604:ILE:HA	1:E:760:VAL:HG11	1.97	0.46
1:F:182:THR:O	1:F:185:LYS:HG3	2.15	0.46
1:F:211:TYR:OH	1:F:223:LEU:N	2.48	0.46
1:A:858:VAL:HG22	1:A:908:ILE:HD11	1.98	0.46
1:B:514:SER:HA	1:B:517:LYS:HZ3	1.81	0.46
1:C:182:THR:O	1:C:185:LYS:HG3	2.16	0.46
1:C:417:MET:HA	1:C:420:LYS:HE3	1.96	0.46
1:C:844:VAL:HG11	1:C:915:LEU:HD22	1.98	0.46
1:D:102:LEU:HD21	1:D:108:PRO:HG3	1.98	0.46
1:D:525:LYS:HA	1:D:528:ILE:HG12	1.97	0.46
1:D:582:ILE:HG13	1:D:652:VAL:O	2.15	0.46
1:D:620:THR:HA	1:D:802:TRP:CE3	2.51	0.46
1:E:45:LYS:C	1:E:47:THR:N	2.74	0.46
1:E:69:TYR:CD2	1:E:254:SER:HA	2.51	0.46
1:E:127:LYS:HA	1:E:127:LYS:HD3	1.54	0.46
1:E:199:LEU:HD12	1:E:200:ASP:N	2.31	0.46
1:E:211:TYR:CG	1:E:256:LEU:HD22	2.51	0.46
1:F:92:SER:HB2	1:F:258:LEU:HD13	1.98	0.46
1:A:433:ASP:OD1	1:A:434:VAL:N	2.48	0.46
1:A:475:GLU:O	1:A:478:SER:OG	2.29	0.46
1:B:21:LEU:HD21	1:B:80:ALA:HB2	1.98	0.46
1:C:413:LEU:HD11	1:C:511:PHE:HE1	1.80	0.46
1:C:509:LYS:HE2	1:C:513:ARG:HE	1.80	0.46
1:D:293:LEU:HD23	1:D:338:LEU:HD23	1.98	0.46
1:D:415:HIS:HB3	1:D:530:GLN:HG3	1.97	0.46
1:D:585:VAL:O	1:D:796:SER:OG	2.31	0.46
1:E:86:GLU:N	1:E:210:LEU:HD12	2.31	0.46
1:E:122:ILE:HD11	1:E:141:PHE:HD2	1.81	0.46
1:E:123:PHE:CD1	1:E:141:PHE:HZ	2.34	0.46
1:E:465:ASN:C	1:E:465:ASN:ND2	2.73	0.46
1:E:31:LEU:HB3	1:E:35:LEU:HD22	1.97	0.45
1:E:706:LYS:HA	1:E:709:VAL:HG22	1.97	0.45
1:F:23:GLU:O	1:F:24:VAL:HB	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:SER:HA	1:A:65:LEU:HB2	1.98	0.45
1:A:87:ARG:HA	1:A:207:PRO:HA	1.98	0.45
1:A:211:TYR:CE1	1:A:256:LEU:HD23	2.51	0.45
1:B:229:LEU:HG	1:B:230:VAL:H	1.80	0.45
1:B:838:PHE:HB2	1:B:865:TRP:CZ3	2.51	0.45
1:C:23:GLU:HB3	1:C:78:GLN:HE22	1.81	0.45
1:D:909:LEU:HD11	1:D:915:LEU:HB3	1.98	0.45
1:F:432:VAL:HB	1:F:536:ARG:HA	1.98	0.45
1:A:171:LYS:HA	1:A:171:LYS:HD3	1.73	0.45
1:A:521:ASP:OD1	1:A:522:SER:N	2.49	0.45
1:C:328:LEU:HD13	1:C:375:LYS:NZ	2.31	0.45
1:E:118:LEU:HA	1:E:182:THR:HG22	1.99	0.45
1:E:485:THR:HG22	1:E:489:LYS:NZ	2.31	0.45
1:E:619:SER:O	1:E:622:ILE:HG12	2.16	0.45
1:F:171:LYS:HA	1:F:171:LYS:HD3	1.77	0.45
1:F:749:THR:HA	1:F:752:ARG:NE	2.22	0.45
1:A:467:ASP:O	1:A:470:HIS:ND1	2.49	0.45
1:A:664:SER:HA	1:A:667:THR:HG22	1.98	0.45
1:D:30:LEU:HD12	1:D:34:GLU:HB2	1.98	0.45
1:D:287:ASP:OD1	1:D:287:ASP:N	2.47	0.45
1:E:72:LEU:HB3	1:E:253:VAL:HG21	1.97	0.45
1:E:158:VAL:CG1	1:E:160:ILE:HD11	2.46	0.45
1:F:20:TYR:CZ	1:F:497:GLU:HG3	2.51	0.45
1:C:157:HIS:CD2	1:C:221:TYR:HE2	2.35	0.45
1:C:705:LEU:O	1:C:709:VAL:HG13	2.17	0.45
1:D:49:ILE:HG23	1:D:58:TYR:HB2	1.99	0.45
1:D:486:GLU:HA	1:D:489:LYS:HG2	1.98	0.45
1:E:187:LEU:HD12	1:E:194:ASN:O	2.17	0.45
1:E:224:LYS:HG2	1:E:225:THR:N	2.31	0.45
1:F:63:THR:O	1:F:66:LEU:HG	2.15	0.45
1:B:94:LEU:O	1:B:95:MET:HE2	2.17	0.45
1:B:602:GLN:HA	1:B:942:TRP:CH2	2.51	0.45
1:C:61:PRO:HD2	1:C:64:GLU:OE2	2.17	0.45
1:C:93:GLY:HA3	1:C:161:PRO:HA	1.99	0.45
1:C:633:LEU:HB3	1:C:755:HIS:HA	1.98	0.45
1:C:634:TRP:O	1:C:735:ALA:HA	2.17	0.45
1:D:406:VAL:HG13	1:D:411:GLY:HA2	1.99	0.45
1:D:413:LEU:HD22	1:D:418:ILE:HD11	1.98	0.45
1:E:223:LEU:HD13	1:E:256:LEU:HD11	1.98	0.45
1:E:485:THR:HG22	1:E:489:LYS:HZ1	1.82	0.45
1:F:315:TYR:CD1	1:F:346:CYS:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:317:GLU:HG3	1:F:319:PRO:HD2	1.97	0.45
1:F:341:TRP:CZ3	1:F:345:LYS:HD2	2.52	0.45
1:A:311:PRO:HB2	1:A:313:GLU:CD	2.42	0.45
1:A:662:ASN:OD1	1:A:664:SER:OG	2.22	0.45
1:B:91:TYR:CD2	1:B:164:LYS:HD3	2.51	0.45
1:C:180:ASP:O	1:C:184:GLN:NE2	2.35	0.45
1:C:485:THR:HA	1:C:488:ILE:HD12	1.98	0.45
1:C:617:TYR:CZ	1:C:632:LEU:HD23	2.52	0.45
1:D:180:ASP:O	1:D:184:GLN:NE2	2.33	0.45
1:D:229:LEU:HG	1:D:230:VAL:H	1.82	0.45
1:D:325:VAL:HA	1:D:328:LEU:HD12	1.99	0.45
1:D:681:MET:HA	1:D:684:LYS:HE2	1.98	0.45
1:E:76:ARG:HG2	1:E:212:GLY:O	2.17	0.45
1:F:830:LYS:NZ	1:F:840:THR:OG1	2.33	0.45
1:A:35:LEU:HB2	1:A:67:ARG:HH22	1.80	0.45
1:A:916:GLN:HG3	1:A:919:GLU:HG2	1.99	0.45
1:B:99:ASP:N	1:B:198:CYS:O	2.38	0.45
1:B:585:VAL:HG13	1:B:586:PRO:CD	2.47	0.45
1:B:946:SER:OG	1:B:948:ASN:O	2.34	0.45
1:C:23:GLU:O	1:C:24:VAL:HB	2.16	0.45
1:D:21:LEU:HD22	1:D:78:GLN:HG2	1.99	0.45
1:E:89:GLY:O	1:E:91:TYR:N	2.49	0.45
1:E:585:VAL:CG1	1:E:586:PRO:HD2	2.46	0.45
1:E:588:ASN:HB3	1:E:590:GLU:HG3	1.99	0.45
1:E:609:ASP:OD1	1:E:610:ALA:N	2.49	0.45
1:F:192:VAL:HG12	1:F:194:ASN:H	1.81	0.45
1:A:229:LEU:HG	1:A:230:VAL:H	1.82	0.45
1:A:347:PRO:HB2	1:A:351:ASN:HD21	1.81	0.45
1:A:641:GLY:HA2	1:A:644:PHE:HB3	1.99	0.45
1:E:70:GLU:HA	1:E:73:GLU:CD	2.42	0.45
1:E:84:PHE:N	1:E:84:PHE:CD1	2.85	0.45
1:E:141:PHE:HA	1:E:160:ILE:CD1	2.46	0.45
1:E:185:LYS:HG2	1:E:186:ILE:HD12	1.98	0.45
1:F:481:MET:SD	1:F:518:ILE:HD13	2.57	0.45
1:F:641:GLY:HA2	1:F:644:PHE:HB3	1.98	0.45
1:B:112:PRO:N	1:B:113:PRO:HD2	2.32	0.45
1:B:166:ALA:HA	1:B:170:LYS:HG3	2.00	0.45
1:B:910:HIS:H	1:B:913:GLU:HG3	1.82	0.45
1:D:95:MET:CE	1:D:159:LEU:HD13	2.47	0.45
1:D:455:GLY:HA3	1:D:579:TYR:CE1	2.52	0.45
1:D:498:SER:HA	1:D:501:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:524:LYS:O	1:E:528:ILE:HG23	2.17	0.45
1:E:653:LEU:HG	1:E:657:TYR:HB2	1.98	0.45
1:E:665:LEU:HD21	1:E:679:ALA:HB3	1.99	0.45
1:A:11:THR:OG1	1:A:13:GLN:OE1	2.30	0.44
1:C:11:THR:OG1	1:C:13:GLN:OE1	2.35	0.44
1:C:67:ARG:O	1:C:70:GLU:HG3	2.17	0.44
1:C:631:MET:O	1:C:754:ARG:N	2.48	0.44
1:C:802:TRP:O	1:C:806:GLN:HG2	2.17	0.44
1:D:157:HIS:CD2	1:D:221:TYR:HE2	2.35	0.44
1:A:93:GLY:O	1:A:170:LYS:NZ	2.50	0.44
1:A:105:ASN:HA	1:A:153:LYS:HD3	1.99	0.44
1:A:170:LYS:O	1:A:174:ILE:HG12	2.17	0.44
1:B:15:THR:O	1:B:18:ARG:HG3	2.16	0.44
1:B:617:TYR:O	1:B:620:THR:OG1	2.27	0.44
1:C:15:THR:HA	1:C:18:ARG:NE	2.32	0.44
1:C:401:ILE:O	1:C:404:GLU:HG2	2.16	0.44
1:C:613:TRP:CE3	1:C:614:ILE:HD13	2.52	0.44
1:E:70:GLU:HA	1:E:73:GLU:OE1	2.17	0.44
1:F:602:GLN:HA	1:F:942:TRP:CH2	2.52	0.44
1:B:62:SER:HA	1:B:65:LEU:HD12	1.99	0.44
1:B:491:HIS:HA	1:B:494:GLN:HG2	1.99	0.44
1:B:615:MET:SD	1:B:616:PHE:N	2.90	0.44
1:C:53:ILE:HG22	1:C:54:THR:HG23	2.00	0.44
1:E:22:ALA:C	1:E:24:VAL:H	2.24	0.44
1:E:199:LEU:HD12	1:E:200:ASP:H	1.83	0.44
1:E:779:ARG:O	1:E:783:GLU:N	2.48	0.44
1:E:939:LYS:HA	1:E:942:TRP:HD1	1.82	0.44
1:F:153:LYS:HG3	1:F:154:TYR:HD1	1.82	0.44
1:F:166:ALA:HA	1:F:170:LYS:HG3	1.99	0.44
1:D:512:GLU:HA	1:D:515:LYS:HG2	1.98	0.44
1:E:481:MET:HE2	1:E:515:LYS:HA	2.00	0.44
1:F:66:LEU:HA	1:F:69:TYR:CD2	2.52	0.44
1:F:121:ARG:HE	1:F:182:THR:HB	1.82	0.44
1:F:350:TRP:HA	1:F:354:GLY:HA3	1.99	0.44
1:A:494:GLN:HB2	1:A:496:HIS:CD2	2.52	0.44
1:B:292:ILE:O	1:B:296:HIS:ND1	2.45	0.44
1:B:834:THR:HG22	1:B:837:ARG:HH22	1.82	0.44
1:C:631:MET:N	1:C:752:ARG:O	2.41	0.44
1:D:417:MET:HA	1:D:420:LYS:HZ3	1.81	0.44
1:D:622:ILE:HG21	1:D:798:LEU:HD13	1.99	0.44
1:E:40:THR:CB	1:E:47:THR:HB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:GLN:HG2	1:E:207:PRO:HA	1.99	0.44
1:E:106:ALA:C	1:E:153:LYS:HG2	2.42	0.44
1:E:215:LYS:CB	1:E:218:HIS:HB2	2.48	0.44
1:F:846:SER:N	1:F:905:GLY:O	2.46	0.44
1:F:870:ILE:HG22	1:F:871:ASN:N	2.33	0.44
1:B:868:THR:OG1	1:B:911:LYS:HE3	2.18	0.44
1:C:328:LEU:HD13	1:C:375:LYS:HZ2	1.82	0.44
1:D:529:ARG:NE	1:E:521:ASP:OD1	2.45	0.44
1:E:36:SER:C	1:E:38:PHE:H	2.24	0.44
1:E:73:GLU:HG2	1:E:252:LEU:CG	2.48	0.44
1:F:360:LYS:HB3	1:F:360:LYS:HE2	1.81	0.44
1:F:496:HIS:N	1:F:497:GLU:OE1	2.50	0.44
1:F:585:VAL:CG1	1:F:586:PRO:CD	2.96	0.44
1:F:743:ASP:N	1:F:743:ASP:OD1	2.50	0.44
1:A:70:GLU:O	1:A:73:GLU:HB2	2.18	0.44
1:A:139:ILE:N	1:A:267:ARG:HH22	2.16	0.44
1:A:564:PRO:HG2	1:A:566:LYS:HE3	2.00	0.44
1:B:27:LEU:HD11	1:B:71:HIS:HB3	1.99	0.44
1:B:339:ALA:HB1	1:B:358:LEU:HD11	2.00	0.44
1:B:433:ASP:HB3	1:B:541:ILE:HG23	2.00	0.44
1:B:549:HIS:CD2	1:B:560:ILE:HG13	2.47	0.44
1:C:699:VAL:HG22	1:C:741:ILE:HB	2.00	0.44
1:D:166:ALA:HA	1:D:170:LYS:HG3	2.00	0.44
1:E:17:GLN:HE22	1:E:81:LEU:HB2	1.81	0.44
1:E:75:CYS:HB3	1:E:82:MET:SD	2.58	0.44
1:E:140:HIS:CE1	1:E:265:LEU:HG	2.53	0.44
1:E:339:ALA:HB1	1:E:358:LEU:HD11	2.00	0.44
1:F:409:TYR:CE2	1:F:417:MET:HG2	2.52	0.44
1:A:215:LYS:HB2	1:A:218:HIS:HB2	1.99	0.44
1:A:523:PHE:O	1:A:527:VAL:HG23	2.18	0.44
1:C:50:ILE:O	1:C:85:LEU:N	2.50	0.44
1:E:700:LEU:HD21	1:E:742:ILE:HG12	2.00	0.44
1:F:97:ASP:OD1	1:F:97:ASP:N	2.51	0.44
1:A:534:LEU:HD23	1:A:534:LEU:HA	1.82	0.44
1:B:530:GLN:HE22	1:C:470:HIS:HE1	1.66	0.44
1:D:470:HIS:NE2	1:D:524:LYS:HD3	2.33	0.44
1:E:250:TYR:CE1	1:E:265:LEU:HD13	2.53	0.44
1:E:314:TYR:CD2	1:E:320:LEU:HB3	2.51	0.44
1:E:414:GLU:CD	1:E:415:HIS:N	2.74	0.44
1:E:525:LYS:O	1:E:528:ILE:HG12	2.17	0.44
1:E:699:VAL:CG1	1:E:700:LEU:N	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ASP:OD1	1:A:287:ASP:N	2.50	0.43
1:D:455:GLY:HA2	1:D:554:GLY:HA2	1.99	0.43
1:E:232:ASP:OD1	1:E:235:ASP:HB2	2.18	0.43
1:A:666:LEU:HB3	1:A:691:PHE:CZ	2.53	0.43
1:D:788:PRO:HA	1:D:791:GLN:OE1	2.18	0.43
1:E:153:LYS:HD2	1:E:153:LYS:HA	1.39	0.43
1:E:227:PHE:CZ	1:E:229:LEU:HB2	2.52	0.43
1:E:302:TYR:O	1:E:306:ILE:HG23	2.18	0.43
1:F:161:PRO:HG2	1:F:266:VAL:HG11	2.00	0.43
1:A:92:SER:HB2	1:A:258:LEU:HD22	2.00	0.43
1:A:219:LYS:HD3	1:A:220:PRO:O	2.19	0.43
1:A:779:ARG:HB3	1:A:784:TYR:CD1	2.54	0.43
1:B:73:GLU:HA	1:B:76:ARG:HE	1.83	0.43
1:B:664:SER:HA	1:B:667:THR:HG22	1.99	0.43
1:C:95:MET:SD	1:C:95:MET:N	2.91	0.43
1:C:112:PRO:HA	1:C:115:LEU:HD12	2.00	0.43
1:C:544:LEU:HD23	1:C:575:PRO:O	2.18	0.43
1:D:25:GLN:HA	1:D:28:GLU:OE2	2.17	0.43
1:D:171:LYS:HA	1:D:171:LYS:HD3	1.67	0.43
1:D:665:LEU:HD23	1:D:665:LEU:HA	1.89	0.43
1:D:689:GLY:N	1:D:731:THR:O	2.35	0.43
1:E:84:PHE:HB3	1:E:210:LEU:HD13	1.99	0.43
1:E:125:HIS:CD2	1:E:177:LEU:HD13	2.53	0.43
1:E:177:LEU:HD13	1:E:177:LEU:HA	1.81	0.43
1:E:263:GLY:CA	1:E:266:VAL:HG23	2.49	0.43
1:E:309:LEU:HD11	1:E:393:ILE:HD12	2.00	0.43
1:E:476:ASN:HA	1:E:479:ARG:HE	1.83	0.43
1:A:66:LEU:O	1:A:70:GLU:HG2	2.19	0.43
1:A:614:ILE:HD11	1:A:634:TRP:CZ2	2.53	0.43
1:B:790:CYS:SG	1:B:791:GLN:N	2.91	0.43
1:E:27:LEU:O	1:E:28:GLU:C	2.62	0.43
1:E:34:GLU:O	1:E:37:VAL:HG23	2.18	0.43
1:E:111:GLU:CD	1:E:111:GLU:H	2.26	0.43
1:E:574:HIS:HB3	1:E:576:ILE:HD11	1.99	0.43
1:A:483:ARG:HA	1:A:486:GLU:CD	2.44	0.43
1:C:267:ARG:CZ	1:C:269:VAL:HG22	2.49	0.43
1:D:52:ARG:HB3	1:D:83:TYR:CD1	2.53	0.43
1:D:72:LEU:HD21	1:D:84:PHE:CE2	2.53	0.43
1:E:18:ARG:NH2	1:E:28:GLU:OE2	2.52	0.43
1:E:21:LEU:HD13	1:E:80:ALA:HB2	2.01	0.43
1:E:51:ASN:HB2	1:E:84:PHE:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:ARG:HD2	1:E:121:ARG:HA	1.65	0.43
1:E:829:ARG:O	1:E:833:ASP:N	2.39	0.43
1:B:146:LYS:HG3	1:B:155:GLY:H	1.84	0.43
1:B:216:LEU:HD22	1:B:216:LEU:HA	1.79	0.43
1:D:107:VAL:HG12	1:D:148:GLU:HG2	2.01	0.43
1:D:574:HIS:HB3	1:D:576:ILE:CD1	2.47	0.43
1:E:75:CYS:HA	1:E:78:GLN:CD	2.44	0.43
1:E:107:VAL:HG22	1:E:148:GLU:HG3	1.99	0.43
1:E:148:GLU:HA	1:E:153:LYS:HE2	2.00	0.43
1:E:700:LEU:HD13	1:E:705:LEU:HD21	2.01	0.43
1:F:146:LYS:HG3	1:F:155:GLY:N	2.32	0.43
1:B:429:LYS:HE2	1:B:430:PHE:CE2	2.54	0.43
1:C:63:THR:O	1:C:66:LEU:HG	2.18	0.43
1:C:315:TYR:HB3	1:C:342:PHE:CE2	2.54	0.43
1:C:807:LYS:HE3	1:C:808:GLU:OE1	2.19	0.43
1:D:316:VAL:HG12	1:D:346:CYS:SG	2.58	0.43
1:E:46:LYS:HD3	1:E:59:ALA:CB	2.47	0.43
1:E:125:HIS:CE1	1:E:176:SER:HB2	2.54	0.43
1:E:211:TYR:CE1	1:E:223:LEU:HB3	2.53	0.43
1:E:219:LYS:HA	1:E:219:LYS:HD3	1.51	0.43
1:F:108:PRO:HG2	1:F:154:TYR:CE1	2.53	0.43
1:F:883:GLU:O	1:F:887:SER:N	2.52	0.43
1:A:164:LYS:NZ	1:A:268:PRO:O	2.52	0.43
1:A:607:GLU:OE1	1:A:607:GLU:N	2.45	0.43
1:B:292:ILE:HG23	1:B:296:HIS:CE1	2.54	0.43
1:B:706:LYS:HA	1:B:709:VAL:HG22	2.01	0.43
1:C:87:ARG:HG3	1:C:207:PRO:HG3	2.00	0.43
1:C:743:ASP:OD1	1:C:743:ASP:N	2.50	0.43
1:E:22:ALA:HA	1:E:25:GLN:CD	2.44	0.43
1:E:88:GLN:HE22	1:E:95:MET:CB	2.31	0.43
1:A:192:VAL:HG12	1:A:194:ASN:H	1.84	0.43
1:A:642:LYS:HG3	1:A:643:THR:N	2.34	0.43
1:A:941:LYS:NZ	1:A:948:ASN:O	2.47	0.43
1:B:26:ALA:HA	1:B:29:THR:HG22	2.00	0.43
1:E:142:PHE:CD2	1:E:159:LEU:HB3	2.52	0.43
1:E:427:GLY:HA2	1:E:535:PHE:CE2	2.54	0.43
1:A:60:LEU:HB3	1:A:64:GLU:CG	2.49	0.43
1:A:226:GLY:H	1:A:247:LEU:HD11	1.84	0.43
1:A:550:LEU:HD22	1:A:576:ILE:HD11	2.00	0.43
1:B:50:ILE:O	1:B:85:LEU:N	2.52	0.43
1:E:89:GLY:O	1:E:90:THR:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:LYS:HA	1:E:221:TYR:CD1	2.54	0.43
1:E:665:LEU:HD23	1:E:665:LEU:HA	1.90	0.43
1:E:705:LEU:HA	1:E:708:MET:HB2	2.01	0.43
1:F:303:LEU:HA	1:F:306:ILE:HG12	2.01	0.43
1:B:20:TYR:CD1	1:B:500:ILE:HG21	2.54	0.42
1:B:76:ARG:HH12	1:B:253:VAL:CG2	2.32	0.42
1:B:320:LEU:HA	1:B:323:ASN:ND2	2.34	0.42
1:C:101:LYS:HA	1:C:152:GLY:O	2.19	0.42
1:C:804:LYS:O	1:C:807:LYS:HB3	2.19	0.42
1:D:146:LYS:HD3	1:D:221:TYR:CE1	2.54	0.42
1:E:76:ARG:HH12	1:E:252:LEU:HB2	1.84	0.42
1:E:118:LEU:HD12	1:E:183:VAL:HG12	2.01	0.42
1:E:252:LEU:HG	1:E:252:LEU:H	1.58	0.42
1:E:647:ARG:HH11	1:E:781:ILE:HD11	1.84	0.42
1:F:830:LYS:NZ	1:F:837:ARG:HA	2.34	0.42
1:B:98:TYR:CE1	1:B:199:LEU:HD13	2.53	0.42
1:D:476:ASN:HA	1:D:479:ARG:HE	1.84	0.42
1:D:805:LEU:O	1:D:809:TYR:N	2.45	0.42
1:E:33:ARG:HG2	1:E:34:GLU:N	2.34	0.42
1:E:51:ASN:HD21	1:E:53:ILE:HG22	1.83	0.42
1:E:209:LEU:HD13	1:E:215:LYS:NZ	2.34	0.42
1:E:414:GLU:OE2	1:F:520:ASN:HA	2.19	0.42
1:E:594:THR:HG23	1:E:797:ILE:HD11	2.00	0.42
1:F:483:ARG:HA	1:F:486:GLU:HG3	2.00	0.42
1:C:540:PHE:O	1:C:543:THR:OG1	2.35	0.42
1:E:27:LEU:HA	1:E:30:LEU:HD23	2.01	0.42
1:E:126:ILE:HD12	1:E:163:LEU:HD21	2.01	0.42
1:E:214:SER:HA	1:E:220:PRO:CA	2.48	0.42
1:E:325:VAL:HA	1:E:328:LEU:HD12	2.02	0.42
1:F:509:LYS:O	1:F:513:ARG:NE	2.50	0.42
1:F:588:ASN:ND2	1:F:590:GLU:OE2	2.45	0.42
1:B:779:ARG:HB3	1:B:784:TYR:CE2	2.54	0.42
1:B:791:GLN:H	1:B:791:GLN:HG3	1.71	0.42
1:C:788:PRO:HA	1:C:791:GLN:OE1	2.18	0.42
1:D:209:LEU:HD21	1:D:215:LYS:NZ	2.35	0.42
1:D:375:LYS:HB3	1:D:379:MET:HE1	2.00	0.42
1:E:86:GLU:H	1:E:210:LEU:HD12	1.84	0.42
1:E:171:LYS:H	1:E:171:LYS:HG2	1.49	0.42
1:E:312:PRO:HA	1:E:315:TYR:CZ	2.55	0.42
1:E:457:ILE:HG13	1:E:458:TRP:CD1	2.54	0.42
1:E:616:PHE:HB3	1:E:805:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:827:ALA:O	1:E:830:LYS:HG3	2.19	0.42
1:F:325:VAL:HA	1:F:328:LEU:HD12	2.01	0.42
1:B:311:PRO:HB2	1:B:313:GLU:OE1	2.20	0.42
1:B:525:LYS:HB3	1:B:529:ARG:NH2	2.35	0.42
1:C:736:SER:HB3	1:C:740:PHE:CE1	2.55	0.42
1:D:54:THR:O	1:D:296:HIS:NE2	2.48	0.42
1:F:54:THR:HA	1:F:295:LEU:HD13	2.02	0.42
1:F:61:PRO:HD2	1:F:64:GLU:OE2	2.19	0.42
1:F:311:PRO:HG3	1:F:385:HIS:NE2	2.34	0.42
1:A:41:GLU:HG3	1:A:42:PRO:HD2	2.02	0.42
1:A:354:GLY:HA2	1:A:357:LYS:HE2	2.02	0.42
1:A:467:ASP:OD1	1:A:467:ASP:N	2.51	0.42
1:B:98:TYR:HE1	1:B:199:LEU:HD13	1.83	0.42
1:C:941:LYS:NZ	1:C:946:SER:OG	2.50	0.42
1:E:219:LYS:HB3	1:E:220:PRO:HD2	2.01	0.42
1:E:911:LYS:HA	1:E:911:LYS:HD3	1.82	0.42
1:F:156:PHE:CE2	1:F:158:VAL:HB	2.54	0.42
1:F:310:LEU:HD23	1:F:310:LEU:HA	1.91	0.42
1:F:444:GLU:HG3	1:F:463:GLU:OE2	2.20	0.42
1:F:478:SER:HA	1:F:481:MET:HG2	2.00	0.42
1:F:844:VAL:HB	1:F:919:GLU:HB3	2.01	0.42
1:C:13:GLN:O	1:C:17:GLN:HG2	2.19	0.42
1:C:153:LYS:HG3	1:C:154:TYR:HD1	1.83	0.42
1:C:750:TRP:CZ2	1:C:833:ASP:HB2	2.54	0.42
1:E:22:ALA:O	1:E:25:GLN:N	2.52	0.42
1:E:94:LEU:HD13	1:E:170:LYS:HD2	2.02	0.42
1:E:96:LEU:CD2	1:E:174:ILE:HG13	2.50	0.42
1:E:105:ASN:HA	1:E:153:LYS:HB2	2.01	0.42
1:E:248:GLU:HA	1:E:252:LEU:CD2	2.49	0.42
1:E:287:ASP:CG	1:E:289:SER:HG	2.28	0.42
1:E:494:GLN:HB2	1:E:496:HIS:NE2	2.34	0.42
1:F:219:LYS:HD2	1:F:220:PRO:O	2.19	0.42
1:A:40:THR:HB	1:A:57:THR:O	2.19	0.42
1:A:468:GLU:HA	1:A:471:ILE:HD12	2.02	0.42
1:B:51:ASN:HB3	1:B:56:LYS:CG	2.50	0.42
1:B:95:MET:CE	1:B:159:LEU:HD13	2.50	0.42
1:C:291:SER:HA	1:C:294:MET:HG3	2.02	0.42
1:C:525:LYS:O	1:C:529:ARG:HG2	2.20	0.42
1:C:609:ASP:OD1	1:C:610:ALA:N	2.53	0.42
1:C:633:LEU:N	1:C:754:ARG:O	2.51	0.42
1:D:41:GLU:OE1	1:D:44:SER:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:SER:HB3	1:D:262:GLN:NE2	2.31	0.42
1:D:485:THR:O	1:D:489:LYS:HE3	2.20	0.42
1:D:616:PHE:O	1:D:619:SER:OG	2.28	0.42
1:E:47:THR:HB	1:E:57:THR:HB	2.01	0.42
1:E:52:ARG:HD2	1:E:216:LEU:H	1.85	0.42
1:E:117:ARG:HH11	1:E:182:THR:HG21	1.85	0.42
1:F:24:VAL:HA	1:F:27:LEU:HD13	2.00	0.42
1:A:617:TYR:O	1:A:620:THR:OG1	2.29	0.42
1:B:916:GLN:HG3	1:B:919:GLU:HG2	2.01	0.42
1:C:457:ILE:HD12	1:C:457:ILE:HA	1.95	0.42
1:E:31:LEU:CA	1:E:35:LEU:HB2	2.48	0.42
1:E:52:ARG:HE	1:E:83:TYR:CB	2.32	0.42
1:E:76:ARG:HD2	1:E:211:TYR:O	2.20	0.42
1:E:263:GLY:HA3	1:E:266:VAL:HG23	2.01	0.42
1:A:13:GLN:O	1:A:17:GLN:HG2	2.20	0.42
1:A:35:LEU:HD12	1:A:67:ARG:NH2	2.35	0.42
1:A:644:PHE:HD2	1:A:645:LEU:HD22	1.83	0.42
1:A:666:LEU:HD23	1:A:691:PHE:CE1	2.55	0.42
1:B:310:LEU:HD23	1:B:310:LEU:HA	1.87	0.42
1:B:453:ASN:HB2	1:B:456:GLU:CD	2.44	0.42
1:C:76:ARG:NH2	1:C:211:TYR:HE1	2.18	0.42
1:D:146:LYS:O	1:D:222:GLN:NE2	2.49	0.42
1:D:663:ILE:O	1:D:666:LEU:HG	2.20	0.42
1:E:65:LEU:HB3	1:E:69:TYR:CZ	2.55	0.42
1:E:419:ALA:HA	1:E:422:ILE:HG22	2.02	0.42
1:F:88:GLN:NE2	1:F:95:MET:HB3	2.34	0.42
1:F:698:GLU:OE2	1:F:736:SER:OG	2.36	0.42
1:A:51:ASN:HB3	1:A:56:LYS:CG	2.49	0.41
1:B:705:LEU:O	1:B:709:VAL:HG13	2.19	0.41
1:C:162:GLY:O	1:C:269:VAL:N	2.53	0.41
1:D:140:HIS:NE2	1:D:265:LEU:O	2.53	0.41
1:D:521:ASP:O	1:D:525:LYS:HG3	2.20	0.41
1:E:100:LEU:HB2	1:E:154:TYR:O	2.19	0.41
1:E:786:MET:SD	1:E:786:MET:N	2.93	0.41
1:F:699:VAL:HG12	1:F:700:LEU:N	2.35	0.41
1:B:357:LYS:HA	1:B:360:LYS:HE2	2.02	0.41
1:C:293:LEU:HD21	1:C:334:ASN:O	2.20	0.41
1:C:525:LYS:HA	1:C:528:ILE:HG12	2.01	0.41
1:D:65:LEU:O	1:D:68:LEU:HG	2.20	0.41
1:E:60:LEU:HD12	1:E:65:LEU:HD23	2.01	0.41
1:E:867:ASN:OD1	1:E:875:HIS:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:940:ASN:HA	1:E:943:TRP:CD1	2.56	0.41
1:F:116:SER:O	1:F:120:HIS:ND1	2.52	0.41
1:A:429:LYS:HG2	1:A:445:PHE:HB3	2.00	0.41
1:B:97:ASP:OD1	1:B:97:ASP:N	2.54	0.41
1:B:252:LEU:HD12	1:B:253:VAL:N	2.35	0.41
1:B:611:ARG:O	1:B:615:MET:HG3	2.19	0.41
1:D:653:LEU:HG	1:D:657:TYR:HB2	2.01	0.41
1:E:51:ASN:HD21	1:E:53:ILE:CG2	2.34	0.41
1:E:110:LEU:HD11	1:E:154:TYR:CE2	2.55	0.41
1:E:122:ILE:CB	1:E:177:LEU:HD21	2.51	0.41
1:A:435:ASP:OD1	1:A:439:LYS:N	2.31	0.41
1:B:73:GLU:CG	1:B:76:ARG:HH21	2.34	0.41
1:B:315:TYR:HB3	1:B:342:PHE:CZ	2.56	0.41
1:B:466:PRO:O	1:B:470:HIS:N	2.40	0.41
1:C:123:PHE:O	1:C:126:ILE:HG22	2.21	0.41
1:C:613:TRP:HD1	1:C:816:VAL:HB	1.85	0.41
1:C:700:LEU:HD21	1:C:742:ILE:HG12	2.02	0.41
1:D:311:PRO:HB2	1:D:313:GLU:CD	2.45	0.41
1:E:83:TYR:HA	1:E:214:SER:O	2.20	0.41
1:E:112:PRO:HG3	1:E:225:THR:HG21	2.02	0.41
1:E:123:PHE:HA	1:E:126:ILE:CD1	2.50	0.41
1:E:140:HIS:ND1	1:E:228:GLU:HG2	2.35	0.41
1:E:430:PHE:HB2	1:E:535:PHE:CE2	2.55	0.41
1:E:704:ARG:O	1:E:708:MET:HG2	2.20	0.41
1:A:23:GLU:O	1:A:78:GLN:NE2	2.39	0.41
1:A:376:ARG:CZ	1:A:428:ASN:HB3	2.49	0.41
1:A:510:ALA:HA	1:A:513:ARG:NH1	2.34	0.41
1:A:604:ILE:HA	1:A:760:VAL:HG11	2.02	0.41
1:A:790:CYS:SG	1:A:791:GLN:N	2.93	0.41
1:A:885:GLU:O	1:A:890:GLU:HB2	2.20	0.41
1:C:97:ASP:HA	1:C:157:HIS:ND1	2.36	0.41
1:C:147:PRO:HG2	1:C:219:LYS:HB3	2.01	0.41
1:C:483:ARG:O	1:C:486:GLU:HG3	2.20	0.41
1:C:613:TRP:CD1	1:C:816:VAL:HB	2.56	0.41
1:D:20:TYR:CE1	1:D:504:TYR:HE2	2.39	0.41
1:D:37:VAL:HG23	1:D:38:PHE:CD1	2.55	0.41
1:D:88:GLN:NE2	1:D:204:ALA:HA	2.35	0.41
1:D:97:ASP:OD1	1:D:97:ASP:N	2.48	0.41
1:E:121:ARG:HB3	1:E:177:LEU:HD11	2.02	0.41
1:E:122:ILE:CG2	1:E:177:LEU:HD21	2.49	0.41
1:F:73:GLU:HB3	1:F:77:LYS:HZ3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ARG:HA	1:A:379:MET:HE2	2.03	0.41
1:B:51:ASN:HB3	1:B:56:LYS:HG3	2.03	0.41
1:B:76:ARG:HH22	1:B:253:VAL:CG2	2.34	0.41
1:B:102:LEU:HD22	1:B:153:LYS:HG2	2.02	0.41
1:C:97:ASP:OD1	1:C:97:ASP:N	2.52	0.41
1:D:110:LEU:HD23	1:D:115:LEU:HD21	2.03	0.41
1:D:750:TRP:CZ2	1:D:833:ASP:HB2	2.55	0.41
1:D:777:ASP:HB3	1:D:780:PHE:CG	2.56	0.41
1:E:65:LEU:HA	1:E:68:LEU:HD23	2.02	0.41
1:E:144:THR:HA	1:E:223:LEU:HB2	2.02	0.41
1:E:145:LEU:HB3	1:E:224:LYS:HZ3	1.84	0.41
1:E:375:LYS:HA	1:E:378:ILE:HD12	2.02	0.41
1:A:85:LEU:HD23	1:A:209:LEU:HB3	2.01	0.41
1:A:418:ILE:HG23	1:A:477:PHE:CE2	2.56	0.41
1:A:780:PHE:CD2	1:A:781:ILE:HG12	2.56	0.41
1:B:427:GLY:HA2	1:B:535:PHE:HE2	1.85	0.41
1:C:125:HIS:NE2	1:C:180:ASP:OD2	2.46	0.41
1:D:125:HIS:NE2	1:D:180:ASP:OD2	2.47	0.41
1:D:294:MET:O	1:D:301:ARG:NH2	2.54	0.41
1:D:388:GLN:O	1:D:391:LYS:N	2.53	0.41
1:E:13:GLN:HG3	1:E:14:LEU:N	2.36	0.41
1:E:86:GLU:CD	1:E:257:SER:HA	2.45	0.41
1:E:161:PRO:O	1:E:162:GLY:C	2.62	0.41
1:E:210:LEU:O	1:E:211:TYR:C	2.64	0.41
1:E:224:LYS:HE3	1:E:224:LYS:HB3	1.51	0.41
1:E:406:VAL:HG23	1:E:411:GLY:HA2	2.03	0.41
1:F:387:PRO:O	1:F:390:TYR:HB3	2.21	0.41
1:F:509:LYS:O	1:F:512:GLU:HG3	2.21	0.41
1:F:513:ARG:O	1:F:517:LYS:HG3	2.20	0.41
1:F:790:CYS:SG	1:F:791:GLN:N	2.94	0.41
1:A:312:PRO:HA	1:A:315:TYR:CZ	2.55	0.41
1:A:624:ARG:HD3	1:A:657:TYR:CD1	2.55	0.41
1:B:587:PHE:HE1	1:B:797:ILE:HG12	1.86	0.41
1:D:47:THR:HA	1:D:59:ALA:HB2	2.02	0.41
1:D:509:LYS:HG2	1:D:513:ARG:NE	2.36	0.41
1:D:910:HIS:ND1	1:D:913:GLU:OE1	2.53	0.41
1:E:85:LEU:CA	1:E:209:LEU:HA	2.40	0.41
1:E:231:PHE:HE2	1:E:269:VAL:HG11	1.85	0.41
1:E:311:PRO:HB2	1:E:313:GLU:OE1	2.20	0.41
1:E:894:GLN:N	1:E:903:LEU:HA	2.36	0.41
1:F:290:LEU:O	1:F:294:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:787:ASP:HB3	1:F:790:CYS:HB3	2.03	0.41
1:A:153:LYS:HG3	1:A:154:TYR:CD1	2.56	0.41
1:A:164:LYS:NZ	1:A:268:PRO:HB2	2.35	0.41
1:A:457:ILE:HG13	1:A:458:TRP:CD1	2.56	0.41
1:A:476:ASN:O	1:A:480:VAL:HG23	2.21	0.41
1:A:525:LYS:HB3	1:A:529:ARG:NH1	2.36	0.41
1:A:613:TRP:CH2	1:A:754:ARG:HG3	2.55	0.41
1:B:184:GLN:NE2	1:B:196:GLU:OE2	2.54	0.41
1:B:699:VAL:HG22	1:B:741:ILE:HD12	2.02	0.41
1:B:813:ILE:HD12	1:B:816:VAL:HG21	2.02	0.41
1:C:372:LYS:HD3	1:C:574:HIS:HD2	1.86	0.41
1:C:602:GLN:HA	1:C:942:TRP:CH2	2.56	0.41
1:D:185:LYS:HA	1:D:188:HIS:HD1	1.85	0.41
1:D:310:LEU:HD23	1:D:310:LEU:HA	1.88	0.41
1:D:534:LEU:HD23	1:D:534:LEU:HA	1.95	0.41
1:E:24:VAL:HG12	1:E:25:GLN:N	2.34	0.41
1:E:147:PRO:O	1:E:148:GLU:HB2	2.21	0.41
1:E:196:GLU:O	1:E:198:CYS:N	2.50	0.41
1:E:250:TYR:HB2	1:E:255:GLU:CG	2.51	0.41
1:E:291:SER:C	1:E:296:HIS:HD1	2.27	0.41
1:E:368:HIS:NE2	1:E:371:LYS:HA	2.35	0.41
1:E:370:GLU:C	1:E:372:LYS:H	2.29	0.41
1:E:491:HIS:HA	1:E:494:GLN:HG2	2.03	0.41
1:F:174:ILE:HD13	1:F:174:ILE:HA	1.95	0.41
1:F:176:SER:O	1:F:180:ASP:N	2.53	0.41
1:F:787:ASP:OD2	1:F:790:CYS:N	2.51	0.41
1:A:132:LEU:HD22	1:A:269:VAL:HG13	2.02	0.41
1:B:56:LYS:HD3	1:B:58:TYR:CZ	2.56	0.41
1:B:107:VAL:HG12	1:B:148:GLU:HG2	2.02	0.41
1:C:47:THR:HA	1:C:59:ALA:HB2	2.02	0.41
1:C:736:SER:OG	1:C:737:ASN:N	2.54	0.41
1:D:429:LYS:HG3	1:D:430:PHE:CE2	2.56	0.41
1:E:76:ARG:NE	1:E:212:GLY:HA3	2.36	0.41
1:E:256:LEU:O	1:E:257:SER:C	2.64	0.41
1:E:895:TRP:HZ2	1:F:757:ARG:HH12	1.69	0.41
1:F:457:ILE:HG13	1:F:458:TRP:CD1	2.56	0.41
1:A:613:TRP:HD1	1:A:816:VAL:HB	1.86	0.40
1:B:529:ARG:HA	1:B:532:GLU:CD	2.46	0.40
1:B:613:TRP:HD1	1:B:816:VAL:HB	1.87	0.40
1:C:17:GLN:O	1:C:20:TYR:HB3	2.21	0.40
1:C:211:TYR:OH	1:C:223:LEU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:GLU:HB2	1:C:417:MET:HE3	2.04	0.40
1:C:416:TYR:CD2	1:C:420:LYS:HE2	2.56	0.40
1:D:17:GLN:HA	1:D:20:TYR:HB2	2.02	0.40
1:D:515:LYS:O	1:D:518:ILE:HG12	2.21	0.40
1:E:76:ARG:HH11	1:E:253:VAL:CG2	2.30	0.40
1:E:118:LEU:HA	1:E:182:THR:CG2	2.51	0.40
1:E:144:THR:HA	1:E:223:LEU:CA	2.47	0.40
1:E:215:LYS:HZ3	1:E:215:LYS:CA	2.34	0.40
1:E:476:ASN:HA	1:E:479:ARG:NE	2.36	0.40
1:F:357:LYS:HA	1:F:360:LYS:HE2	2.03	0.40
1:F:432:VAL:O	1:F:536:ARG:HD2	2.21	0.40
1:F:762:PHE:CD2	1:F:776:GLU:HA	2.56	0.40
1:A:20:TYR:HE1	1:A:500:ILE:HG21	1.86	0.40
1:A:779:ARG:NH2	1:A:784:TYR:HA	2.35	0.40
1:B:171:LYS:HA	1:B:171:LYS:HD3	1.73	0.40
1:B:757:ARG:HD2	1:B:758:SER:O	2.20	0.40
1:C:167:ALA:H	1:C:170:LYS:HG3	1.85	0.40
1:C:794:PHE:O	1:C:798:LEU:HD23	2.21	0.40
1:D:609:ASP:OD1	1:D:610:ALA:N	2.54	0.40
1:E:33:ARG:HE	1:E:33:ARG:HB3	1.56	0.40
1:E:53:ILE:HG13	1:E:83:TYR:CE2	2.56	0.40
1:E:563:ILE:HG12	1:E:803:GLU:HG2	2.02	0.40
1:E:759:LYS:NZ	1:E:824:GLU:OE2	2.53	0.40
1:F:416:TYR:CE2	1:F:420:LYS:HE3	2.55	0.40
1:F:483:ARG:O	1:F:486:GLU:HG3	2.21	0.40
1:F:510:ALA:HA	1:F:513:ARG:HH21	1.86	0.40
1:F:736:SER:OG	1:F:737:ASN:N	2.52	0.40
1:F:777:ASP:OD1	1:F:779:ARG:NE	2.49	0.40
1:F:867:ASN:HA	1:F:872:VAL:HA	2.03	0.40
1:A:443:PHE:CE1	1:A:462:LYS:HB3	2.56	0.40
1:C:56:LYS:HD3	1:C:58:TYR:CE2	2.56	0.40
1:D:293:LEU:HD21	1:D:335:TYR:HD1	1.87	0.40
1:E:49:ILE:HD12	1:E:49:ILE:HA	1.93	0.40
1:E:156:PHE:HE1	1:E:224:LYS:HZ2	1.69	0.40
1:E:343:SER:OG	1:E:358:LEU:HD22	2.22	0.40
1:E:777:ASP:CG	1:E:779:ARG:HH21	2.29	0.40
1:F:18:ARG:HG2	1:F:25:GLN:NE2	2.36	0.40
1:F:107:VAL:HA	1:F:108:PRO:HD3	1.95	0.40
1:F:147:PRO:HA	1:F:222:GLN:HE22	1.85	0.40
1:A:254:SER:C	1:A:260:ASN:HD22	2.30	0.40
1:A:757:ARG:NH2	1:A:759:LYS:HG3	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:LEU:HD11	1:A:813:ILE:HD13	2.03	0.40
1:C:30:LEU:HD11	1:C:67:ARG:HE	1.86	0.40
1:C:146:LYS:HD3	1:C:221:TYR:CE1	2.56	0.40
1:C:321:TRP:HD1	1:C:342:PHE:CE2	2.39	0.40
1:C:460:TRP:CD1	1:C:575:PRO:HA	2.57	0.40
1:C:541:ILE:O	1:C:544:LEU:HB2	2.21	0.40
1:C:613:TRP:HE3	1:C:614:ILE:HD13	1.85	0.40
1:D:630:LEU:HD23	1:D:630:LEU:HA	1.94	0.40
1:E:24:VAL:O	1:E:28:GLU:HG3	2.21	0.40
1:E:86:GLU:O	1:E:86:GLU:HG2	2.20	0.40
1:F:617:TYR:O	1:F:620:THR:OG1	2.23	0.40
1:F:846:SER:OG	1:F:907:ARG:HB2	2.21	0.40
1:A:452:MET:HE1	1:A:456:GLU:H	1.87	0.40
1:A:634:TRP:HE3	1:A:642:LYS:HB2	1.87	0.40
1:B:895:TRP:HE1	1:C:757:ARG:HH12	1.69	0.40
1:E:76:ARG:NH1	1:E:252:LEU:HB2	2.36	0.40
1:E:107:VAL:HG22	1:E:153:LYS:HE3	2.03	0.40
1:E:139:ILE:HG23	1:E:140:HIS:N	2.37	0.40
1:E:184:GLN:HB3	1:E:195:PRO:CB	2.51	0.40
1:E:247:LEU:HA	1:E:250:TYR:CE1	2.56	0.40
1:E:584:TYR:HB2	1:E:795:PHE:HE2	1.86	0.40
1:F:97:ASP:O	1:F:199:LEU:HA	2.22	0.40
1:F:644:PHE:CD2	1:F:645:LEU:HD22	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	838/972 (86%)	794 (95%)	43 (5%)	1 (0%)	48 81
1	B	837/972 (86%)	794 (95%)	42 (5%)	1 (0%)	48 81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	838/972 (86%)	798 (95%)	37 (4%)	3 (0%)	30	65
1	D	840/972 (86%)	806 (96%)	33 (4%)	1 (0%)	48	81
1	E	840/972 (86%)	787 (94%)	53 (6%)	0	100	100
1	F	840/972 (86%)	803 (96%)	33 (4%)	4 (0%)	24	60
All	All	5033/5832 (86%)	4782 (95%)	241 (5%)	10 (0%)	44	75

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	B	24	VAL
1	C	24	VAL
1	D	24	VAL
1	F	24	VAL
1	F	890	GLU
1	C	901	ARG
1	F	108	PRO
1	F	370	GLU
1	C	370	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	717/879 (82%)	711 (99%)	6 (1%)	73	77
1	B	716/879 (82%)	705 (98%)	11 (2%)	57	70
1	C	717/879 (82%)	707 (99%)	10 (1%)	59	71
1	D	719/879 (82%)	709 (99%)	10 (1%)	59	71
1	E	719/879 (82%)	606 (84%)	113 (16%)	2	15
1	F	720/879 (82%)	705 (98%)	15 (2%)	47	65
All	All	4308/5274 (82%)	4143 (96%)	165 (4%)	30	51

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	582	ILE
1	A	583	CYS
1	A	585	VAL
1	A	789	ASP
1	A	790	CYS
1	A	791	GLN
1	B	183	VAL
1	B	185	LYS
1	B	202	HIS
1	B	213	SER
1	B	216	LEU
1	B	366	SER
1	B	367	HIS
1	B	370	GLU
1	B	547	ASN
1	B	789	ASP
1	B	790	CYS
1	C	369	THR
1	C	370	GLU
1	C	410	ASN
1	C	557	VAL
1	C	558	LEU
1	C	559	SER
1	C	560	ILE
1	C	789	ASP
1	C	790	CYS
1	C	791	GLN
1	D	370	GLU
1	D	372	LYS
1	D	569	ASN
1	D	574	HIS
1	D	577	HIS
1	D	578	GLN
1	D	582	ILE
1	D	583	CYS
1	D	789	ASP
1	D	790	CYS
1	E	11	THR
1	E	12	ILE
1	E	14	LEU
1	E	18	ARG
1	E	19	LYS

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Mol	Chain	Res	Type
1	E	21	LEU
1	E	23	GLU
1	E	24	VAL
1	E	25	GLN
1	E	27	LEU
1	E	30	LEU
1	E	33	ARG
1	E	37	VAL
1	E	39	LEU
1	E	45	LYS
1	E	47	THR
1	E	49	ILE
1	E	52	ARG
1	E	53	ILE
1	E	54	THR
1	E	60	LEU
1	E	62	SER
1	E	63	THR
1	E	66	LEU
1	E	68	LEU
1	E	72	LEU
1	E	75	CYS
1	E	76	ARG
1	E	77	LYS
1	E	82	MET
1	E	86	GLU
1	E	87	ARG
1	E	90	THR
1	E	96	LEU
1	E	97	ASP
1	E	98	TYR
1	E	99	ASP
1	E	101	LYS
1	E	103	ASN
1	E	104	THR
1	E	105	ASN
1	E	107	VAL
1	E	110	LEU
1	E	111	GLU
1	E	115	LEU
1	E	117	ARG
1	E	118	LEU

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Mol	Chain	Res	Type
1	E	122	ILE
1	E	126	ILE
1	E	127	LYS
1	E	131	VAL
1	E	132	LEU
1	E	139	ILE
1	E	144	THR
1	E	145	LEU
1	E	149	VAL
1	E	150	VAL
1	E	151	GLN
1	E	153	LYS
1	E	158	VAL
1	E	159	LEU
1	E	160	ILE
1	E	163	LEU
1	E	164	LYS
1	E	165	LEU
1	E	169	THR
1	E	171	LYS
1	E	173	ILE
1	E	174	ILE
1	E	177	LEU
1	E	178	GLN
1	E	180	ASP
1	E	183	VAL
1	E	184	GLN
1	E	185	LYS
1	E	186	ILE
1	E	187	LEU
1	E	189	GLU
1	E	193	THR
1	E	196	GLU
1	E	197	SER
1	E	205	SER
1	E	209	LEU
1	E	213	SER
1	E	214	SER
1	E	215	LYS
1	E	216	LEU
1	E	219	LYS
1	E	223	LEU

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Mol	Chain	Res	Type
1	E	224	LYS
1	E	227	PHE
1	E	232	ASP
1	E	233	SER
1	E	235	ASP
1	E	247	LEU
1	E	248	GLU
1	E	250	TYR
1	E	251	ASN
1	E	252	LEU
1	E	255	GLU
1	E	258	LEU
1	E	259	THR
1	E	260	ASN
1	E	262	GLN
1	E	265	LEU
1	E	266	VAL
1	E	267	ARG
1	E	287	ASP
1	E	369	THR
1	E	465	ASN
1	E	789	ASP
1	E	790	CYS
1	E	791	GLN
1	F	107	VAL
1	F	251	ASN
1	F	252	LEU
1	F	254	SER
1	F	258	LEU
1	F	259	THR
1	F	369	THR
1	F	370	GLU
1	F	751	ARG
1	F	752	ARG
1	F	754	ARG
1	F	789	ASP
1	F	790	CYS
1	F	898	ASN
1	F	900	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
1	A	260	ASN
1	A	351	ASN
1	A	367	HIS
1	A	530	GLN
1	A	747	HIS
1	A	764	HIS
1	A	810	ASN
1	A	898	ASN
1	A	910	HIS
1	B	78	GLN
1	B	184	GLN
1	B	188	HIS
1	B	262	GLN
1	B	363	ASN
1	B	389	GLN
1	B	530	GLN
1	B	549	HIS
1	B	810	ASN
1	B	894	GLN
1	C	105	ASN
1	C	218	HIS
1	C	363	ASN
1	C	470	HIS
1	C	701	ASN
1	C	806	GLN
1	C	812	GLN
1	D	260	ASN
1	D	428	ASN
1	D	491	HIS
1	D	549	HIS
1	D	581	HIS
1	D	695	ASN
1	D	792	ASN
1	E	51	ASN
1	E	78	GLN
1	E	120	HIS
1	E	188	HIS
1	E	194	ASN
1	E	260	ASN
1	E	262	GLN
1	E	415	HIS
1	E	465	ASN

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Mol	Chain	Res	Type
1	E	476	ASN
1	E	499	ASN
1	E	530	GLN
1	E	549	HIS
1	E	810	ASN
1	E	910	HIS
1	F	78	GLN
1	F	105	ASN
1	F	190	GLN
1	F	202	HIS
1	F	296	HIS
1	F	363	ASN
1	F	494	GLN
1	F	502	ASN
1	F	549	HIS
1	F	894	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 ⓘ

There are no chain breaks in this entry.

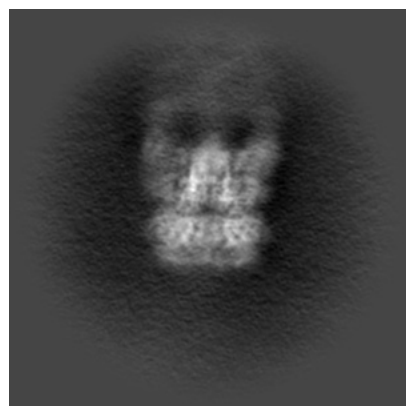
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37884. These allow visual inspection of the internal detail of the map and identification of artifacts.

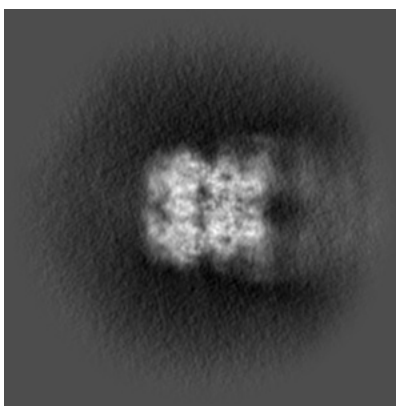
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

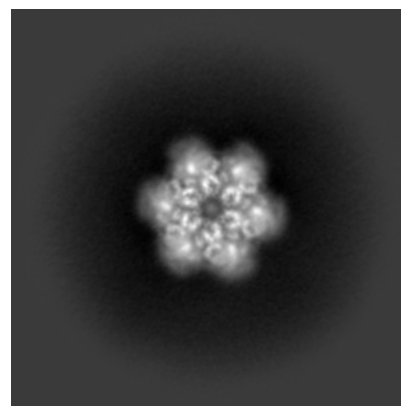
6.1.1 Primary map



X

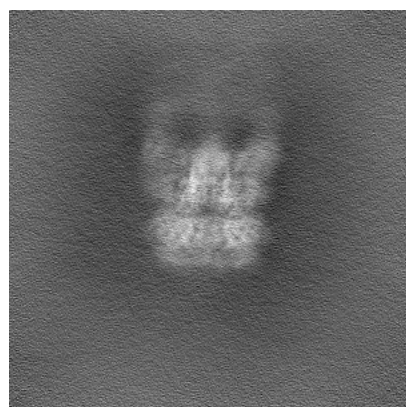


Y

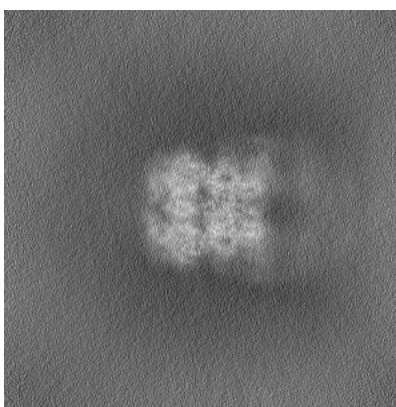


Z

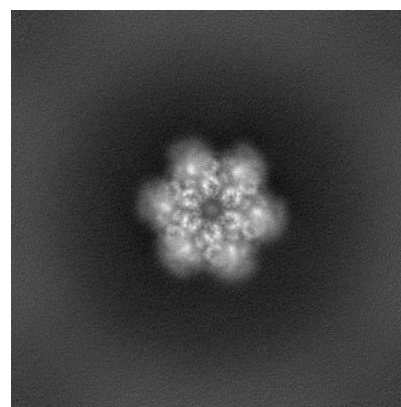
6.1.2 Raw map



X



Y

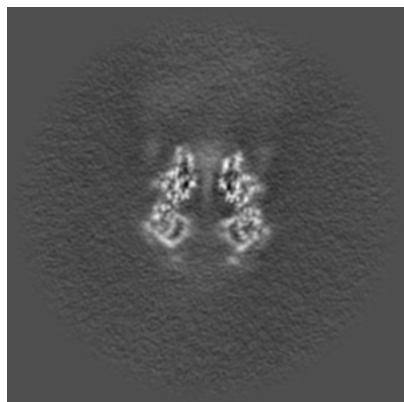


Z

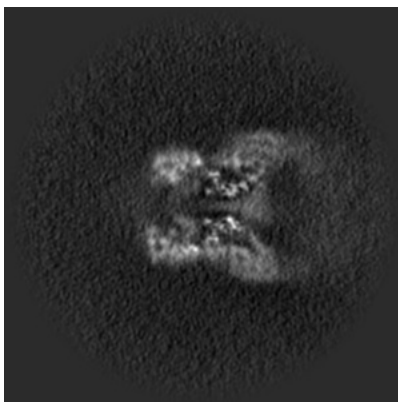
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

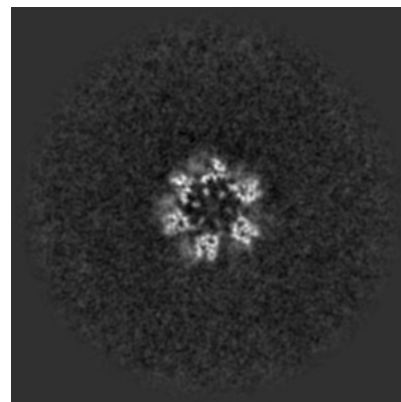
6.2.1 Primary map



X Index: 192

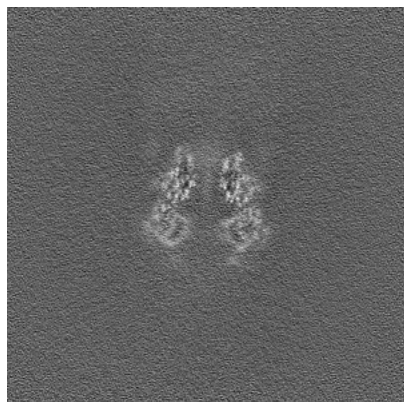


Y Index: 192

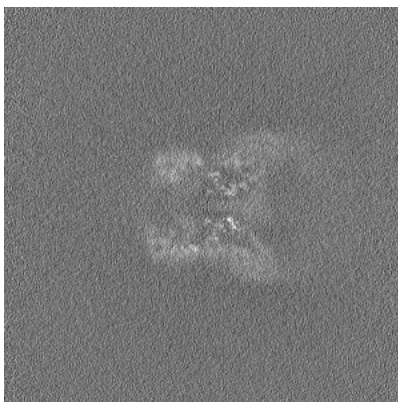


Z Index: 192

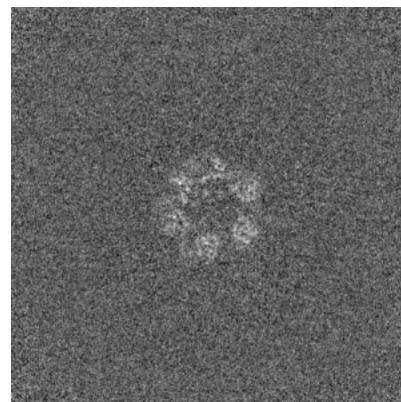
6.2.2 Raw map



X Index: 192



Y Index: 192

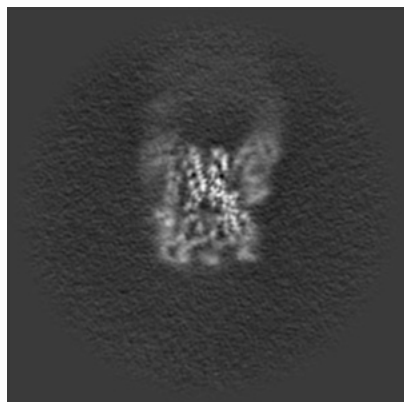


Z Index: 192

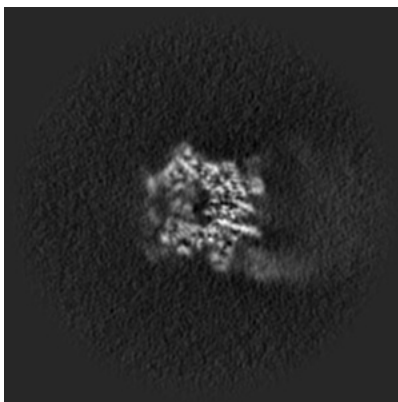
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

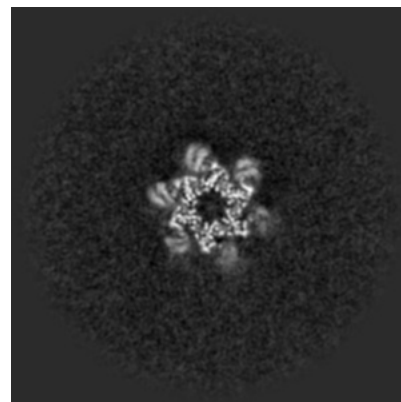
6.3.1 Primary map



X Index: 169

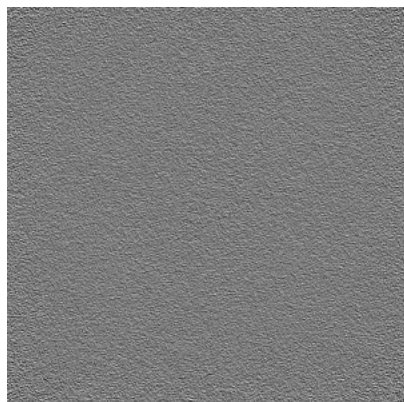


Y Index: 209

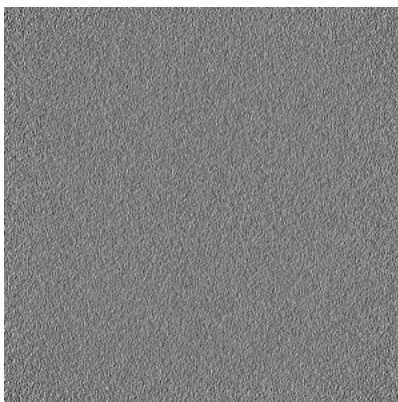


Z Index: 202

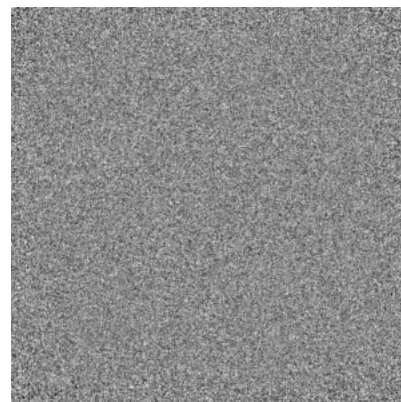
6.3.2 Raw map



X Index: 0



Y Index: 0

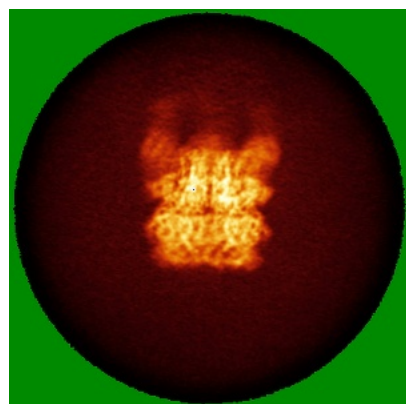


Z Index: 0

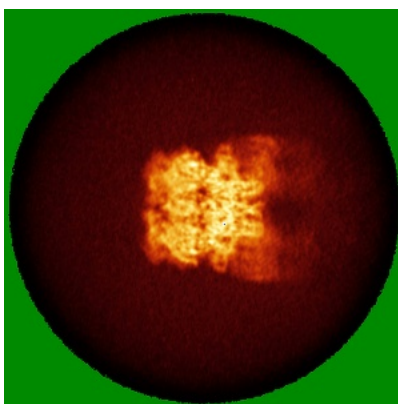
The images above show the largest variance slices of the map in three orthogonal directions.

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

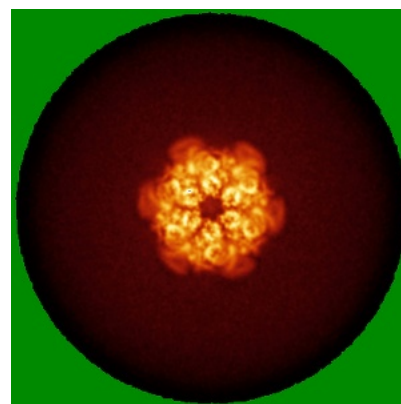
6.4.1 Primary map



X

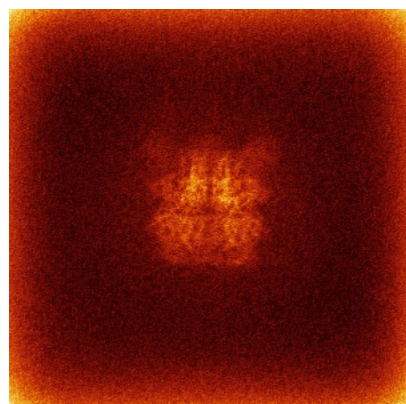


Y

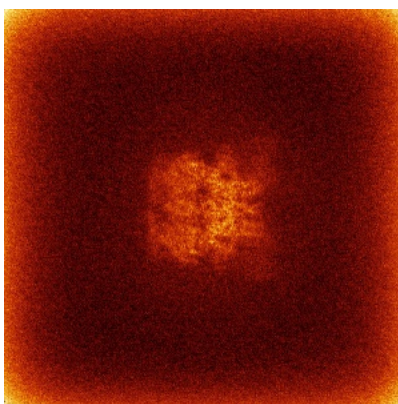


Z

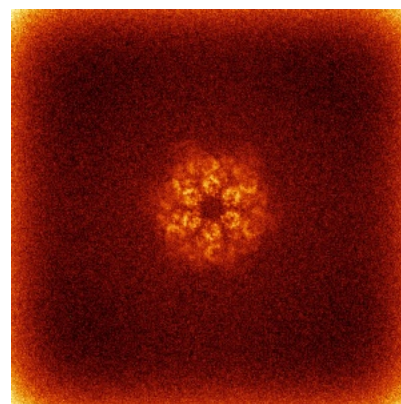
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



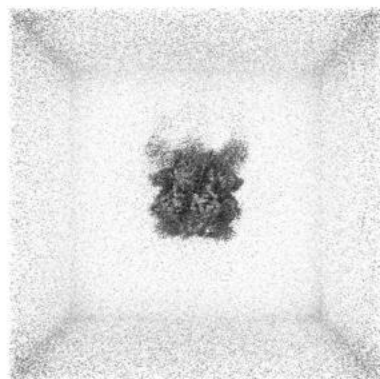
Y



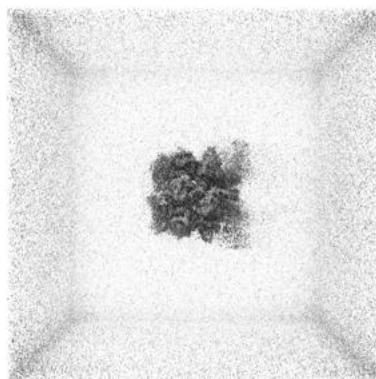
Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

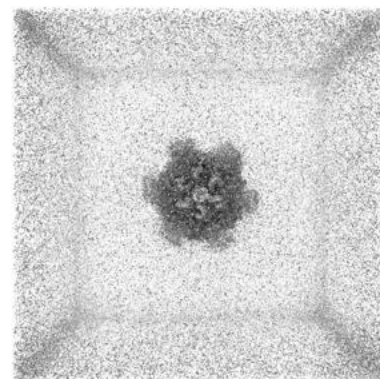
6.5.2 Raw map



X



Y



Z

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

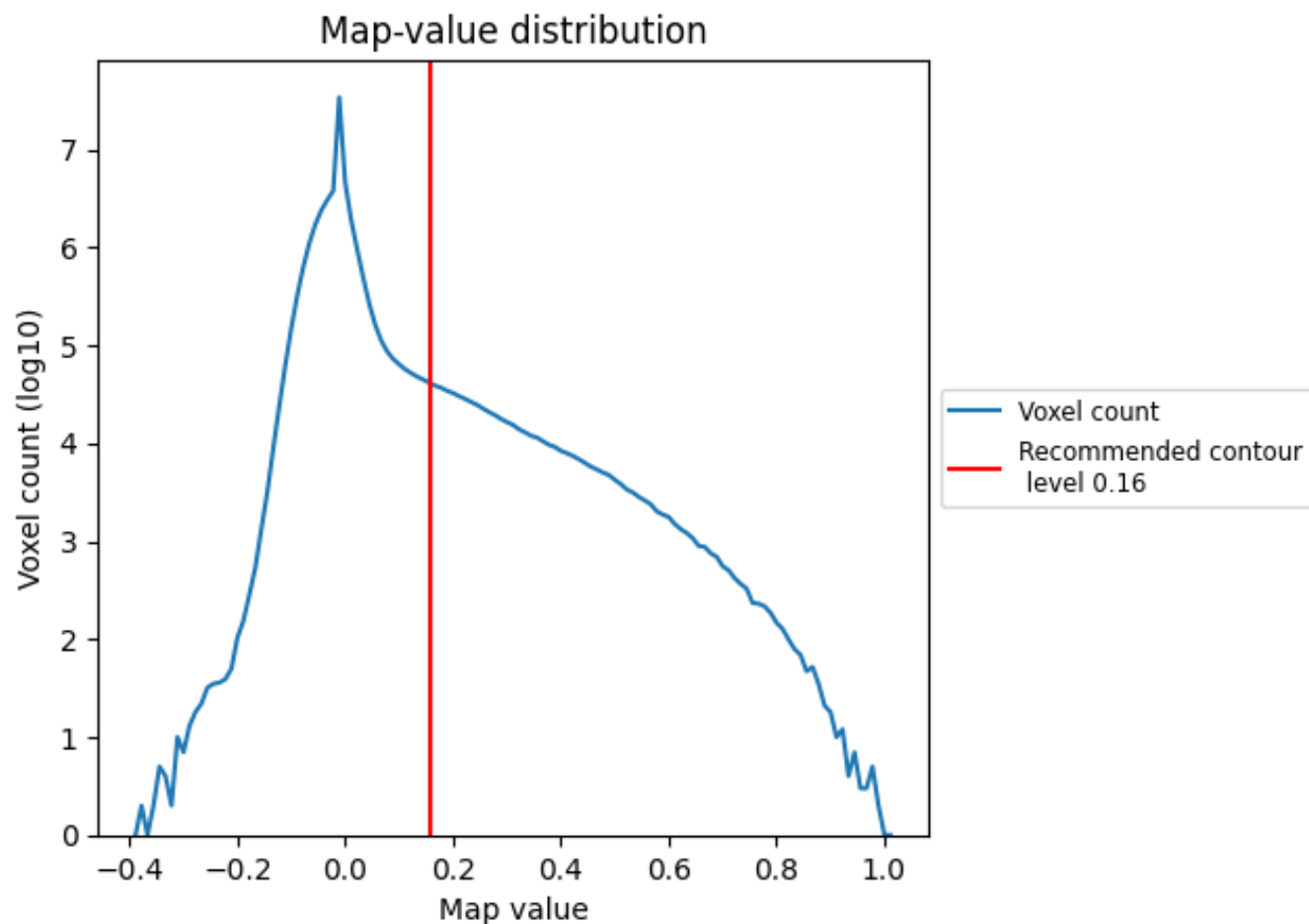
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

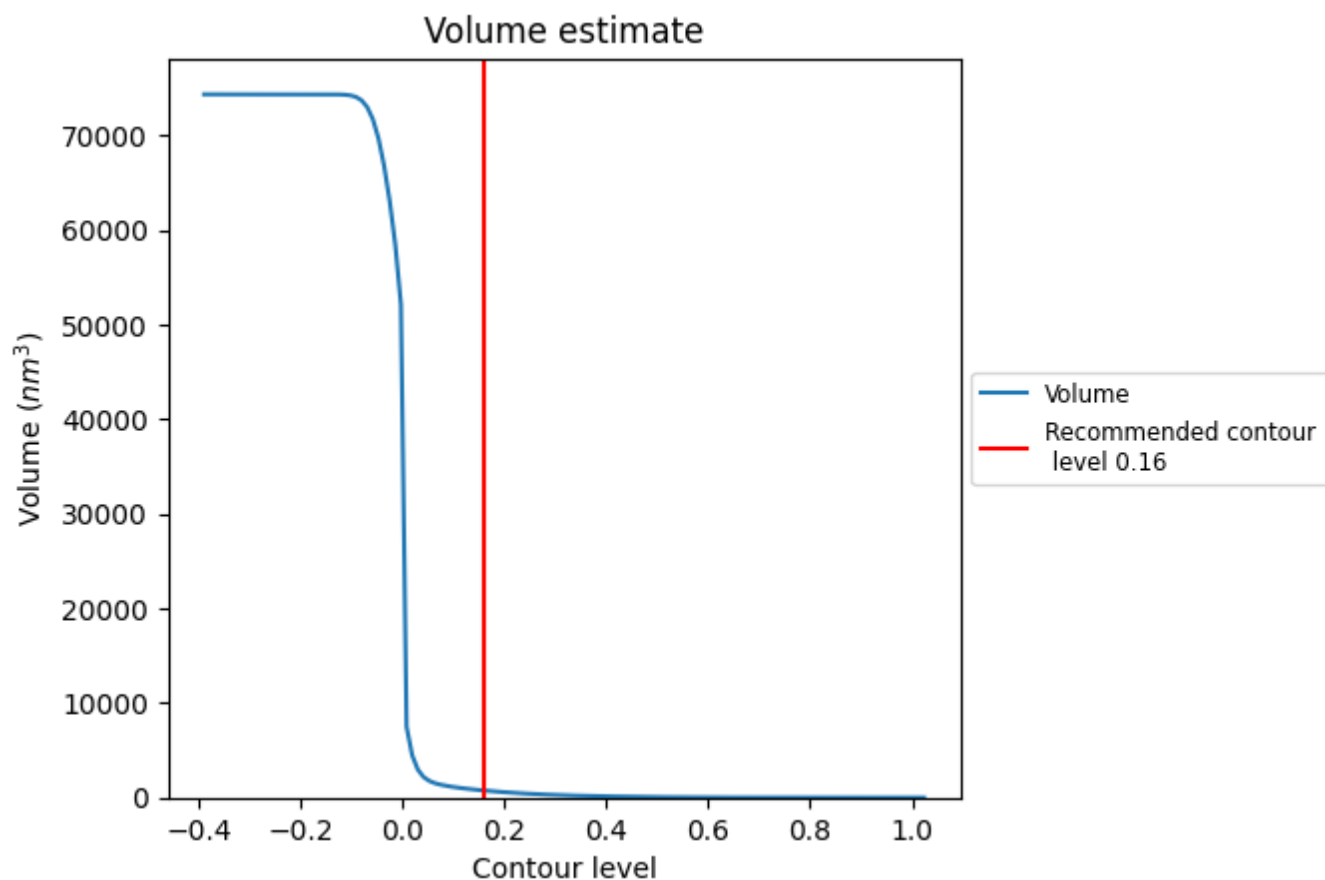
This section contains the results of statistical analysis of the map.

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.

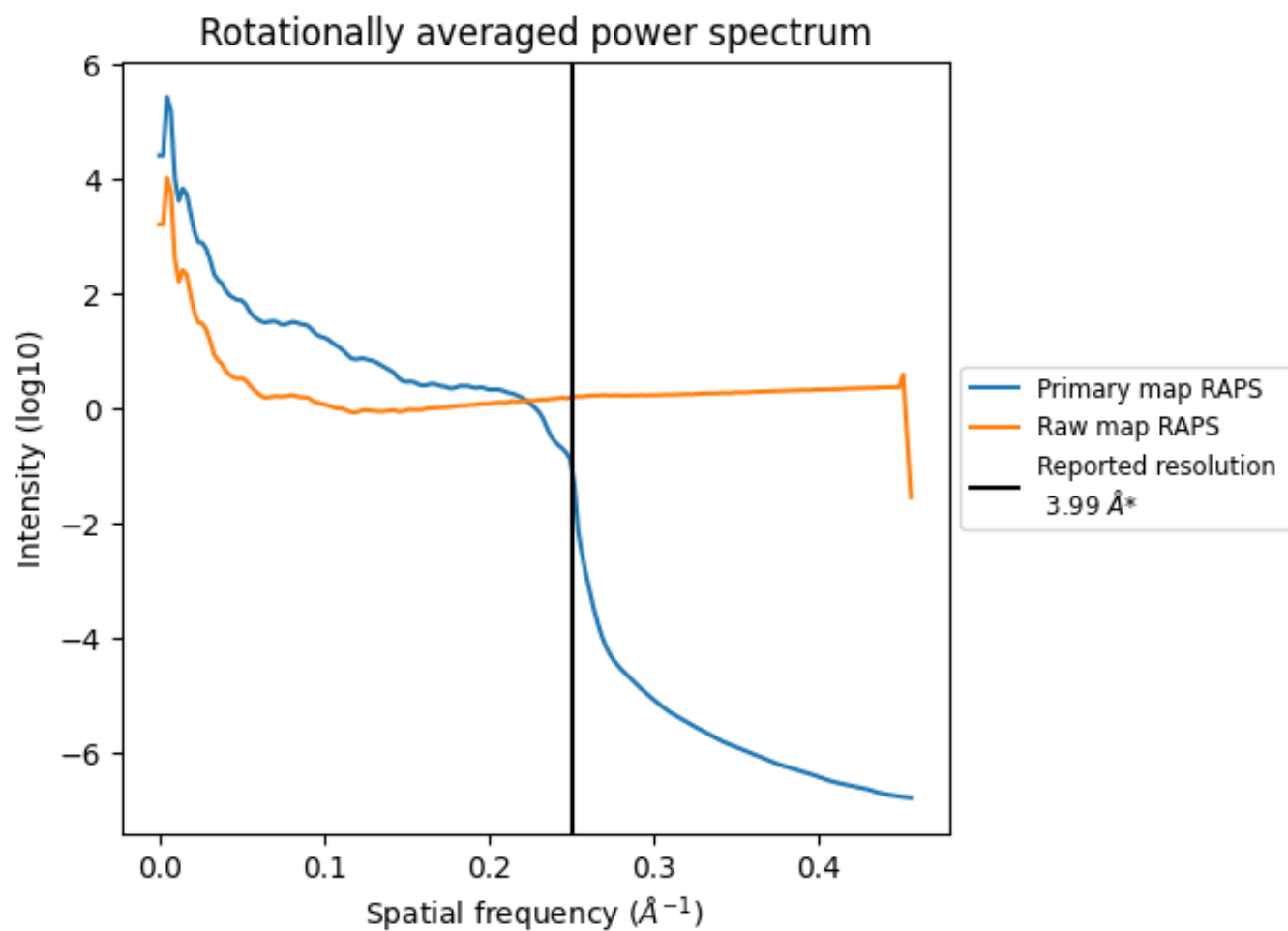
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 746 nm³; this corresponds to an approximate mass of 673 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 [i](#)

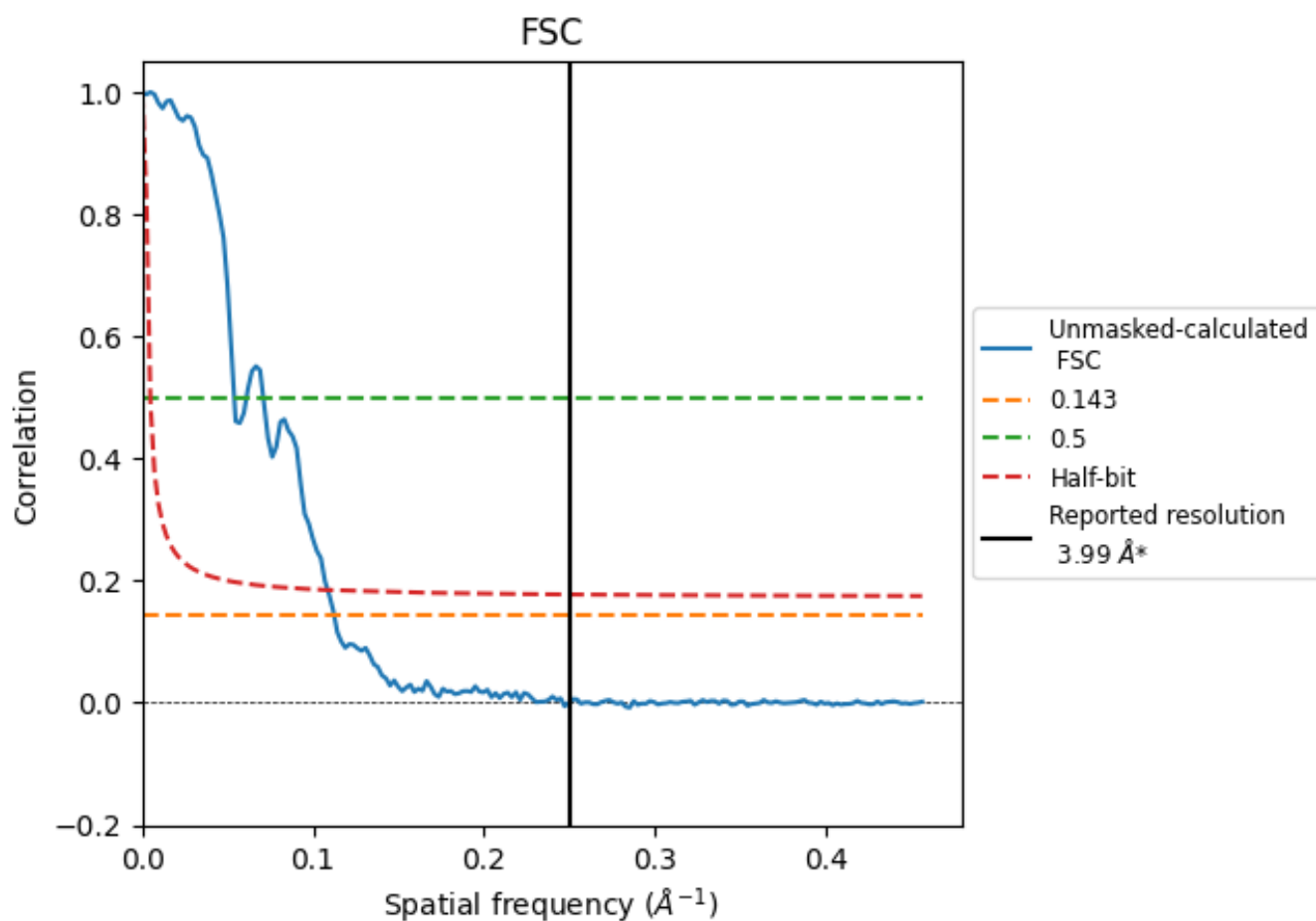


*Reported resolution corresponds to spatial frequency of 0.251 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.251 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

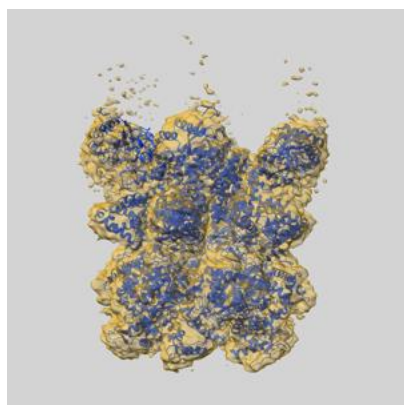
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.99	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.90	18.55	9.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.90 differs from the reported value 3.99 by more than 10 %

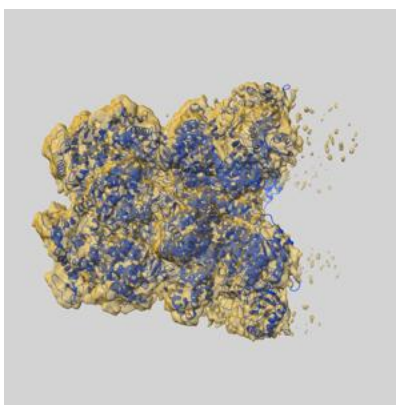
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37884 and PDB model 8WW8. Per-residue inclusion information can be found in section 3 on page 6.

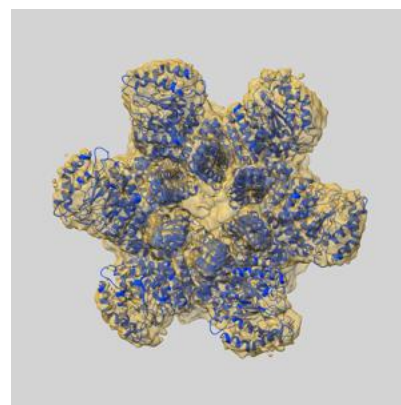
9.1 Map-model overlay [i](#)



X



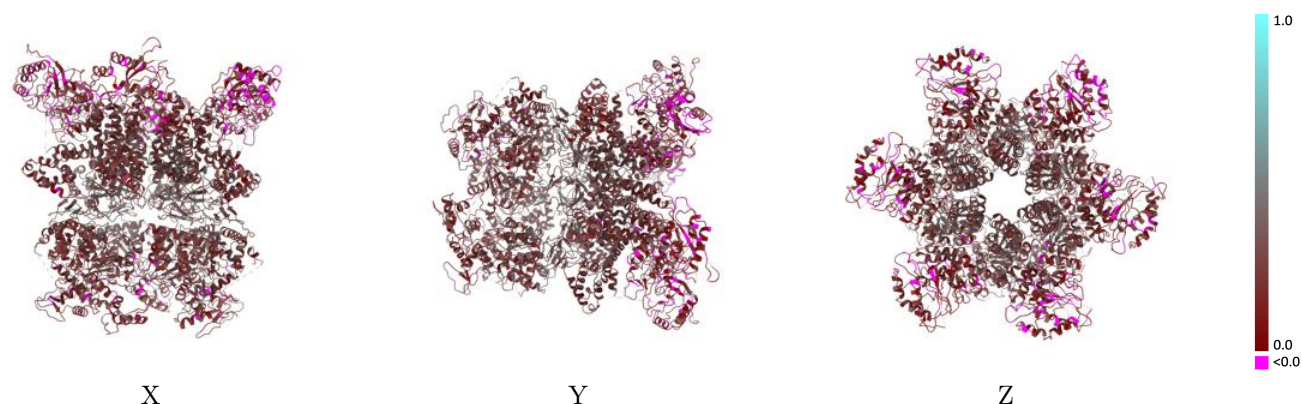
Y



Z

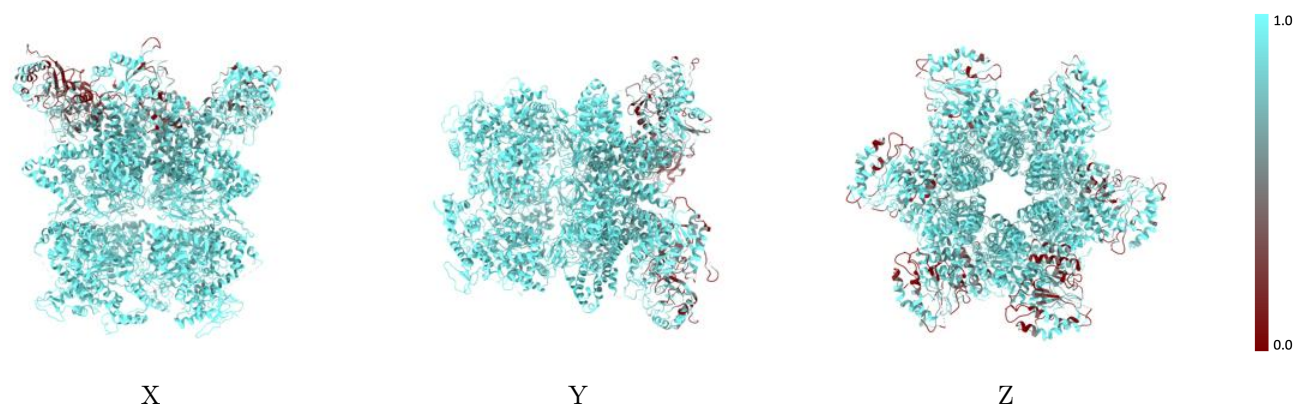
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



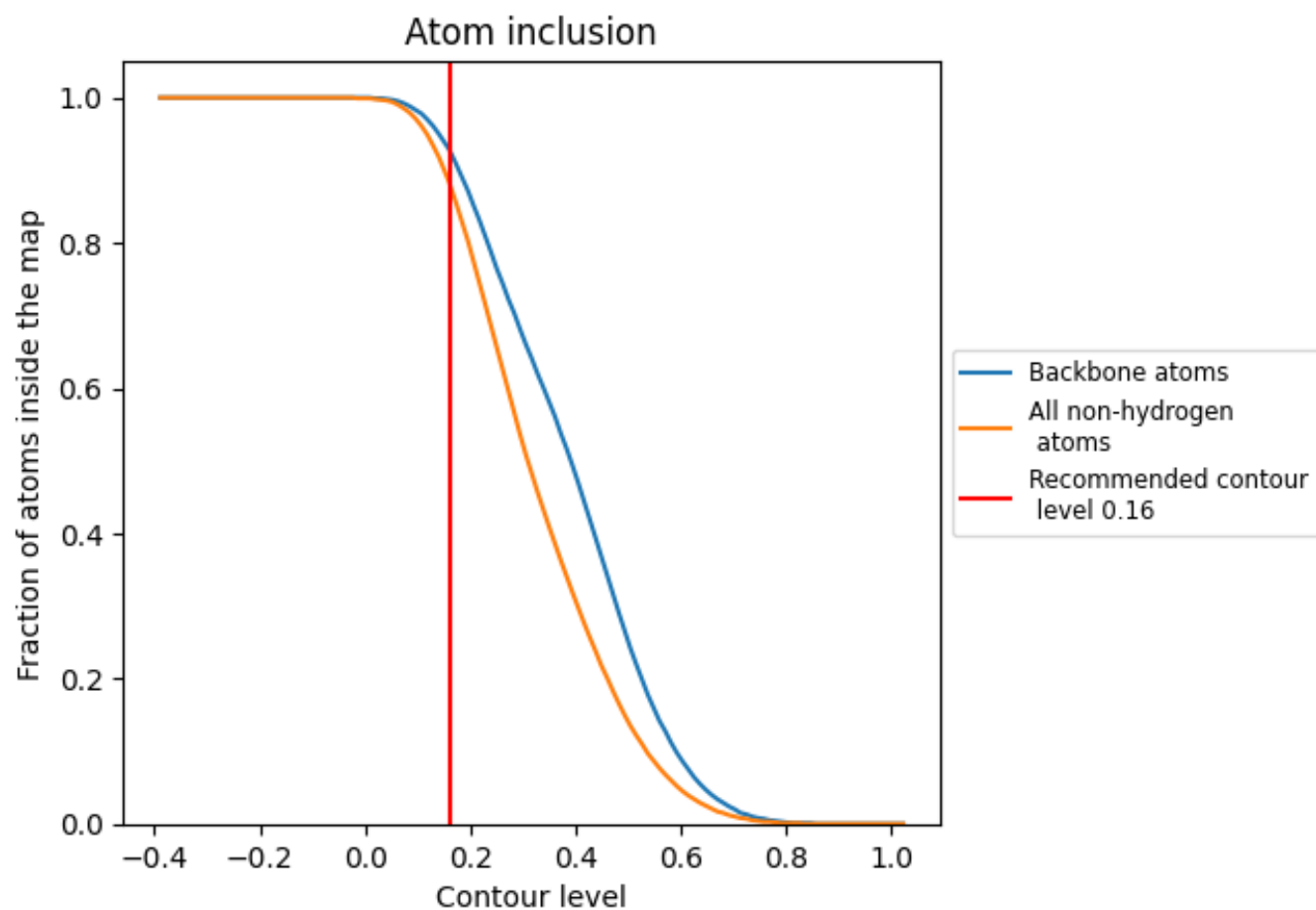
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 88% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8840	0.2380
A	0.8890	0.2410
B	0.8530	0.2440
C	0.8230	0.2390
D	0.8810	0.2340
E	0.9360	0.2260
F	0.9190	0.2430

1.0

0.0

<0.0