



Full wwPDB EM Validation Report ⓘ

Apr 21, 2025 – 12:25 AM JST

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.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

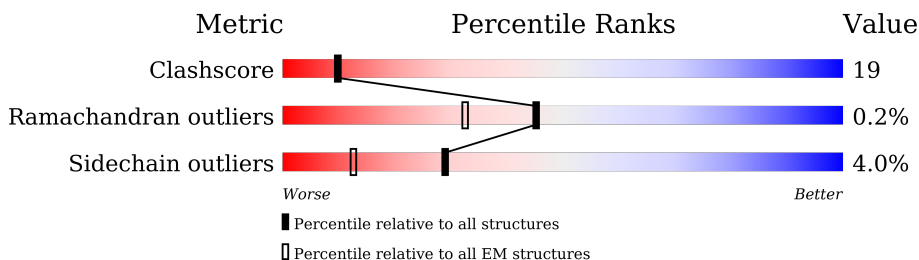
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.99 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	
1	B	972	
1	C	972	
1	D	972	
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		

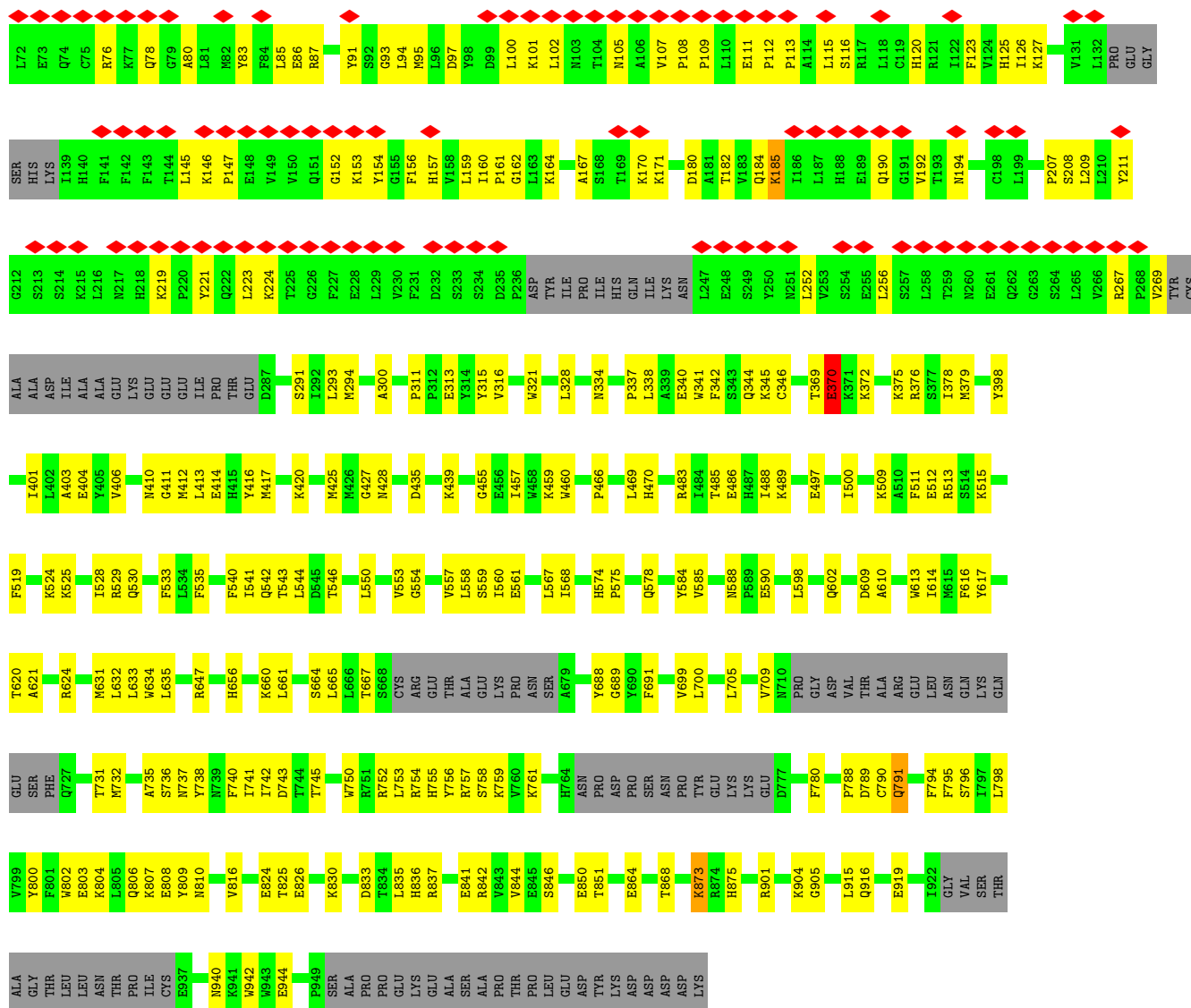
There are 60 discrepancies between the modelled and reference sequences:

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

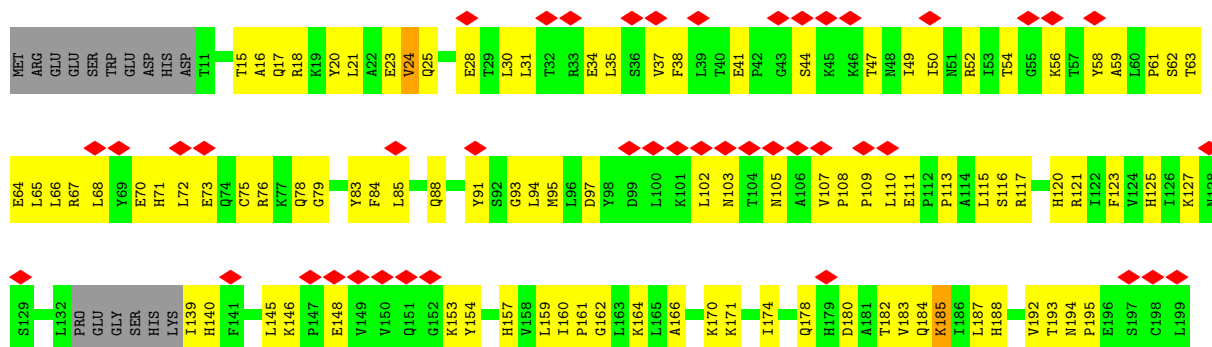
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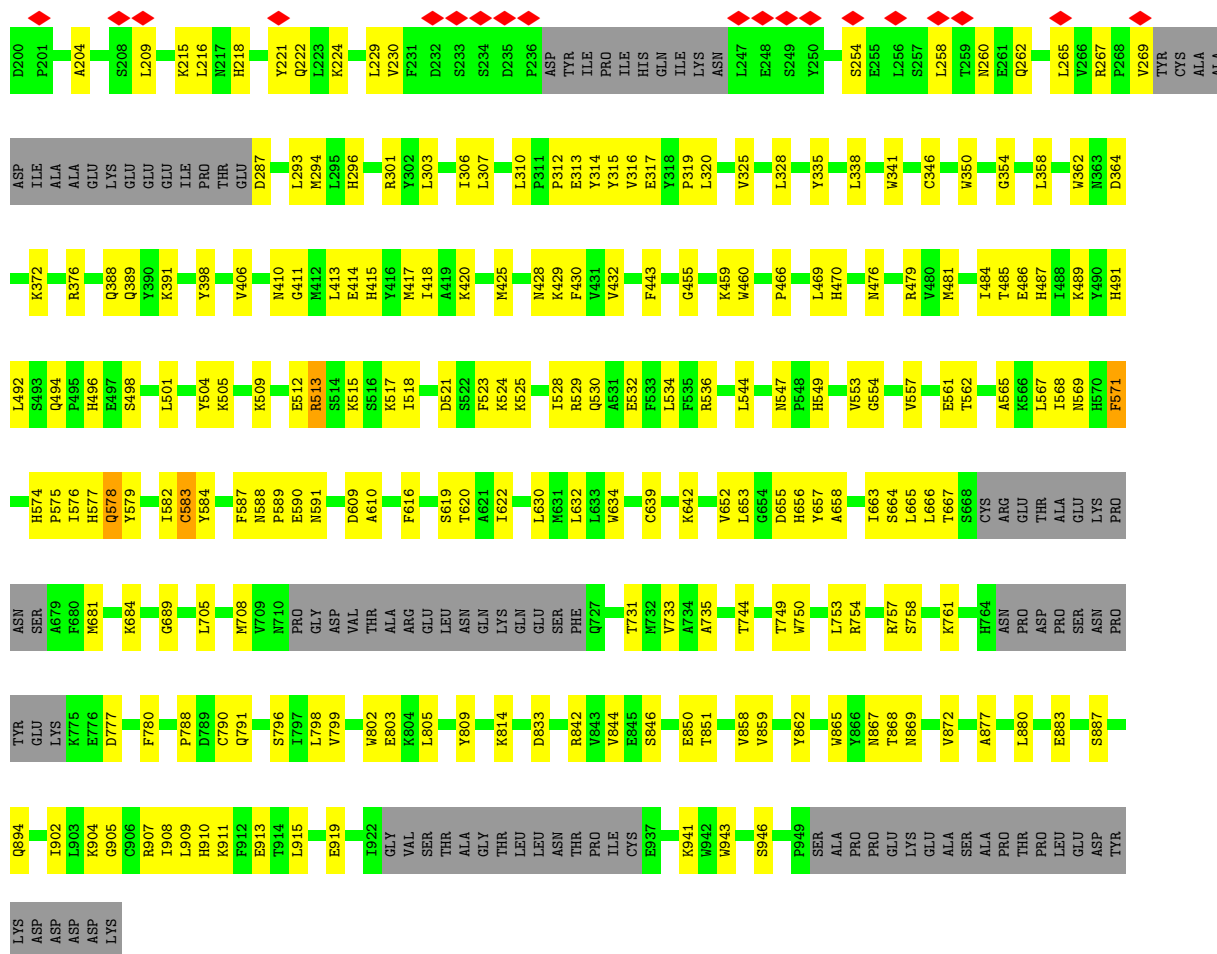
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Chain	Residue	Modelled	Actual	Comment	Reference
B	971	ASP	-	expression tag	UNP A0A2X0TKI6
B	972	LYS	-	expression tag	UNP A0A2X0TKI6
C	963	LEU	-	expression tag	UNP A0A2X0TKI6
C	964	GLU	-	expression tag	UNP A0A2X0TKI6
C	965	ASP	-	expression tag	UNP A0A2X0TKI6
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

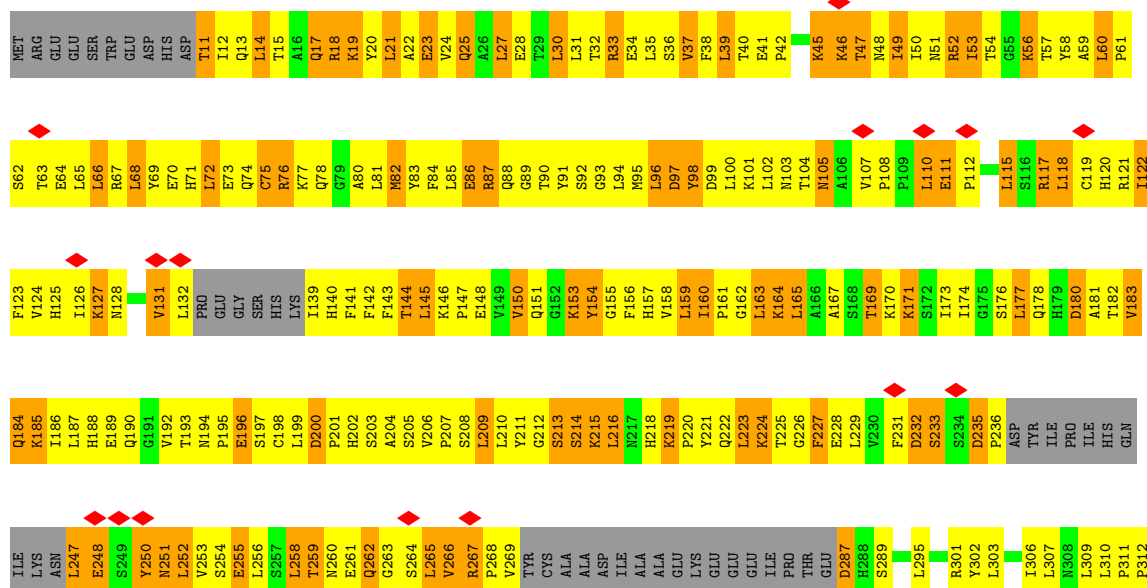


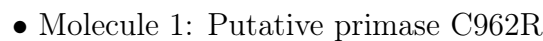
• Molecule 1: Putative primase C962R





• Molecule 1: Putative primase C962R





R624	GLN	R837	LEU
L630	GLU	R842	ASN
G641	SER	V843	THR
F644	PHE	V844	PRO
L645	M727	E845	ILE
M646	M728	S846	CYS
R647	W732	T851	E937
L653	S736	N854	W942
H656	N737	V858	P949
Y657	Y738	E864	SER
A658	I742	N867	ALA
S659	D743	T868	PRO
K660	T744	R869	PRO
L661	T745	I870	GLU
S664	T749	N871	LYS
L665	W750	V872	ALA
L666	R751	E883	SER
T667	R752	V887	ALA
S668	L753	L889	PRO
CYS	R754	E890	THR
ARG	R757	K891	PRO
GLU	S758	Y892	PRO
THR	K759	W895	LEU
ALA	V760	P897	GLU
GLU	K761	N898	ASP
LYS	F762	K899	ASP
PRO	C763	T900	ASP
ASN	H764	K904	ASP
ASN	ASN	G905	LYS
SER	PRO	C966	
A679	ASP	R907	
Y688	PRO	I908	
K696	SER	L909	
V699	ASN	H910	
L700	ASN	K911	
N701	TYR	E919	
T702	GLU	I922	
S703	LYS	GLY	
N710	K775	VAL	
PRO	E776	SER	
GLY	D777	THR	
ASP	R779	ALA	
VAL	D787	GLY	
THR	F788	THR	
ALA	D789	ALA	
ARG	C790	GLY	
GLU	Q791	THR	
LEU	K814	LEU	
ASN	E826		
GLN	K830		
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	0.25	0/6985	0.48	0/9482
1	B	0.25	0/6974	0.47	0/9467
1	C	0.25	0/6985	0.47	0/9482
1	D	0.25	0/7003	0.46	0/9505
1	E	0.25	0/7003	0.44	0/9505
1	F	0.25	0/7009	0.46	0/9512
All	All	0.25	0/41959	0.46	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	197	0
1	B	6796	0	6539	208	0
1	C	6806	0	6546	202	0
1	D	6824	0	6565	203	0
1	E	6824	0	6565	532	0
1	F	6830	0	6576	214	0
All	All	40886	0	39337	1539	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1539) 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: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: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:145:LEU:HB3	1:E:224:LYS:HZ1	1.45	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
1:B:183:VAL:HG23	1:B:184:GLN:HE21	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:107:VAL:HA	1:E:153:LYS:HZ2	1.51	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:459:LYS:NZ	1:D:553:VAL:O	2.23	0.66
1:E:124:VAL:HG13	1:E:236:PRO:HB2	1.75	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:414:GLU:CD	1:E:415:HIS:H	2.02	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:866:TYR:HE2	1:B:873:LYS:HZ3	1.47	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:481:MET:HE1	1:D:515:LYS:HA	1.83	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: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:22:ALA:C	1:E:24:VAL:N	2.54	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:398:TYR:CZ	1:A:425:MET:HA	2.39	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:459:LYS:NZ	1:E:556:GLY:O	2.32	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: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: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
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:321:TRP:HE1	1:E:358:LEU:HD13	1.70	0.56
1:E:465:ASN:C	1:E:465:ASN:HD22	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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:C:519:PHE:HA	1:C:524:LYS:HZ1	1.72	0.55
1:D:56:LYS:HD3	1:D:58:TYR:HE2	1.71	0.55
1:B:486:GLU:HA	1:B:489:LYS:HE2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:82:MET:O	1:F:214:SER:N	2.41	0.54
1:B:891:LYS:HA	1:C:761:LYS:HZ1	1.72	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:A:52:ARG:HH22	1:A:215:LYS:HA	1.72	0.54
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:145:LEU:HB3	1:E:224:LYS:NZ	2.21	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:A:842:ARG:HA	1:A:909:LEU:HB2	1.91	0.53
1:B:356:GLU:HB3	1:B:360:LYS:NZ	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:485:THR:HG22	1:B:489:LYS:NZ	2.23	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
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:A:375:LYS:HD2	1:A:379:MET:HE1	1.91	0.52
1:B:107:VAL:O	1:B:109:PRO:HD3	2.09	0.52
1:E:22:ALA:O	1:E:23:GLU:C	2.45	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:D:941:LYS:HZ3	1:D:946:SER:H	1.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:121:ARG:HG2	1:E:180:ASP:CG	2.30	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: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
1:C:660:LYS:HE2	1:C:691:PHE:HA	1.91	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:E:45:LYS:C	1:E:47:THR:H	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ASP:OD2	1:B:335:TYR:OH	2.28	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: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: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: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
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: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: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:154:TYR:HH	1:E:190:GLN:HG3	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:941:LYS:NZ	1:B:948:ASN:O	2.45	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
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:E:153:LYS:HZ3	1:E:154:TYR:H	1.59	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:262:GLN:CD	1:E:262:GLN:H	2.14	0.50
1:E:40:THR:HG21	1:E:47:THR:CG2	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: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:915:LEU:HD13	1:C:919:GLU:HB2	1.92	0.49
1:E:154:TYR:OH	1:E:190:GLN:HG3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:369:THR:O	1:F:370:GLU:C	2.50	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:84:PHE:H	1:E:84:PHE:HD1	1.61	0.49
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:147:PRO:HA	1:B:222:GLN:HE22	1.78	0.48
1:E:485:THR:HG22	1:E:489:LYS:HZ1	1.79	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:153:LYS:HZ3	1:E:154:TYR:HB3	1.78	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:F:617:TYR:O	1:F:620:THR:OG1	2.23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:B:369:THR:O	1:B:370:GLU:C	2.52	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:PRO:O	1:C:470:HIS:N	2.42	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
1:E:119:CYS:HB3	1:E:141:PHE:CD2	2.50	0.47
1:E:196:GLU:C	1:E:198:CYS:H	2.17	0.47
1:E:548:PRO:HA	1:E:624:ARG:NH1	2.29	0.47
1:F:405:TYR:OH	1:F:420:LYS:HD2	2.15	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: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:51:ASN:HA	1:E:83:TYR:C	2.35	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: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: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:C:560:ILE:O	1:C:561:GLU:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:787:ASP:CG	1:E:790:CYS:HB3	2.35	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:E:89:GLY:C	1:E:91:TYR:N	2.69	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:180:ASP:CG	1:E:182:THR:H	2.19	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
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:427:GLY:HA2	1:C:535:PHE:HE2	1.81	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:TYR:O	1:B:620:THR:OG1	2.27	0.45
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
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:A:941:LYS:NZ	1:A:948:ASN:O	2.47	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:LEU:HD22	1:D:418:ILE:HD11	1.98	0.45
1:E:92:SER:C	1:E:164:LYS:HA	2.37	0.45
1:E:223:LEU:HD13	1:E:256:LEU:HD11	1.98	0.45
1:F:315:TYR:CD1	1:F:346:CYS:HB2	2.52	0.45
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: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: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:C:759:LYS:NZ	1:C:824:GLU:OE2	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:49:ILE:C	1:E:50:ILE:HG13	2.38	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: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:C:873:LYS:HZ2	1:C:875:HIS:HA	1.82	0.44
1:E:36:SER:C	1:E:38:PHE:N	2.71	0.44
1:E:70:GLU:HA	1:E:73:GLU:OE1	2.17	0.44
1:F:106:ALA:C	1:F:153:LYS:HZ3	2.21	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: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: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:467:ASP:N	1:A:467:ASP:OD1	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:88:GLN:HG2	1:E:207:PRO:HA	1.99	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:D:529:ARG:NE	1:E:521:ASP:OD1	2.45	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:485:THR:HG22	1:C:489:LYS:HZ2	1.82	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:82:MET:C	1:E:83:TYR:HD1	2.21	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:525:LYS:O	1:E:528:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:699:VAL:CG1	1:E:700:LEU:N	2.81	0.44
1:A:287:ASP:OD1	1:A:287:ASP:N	2.50	0.43
1:B:883:GLU:OE1	1:C:738:TYR:OH	2.27	0.43
1:D:455:GLY:HA2	1:D:554:GLY:HA2	1.99	0.43
1:E:213:SER:C	1:E:220:PRO:HB3	2.38	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:93:GLY:O	1:A:170:LYS:NZ	2.50	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:91:TYR:C	1:E:164:LYS:HB2	2.39	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:E:481:MET:HE2	1:E:515:LYS:HA	2.00	0.43
1:A:66:LEU:O	1:A:70:GLU:HG2	2.19	0.43
1:A:519:PHE:HZ	1:F:409:TYR:HH	1.65	0.43
1:A:614:ILE:HD11	1:A:634:TRP:CZ2	2.53	0.43
1:B:485:THR:HG22	1:B:489:LYS:HZ3	1.82	0.43
1:B:790:CYS:SG	1:B:791:GLN:N	2.91	0.43
1:E:34:GLU:O	1:E:37:VAL:HG23	2.18	0.43
1:E:574:HIS:HB3	1:E:576:ILE:HD11	1.99	0.43
1:C:267:ARG:CZ	1:C:269:VAL:HG22	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:73:GLU:HB3	1:F:77:LYS:HZ3	1.82	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: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:369:THR:O	1:C:370:GLU:C	2.57	0.43
1:C:743:ASP:OD1	1:C:743:ASP:N	2.50	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:B:26:ALA:HA	1:B:29:THR:HG22	2.00	0.43
1:B:485:THR:C	1:B:489:LYS:HZ3	2.23	0.43
1:E:73:GLU:HB3	1:E:77:LYS:HZ3	1.84	0.43
1:E:142:PHE:CD2	1:E:159:LEU:HB3	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:455:GLY:O	1:D:459:LYS:NZ	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:287:ASP:CG	1:E:289:SER:HG	2.22	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
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:B:98:TYR:HE1	1:B:199:LEU:HD13	1.83	0.42
1:E:101:LYS:C	1:E:192:VAL:HG13	2.40	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:GLU:HB2	1:C:417:MET:HE3	2.00	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
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:E:156:PHE:HE1	1:E:224:LYS:HZ3	1.66	0.42
1:E:174:ILE:HG21	1:E:200:ASP:C	2.39	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:403:ALA:C	1:B:405:TYR:H	2.24	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:139:ILE:HD11	1:E:162:GLY:C	2.40	0.42
1:E:263:GLY:HA3	1:E:266:VAL:HG23	2.01	0.42
1:F:736:SER:OG	1:F:737:ASN:N	2.52	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:C:76:ARG:NH2	1:C:211:TYR:HE1	2.18	0.42
1:C:376:ARG:HA	1:C:379:MET:HE2	2.01	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:45:LYS:C	1:E:47:THR:N	2.74	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:660:LYS:NZ	1:F:661:LEU:O	2.39	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:311:PRO:HB2	1:C:313:GLU:CD	2.41	0.41
1:D:110:LEU:HD23	1:D:115:LEU:HD21	2.03	0.41
1:D:389:GLN:H	1:D:389:GLN:CD	2.24	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:667:THR:OG1	1:B:699:VAL:O	2.27	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:485:THR:C	1:C:489:LYS:HZ3	2.24	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:153:LYS:HZ3	1:E:153:LYS:HG3	1.65	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:368:HIS:NE2	1:E:371:LYS:HA	2.35	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:895:TRP:HZ2	1:F:757:ARG:HH12	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:214:SER:OG	1:E:218:HIS:O	2.38	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: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:343:SER:OG	1:E:358:LEU:HD22	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:PRO:HB2	1:A:313:GLU:CD	2.42	0.40
1:A:757:ARG:NH2	1:A:759:LYS:HG3	2.37	0.40
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:846:SER:OG	1:F:907:ARG:HB2	2.21	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	66
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%)	25	61
All	All	5033/5832 (86%)	4782 (95%)	241 (5%)	10 (0%)	45	76

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%)	707 (99%)	10 (1%)	62	75
1	B	716/879 (82%)	702 (98%)	14 (2%)	50	68
1	C	717/879 (82%)	707 (99%)	10 (1%)	62	75
1	D	719/879 (82%)	707 (98%)	12 (2%)	56	72
1	E	719/879 (82%)	612 (85%)	107 (15%)	2	14
1	F	720/879 (82%)	699 (97%)	21 (3%)	37	58
All	All	4308/5274 (82%)	4134 (96%)	174 (4%)	29	49

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	LYS
1	A	267	ARG
1	A	375	LYS
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	A	814	LYS
1	B	183	VAL
1	B	185	LYS
1	B	213	SER
1	B	215	LYS
1	B	216	LEU
1	B	267	ARG
1	B	366	SER
1	B	367	HIS
1	B	370	GLU
1	B	375	LYS
1	B	547	ASN
1	B	789	ASP
1	B	790	CYS
1	B	814	LYS
1	C	185	LYS
1	C	370	GLU
1	C	410	ASN
1	C	412	MET
1	C	558	LEU
1	C	559	SER
1	C	789	ASP
1	C	790	CYS
1	C	791	GLN
1	C	873	LYS
1	D	185	LYS
1	D	267	ARG
1	D	364	ASP
1	D	372	LYS
1	D	513	ARG
1	D	536	ARG
1	D	569	ASN
1	D	571	PHE

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Mol	Chain	Res	Type
1	D	578	GLN
1	D	583	CYS
1	D	790	CYS
1	D	814	LYS
1	E	11	THR
1	E	14	LEU
1	E	17	GLN
1	E	18	ARG
1	E	19	LYS
1	E	21	LEU
1	E	23	GLU
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	46	LYS
1	E	47	THR
1	E	49	ILE
1	E	52	ARG
1	E	53	ILE
1	E	54	THR
1	E	56	LYS
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	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	103	ASN

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Mol	Chain	Res	Type
1	E	104	THR
1	E	105	ASN
1	E	110	LEU
1	E	111	GLU
1	E	115	LEU
1	E	117	ARG
1	E	118	LEU
1	E	122	ILE
1	E	127	LYS
1	E	131	VAL
1	E	132	LEU
1	E	144	THR
1	E	145	LEU
1	E	150	VAL
1	E	151	GLN
1	E	153	LYS
1	E	154	TYR
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	177	LEU
1	E	178	GLN
1	E	180	ASP
1	E	183	VAL
1	E	184	GLN
1	E	185	LYS
1	E	189	GLU
1	E	193	THR
1	E	196	GLU
1	E	197	SER
1	E	200	ASP
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

Continued on next page...

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Mol	Chain	Res	Type
1	E	223	LEU
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	262	GLN
1	E	265	LEU
1	E	266	VAL
1	E	267	ARG
1	E	287	ASP
1	E	369	THR
1	E	370	GLU
1	E	465	ASN
1	E	786	MET
1	E	789	ASP
1	E	790	CYS
1	E	814	LYS
1	E	830	LYS
1	F	107	VAL
1	F	117	ARG
1	F	185	LYS
1	F	251	ASN
1	F	252	LEU
1	F	254	SER
1	F	258	LEU
1	F	259	THR
1	F	267	ARG
1	F	369	THR
1	F	370	GLU
1	F	376	ARG
1	F	728	MET
1	F	751	ARG
1	F	752	ARG

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Continued from previous page...

Mol	Chain	Res	Type
1	F	754	ARG
1	F	789	ASP
1	F	790	CYS
1	F	814	LYS
1	F	898	ASN
1	F	900	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) 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	B	184	GLN
1	B	188	HIS
1	B	262	GLN
1	B	367	HIS
1	B	530	GLN
1	B	549	HIS
1	C	218	HIS
1	C	363	ASN
1	C	465	ASN
1	C	470	HIS
1	D	260	ASN
1	D	491	HIS
1	D	549	HIS
1	D	569	ASN
1	D	581	HIS
1	E	78	GLN
1	E	120	HIS
1	E	125	HIS
1	E	188	HIS
1	E	194	ASN
1	E	251	ASN
1	E	260	ASN
1	E	262	GLN
1	E	476	ASN
1	E	530	GLN
1	E	549	HIS
1	F	363	ASN
1	F	549	HIS

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Mol	Chain	Res	Type
1	F	791	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

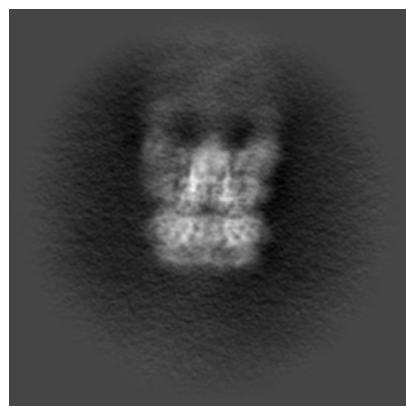
6 Map visualisation [i](#)

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

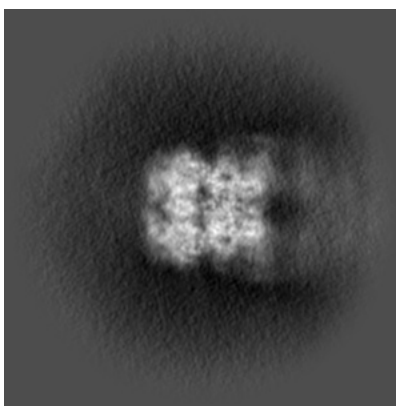
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

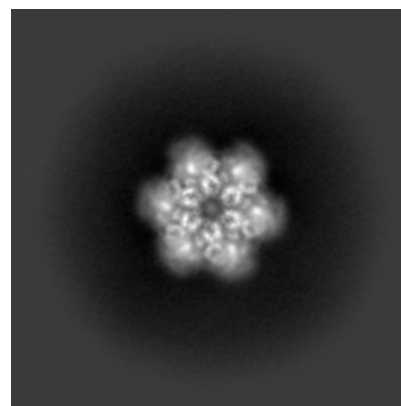
6.1.1 Primary map



X

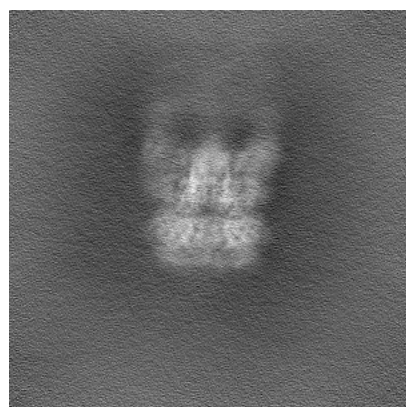


Y

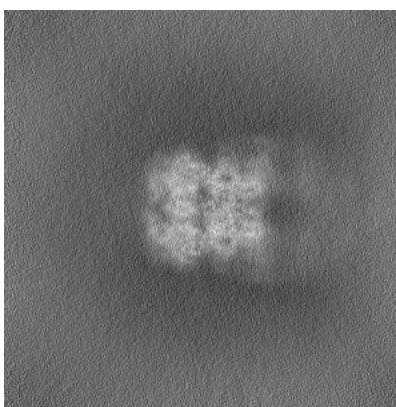


Z

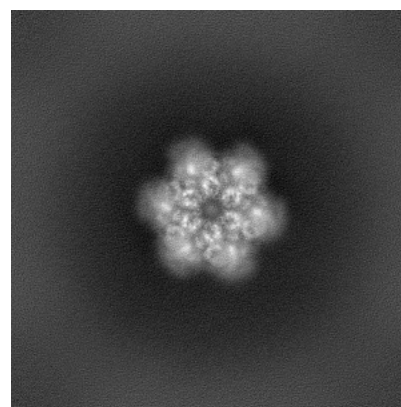
6.1.2 Raw map



X



Y

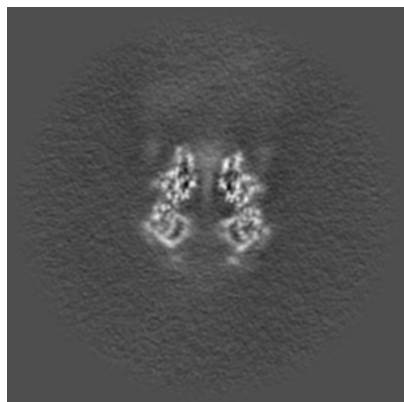


Z

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

6.2 Central slices [i](#)

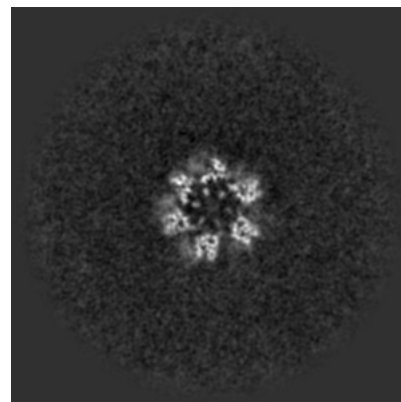
6.2.1 Primary map



X Index: 192

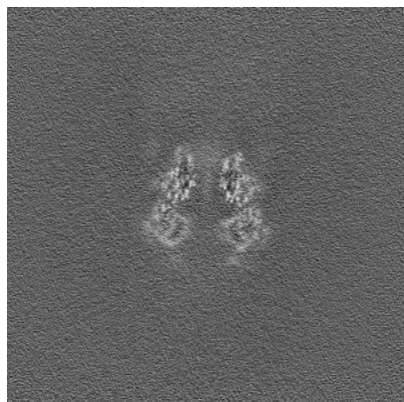


Y Index: 192

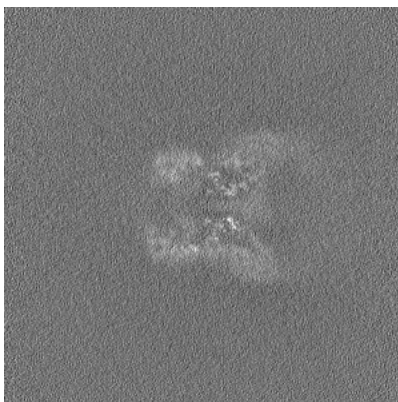


Z Index: 192

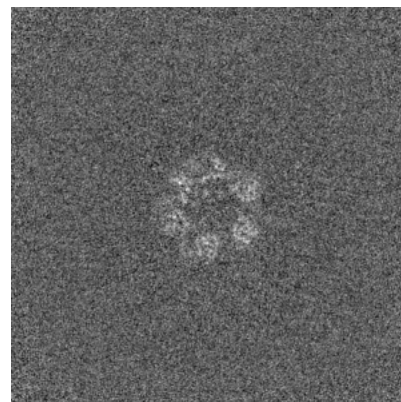
6.2.2 Raw map



X Index: 192



Y Index: 192

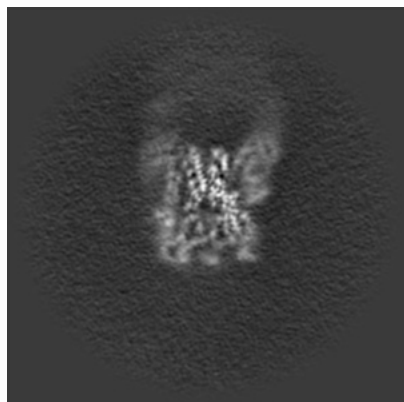


Z Index: 192

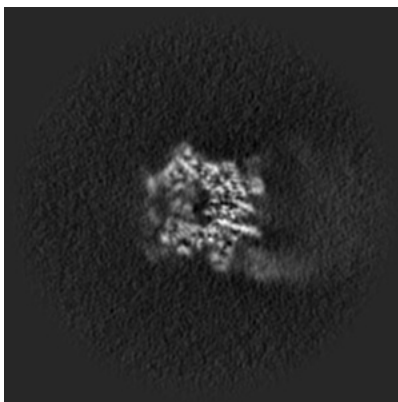
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

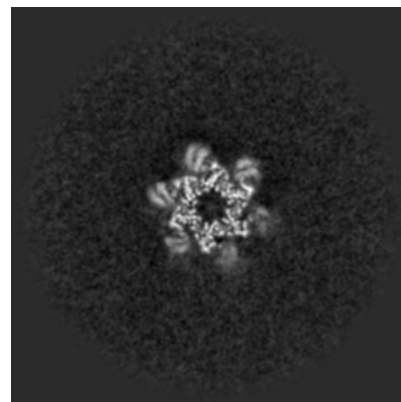
6.3.1 Primary map



X Index: 169

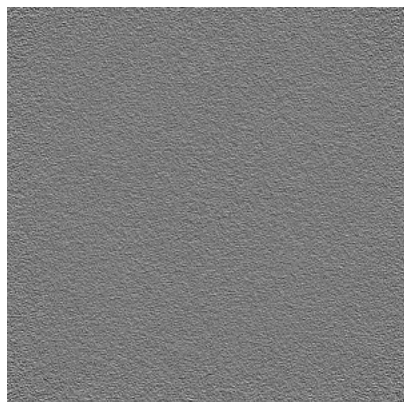


Y Index: 209

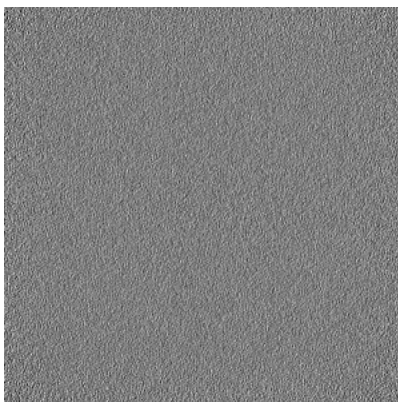


Z Index: 202

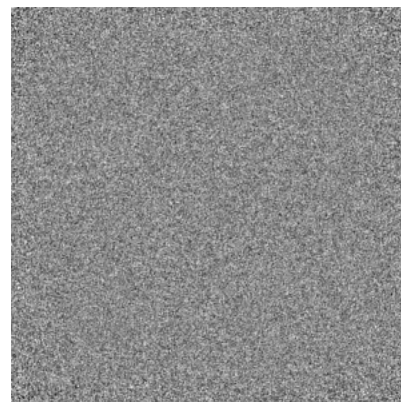
6.3.2 Raw map



X Index: 0



Y Index: 0

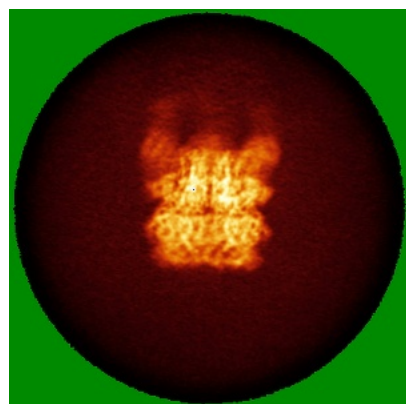


Z Index: 0

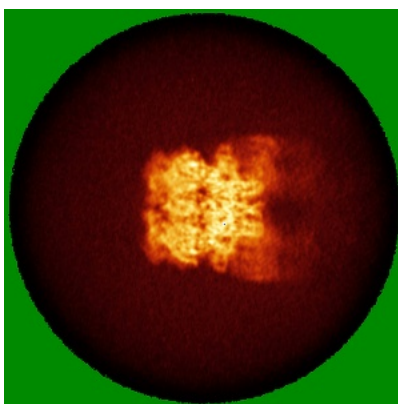
The images above show the largest variance slices of the map in three orthogonal directions.

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

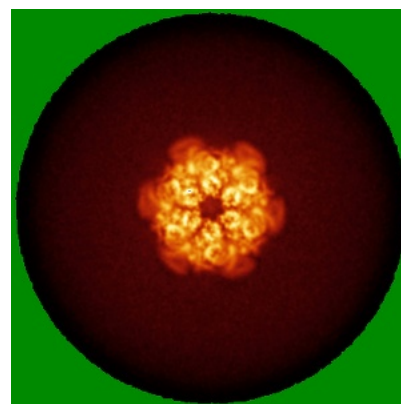
6.4.1 Primary map



X

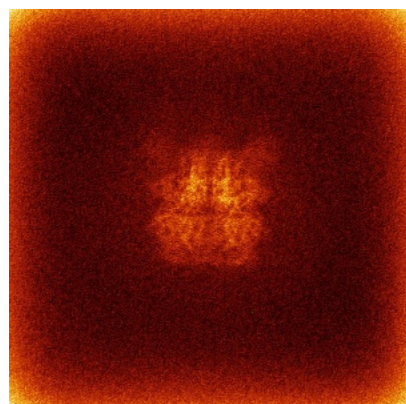


Y

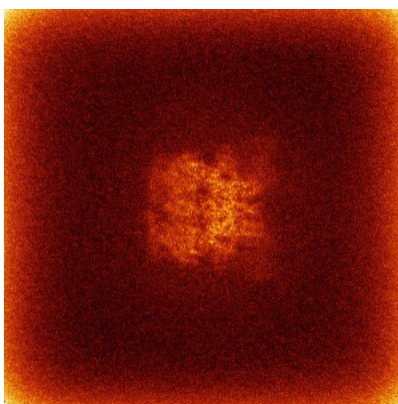


Z

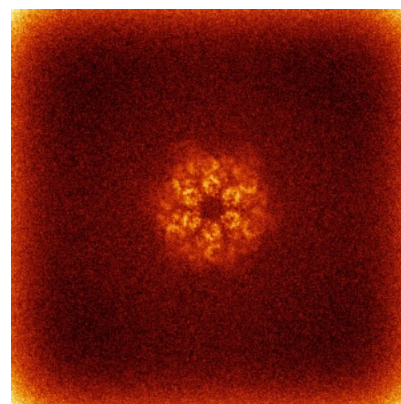
6.4.2 Raw map



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



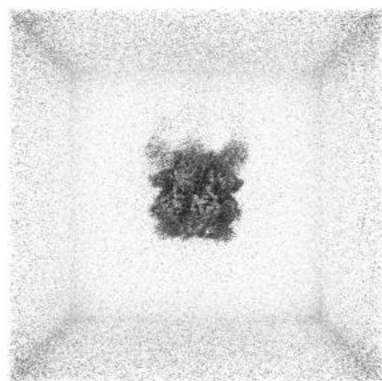
Y



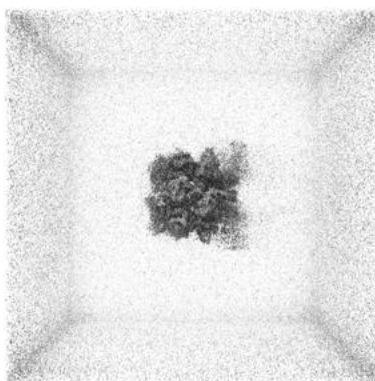
Z

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.

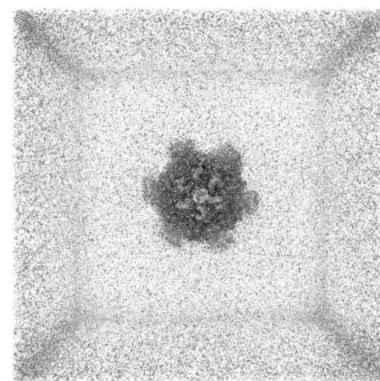
6.5.2 Raw map



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.

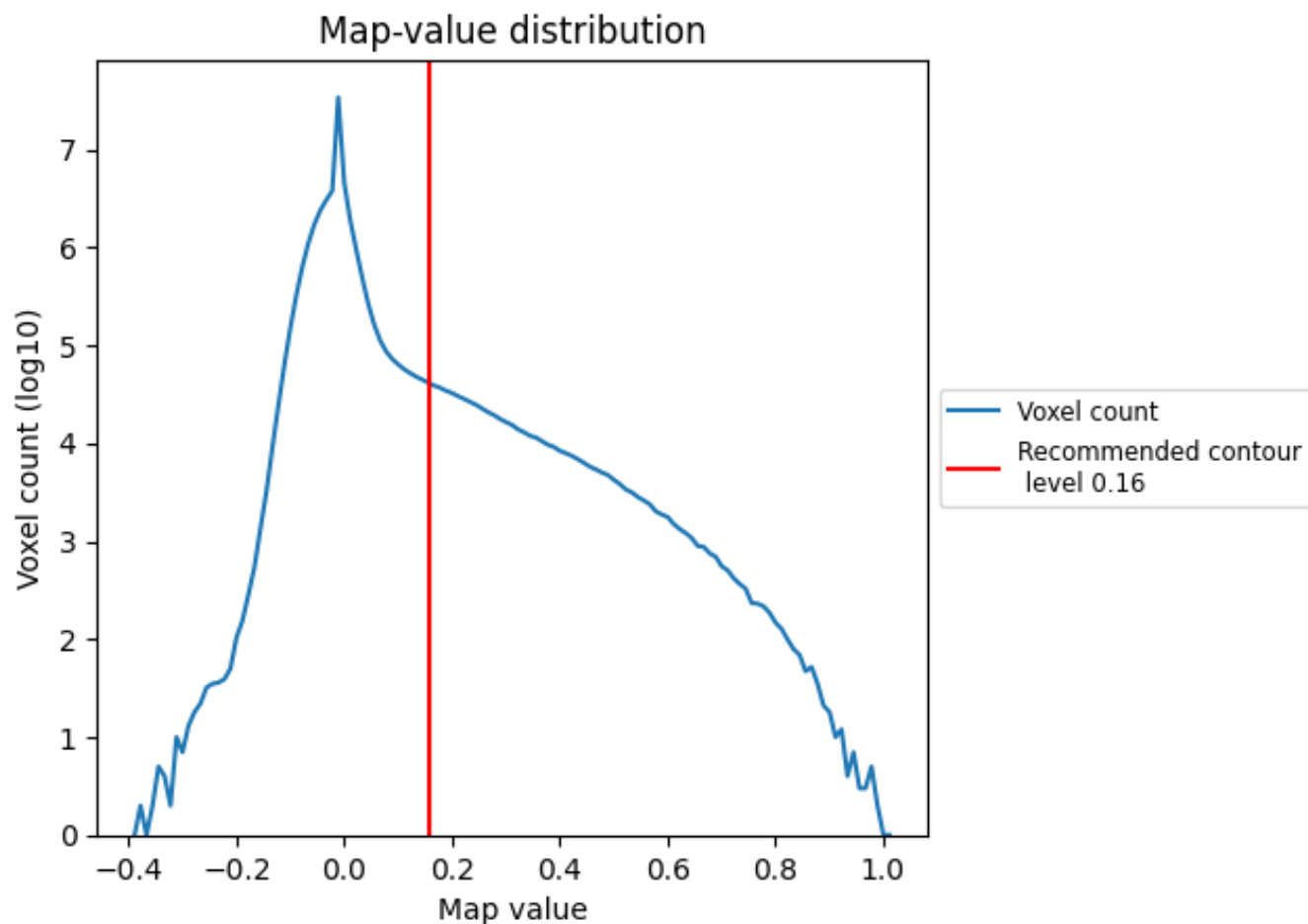
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

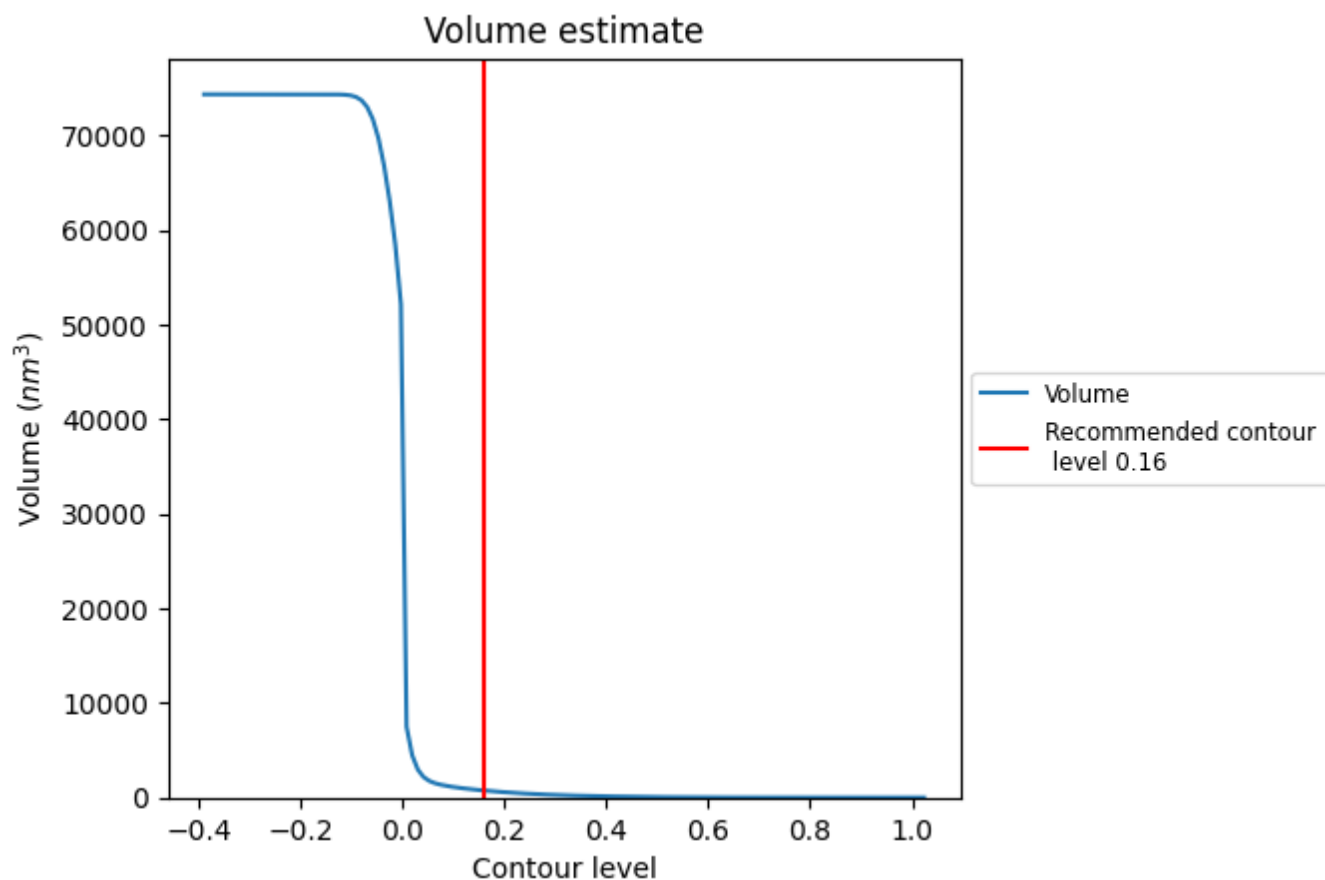
This section contains the results of statistical analysis of the map.

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.

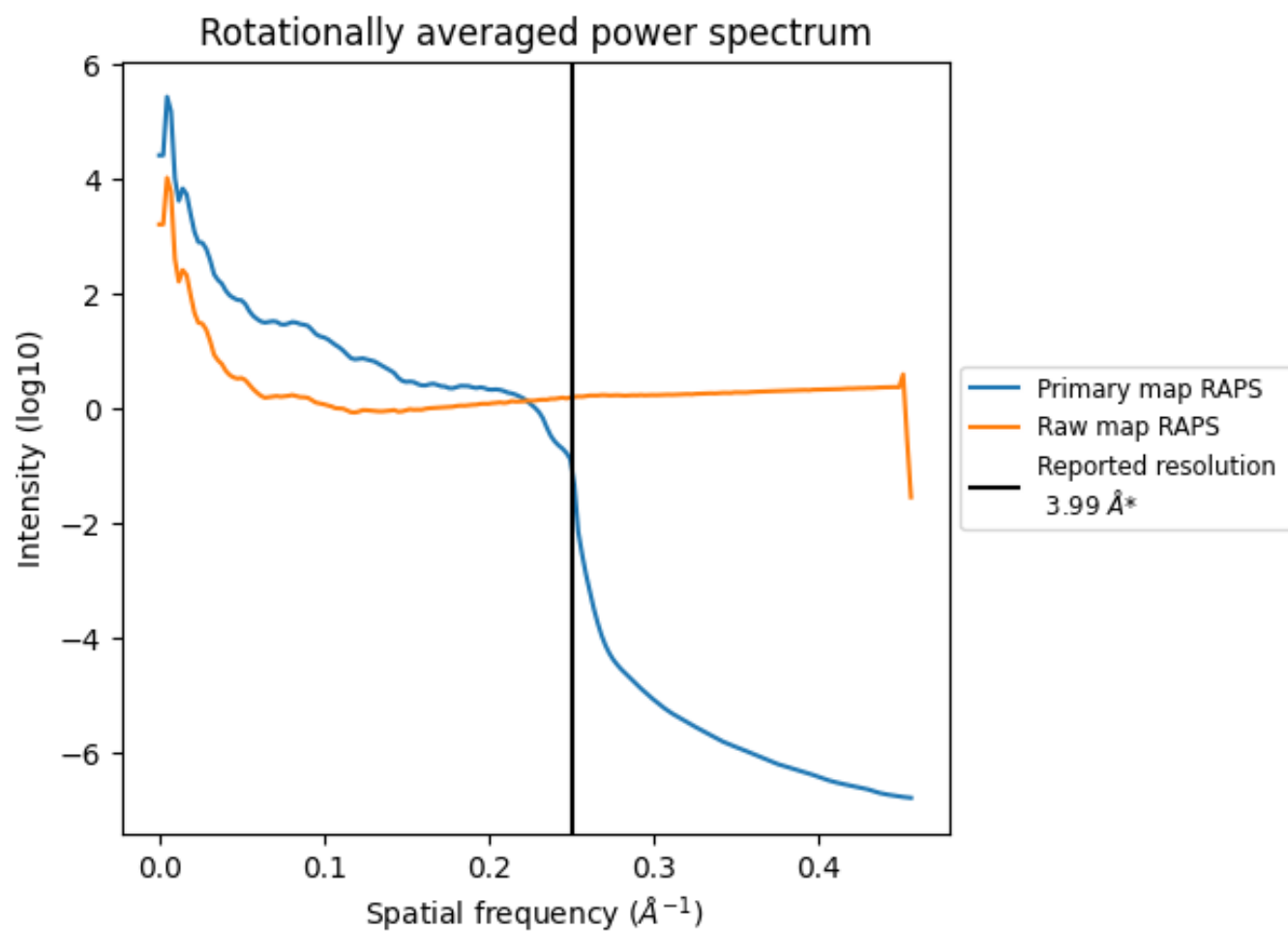
7.2 Volume estimate [i](#)



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](#)

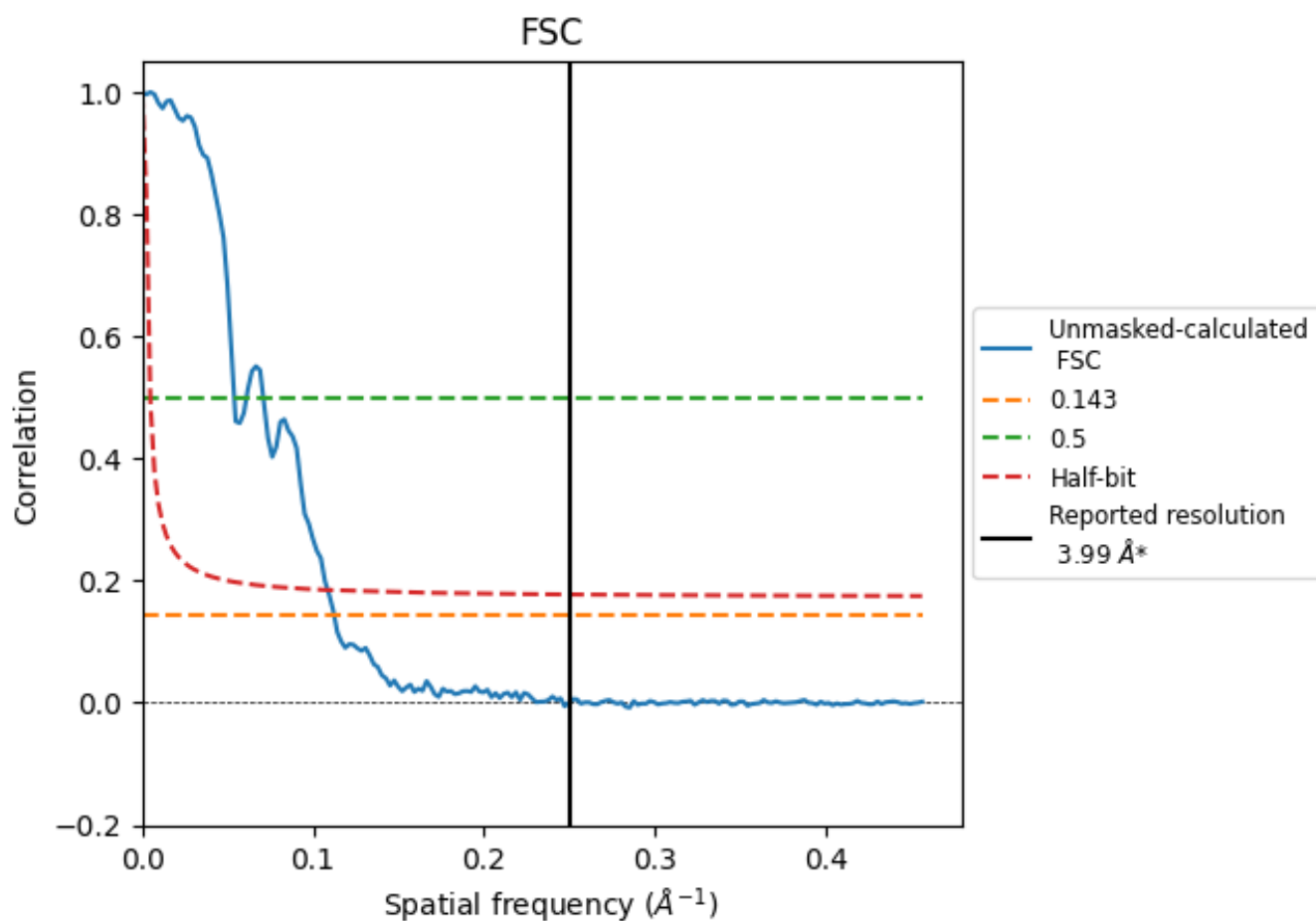


*Reported resolution corresponds to spatial frequency of 0.251 \AA^{-1}

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 \AA^{-1}

8.2 Resolution estimates [i](#)

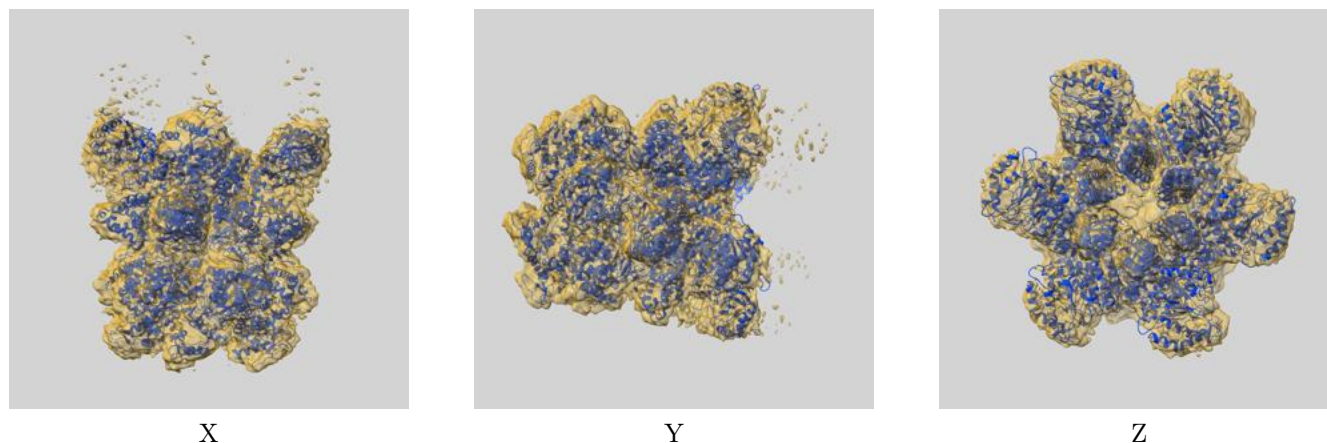
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.99	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.90	18.55	9.21

*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](#)

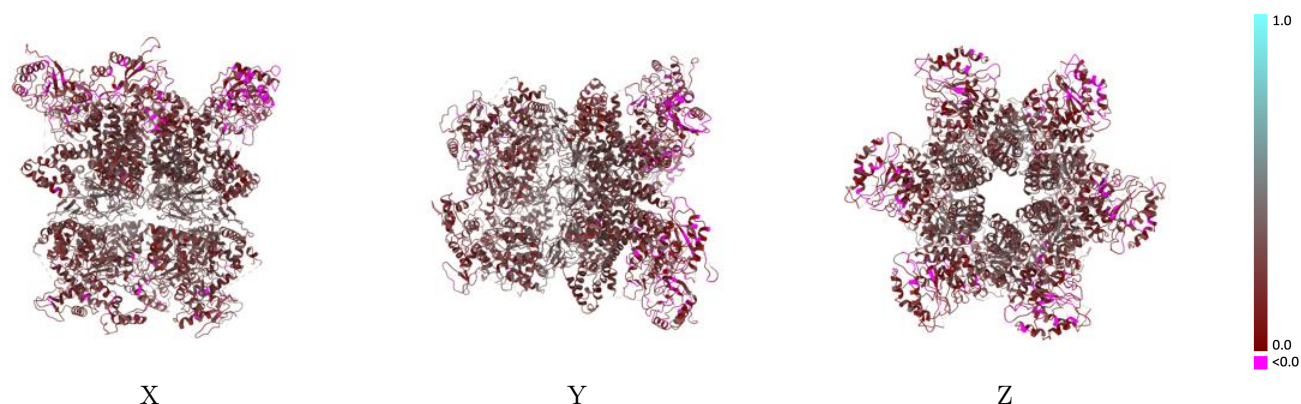
This section contains information regarding the fit between EMDB map EMD-37884 and PDB model 8WW8. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



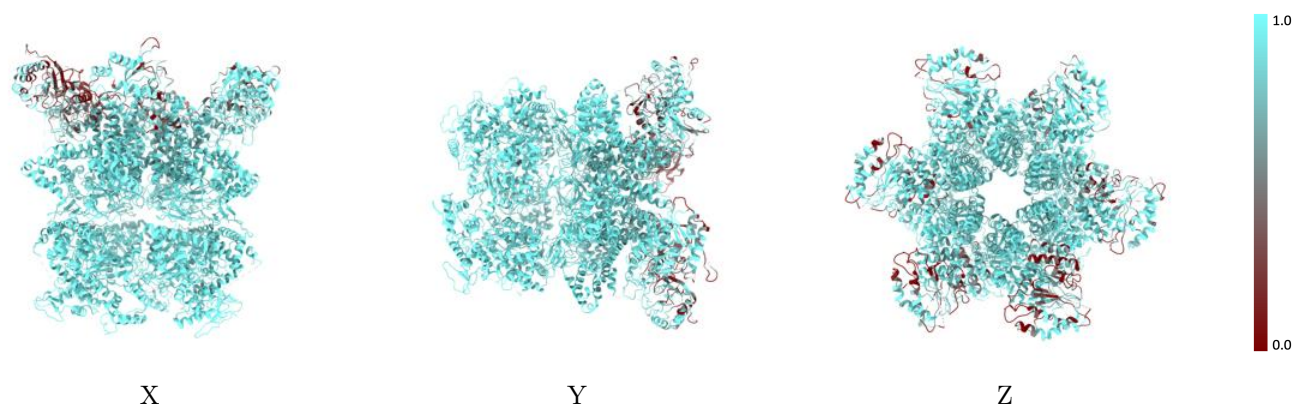
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



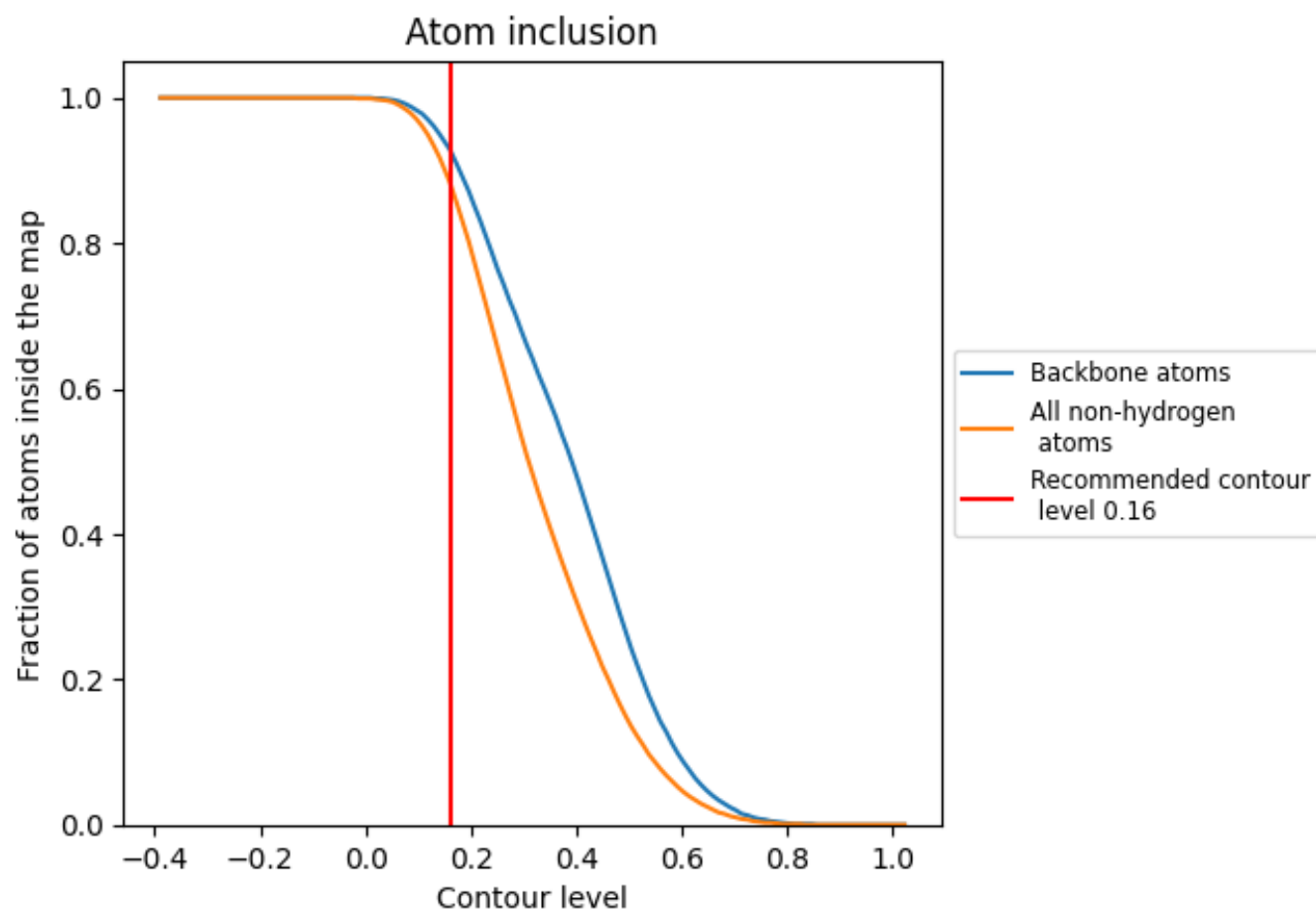
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div></div> 0.8840	<div></div> 0.2380
A	<div></div> 0.8890	<div></div> 0.2410
B	<div></div> 0.8530	<div></div> 0.2440
C	<div></div> 0.8230	<div></div> 0.2390
D	<div></div> 0.8810	<div></div> 0.2340
E	<div></div> 0.9360	<div></div> 0.2260
F	<div></div> 0.9190	<div></div> 0.2430

