



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:40 PM UTC

PDB ID : 8H35 / pdb_00008h35
EMDB ID : EMD-34451
Title : Cryo-EM Structure of the KBTBD2-Cul3-Rbx1 octameric complex
Authors : Hu, Y.; Mao, Q.; Chen, Z.; Sun, L.
Deposited on : 2022-10-08
Resolution : 7.41 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

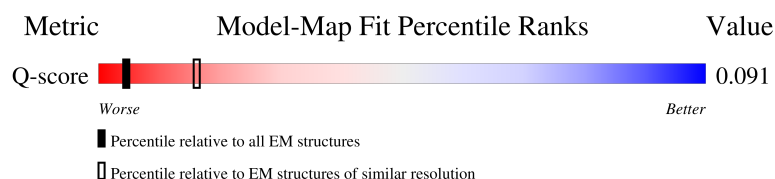
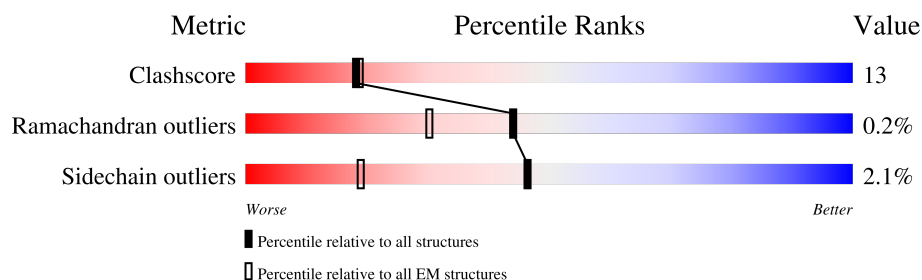
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.41 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



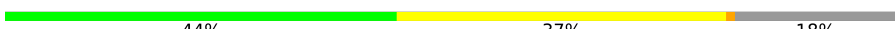
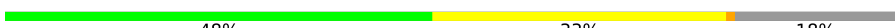
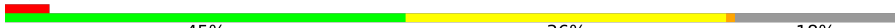
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	381 (6.91 - 7.90)

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	C	768	
1	F	768	
1	H	768	
1	I	768	

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Mol	Chain	Length	Quality of chain
1	M	768	
1	O	768	
1	T	768	
1	V	768	
2	A	623	
2	B	623	
2	G	623	
2	J	623	
2	N	623	
2	P	623	
2	S	623	
2	U	623	
3	D	108	
3	E	108	
3	K	108	
3	L	108	
3	Q	108	
3	R	108	
3	W	108	
3	X	108	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 86872 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 Cullin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	720	Total	C	N	O	S	0	0
			5654	3541	1003	1073	37		
1	F	720	Total	C	N	O	S	0	0
			5801	3645	1026	1092	38		
1	I	720	Total	C	N	O	S	0	0
			5764	3618	1021	1087	38		
1	H	720	Total	C	N	O	S	0	0
			5703	3581	1002	1084	36		
1	M	720	Total	C	N	O	S	0	0
			5708	3582	1003	1087	36		
1	O	720	Total	C	N	O	S	0	0
			5746	3608	1018	1082	38		
1	T	720	Total	C	N	O	S	0	0
			5770	3623	1024	1085	38		
1	V	720	Total	C	N	O	S	0	0
			5657	3549	1000	1072	36		

- Molecule 2 is a protein called Kelch repeat and BTB domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	561	Total	C	N	O	S	0	0
			4380	2798	730	819	33		
2	B	563	Total	C	N	O	S	0	0
			4405	2810	736	824	35		
2	G	561	Total	C	N	O	S	0	0
			4424	2829	736	823	36		
2	J	563	Total	C	N	O	S	0	0
			4393	2808	730	818	37		
2	P	561	Total	C	N	O	S	0	0
			4387	2805	726	820	36		
2	N	563	Total	C	N	O	S	0	0
			4427	2828	736	827	36		
2	S	561	Total	C	N	O	S	0	0
			4435	2838	733	827	37		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	563	Total	C	N	O	S	0	0
			4398	2805	734	822	37		

- Molecule 3 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	89	Total	C	N	O	S	0	0
			733	463	134	127	9		
3	D	89	Total	C	N	O	S	0	0
			731	463	132	127	9		
3	L	89	Total	C	N	O	S	0	0
			705	448	127	122	8		
3	K	89	Total	C	N	O	S	0	0
			729	460	133	127	9		
3	R	89	Total	C	N	O	S	0	0
			733	463	134	127	9		
3	Q	89	Total	C	N	O	S	0	0
			695	442	123	122	8		
3	W	89	Total	C	N	O	S	0	0
			737	466	135	127	9		
3	X	89	Total	C	N	O	S	0	0
			733	463	134	127	9		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

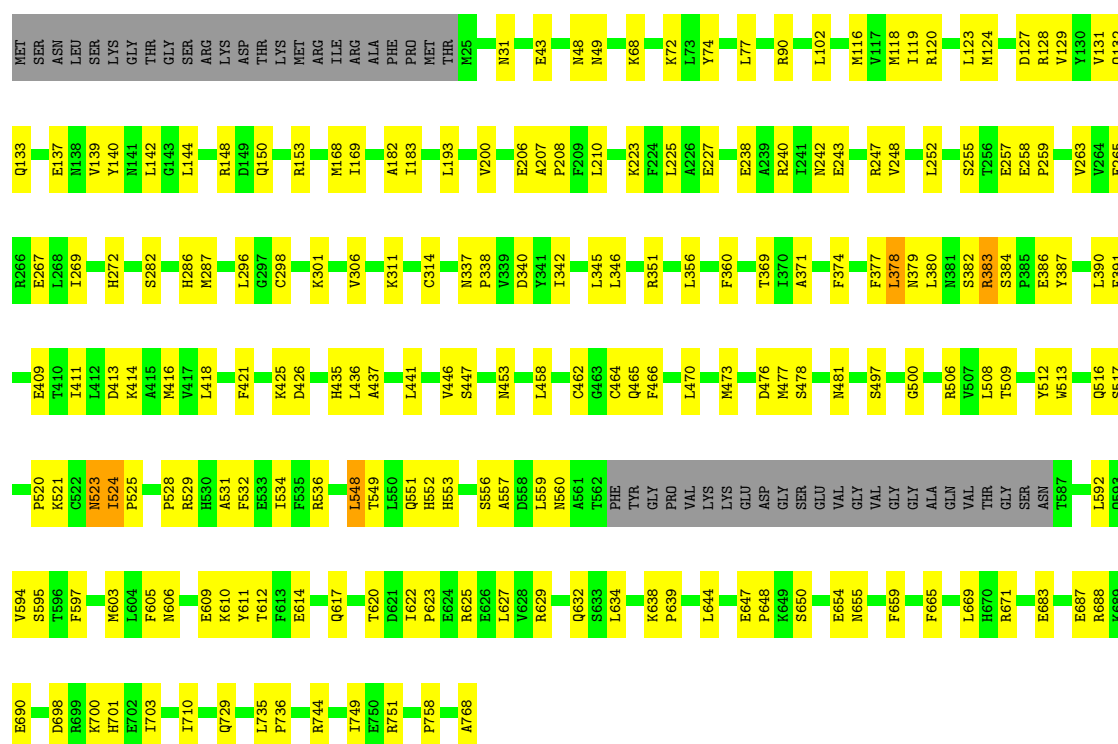
Mol	Chain	Residues	Atoms		AltConf
4	E	3	Total	Zn	0
			3	3	
4	D	3	Total	Zn	0
			3	3	
4	L	3	Total	Zn	0
			3	3	
4	K	3	Total	Zn	0
			3	3	
4	R	3	Total	Zn	0
			3	3	
4	Q	3	Total	Zn	0
			3	3	
4	W	3	Total	Zn	0
			3	3	
4	X	3	Total	Zn	0
			3	3	

3 Residue-property plots

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

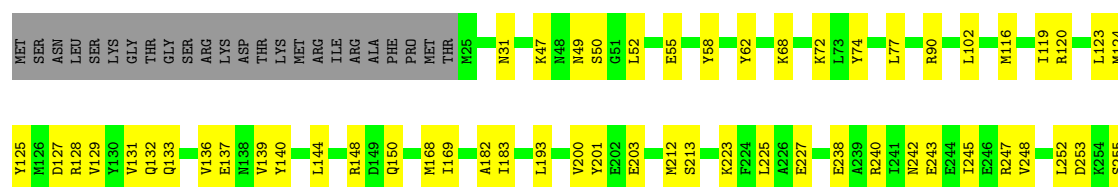
• Molecule 1: Cullin-3

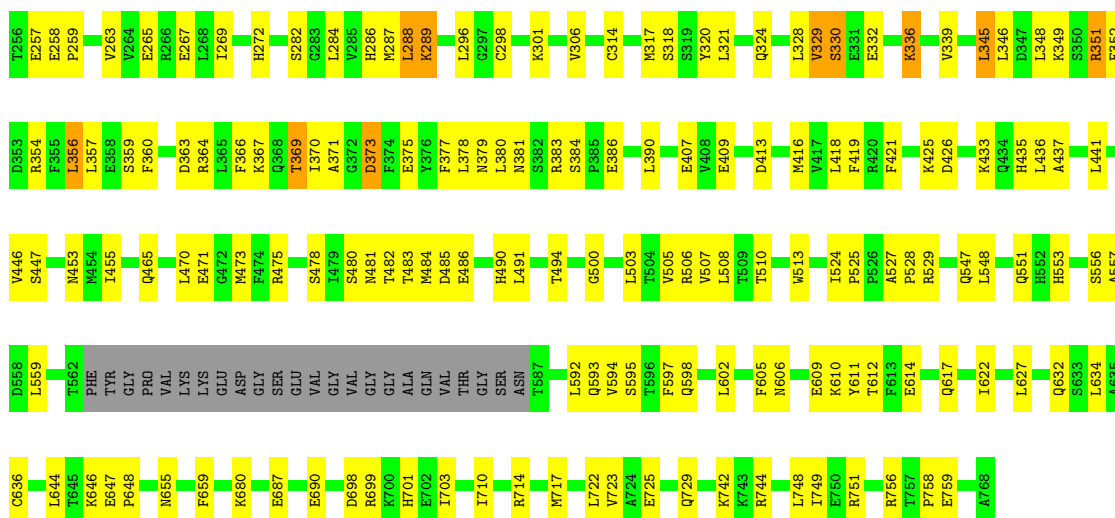
Chain C: 



• Molecule 1: Cullin-3

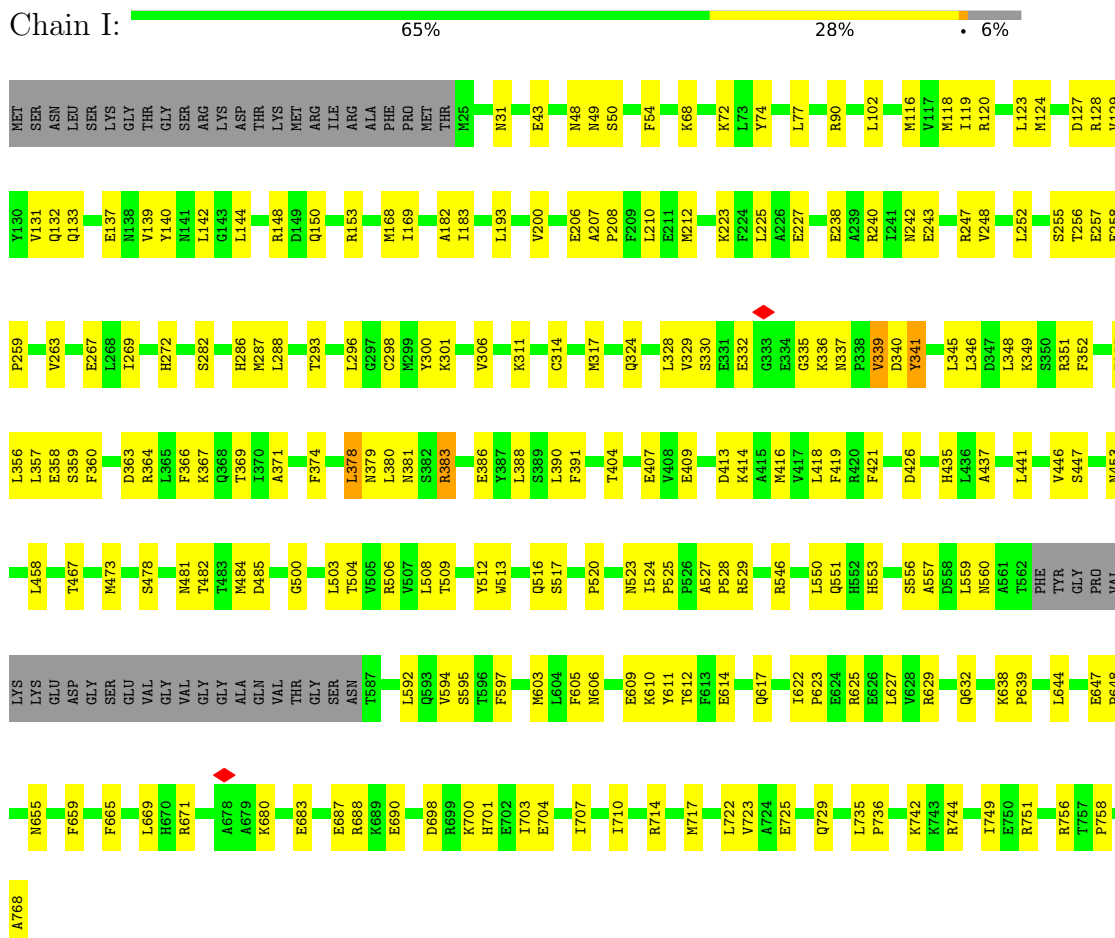
Chain F: 





• Molecule 1: Cullin-3

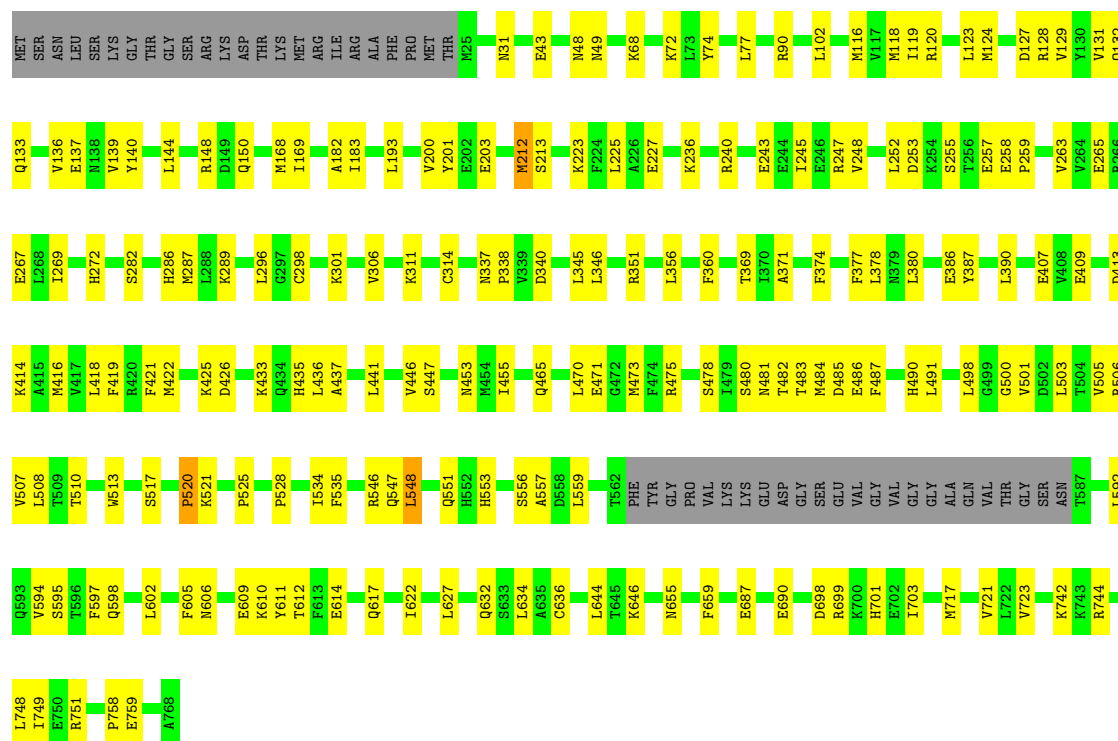
Chain I:



• Molecule 1: Cullin-3

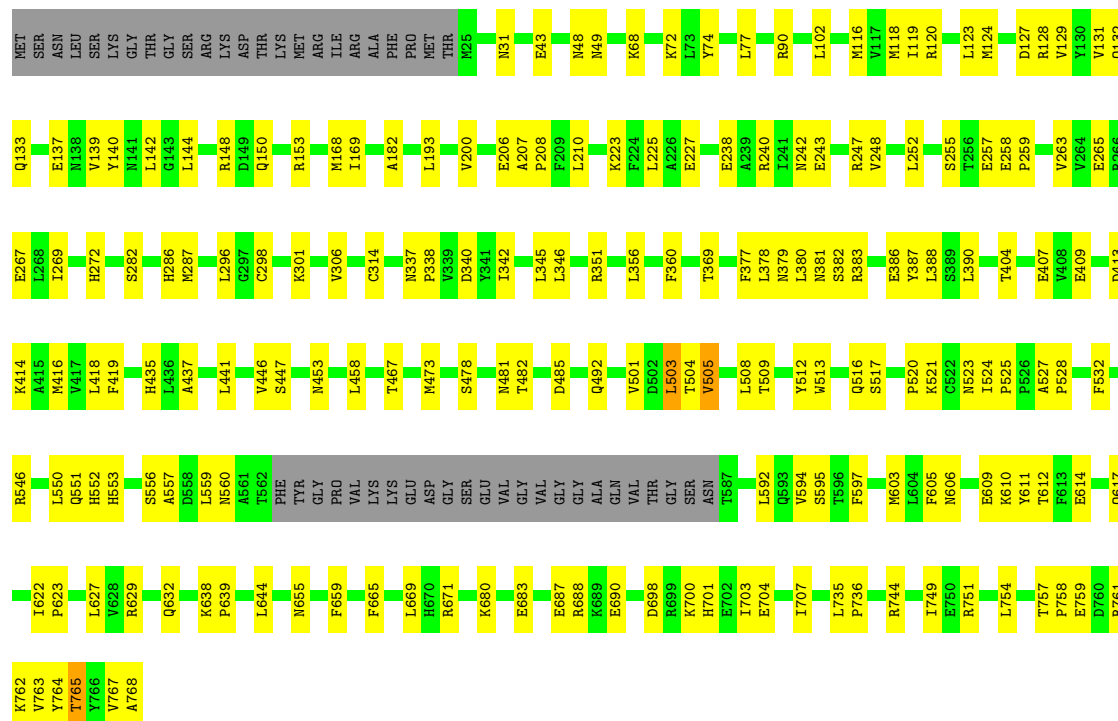
Chain H:





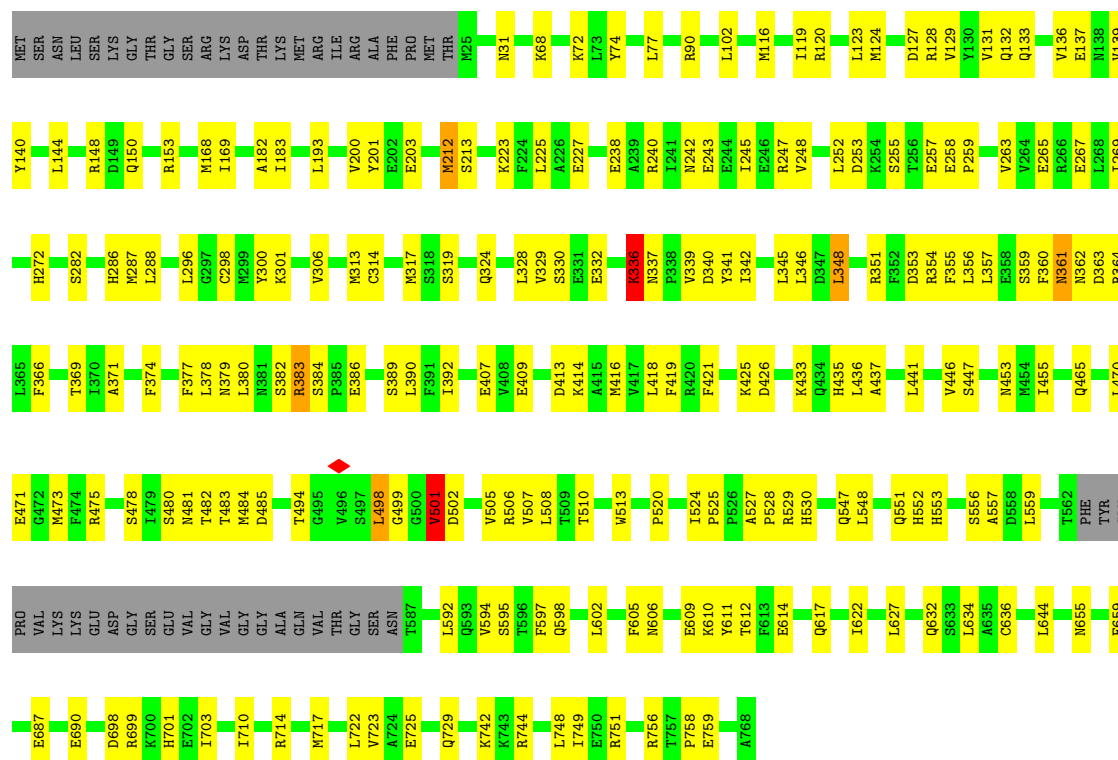
• Molecule 1: Cullin-3

Chain M: 69% 24% 6%



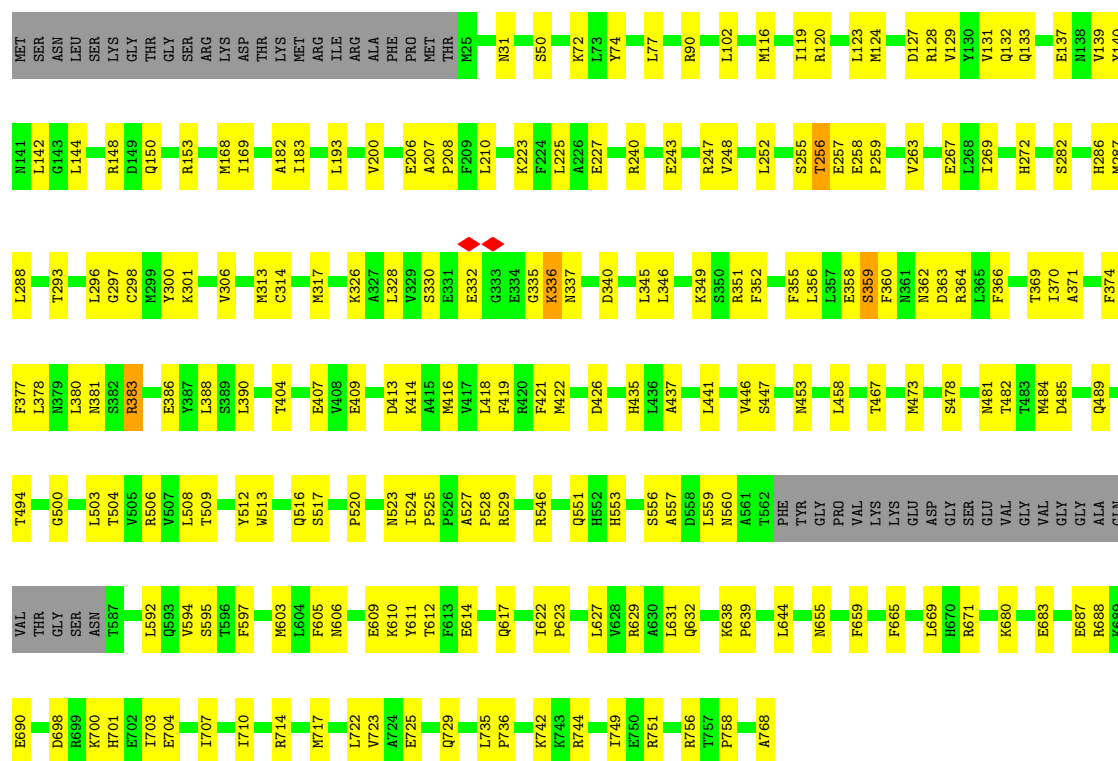
• Molecule 1: Cullin-3

Chain O: 66% 27% 6%



• Molecule 1: Cullin-3

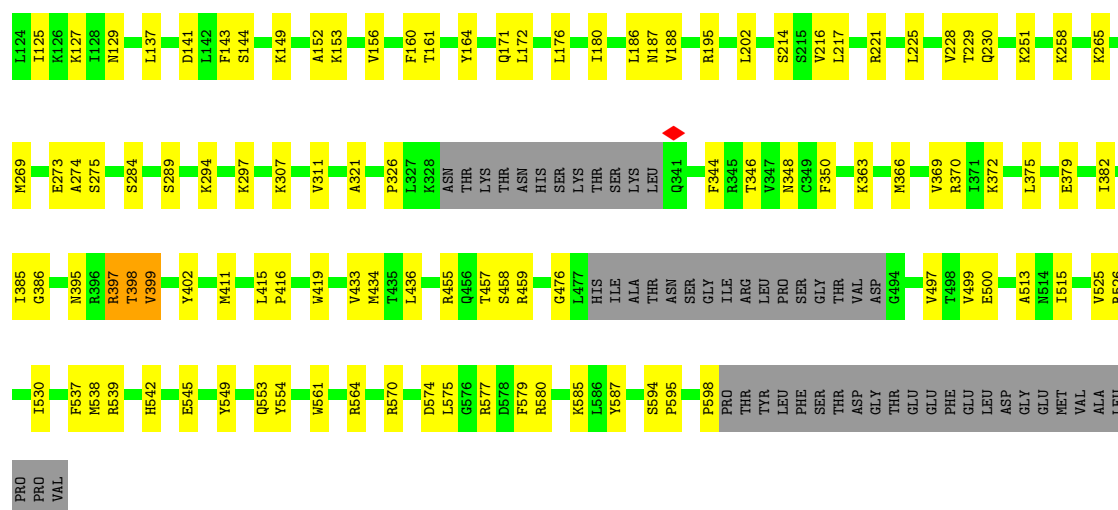
Chain T: 67% 26% • 6%



• Molecule 1: Cullin-3

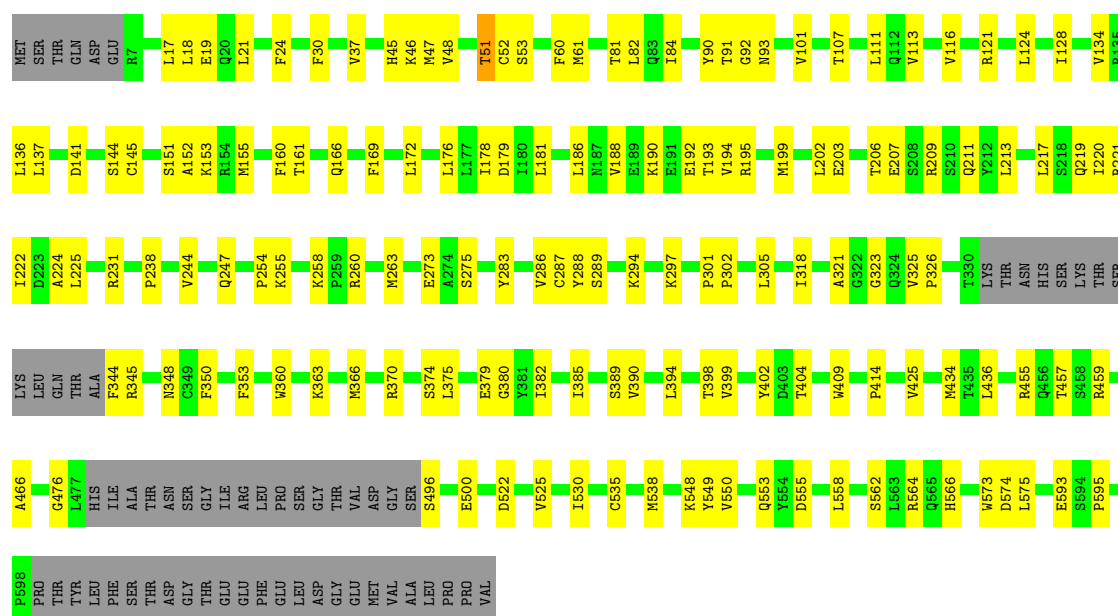






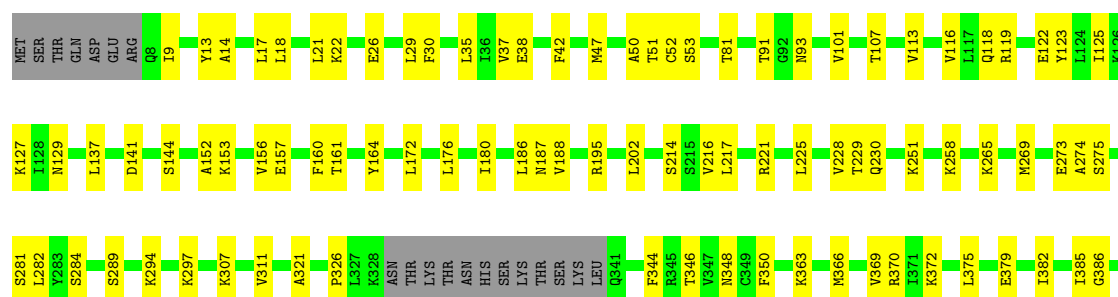
- Molecule 2: Kelch repeat and BTB domain-containing protein 2

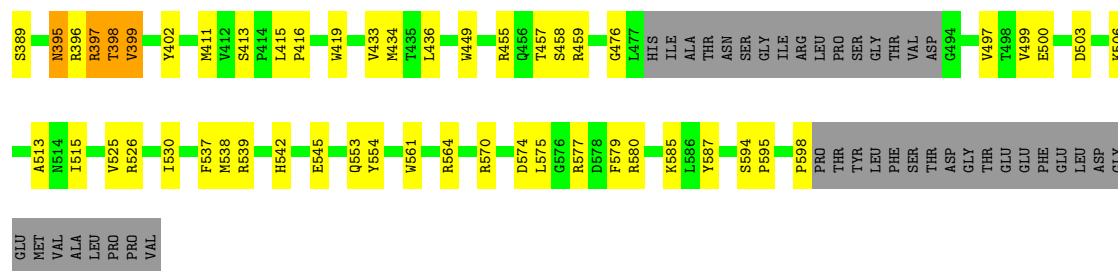
Chain P: 66% 24% 10%



- Molecule 2: Kelch repeat and BTB domain-containing protein 2

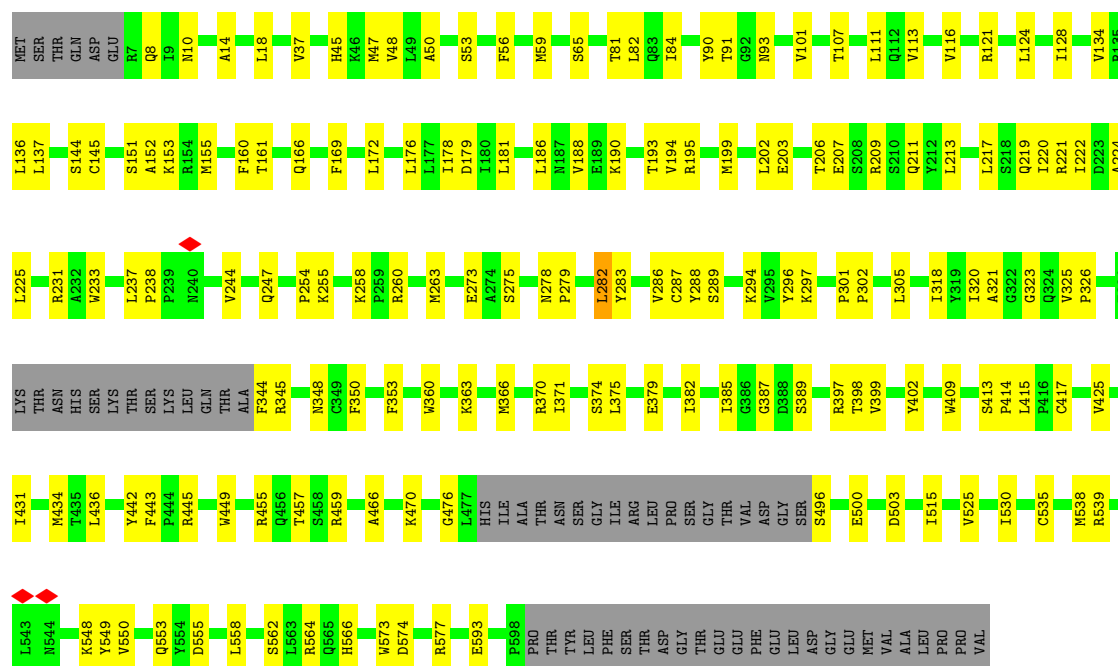
Chain N: 68% 22% 10%





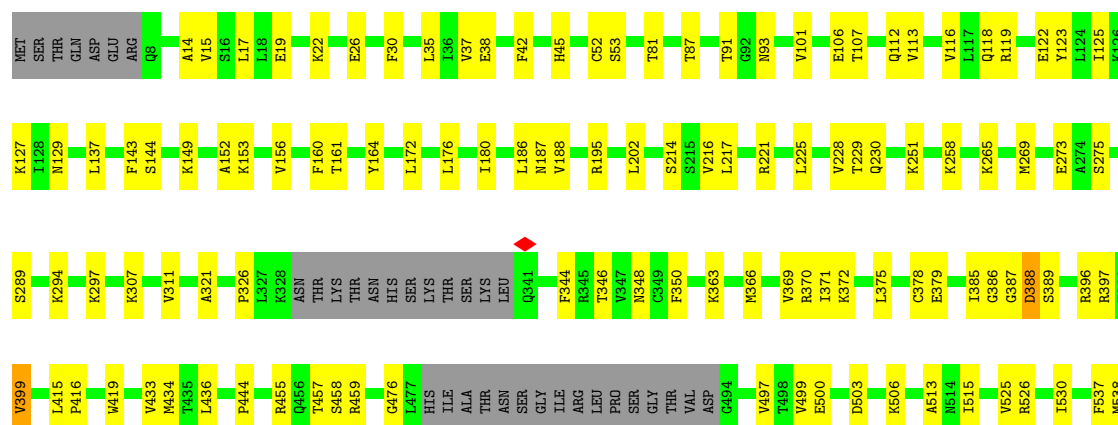
• Molecule 2: Kelch repeat and BTB domain-containing protein 2

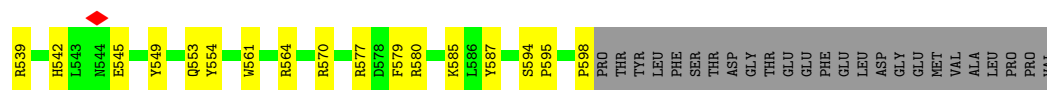
Chain S: 64% 26% 10%



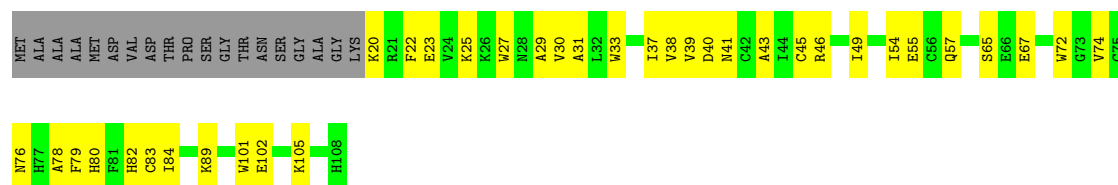
• Molecule 2: Kelch repeat and BTB domain-containing protein 2

Chain U: 69% 21% 10%





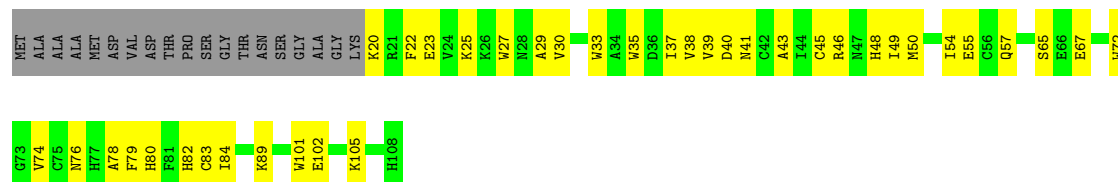
• Molecule 3: E3 ubiquitin-protein ligase RBX1



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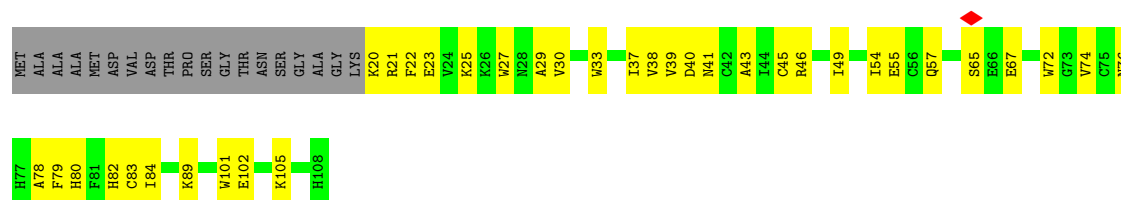


• Molecule 3: E3 ubiquitin-protein ligase RBX1

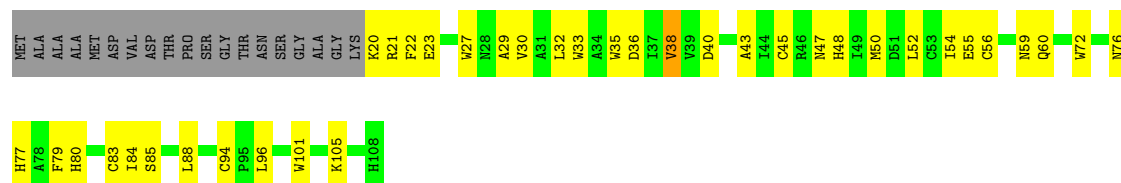


• Molecule 3: E3 ubiquitin-protein ligase RBX1

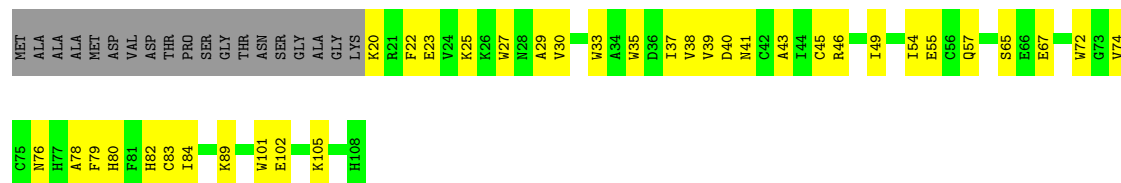




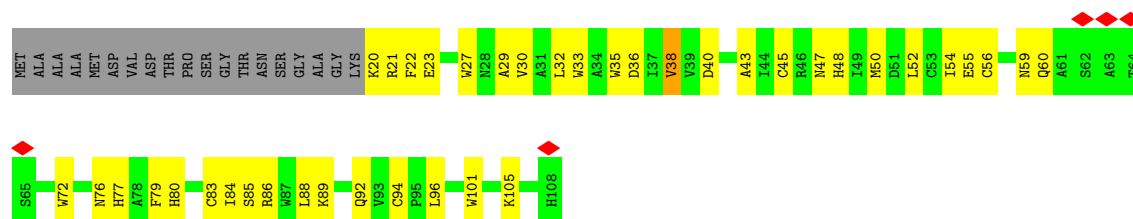
• Molecule 3: E3 ubiquitin-protein ligase RBX1



• Molecule 3: E3 ubiquitin-protein ligase RBX1



• Molecule 3: E3 ubiquitin-protein ligase RBX1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	30204	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.454	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.001	Depositor
Map size ($\text{\AA}$)	511.488, 511.488, 511.488	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.664, 2.664, 2.664	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	C	0.33	0/5736	0.47	0/7726
1	F	0.36	0/5891	0.52	0/7919
1	H	0.30	0/5788	0.44	0/7793
1	I	0.25	0/5850	0.40	0/7865
1	M	0.30	0/5793	0.45	0/7799
1	O	0.32	0/5832	0.47	0/7843
1	T	0.23	0/5858	0.39	0/7875
1	V	0.32	0/5742	0.46	0/7735
2	A	0.31	0/4476	0.48	0/6083
2	B	0.24	0/4503	0.37	0/6117
2	G	0.27	0/4524	0.42	0/6143
2	J	0.25	0/4491	0.39	0/6100
2	N	0.21	0/4526	0.35	0/6146
2	P	0.23	0/4485	0.40	0/6095
2	S	0.19	0/4537	0.35	0/6161
2	U	0.28	0/4493	0.41	0/6100
3	D	0.39	0/753	0.58	0/1022
3	E	0.16	0/755	0.48	1/1025 (0.1%)
3	K	0.14	0/751	0.46	0/1021
3	L	0.16	0/726	0.49	1/986 (0.1%)
3	Q	0.14	0/716	0.47	0/975
3	R	0.15	0/755	0.48	1/1025 (0.1%)
3	W	0.15	0/759	0.48	1/1029 (0.1%)
3	X	0.14	0/755	0.46	0/1025
All	All	0.28	0/88495	0.43	4/119608 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
-----	-------	-----	------	-------	---	-------------	----------

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	65	SER	CB-CA-C	-5.07	110.34	117.23
3	L	65	SER	CB-CA-C	-5.04	110.37	117.23
3	E	65	SER	CB-CA-C	-5.03	110.39	117.23
3	W	65	SER	CB-CA-C	-5.02	110.40	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5654	0	5513	148	0
1	F	5801	0	5790	148	0
1	H	5703	0	5614	135	0
1	I	5764	0	5731	181	0
1	M	5708	0	5611	128	0
1	O	5746	0	5703	204	0
1	T	5770	0	5727	220	0
1	V	5657	0	5503	143	0
2	A	4380	0	4183	117	0
2	B	4405	0	4201	117	0
2	G	4424	0	4237	120	0
2	J	4393	0	4189	110	0
2	N	4427	0	4256	126	0
2	P	4387	0	4183	144	0
2	S	4435	0	4253	121	0
2	U	4398	0	4205	93	0
3	D	731	0	675	27	0
3	E	733	0	675	27	0
3	K	729	0	664	34	0
3	L	705	0	623	30	0
3	Q	695	0	601	30	0
3	R	733	0	675	27	0
3	W	737	0	686	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	X	733	0	675	33	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	K	3	0	0	0	0
4	L	3	0	0	0	0
4	Q	3	0	0	0	0
4	R	3	0	0	0	0
4	W	3	0	0	0	0
4	X	3	0	0	0	0
All	All	86872	0	84173	2261	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 13.

All (2261) 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:T:288:LEU:HD21	1:T:352:PHE:CZ	1.45	1.52
1:T:378:LEU:CD2	1:T:422:MET:HG2	1.43	1.47
1:O:346:LEU:HD21	1:O:414:LYS:CB	1.41	1.47
1:O:346:LEU:CD2	1:O:414:LYS:HB3	1.53	1.38
1:T:288:LEU:HD21	1:T:352:PHE:CE2	1.60	1.34
1:T:288:LEU:CD2	1:T:352:PHE:CZ	2.23	1.20
2:P:47:MET:HG2	2:N:21:LEU:HD22	1.21	1.19
2:A:18:LEU:HD22	2:B:14:ALA:CA	1.74	1.18
1:T:378:LEU:CD2	1:T:422:MET:CG	2.21	1.18
1:T:378:LEU:CD1	1:T:422:MET:HG2	1.75	1.17
1:C:129:VAL:HG23	2:A:144:SER:HB2	1.25	1.15
1:T:349:LYS:HB2	1:T:374:PHE:CZ	1.83	1.13
2:P:144:SER:HB2	1:M:129:VAL:HG23	1.25	1.12
2:P:18:LEU:HD22	2:N:14:ALA:CA	1.78	1.12
1:O:345:LEU:HD13	1:O:377:PHE:CZ	1.84	1.12
1:O:328:LEU:HG	1:O:341:TYR:CD1	1.84	1.12
1:O:328:LEU:HG	1:O:341:TYR:HD1	1.08	1.12
1:V:505:VAL:HG11	1:V:535:PHE:CE1	1.84	1.11
2:P:18:LEU:HD22	2:N:14:ALA:HA	1.28	1.11
1:T:345:LEU:HD21	1:T:377:PHE:CZ	1.84	1.10
1:C:473:MET:HE1	1:C:513:TRP:CE3	1.86	1.10
1:O:288:LEU:HD12	1:O:355:PHE:CE2	1.87	1.09
1:T:378:LEU:CG	1:T:422:MET:HG2	1.82	1.09
1:T:378:LEU:HD22	1:T:422:MET:HG2	1.24	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:18:LEU:HD22	2:B:14:ALA:HA	1.23	1.08
2:A:17:LEU:HD22	2:B:18:LEU:HD13	1.32	1.08
1:T:345:LEU:CD2	1:T:377:PHE:HZ	1.67	1.08
1:I:288:LEU:HD21	1:I:352:PHE:CE2	1.87	1.08
2:P:18:LEU:HD23	2:N:14:ALA:HB2	1.34	1.07
1:F:317:MET:SD	1:F:352:PHE:HE2	1.77	1.07
1:T:349:LYS:HB2	1:T:374:PHE:HZ	1.09	1.06
1:V:436:LEU:HD11	1:V:470:LEU:CD1	1.84	1.06
1:I:288:LEU:HD21	1:I:352:PHE:CZ	1.91	1.06
1:O:345:LEU:HD21	1:O:378:LEU:HD11	1.33	1.06
1:T:378:LEU:HD22	1:T:422:MET:CG	1.83	1.05
1:T:378:LEU:HD21	1:T:422:MET:HE3	1.34	1.04
1:F:317:MET:CG	1:F:352:PHE:HE2	1.70	1.04
1:I:349:LYS:HD3	1:I:374:PHE:CE1	1.93	1.03
2:A:18:LEU:HD23	2:B:14:ALA:HB2	1.36	1.03
2:P:17:LEU:HD22	2:N:18:LEU:HD13	1.37	1.03
1:F:346:LEU:HD12	1:F:418:LEU:HD13	1.36	1.03
2:P:18:LEU:CD2	2:N:14:ALA:HB2	1.88	1.02
1:I:324:GLN:HG2	1:I:348:LEU:HD22	1.41	1.02
2:P:45:HIS:CD2	2:N:47:MET:HE3	1.93	1.02
1:T:378:LEU:CD1	1:T:422:MET:CG	2.35	1.02
1:V:436:LEU:CD1	1:V:470:LEU:HD11	1.90	1.02
1:I:374:PHE:HB3	1:I:421:PHE:CB	1.89	1.02
1:O:345:LEU:HD13	1:O:377:PHE:HZ	1.19	1.02
1:C:473:MET:HE1	1:C:513:TRP:CZ3	1.94	1.02
1:C:477:MET:SD	1:C:506:ARG:NH2	2.31	1.02
1:H:487:PHE:HE1	1:H:534:ILE:HG22	1.23	1.01
2:G:10:ASN:HB3	2:J:15:VAL:CG1	1.90	1.01
1:O:345:LEU:CD2	1:O:378:LEU:HD11	1.89	1.01
1:C:473:MET:SD	1:C:513:TRP:CE2	2.53	1.01
1:T:349:LYS:HD3	1:T:374:PHE:CE1	1.95	1.01
1:V:345:LEU:HG	1:V:418:LEU:HD11	1.43	1.01
1:V:436:LEU:HD11	1:V:470:LEU:HD11	1.03	1.01
1:O:288:LEU:HD12	1:O:355:PHE:HE2	1.19	1.00
1:O:288:LEU:CD1	1:O:355:PHE:CE2	2.44	1.00
1:T:378:LEU:HD21	1:T:422:MET:CE	1.91	1.00
2:P:47:MET:HG2	2:N:21:LEU:CD2	1.91	1.00
1:T:346:LEU:HD13	1:T:418:LEU:HB2	1.40	1.00
1:T:345:LEU:HD21	1:T:377:PHE:HZ	1.17	0.99
2:A:18:LEU:CD2	2:B:14:ALA:HB2	1.92	0.98
1:C:345:LEU:HG	1:C:418:LEU:HD11	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:346:LEU:HD21	1:T:414:LYS:C	1.89	0.97
1:T:374:PHE:HB3	1:T:421:PHE:CB	1.94	0.97
1:O:346:LEU:HD21	1:O:414:LYS:HB2	1.47	0.96
1:T:345:LEU:CD2	1:T:377:PHE:CZ	2.44	0.96
1:C:525:PRO:HA	1:C:603:MET:HE2	1.47	0.96
1:F:317:MET:CG	1:F:352:PHE:CE2	2.49	0.95
1:T:129:VAL:HG23	2:S:144:SER:HB2	1.47	0.95
2:P:60:PHE:HB2	2:N:30:PHE:CZ	2.03	0.94
1:O:345:LEU:HD11	1:O:374:PHE:CE2	2.01	0.94
2:P:47:MET:CG	2:N:21:LEU:HD22	1.97	0.93
1:C:532:PHE:HB2	3:E:27:TRP:CH2	2.04	0.93
1:C:346:LEU:HD11	1:C:414:LYS:HB3	1.51	0.92
1:T:288:LEU:CD2	1:T:352:PHE:HZ	1.82	0.92
1:V:346:LEU:HD11	1:V:414:LYS:HB3	1.51	0.92
1:I:374:PHE:HB3	1:I:421:PHE:HB3	1.51	0.91
1:F:346:LEU:HD12	1:F:418:LEU:CD1	2.00	0.91
1:T:374:PHE:HB3	1:T:421:PHE:HB3	1.53	0.91
1:V:473:MET:HE3	1:V:513:TRP:CH2	2.06	0.90
1:T:378:LEU:HD22	1:T:422:MET:CB	2.00	0.90
1:F:317:MET:SD	1:F:352:PHE:CE2	2.64	0.90
1:T:378:LEU:HD13	1:T:422:MET:CG	2.01	0.89
1:I:349:LYS:HB2	1:I:374:PHE:HZ	1.37	0.89
1:T:378:LEU:HD21	1:T:422:MET:CG	2.03	0.89
1:V:505:VAL:CG1	1:V:535:PHE:CE1	2.56	0.89
2:P:141:ASP:O	1:M:68:LYS:HE3	1.72	0.88
1:O:345:LEU:CD1	1:O:377:PHE:CZ	2.56	0.88
2:A:17:LEU:HD22	2:B:18:LEU:CD1	2.03	0.88
1:O:374:PHE:HB3	1:O:421:PHE:CB	2.03	0.88
1:M:525:PRO:HA	1:M:603:MET:HE2	1.55	0.87
1:O:345:LEU:CD1	1:O:377:PHE:HZ	1.87	0.87
1:C:497:SER:O	1:C:534:ILE:CB	2.22	0.87
1:H:505:VAL:HG11	1:H:535:PHE:CD1	2.09	0.87
1:O:346:LEU:HD21	1:O:414:LYS:HB3	0.89	0.87
1:I:324:GLN:HG2	1:I:348:LEU:CD2	2.04	0.87
1:H:378:LEU:HD22	1:H:422:MET:HG2	1.54	0.87
1:T:133:GLN:CD	2:S:144:SER:HB3	2.00	0.87
1:O:346:LEU:CD2	1:O:414:LYS:CB	2.30	0.87
1:V:505:VAL:HG11	1:V:535:PHE:CD1	2.11	0.86
1:O:356:LEU:HA	1:O:360:PHE:HB2	1.57	0.86
1:V:436:LEU:CD1	1:V:470:LEU:CD1	2.50	0.85
2:G:8:GLN:HG3	2:J:19:GLU:HB3	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:345:LEU:HD11	1:T:377:PHE:CZ	2.10	0.85
1:H:507:VAL:HG23	1:H:535:PHE:HZ	1.40	0.85
2:P:144:SER:HB2	1:M:129:VAL:CG2	2.07	0.85
1:O:374:PHE:HB3	1:O:421:PHE:HB2	1.59	0.85
2:P:18:LEU:HD22	2:N:14:ALA:CB	2.05	0.85
1:T:378:LEU:HD21	1:T:422:MET:SD	2.16	0.84
2:P:18:LEU:CD2	2:N:14:ALA:CB	2.55	0.84
1:M:345:LEU:HG	1:M:418:LEU:HD11	1.59	0.84
1:C:68:LYS:HE3	2:A:141:ASP:O	1.77	0.84
2:P:47:MET:SD	2:N:21:LEU:HD13	2.18	0.84
1:O:371:ALA:CB	1:O:421:PHE:HE1	1.91	0.84
1:I:349:LYS:HD3	1:I:374:PHE:CZ	2.13	0.83
1:H:487:PHE:CE1	1:H:534:ILE:HG22	2.12	0.83
1:V:505:VAL:HG11	1:V:535:PHE:CZ	2.13	0.83
1:C:525:PRO:HB2	1:C:528:PRO:HD2	1.60	0.83
1:I:328:LEU:CD2	1:I:345:LEU:HB2	2.08	0.83
1:T:288:LEU:CD2	1:T:352:PHE:CE2	2.52	0.83
1:F:346:LEU:CD1	1:F:418:LEU:HD13	2.08	0.83
2:G:47:MET:HE3	2:J:45:HIS:CD2	2.13	0.83
1:I:346:LEU:HD21	1:I:414:LYS:CB	2.09	0.83
1:O:345:LEU:CD1	1:O:374:PHE:CE2	2.62	0.83
1:O:346:LEU:CG	1:O:414:LYS:HB3	2.08	0.82
1:I:346:LEU:HD21	1:I:414:LYS:HB3	1.62	0.82
1:H:345:LEU:HG	1:H:418:LEU:HD11	1.61	0.82
1:V:505:VAL:CG1	1:V:535:PHE:CZ	2.61	0.82
2:G:10:ASN:HB3	2:J:15:VAL:HG11	1.62	0.82
2:A:18:LEU:CD2	2:B:14:ALA:CB	2.57	0.82
2:S:10:ASN:HB3	2:U:15:VAL:CG1	2.08	0.82
2:A:18:LEU:HD22	2:B:14:ALA:CB	2.09	0.82
2:G:50:ALA:HB2	2:J:30:PHE:CZ	2.15	0.82
1:M:338:PRO:HB3	1:M:387:TYR:CD1	2.15	0.82
1:T:356:LEU:HD12	1:T:360:PHE:HB2	1.60	0.82
1:V:124:MET:HA	1:V:127:ASP:HB2	1.62	0.82
1:O:124:MET:HA	1:O:127:ASP:HB2	1.62	0.82
1:C:124:MET:HA	1:C:127:ASP:HB2	1.62	0.81
1:T:124:MET:HA	1:T:127:ASP:HB2	1.62	0.81
1:V:436:LEU:HD13	1:V:470:LEU:HG	1.61	0.81
1:C:133:GLN:CD	2:A:144:SER:HB3	2.05	0.81
1:H:124:MET:HA	1:H:127:ASP:HB2	1.62	0.81
1:M:124:MET:HA	1:M:127:ASP:HB2	1.62	0.81
1:H:507:VAL:CG2	1:H:535:PHE:HZ	1.93	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:17:LEU:CD2	2:B:18:LEU:HD13	2.09	0.81
1:I:349:LYS:HB2	1:I:374:PHE:CZ	2.14	0.81
2:G:47:MET:HE3	2:J:45:HIS:NE2	1.95	0.81
2:P:17:LEU:HD22	2:N:18:LEU:CD1	2.09	0.81
1:C:129:VAL:CG2	2:A:144:SER:HB2	2.09	0.81
1:I:356:LEU:HD13	1:I:366:PHE:CB	2.11	0.81
1:F:124:MET:HA	1:F:127:ASP:HB2	1.62	0.81
1:I:346:LEU:HD13	1:I:418:LEU:HB2	1.63	0.80
2:P:17:LEU:CD2	2:N:18:LEU:HD13	2.10	0.80
1:I:356:LEU:HD13	1:I:366:PHE:HB2	1.64	0.80
1:C:500:GLY:H	1:C:531:ALA:HB2	1.47	0.80
1:I:124:MET:HA	1:I:127:ASP:HB2	1.62	0.80
1:I:374:PHE:HB3	1:I:421:PHE:HB2	1.61	0.80
1:T:378:LEU:HD21	1:T:422:MET:HG2	1.55	0.80
1:F:494:THR:O	1:H:498:LEU:HD11	1.80	0.80
2:P:60:PHE:HB2	2:N:30:PHE:HZ	1.45	0.80
1:O:371:ALA:CB	1:O:421:PHE:CE1	2.63	0.80
1:I:288:LEU:CD2	1:I:352:PHE:CZ	2.65	0.80
1:F:321:LEU:CD2	1:F:348:LEU:HD21	2.12	0.79
1:T:346:LEU:HB2	1:T:418:LEU:CD1	2.11	0.79
1:H:346:LEU:HD11	1:H:414:LYS:HB3	1.64	0.79
1:C:473:MET:SD	1:C:513:TRP:CZ2	2.75	0.79
2:J:141:ASP:O	1:H:68:LYS:HE3	1.83	0.79
1:T:345:LEU:CD1	1:T:377:PHE:CZ	2.65	0.78
1:T:378:LEU:HD13	1:T:422:MET:HG3	1.66	0.78
1:T:120:ARG:HG3	1:T:140:TYR:HB2	1.66	0.78
2:A:18:LEU:CD2	2:B:14:ALA:CA	2.60	0.78
1:C:120:ARG:HG3	1:C:140:TYR:HB2	1.66	0.78
1:T:378:LEU:CD2	1:T:422:MET:HE3	2.12	0.78
1:O:288:LEU:CD1	1:O:355:PHE:CD2	2.66	0.78
1:O:345:LEU:HD21	1:O:378:LEU:CD1	2.14	0.78
1:I:120:ARG:HG3	1:I:140:TYR:HB2	1.66	0.77
1:O:346:LEU:CD1	1:O:414:LYS:HB3	2.13	0.77
1:C:129:VAL:HG23	2:A:144:SER:CB	2.11	0.77
1:C:436:LEU:HD13	1:C:470:LEU:HD13	1.66	0.77
2:A:21:LEU:HD12	2:B:17:LEU:HD21	1.65	0.77
1:O:288:LEU:CD1	1:O:355:PHE:HE2	1.86	0.77
1:O:345:LEU:HG	1:O:374:PHE:HE2	1.48	0.77
2:P:144:SER:HB3	1:M:133:GLN:CD	2.10	0.76
1:M:120:ARG:HG3	1:M:140:TYR:HB2	1.66	0.76
2:P:30:PHE:CZ	2:N:50:ALA:HB1	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:505:VAL:HG21	1:V:535:PHE:CD2	2.20	0.76
2:A:30:PHE:CZ	2:B:50:ALA:HB1	2.21	0.76
2:P:144:SER:CB	1:M:129:VAL:HG23	2.12	0.76
1:O:120:ARG:HG3	1:O:140:TYR:HB2	1.68	0.76
1:T:378:LEU:HD13	1:T:422:MET:HG2	1.61	0.76
1:O:371:ALA:HA	1:O:421:PHE:CE1	2.21	0.76
1:F:321:LEU:HD23	1:F:348:LEU:HD21	1.66	0.76
2:P:45:HIS:CD2	2:N:47:MET:CE	2.68	0.76
1:O:328:LEU:HD11	1:O:341:TYR:HA	1.68	0.76
1:M:346:LEU:HD11	1:M:414:LYS:HB3	1.68	0.76
1:T:345:LEU:CD1	1:T:377:PHE:HZ	1.99	0.76
1:I:123:LEU:HB3	1:I:139:VAL:HG11	1.69	0.75
1:C:532:PHE:HB2	3:E:27:TRP:HH2	1.49	0.75
1:V:473:MET:HE3	1:V:513:TRP:CZ2	2.20	0.75
1:F:120:ARG:HG3	1:F:140:TYR:HB2	1.68	0.75
1:H:120:ARG:HG3	1:H:140:TYR:HB2	1.68	0.75
1:O:371:ALA:HB1	1:O:421:PHE:HE1	1.52	0.75
2:P:141:ASP:O	1:M:68:LYS:CE	2.34	0.75
1:I:328:LEU:HD23	1:I:345:LEU:HB2	1.69	0.74
1:M:123:LEU:HB3	1:M:139:VAL:HG11	1.69	0.74
1:C:473:MET:CE	1:C:513:TRP:CZ3	2.70	0.74
1:M:206:GLU:O	1:M:210:LEU:N	2.20	0.74
1:V:120:ARG:HG3	1:V:140:TYR:HB2	1.68	0.74
1:O:288:LEU:HD11	1:O:355:PHE:CD2	2.23	0.74
1:I:206:GLU:O	1:I:210:LEU:N	2.20	0.73
1:T:123:LEU:HB3	1:T:139:VAL:HG11	1.69	0.73
1:C:123:LEU:HB3	1:C:139:VAL:HG11	1.69	0.73
1:F:123:LEU:HB3	1:F:139:VAL:HG11	1.70	0.73
2:P:18:LEU:CD2	2:N:14:ALA:CA	2.64	0.73
1:T:356:LEU:HD13	1:T:366:PHE:HB2	1.69	0.73
1:H:378:LEU:CD2	1:H:422:MET:HG2	2.18	0.73
1:T:374:PHE:HB3	1:T:421:PHE:HB2	1.69	0.73
1:C:532:PHE:HB2	3:E:27:TRP:CZ3	2.24	0.73
1:T:378:LEU:HD11	1:T:422:MET:CG	2.17	0.73
1:C:68:LYS:CE	2:A:141:ASP:O	2.37	0.73
1:I:356:LEU:CD1	1:I:366:PHE:HB2	2.19	0.73
2:S:10:ASN:HB3	2:U:15:VAL:HG11	1.69	0.73
1:C:206:GLU:O	1:C:210:LEU:N	2.20	0.72
1:H:123:LEU:HB3	1:H:139:VAL:HG11	1.70	0.72
1:O:300:TYR:CG	1:O:360:PHE:HA	2.25	0.72
1:T:50:SER:O	2:S:65:SER:CB	2.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:317:MET:HG3	1:F:352:PHE:CE2	2.24	0.72
1:V:123:LEU:HB3	1:V:139:VAL:HG11	1.70	0.72
1:O:328:LEU:HD21	1:O:341:TYR:O	1.89	0.72
1:C:516:GLN:HG2	1:C:517:SER:H	1.55	0.72
1:O:123:LEU:HB3	1:O:139:VAL:HG11	1.70	0.72
2:S:397:ARG:HB2	2:S:415:LEU:HB2	1.71	0.72
2:G:397:ARG:HB2	2:G:415:LEU:HB2	1.71	0.72
1:T:293:THR:HG22	1:T:355:PHE:CE1	2.24	0.72
1:T:346:LEU:HD21	1:T:414:LYS:HB3	1.71	0.72
1:V:505:VAL:HG21	1:V:535:PHE:CE2	2.24	0.72
1:T:346:LEU:HB2	1:T:418:LEU:HD13	1.69	0.71
1:T:516:GLN:HG2	1:T:517:SER:H	1.55	0.71
2:A:18:LEU:HD13	2:B:17:LEU:HD23	1.72	0.71
1:T:206:GLU:O	1:T:210:LEU:N	2.20	0.71
1:M:516:GLN:HG2	1:M:517:SER:H	1.55	0.71
1:O:300:TYR:CD2	1:O:360:PHE:HA	2.26	0.71
1:T:516:GLN:HG3	1:T:553:HIS:HB2	1.73	0.71
2:B:297:LYS:HZ1	2:B:595:PRO:HD3	1.56	0.70
1:V:433:LYS:HD3	1:V:469:LYS:NZ	2.06	0.70
1:M:516:GLN:HG3	1:M:553:HIS:HB2	1.73	0.70
1:O:356:LEU:HD11	1:O:363:ASP:H	1.56	0.70
1:O:346:LEU:HD11	1:O:414:LYS:HB3	1.73	0.70
1:C:516:GLN:HG3	1:C:553:HIS:HB2	1.74	0.70
2:P:390:VAL:CB	2:P:394:LEU:CB	2.70	0.70
1:T:317:MET:HG3	1:T:352:PHE:HE2	1.57	0.70
1:I:516:GLN:HG2	1:I:517:SER:H	1.55	0.70
1:F:345:LEU:HB3	1:F:418:LEU:HD11	1.74	0.69
1:I:516:GLN:HG3	1:I:553:HIS:HB2	1.73	0.69
2:U:378:CYS:SG	2:U:444:PRO:CB	2.81	0.69
1:F:133:GLN:CD	2:B:144:SER:HB3	2.17	0.69
2:G:50:ALA:CB	2:J:30:PHE:CZ	2.76	0.69
1:I:374:PHE:CB	1:I:421:PHE:HB3	2.22	0.69
1:T:288:LEU:HD23	1:T:352:PHE:HZ	1.58	0.68
1:T:300:TYR:HB2	1:T:360:PHE:HD1	1.58	0.68
1:V:632:GLN:HG2	1:V:636:CYS:HB3	1.76	0.68
2:G:50:ALA:HB2	2:J:30:PHE:CE2	2.28	0.68
1:H:632:GLN:HG2	1:H:636:CYS:HB3	1.76	0.68
2:G:10:ASN:HB3	2:J:15:VAL:HG12	1.74	0.68
1:O:632:GLN:HG2	1:O:636:CYS:HB3	1.76	0.68
1:F:133:GLN:NE2	2:B:144:SER:HB3	2.09	0.68
2:U:22:LYS:NZ	2:U:26:GLU:OE2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:546:ARG:HB2	3:K:33:TRP:HB2	1.76	0.68
2:N:22:LYS:NZ	2:N:26:GLU:OE2	2.27	0.68
1:O:329:VAL:HG23	1:O:341:TYR:CZ	2.29	0.68
1:C:477:MET:CE	1:C:506:ARG:NH2	2.56	0.67
3:L:33:TRP:O	3:L:76:ASN:ND2	2.27	0.67
3:W:33:TRP:O	3:W:76:ASN:ND2	2.27	0.67
1:I:371:ALA:HA	1:I:421:PHE:CE1	2.29	0.67
2:P:21:LEU:HD12	2:N:17:LEU:HD21	1.75	0.67
2:A:161:THR:HB	2:A:188:VAL:HG13	1.77	0.67
2:S:161:THR:HB	2:S:188:VAL:HG13	1.77	0.67
2:J:22:LYS:NZ	2:J:26:GLU:OE2	2.27	0.67
2:B:22:LYS:NZ	2:B:26:GLU:OE2	2.27	0.67
2:G:161:THR:HB	2:G:188:VAL:HG13	1.77	0.67
1:V:338:PRO:HB3	1:V:387:TYR:CD1	2.30	0.67
1:F:632:GLN:HG2	1:F:636:CYS:HB3	1.76	0.67
2:U:144:SER:HB3	1:V:133:GLN:NE2	2.10	0.67
3:R:33:TRP:O	3:R:76:ASN:ND2	2.27	0.67
2:P:45:HIS:HD1	2:P:90:TYR:HH	1.41	0.66
2:G:65:SER:CB	1:I:50:SER:O	2.43	0.66
2:P:161:THR:HB	2:P:188:VAL:HG13	1.77	0.66
1:I:328:LEU:HD21	1:I:345:LEU:HB2	1.76	0.66
1:I:374:PHE:CB	1:I:421:PHE:CB	2.70	0.66
1:O:371:ALA:HB1	1:O:421:PHE:CE1	2.30	0.66
1:T:349:LYS:CB	1:T:374:PHE:CZ	2.73	0.66
3:E:33:TRP:O	3:E:76:ASN:ND2	2.27	0.66
1:T:374:PHE:CB	1:T:421:PHE:HB3	2.25	0.66
2:J:297:LYS:HZ1	2:J:595:PRO:HD3	1.60	0.66
2:S:45:HIS:HD1	2:S:90:TYR:HH	1.40	0.66
2:G:47:MET:CE	2:J:45:HIS:CD2	2.78	0.66
1:V:248:VAL:HG23	1:V:252:LEU:HD12	1.78	0.66
2:J:187:ASN:ND2	2:J:587:TYR:OH	2.29	0.66
2:N:187:ASN:ND2	2:N:587:TYR:OH	2.29	0.66
2:U:187:ASN:ND2	2:U:587:TYR:OH	2.29	0.66
1:I:346:LEU:HD21	1:I:414:LYS:C	2.21	0.65
1:F:248:VAL:HG23	1:F:252:LEU:HD12	1.78	0.65
2:B:187:ASN:ND2	2:B:587:TYR:OH	2.29	0.65
2:G:530:ILE:HD12	2:G:535:CYS:HB2	1.79	0.65
3:L:67:GLU:O	3:L:82:HIS:NE2	2.29	0.65
1:M:501:VAL:HG13	1:T:494:THR:CB	2.25	0.65
1:I:324:GLN:CG	1:I:348:LEU:HD22	2.22	0.65
2:P:530:ILE:HD12	2:P:535:CYS:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:MET:SD	1:C:512:TYR:HB3	2.37	0.65
1:H:248:VAL:HG23	1:H:252:LEU:HD12	1.78	0.65
3:R:72:TRP:HB2	3:R:105:LYS:HB3	1.79	0.65
2:A:30:PHE:CZ	2:B:50:ALA:CB	2.79	0.65
1:F:494:THR:O	1:H:498:LEU:CD1	2.45	0.65
1:I:371:ALA:CB	1:I:421:PHE:HE1	2.10	0.65
1:I:749:ILE:HD13	1:I:758:PRO:HD3	1.79	0.65
1:V:505:VAL:HG13	1:V:535:PHE:CZ	2.29	0.65
2:G:45:HIS:HD1	2:G:90:TYR:HH	1.42	0.65
2:G:207:GLU:HG3	2:G:238:PRO:HG3	1.79	0.65
2:S:530:ILE:HD12	2:S:535:CYS:HB2	1.78	0.65
1:O:288:LEU:HD11	1:O:355:PHE:CE2	2.31	0.65
1:T:345:LEU:HD11	1:T:377:PHE:HZ	1.59	0.65
2:P:45:HIS:CG	2:N:47:MET:HE3	2.31	0.65
1:C:749:ILE:HD13	1:C:758:PRO:HD3	1.79	0.64
2:P:18:LEU:HD13	2:N:17:LEU:HD23	1.77	0.64
3:W:67:GLU:O	3:W:82:HIS:NE2	2.29	0.64
3:D:36:ASP:HB2	3:D:77:HIS:HE2	1.62	0.64
2:J:141:ASP:O	1:H:68:LYS:CE	2.45	0.64
3:K:36:ASP:HB2	3:K:77:HIS:HE2	1.62	0.64
2:N:297:LYS:HZ1	2:N:595:PRO:HD3	1.62	0.64
3:X:45:CYS:SG	3:X:80:HIS:HE1	2.20	0.64
2:P:45:HIS:CG	2:N:47:MET:CE	2.80	0.64
3:R:67:GLU:O	3:R:82:HIS:NE2	2.29	0.64
1:T:337:ASN:HB3	1:T:340:ASP:HB2	1.78	0.64
3:X:36:ASP:HB2	3:X:77:HIS:HE2	1.62	0.64
2:A:207:GLU:HG3	2:A:238:PRO:HG3	1.79	0.64
2:P:222:ILE:HA	2:P:225:LEU:HB2	1.80	0.64
1:C:338:PRO:HB3	1:C:387:TYR:CD1	2.32	0.64
1:C:669:LEU:HG	1:C:671:ARG:H	1.62	0.64
1:H:371:ALA:HB1	1:H:421:PHE:CE1	2.33	0.64
1:M:669:LEU:HG	1:M:671:ARG:H	1.62	0.64
2:S:222:ILE:HA	2:S:225:LEU:HB2	1.80	0.64
2:U:144:SER:HB2	1:V:129:VAL:HB	1.78	0.64
3:E:67:GLU:O	3:E:82:HIS:NE2	2.29	0.64
1:I:346:LEU:CD2	1:I:414:LYS:HB3	2.27	0.64
3:L:72:TRP:HB2	3:L:105:LYS:HB3	1.79	0.64
3:Q:45:CYS:SG	3:Q:80:HIS:HE1	2.20	0.64
1:I:669:LEU:HG	1:I:671:ARG:H	1.62	0.64
3:Q:36:ASP:HB2	3:Q:77:HIS:HE2	1.62	0.64
2:A:222:ILE:HA	2:A:225:LEU:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:530:ILE:HD12	2:A:535:CYS:HB2	1.79	0.64
3:E:72:TRP:HB2	3:E:105:LYS:HB3	1.79	0.64
1:T:669:LEU:HG	1:T:671:ARG:H	1.62	0.64
2:J:144:SER:HB3	1:H:133:GLN:NE2	2.13	0.63
2:P:207:GLU:HG3	2:P:238:PRO:HG3	1.79	0.63
2:S:207:GLU:HG3	2:S:238:PRO:HG3	1.79	0.63
3:W:72:TRP:HB2	3:W:105:LYS:HB3	1.79	0.63
2:G:222:ILE:HA	2:G:225:LEU:HB2	1.80	0.63
1:O:248:VAL:HG23	1:O:252:LEU:HD12	1.78	0.63
1:O:282:SER:HA	1:O:286:HIS:HB3	1.80	0.63
1:T:749:ILE:HD13	1:T:758:PRO:HD3	1.79	0.63
1:I:356:LEU:HD12	1:I:360:PHE:HB2	1.80	0.63
2:N:553:GLN:HB2	2:N:564:ARG:HB2	1.81	0.63
1:T:300:TYR:CG	1:T:360:PHE:HA	2.34	0.63
1:V:282:SER:HA	1:V:286:HIS:HB3	1.80	0.63
1:V:480:SER:O	1:V:484:MET:HG3	1.99	0.63
3:K:45:CYS:SG	3:K:80:HIS:HE1	2.20	0.63
1:V:371:ALA:HB1	1:V:421:PHE:CE1	2.34	0.63
1:I:356:LEU:HA	1:I:360:PHE:CD2	2.34	0.63
2:U:214:SER:O	2:U:251:LYS:NZ	2.32	0.63
1:F:282:SER:HA	1:F:286:HIS:HB3	1.80	0.63
2:J:553:GLN:HB2	2:J:564:ARG:HB2	1.81	0.63
2:G:9:ILE:HG22	2:J:91:THR:O	1.99	0.62
2:P:30:PHE:CZ	2:N:50:ALA:CB	2.82	0.62
1:V:551:GLN:NE2	3:X:30:VAL:O	2.32	0.62
2:B:539:ARG:HH22	2:B:577:ARG:HD3	1.64	0.62
1:H:378:LEU:HD21	1:H:422:MET:HE3	1.79	0.62
1:T:346:LEU:HD21	1:T:414:LYS:CB	2.29	0.62
2:B:553:GLN:HB2	2:B:564:ARG:HB2	1.81	0.62
2:G:18:LEU:HD13	2:J:17:LEU:CD2	2.28	0.62
2:N:539:ARG:HH22	2:N:577:ARG:HD3	1.64	0.62
1:O:345:LEU:CG	1:O:374:PHE:CE2	2.82	0.62
1:O:371:ALA:CA	1:O:421:PHE:CE1	2.83	0.62
2:U:553:GLN:HB2	2:U:564:ARG:HB2	1.81	0.62
1:F:90:ARG:NH2	1:F:150:GLN:OE1	2.33	0.62
2:J:214:SER:O	2:J:251:LYS:NZ	2.32	0.62
1:H:505:VAL:HG11	1:H:535:PHE:CE1	2.34	0.62
1:V:473:MET:CE	1:V:513:TRP:CH2	2.81	0.62
1:F:551:GLN:NE2	3:D:30:VAL:O	2.32	0.62
1:H:480:SER:O	1:H:484:MET:HG3	1.99	0.62
2:B:214:SER:O	2:B:251:LYS:NZ	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:370:ARG:NH1	2:B:386:GLY:O	2.33	0.62
2:G:8:GLN:CG	2:J:19:GLU:HB3	2.28	0.62
1:H:90:ARG:NH2	1:H:150:GLN:OE1	2.33	0.62
1:H:282:SER:HA	1:H:286:HIS:HB3	1.81	0.62
2:N:214:SER:O	2:N:251:LYS:NZ	2.32	0.62
1:O:296:LEU:HD12	1:O:360:PHE:CZ	2.34	0.62
1:O:551:GLN:NE2	3:Q:30:VAL:O	2.32	0.62
1:T:133:GLN:HG2	2:S:144:SER:OG	2.00	0.62
2:G:535:CYS:SG	2:G:564:ARG:NH1	2.73	0.62
1:O:90:ARG:NH2	1:O:150:GLN:OE1	2.33	0.62
1:O:480:SER:O	1:O:484:MET:HG3	1.99	0.62
1:C:90:ARG:NH2	1:C:150:GLN:OE1	2.33	0.62
1:C:525:PRO:HB3	1:C:603:MET:HG3	1.81	0.62
1:F:480:SER:O	1:F:484:MET:HG3	1.99	0.62
1:I:248:VAL:HG23	1:I:252:LEU:HD12	1.81	0.62
1:H:486:GLU:O	1:H:490:HIS:ND1	2.30	0.62
2:S:50:ALA:HB2	2:U:30:PHE:CZ	2.34	0.62
2:S:382:ILE:HB	2:S:402:TYR:HB3	1.82	0.62
2:A:382:ILE:HB	2:A:402:TYR:HB3	1.82	0.62
1:I:90:ARG:NH2	1:I:150:GLN:OE1	2.33	0.62
1:T:317:MET:HG3	1:T:352:PHE:CE2	2.35	0.62
1:T:374:PHE:CB	1:T:421:PHE:CB	2.76	0.62
1:C:314:CYS:HB3	1:C:369:THR:HG21	1.82	0.61
1:F:288:LEU:HG	1:F:351:ARG:NH2	2.15	0.61
1:T:346:LEU:HB2	1:T:418:LEU:HD12	1.81	0.61
2:S:273:GLU:HA	2:S:283:TYR:HB3	1.81	0.61
1:F:223:LYS:HE3	1:F:227:GLU:HG3	1.82	0.61
1:I:314:CYS:HB3	1:I:369:THR:HG21	1.82	0.61
1:I:371:ALA:HA	1:I:421:PHE:CD1	2.36	0.61
1:H:551:GLN:NE2	3:K:30:VAL:O	2.32	0.61
2:P:382:ILE:HB	2:P:402:TYR:HB3	1.82	0.61
1:M:90:ARG:NH2	1:M:150:GLN:OE1	2.33	0.61
1:O:296:LEU:HD12	1:O:360:PHE:CE1	2.36	0.61
1:F:749:ILE:HD13	1:F:758:PRO:HD3	1.83	0.61
2:G:9:ILE:CG2	2:J:92:GLY:HA3	2.31	0.61
1:O:345:LEU:HG	1:O:374:PHE:CE2	2.32	0.61
1:O:356:LEU:HA	1:O:360:PHE:CB	2.28	0.61
1:T:314:CYS:HB3	1:T:369:THR:HG21	1.82	0.61
2:A:273:GLU:HA	2:A:283:TYR:HB3	1.81	0.61
2:G:8:GLN:HE22	2:J:22:LYS:CD	2.13	0.61
1:T:90:ARG:NH2	1:T:150:GLN:OE1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:221:ARG:HH11	2:G:258:LYS:H	1.48	0.61
1:M:314:CYS:HB3	1:M:369:THR:HG21	1.82	0.61
2:S:535:CYS:SG	2:S:564:ARG:NH1	2.73	0.61
1:V:223:LYS:HE3	1:V:227:GLU:HG3	1.82	0.61
1:H:314:CYS:HB3	1:H:369:THR:HG21	1.83	0.61
1:H:703:ILE:HD11	1:H:744:ARG:HD3	1.83	0.61
1:M:248:VAL:HG23	1:M:252:LEU:HD12	1.81	0.61
1:O:314:CYS:HB3	1:O:369:THR:HG21	1.83	0.61
1:O:703:ILE:HD11	1:O:744:ARG:HD3	1.83	0.61
1:O:749:ILE:HD13	1:O:758:PRO:HD3	1.83	0.61
1:V:90:ARG:NH2	1:V:150:GLN:OE1	2.33	0.61
1:F:703:ILE:HD11	1:F:744:ARG:HD3	1.83	0.61
2:J:539:ARG:HH22	2:J:577:ARG:HD3	1.64	0.61
2:P:273:GLU:HA	2:P:283:TYR:HB3	1.81	0.61
1:T:129:VAL:HG23	2:S:144:SER:CB	2.29	0.61
2:U:539:ARG:HH22	2:U:577:ARG:HD3	1.64	0.61
2:P:535:CYS:SG	2:P:564:ARG:NH1	2.73	0.61
1:O:223:LYS:HE3	1:O:227:GLU:HG3	1.82	0.61
1:V:409:GLU:OE2	1:V:453:ASN:ND2	2.34	0.61
1:I:703:ILE:HD11	1:I:744:ARG:HD3	1.83	0.60
1:M:77:LEU:HD22	1:M:123:LEU:HD22	1.83	0.60
3:Q:85:SER:HA	3:Q:88:LEU:HD12	1.83	0.60
1:T:378:LEU:CD1	1:T:422:MET:HG3	2.24	0.60
1:C:248:VAL:HG23	1:C:252:LEU:HD12	1.81	0.60
1:F:409:GLU:OE2	1:F:453:ASN:ND2	2.34	0.60
2:J:144:SER:HB3	1:H:133:GLN:CD	2.26	0.60
2:U:297:LYS:HZ1	2:U:595:PRO:HD3	1.66	0.60
1:V:314:CYS:HB3	1:V:369:THR:HG21	1.83	0.60
1:V:436:LEU:HD13	1:V:470:LEU:CG	2.29	0.60
1:C:77:LEU:HD22	1:C:123:LEU:HD22	1.83	0.60
1:F:120:ARG:O	1:F:124:MET:CB	2.50	0.60
1:V:441:LEU:HD21	1:V:508:LEU:HD11	1.84	0.60
1:V:749:ILE:HD13	1:V:758:PRO:HD3	1.83	0.60
1:C:473:MET:SD	1:C:513:TRP:CD2	2.94	0.60
2:A:535:CYS:SG	2:A:564:ARG:NH1	2.73	0.60
1:I:296:LEU:HD12	1:I:360:PHE:CZ	2.36	0.60
1:H:120:ARG:O	1:H:124:MET:CB	2.50	0.60
1:H:441:LEU:HD21	1:H:508:LEU:HD11	1.84	0.60
1:H:749:ILE:HD13	1:H:758:PRO:HD3	1.83	0.60
1:T:248:VAL:HG23	1:T:252:LEU:HD12	1.81	0.60
1:V:346:LEU:HD11	1:V:414:LYS:CB	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:221:ARG:HH11	2:S:258:LYS:H	1.48	0.60
1:M:644:LEU:HD11	1:M:659:PHE:HB3	1.84	0.60
1:C:703:ILE:HD11	1:C:744:ARG:HD3	1.83	0.60
1:F:441:LEU:HD21	1:F:508:LEU:HD11	1.84	0.60
1:I:644:LEU:HD11	1:I:659:PHE:HB3	1.84	0.60
1:H:223:LYS:HE3	1:H:227:GLU:HG3	1.82	0.60
1:H:409:GLU:OE2	1:H:453:ASN:ND2	2.34	0.60
2:P:434:MET:HE2	2:P:455:ARG:HE	1.67	0.60
2:G:434:MET:HE2	2:G:455:ARG:HE	1.67	0.60
1:I:223:LYS:HE3	1:I:227:GLU:HG3	1.84	0.60
1:V:556:SER:HA	1:V:595:SER:HA	1.84	0.60
3:X:85:SER:HA	3:X:88:LEU:HD12	1.83	0.60
1:C:644:LEU:HD11	1:C:659:PHE:HB3	1.84	0.60
2:A:221:ARG:HH11	2:A:258:LYS:H	1.48	0.60
1:H:338:PRO:HB3	1:H:387:TYR:CD1	2.36	0.60
1:M:551:GLN:NE2	3:R:30:VAL:O	2.35	0.60
1:O:409:GLU:OE2	1:O:453:ASN:ND2	2.34	0.60
1:O:441:LEU:HD21	1:O:508:LEU:HD11	1.84	0.60
2:A:434:MET:HE2	2:A:455:ARG:HE	1.67	0.59
2:P:128:ILE:HG23	2:P:136:LEU:HD21	1.84	0.59
1:O:345:LEU:CG	1:O:374:PHE:HE2	2.15	0.59
1:V:557:ALA:HB3	1:V:594:VAL:HG23	1.84	0.59
1:V:703:ILE:HD11	1:V:744:ARG:HD3	1.83	0.59
1:I:525:PRO:HB2	1:I:528:PRO:HD2	1.84	0.59
3:K:85:SER:HA	3:K:88:LEU:HD12	1.83	0.59
1:T:77:LEU:HD22	1:T:123:LEU:HD22	1.83	0.59
1:T:551:GLN:NE2	3:W:30:VAL:O	2.35	0.59
2:G:382:ILE:HB	2:G:402:TYR:HB3	1.82	0.59
1:H:356:LEU:HD12	1:H:360:PHE:HB2	1.84	0.59
1:O:346:LEU:HD21	1:O:414:LYS:CG	2.28	0.59
1:F:525:PRO:HB2	1:F:528:PRO:HD2	1.85	0.59
2:P:555:ASP:HB3	2:P:558:LEU:HB2	1.85	0.59
1:M:492:GLN:HE22	1:T:489:GLN:C	2.07	0.59
1:M:703:ILE:HD11	1:M:744:ARG:HD3	1.83	0.59
1:O:525:PRO:HB2	1:O:528:PRO:HD2	1.85	0.59
1:T:346:LEU:HD21	1:T:414:LYS:O	2.03	0.59
1:T:703:ILE:HD11	1:T:744:ARG:HD3	1.83	0.59
2:S:434:MET:HE2	2:S:455:ARG:HE	1.67	0.59
2:U:214:SER:OG	2:U:251:LYS:NZ	2.33	0.59
1:C:551:GLN:NE2	3:E:30:VAL:O	2.35	0.59
1:I:371:ALA:CB	1:I:421:PHE:CE1	2.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:221:ARG:HH11	2:P:258:LYS:H	1.48	0.59
1:O:374:PHE:HB3	1:O:421:PHE:HB3	1.83	0.59
1:V:120:ARG:O	1:V:124:MET:CB	2.50	0.59
1:F:317:MET:HG2	1:F:352:PHE:CE2	2.36	0.59
1:I:77:LEU:HD22	1:I:123:LEU:HD22	1.83	0.59
1:V:506:ARG:HB2	3:X:30:VAL:HG22	1.84	0.59
2:P:47:MET:O	2:P:51:THR:HG22	2.01	0.59
1:M:525:PRO:HB3	1:M:603:MET:HG3	1.84	0.59
1:T:223:LYS:HE3	1:T:227:GLU:HG3	1.84	0.59
1:T:349:LYS:HE2	1:T:370:ILE:HD12	1.84	0.59
1:C:223:LYS:HE3	1:C:227:GLU:HG3	1.84	0.59
2:P:60:PHE:CB	2:N:30:PHE:CZ	2.84	0.59
1:O:120:ARG:O	1:O:124:MET:CB	2.50	0.59
1:T:644:LEU:HD11	1:T:659:PHE:HB3	1.84	0.59
1:V:505:VAL:CG2	1:V:535:PHE:CE2	2.86	0.59
1:H:557:ALA:HB3	1:H:594:VAL:HG23	1.84	0.59
1:O:556:SER:HA	1:O:595:SER:HA	1.84	0.59
1:T:345:LEU:CG	1:T:377:PHE:HZ	2.15	0.59
1:I:356:LEU:HD21	1:I:367:LYS:CG	2.33	0.59
1:H:556:SER:HA	1:H:595:SER:HA	1.84	0.59
2:U:153:LYS:HE3	2:U:180:ILE:HA	1.85	0.59
2:U:225:LEU:O	2:U:230:GLN:NE2	2.36	0.59
2:B:225:LEU:O	2:B:230:GLN:NE2	2.36	0.58
2:J:214:SER:OG	2:J:251:LYS:NZ	2.33	0.58
2:N:370:ARG:NH1	2:N:386:GLY:O	2.33	0.58
2:U:370:ARG:NH1	2:U:386:GLY:O	2.33	0.58
1:C:120:ARG:O	1:C:124:MET:CB	2.51	0.58
1:C:622:ILE:HD12	1:C:623:PRO:HD2	1.86	0.58
1:F:77:LEU:HD22	1:F:123:LEU:HD22	1.85	0.58
3:D:85:SER:HA	3:D:88:LEU:HD12	1.83	0.58
1:M:120:ARG:O	1:M:124:MET:CB	2.51	0.58
1:O:346:LEU:HD11	1:O:414:LYS:CB	2.33	0.58
1:O:499:GLY:HA3	1:O:530:HIS:HB2	1.85	0.58
1:T:293:THR:HG22	1:T:355:PHE:HE1	1.68	0.58
2:A:128:ILE:HG23	2:A:136:LEU:HD21	1.84	0.58
2:B:350:PHE:HD2	2:B:363:LYS:HB2	1.69	0.58
2:G:128:ILE:HG23	2:G:136:LEU:HD21	1.84	0.58
1:I:120:ARG:O	1:I:124:MET:CB	2.51	0.58
1:I:356:LEU:HD13	1:I:366:PHE:HB3	1.85	0.58
1:I:551:GLN:NE2	3:L:30:VAL:O	2.35	0.58
2:N:350:PHE:HD2	2:N:363:LYS:HB2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:683:GLU:HG3	1:M:688:ARG:HH21	1.69	0.58
1:T:296:LEU:HD12	1:T:360:PHE:CZ	2.37	0.58
2:S:374:SER:OG	2:S:385:ILE:O	2.21	0.58
1:V:356:LEU:HD12	1:V:360:PHE:HB2	1.84	0.58
1:F:556:SER:HA	1:F:595:SER:HA	1.84	0.58
1:H:77:LEU:HD22	1:H:123:LEU:HD22	1.85	0.58
2:S:286:VAL:HG11	2:S:573:TRP:HH2	1.69	0.58
2:U:434:MET:HE2	2:U:455:ARG:HE	1.69	0.58
2:A:555:ASP:HB3	2:A:558:LEU:HB2	1.85	0.58
2:G:525:VAL:HA	2:G:538:MET:HG2	1.85	0.58
2:N:225:LEU:O	2:N:230:GLN:NE2	2.36	0.58
1:M:622:ILE:HD12	1:M:623:PRO:HD2	1.85	0.58
1:T:525:PRO:HB2	1:T:528:PRO:HD2	1.84	0.58
1:V:77:LEU:HD22	1:V:123:LEU:HD22	1.85	0.58
1:F:557:ALA:HB3	1:F:594:VAL:HG23	1.84	0.58
2:A:385:ILE:HA	2:A:399:VAL:HG12	1.85	0.58
2:J:153:LYS:HE3	2:J:180:ILE:HA	1.85	0.58
2:J:370:ARG:NH1	2:J:386:GLY:O	2.33	0.58
2:J:434:MET:HE2	2:J:455:ARG:HE	1.69	0.58
1:M:383:ARG:HB3	1:M:688:ARG:HH12	1.68	0.58
1:M:478:SER:HA	1:M:481:ASN:HD21	1.69	0.58
1:O:557:ALA:HB3	1:O:594:VAL:HG23	1.84	0.58
1:T:120:ARG:O	1:T:124:MET:CB	2.51	0.58
2:U:350:PHE:HD2	2:U:363:LYS:HB2	1.69	0.58
2:G:385:ILE:HA	2:G:399:VAL:HG12	1.85	0.58
1:I:441:LEU:HD21	1:I:508:LEU:HD11	1.86	0.58
1:M:282:SER:HA	1:M:286:HIS:HB3	1.85	0.58
1:O:506:ARG:HB2	3:Q:30:VAL:HG22	1.84	0.58
1:F:506:ARG:HB2	3:D:30:VAL:HG22	1.84	0.58
2:A:525:VAL:HA	2:A:538:MET:HG2	1.86	0.58
2:B:214:SER:OG	2:B:251:LYS:NZ	2.33	0.58
2:G:286:VAL:HG11	2:G:573:TRP:HH2	1.69	0.58
2:G:555:ASP:HB3	2:G:558:LEU:HB2	1.85	0.58
2:J:225:LEU:O	2:J:230:GLN:NE2	2.36	0.58
1:I:683:GLU:HG3	1:I:688:ARG:HH21	1.68	0.58
1:I:698:ASP:HA	1:I:701:HIS:HD2	1.69	0.58
1:M:754:LEU:HD11	1:M:764:TYR:HB3	1.85	0.58
1:C:698:ASP:HA	1:C:701:HIS:HD2	1.69	0.58
1:I:282:SER:HA	1:I:286:HIS:HB3	1.85	0.58
1:I:768:ALA:HB1	3:L:89:LYS:HB3	1.85	0.58
2:P:436:LEU:O	2:P:455:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:223:LYS:HE3	1:M:227:GLU:HG3	1.84	0.58
1:M:525:PRO:HB2	1:M:528:PRO:HD2	1.85	0.58
2:S:18:LEU:HD13	2:U:17:LEU:CD2	2.33	0.58
2:S:436:LEU:O	2:S:455:ARG:NH2	2.37	0.58
2:G:30:PHE:CZ	2:J:61:MET:HB2	2.39	0.58
1:H:506:ARG:HB2	3:K:30:VAL:HG22	1.84	0.58
2:N:153:LYS:HE3	2:N:180:ILE:HA	1.85	0.58
1:M:768:ALA:HB1	3:R:89:LYS:HB3	1.85	0.58
1:T:356:LEU:HD12	1:T:360:PHE:CB	2.33	0.58
2:S:555:ASP:HB3	2:S:558:LEU:HB2	1.85	0.58
2:U:52:CYS:SG	2:U:53:SER:N	2.77	0.58
1:C:43:GLU:OE2	1:C:48:ASN:ND2	2.33	0.57
2:A:286:VAL:HG11	2:A:573:TRP:HH2	1.69	0.57
2:A:297:LYS:HZ1	2:A:595:PRO:HD3	1.69	0.57
2:B:153:LYS:HE3	2:B:180:ILE:HA	1.85	0.57
2:G:9:ILE:HG21	2:J:92:GLY:HA3	1.86	0.57
1:I:293:THR:HG22	1:I:355:PHE:CE1	2.39	0.57
1:I:478:SER:HA	1:I:481:ASN:HD21	1.69	0.57
2:P:525:VAL:HA	2:P:538:MET:HG2	1.86	0.57
1:M:698:ASP:HA	1:M:701:HIS:HD2	1.68	0.57
1:O:127:ASP:O	1:O:131:VAL:HG22	2.04	0.57
1:T:698:ASP:HA	1:T:701:HIS:HD2	1.69	0.57
2:G:47:MET:HE3	2:J:45:HIS:CE1	2.39	0.57
1:T:622:ILE:HD12	1:T:623:PRO:HD2	1.86	0.57
2:A:17:LEU:CD2	2:B:18:LEU:CD1	2.77	0.57
2:P:60:PHE:HB2	2:N:30:PHE:CE2	2.39	0.57
2:P:286:VAL:HG11	2:P:573:TRP:HH2	1.69	0.57
2:S:128:ILE:HG23	2:S:136:LEU:HD21	1.84	0.57
2:S:459:ARG:HB3	2:S:476:GLY:HA3	1.86	0.57
1:C:282:SER:HA	1:C:286:HIS:HB3	1.85	0.57
1:C:356:LEU:HD12	1:C:360:PHE:HB2	1.87	0.57
2:B:434:MET:HE2	2:B:455:ARG:HE	1.69	0.57
1:I:622:ILE:HD12	1:I:623:PRO:HD2	1.85	0.57
2:P:385:ILE:HA	2:P:399:VAL:HG12	1.85	0.57
2:N:161:THR:HB	2:N:188:VAL:HG13	1.86	0.57
2:N:434:MET:HE2	2:N:455:ARG:HE	1.69	0.57
1:O:77:LEU:HD22	1:O:123:LEU:HD22	1.85	0.57
1:O:345:LEU:CD1	1:O:377:PHE:CE1	2.88	0.57
1:T:441:LEU:HD21	1:T:508:LEU:HD11	1.86	0.57
1:C:478:SER:HA	1:C:481:ASN:HD21	1.69	0.57
2:A:153:LYS:NZ	2:A:179:ASP:OD1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:436:LEU:O	2:A:455:ARG:NH2	2.37	0.57
2:B:161:THR:HG21	2:B:186:LEU:HB2	1.86	0.57
1:T:282:SER:HA	1:T:286:HIS:HB3	1.85	0.57
2:J:52:CYS:SG	2:J:53:SER:N	2.77	0.57
1:H:507:VAL:CG2	1:H:535:PHE:CZ	2.81	0.57
2:S:8:GLN:HG3	2:U:19:GLU:HB3	1.86	0.57
2:S:455:ARG:NH1	2:S:500:GLU:OE2	2.38	0.57
2:U:35:LEU:HB2	2:U:42:PHE:HB2	1.87	0.57
2:U:161:THR:HB	2:U:188:VAL:HG13	1.86	0.57
1:C:683:GLU:HG3	1:C:688:ARG:HH21	1.69	0.57
1:C:768:ALA:HB1	3:E:89:LYS:HB3	1.85	0.57
1:F:486:GLU:O	1:F:490:HIS:ND1	2.30	0.57
1:H:43:GLU:OE2	1:H:48:ASN:ND2	2.33	0.57
1:H:127:ASP:O	1:H:131:VAL:HG22	2.05	0.57
2:P:455:ARG:NH1	2:P:500:GLU:OE2	2.38	0.57
2:P:459:ARG:HB3	2:P:476:GLY:HA3	1.86	0.57
2:N:214:SER:OG	2:N:251:LYS:NZ	2.33	0.57
1:M:356:LEU:HD12	1:M:360:PHE:HB2	1.87	0.57
1:O:371:ALA:HA	1:O:421:PHE:CD1	2.40	0.57
1:F:127:ASP:O	1:F:131:VAL:HG22	2.05	0.57
2:A:455:ARG:NH1	2:A:500:GLU:OE2	2.38	0.57
2:G:289:SER:HG	2:G:294:LYS:H	1.52	0.57
1:O:324:GLN:HG2	1:O:348:LEU:HD21	1.87	0.57
2:S:153:LYS:NZ	2:S:179:ASP:OD1	2.38	0.57
1:T:371:ALA:HA	1:T:421:PHE:CE1	2.40	0.57
2:U:161:THR:HG21	2:U:186:LEU:HB2	1.86	0.57
1:M:43:GLU:OE2	1:M:48:ASN:ND2	2.33	0.57
1:M:441:LEU:HD21	1:M:508:LEU:HD11	1.86	0.57
1:M:557:ALA:HB3	1:M:594:VAL:HG23	1.87	0.57
1:T:478:SER:HA	1:T:481:ASN:HD21	1.69	0.57
2:S:525:VAL:HA	2:S:538:MET:HG2	1.85	0.57
2:U:112:GLN:NE2	1:V:125:TYR:CD1	2.72	0.57
1:C:525:PRO:HB2	1:C:528:PRO:CD	2.32	0.56
2:G:8:GLN:HE22	2:J:22:LYS:HD3	1.70	0.56
2:N:52:CYS:SG	2:N:53:SER:N	2.77	0.56
2:N:160:PHE:O	2:N:164:TYR:N	2.38	0.56
2:S:385:ILE:HA	2:S:399:VAL:HG12	1.85	0.56
1:V:127:ASP:O	1:V:131:VAL:HG22	2.04	0.56
1:V:371:ALA:CB	1:V:421:PHE:CE1	2.88	0.56
2:A:459:ARG:HB3	2:A:476:GLY:HA3	1.86	0.56
2:B:52:CYS:SG	2:B:53:SER:N	2.77	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:370:ARG:HG2	2:G:389:SER:HA	1.87	0.56
2:G:455:ARG:NH1	2:G:500:GLU:OE2	2.38	0.56
2:J:350:PHE:HD2	2:J:363:LYS:HB2	1.69	0.56
2:N:161:THR:HG21	2:N:186:LEU:HB2	1.86	0.56
1:M:749:ILE:HD13	1:M:758:PRO:HD3	1.87	0.56
1:T:683:GLU:HG3	1:T:688:ARG:HH21	1.69	0.56
2:U:455:ARG:NH1	2:U:500:GLU:OE2	2.38	0.56
1:C:441:LEU:HD21	1:C:508:LEU:HD11	1.86	0.56
1:F:144:LEU:HD12	1:F:193:LEU:HA	1.87	0.56
2:B:275:SER:OG	2:B:574:ASP:O	2.24	0.56
2:B:398:THR:HB	2:B:411:MET:HE1	1.87	0.56
2:G:153:LYS:NZ	2:G:179:ASP:OD1	2.38	0.56
2:G:254:PRO:O	2:G:255:LYS:HG2	2.06	0.56
2:G:436:LEU:O	2:G:455:ARG:NH2	2.37	0.56
2:G:459:ARG:HB3	2:G:476:GLY:HA3	1.86	0.56
1:H:144:LEU:HD12	1:H:193:LEU:HA	1.87	0.56
2:P:153:LYS:NZ	2:P:179:ASP:OD1	2.38	0.56
1:M:698:ASP:HA	1:M:701:HIS:CD2	2.40	0.56
1:T:768:ALA:HB1	3:W:89:LYS:HB3	1.85	0.56
2:S:370:ARG:HG2	2:S:389:SER:HA	1.87	0.56
2:B:455:ARG:NH1	2:B:500:GLU:OE2	2.38	0.56
2:J:455:ARG:NH1	2:J:500:GLU:OE2	2.38	0.56
2:J:459:ARG:HB3	2:J:476:GLY:HA3	1.88	0.56
2:N:398:THR:HB	2:N:411:MET:HE1	1.87	0.56
1:C:127:ASP:O	1:C:131:VAL:HG22	2.06	0.56
2:B:35:LEU:HB2	2:B:42:PHE:HB2	1.87	0.56
2:G:374:SER:OG	2:G:385:ILE:O	2.21	0.56
2:J:35:LEU:HB2	2:J:42:PHE:HB2	1.87	0.56
2:J:161:THR:HG21	2:J:186:LEU:HB2	1.86	0.56
2:J:398:THR:HB	2:J:411:MET:HE1	1.87	0.56
2:N:35:LEU:HB2	2:N:42:PHE:HB2	1.87	0.56
1:M:404:THR:OG1	1:M:407:GLU:OE1	2.24	0.56
1:T:698:ASP:HA	1:T:701:HIS:CD2	2.40	0.56
1:V:478:SER:HA	1:V:481:ASN:ND2	2.21	0.56
2:B:161:THR:HB	2:B:188:VAL:HG13	1.86	0.56
2:J:161:THR:HB	2:J:188:VAL:HG13	1.86	0.56
2:J:436:LEU:O	2:J:455:ARG:NH2	2.39	0.56
1:T:133:GLN:CD	2:S:144:SER:CB	2.76	0.56
1:T:546:ARG:HH21	3:W:35:TRP:HE1	1.53	0.56
2:P:91:THR:HG23	2:P:93:ASN:H	1.71	0.56
2:N:455:ARG:NH1	2:N:500:GLU:OE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:127:ASP:O	1:T:131:VAL:HG22	2.06	0.56
1:T:557:ALA:HB3	1:T:594:VAL:HG23	1.87	0.56
2:B:436:LEU:O	2:B:455:ARG:NH2	2.39	0.56
1:I:127:ASP:O	1:I:131:VAL:HG22	2.06	0.56
1:I:300:TYR:HB2	1:I:360:PHE:HD1	1.70	0.56
1:I:404:THR:OG1	1:I:407:GLU:OE1	2.24	0.56
1:I:557:ALA:HB3	1:I:594:VAL:HG23	1.87	0.56
1:F:478:SER:HA	1:F:481:ASN:ND2	2.21	0.56
2:A:91:THR:HG23	2:A:93:ASN:H	1.71	0.56
1:I:356:LEU:HD21	1:I:367:LYS:HG3	1.86	0.56
1:I:698:ASP:HA	1:I:701:HIS:CD2	2.40	0.56
1:H:478:SER:HA	1:H:481:ASN:ND2	2.21	0.56
1:H:505:VAL:CG1	1:H:535:PHE:CE1	2.89	0.56
2:N:459:ARG:HB3	2:N:476:GLY:HA3	1.88	0.56
1:M:127:ASP:O	1:M:131:VAL:HG22	2.06	0.56
2:S:47:MET:HE3	2:U:45:HIS:NE2	2.21	0.56
2:U:144:SER:HB3	1:V:133:GLN:CD	2.31	0.56
1:C:560:ASN:HB2	3:E:25:LYS:HG2	1.88	0.56
1:F:62:TYR:CB	2:B:110:PHE:HE1	2.19	0.56
1:I:317:MET:HG3	1:I:352:PHE:HE2	1.71	0.56
1:I:560:ASN:HB2	3:L:25:LYS:HG2	1.88	0.56
1:M:144:LEU:HD12	1:M:193:LEU:HA	1.88	0.56
3:X:45:CYS:SG	3:X:47:ASN:ND2	2.79	0.56
1:C:476:ASP:OD1	1:C:508:LEU:HA	2.06	0.55
1:C:698:ASP:HA	1:C:701:HIS:CD2	2.40	0.55
1:O:288:LEU:HD11	1:O:355:PHE:HD2	1.70	0.55
3:Q:43:ALA:HB3	3:Q:79:PHE:HE1	1.71	0.55
3:Q:45:CYS:SG	3:Q:47:ASN:ND2	2.79	0.55
1:T:346:LEU:CD2	1:T:414:LYS:HB3	2.34	0.55
1:C:144:LEU:HD12	1:C:193:LEU:HA	1.88	0.55
2:J:160:PHE:O	2:J:164:TYR:N	2.38	0.55
1:M:559:LEU:O	1:M:592:LEU:N	2.39	0.55
1:V:144:LEU:HD12	1:V:193:LEU:HA	1.87	0.55
1:V:469:LYS:HA	1:V:512:TYR:HE1	1.71	0.55
2:B:137:LEU:HG	2:B:176:LEU:HD21	1.88	0.55
1:I:363:ASP:HB3	1:I:366:PHE:HD1	1.71	0.55
2:N:436:LEU:O	2:N:455:ARG:NH2	2.39	0.55
1:M:560:ASN:HB2	3:R:25:LYS:HG2	1.88	0.55
1:T:560:ASN:HB2	3:W:25:LYS:HG2	1.88	0.55
2:S:91:THR:HG23	2:S:93:ASN:H	1.71	0.55
2:U:160:PHE:O	2:U:164:TYR:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:92:GLY:CA	2:B:13:TYR:CB	2.84	0.55
1:I:144:LEU:HD12	1:I:193:LEU:HA	1.88	0.55
3:K:45:CYS:SG	3:K:47:ASN:ND2	2.79	0.55
1:C:524:ILE:HB	1:C:529:ARG:HG3	1.87	0.55
2:A:254:PRO:O	2:A:255:LYS:HG2	2.06	0.55
2:J:275:SER:OG	2:J:574:ASP:O	2.23	0.55
1:O:345:LEU:HD22	1:O:377:PHE:CZ	2.40	0.55
2:S:476:GLY:O	2:S:496:SER:N	2.40	0.55
2:U:436:LEU:O	2:U:455:ARG:NH2	2.39	0.55
3:X:43:ALA:HB3	3:X:79:PHE:HE1	1.71	0.55
2:P:47:MET:HE2	2:N:21:LEU:HB3	1.88	0.55
1:O:144:LEU:HD12	1:O:193:LEU:HA	1.87	0.55
1:T:404:THR:OG1	1:T:407:GLU:OE1	2.24	0.55
1:T:546:ARG:HB3	3:W:35:TRP:HD1	1.72	0.55
2:B:160:PHE:O	2:B:164:TYR:N	2.38	0.55
2:N:37:VAL:HG12	2:N:38:GLU:HG2	1.88	0.55
2:N:275:SER:OG	2:N:574:ASP:O	2.23	0.55
1:C:557:ALA:HB3	1:C:594:VAL:HG23	1.87	0.55
2:A:476:GLY:O	2:A:496:SER:N	2.40	0.55
3:D:52:LEU:HD21	3:D:59:ASN:HB3	1.88	0.55
1:H:759:GLU:OE1	1:H:759:GLU:N	2.37	0.55
3:K:43:ALA:HB3	3:K:79:PHE:HE1	1.71	0.55
1:V:536:ARG:HA	1:V:548:LEU:HD12	1.88	0.55
1:C:506:ARG:HB2	3:E:30:VAL:HG22	1.89	0.55
2:B:297:LYS:HB3	2:B:594:SER:HB2	1.89	0.55
2:B:459:ARG:HB3	2:B:476:GLY:HA3	1.88	0.55
2:G:30:PHE:CE1	2:J:61:MET:HB2	2.41	0.55
2:G:91:THR:HG23	2:G:93:ASN:H	1.71	0.55
2:P:476:GLY:O	2:P:496:SER:N	2.40	0.55
2:P:522:ASP:OD1	2:P:522:ASP:N	2.40	0.55
1:T:144:LEU:HD12	1:T:193:LEU:HA	1.88	0.55
2:U:137:LEU:HG	2:U:176:LEU:HD21	1.88	0.55
2:U:459:ARG:HB3	2:U:476:GLY:HA3	1.88	0.55
2:A:217:LEU:HG	2:A:225:LEU:HD21	1.89	0.55
2:J:137:LEU:HG	2:J:176:LEU:HD21	1.88	0.55
1:I:409:GLU:OE2	1:I:453:ASN:ND2	2.40	0.55
2:P:254:PRO:O	2:P:255:LYS:HG2	2.06	0.55
2:S:217:LEU:HG	2:S:225:LEU:HD21	1.89	0.55
2:S:414:PRO:O	2:S:449:TRP:NE1	2.41	0.55
2:B:122:GLU:O	2:B:125:ILE:HG22	2.07	0.54
2:G:455:ARG:NH1	2:G:457:THR:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:527:ALA:HB3	1:M:528:PRO:HD3	1.89	0.54
1:O:478:SER:HA	1:O:481:ASN:ND2	2.21	0.54
1:T:409:GLU:OE2	1:T:453:ASN:ND2	2.40	0.54
2:J:122:GLU:O	2:J:125:ILE:HG22	2.07	0.54
1:I:546:ARG:HH21	3:L:35:TRP:HE1	1.53	0.54
1:I:735:LEU:HD13	1:I:736:PRO:HD2	1.90	0.54
2:P:60:PHE:CB	2:N:30:PHE:CE2	2.91	0.54
2:P:455:ARG:NH1	2:P:457:THR:O	2.41	0.54
1:O:559:LEU:O	1:O:592:LEU:N	2.38	0.54
2:U:122:GLU:O	2:U:125:ILE:HG22	2.07	0.54
1:C:409:GLU:OE2	1:C:453:ASN:ND2	2.40	0.54
2:S:254:PRO:O	2:S:255:LYS:HG2	2.06	0.54
2:S:455:ARG:NH1	2:S:457:THR:O	2.41	0.54
2:U:37:VAL:HG12	2:U:38:GLU:HG2	1.88	0.54
1:F:717:MET:HB3	1:F:722:LEU:HG	1.89	0.54
2:A:455:ARG:NH1	2:A:457:THR:O	2.41	0.54
2:N:137:LEU:HG	2:N:176:LEU:HD21	1.88	0.54
2:B:37:VAL:HG12	2:B:38:GLU:HG2	1.88	0.54
2:B:321:ALA:HB3	2:B:375:LEU:HD11	1.90	0.54
1:I:506:ARG:HB2	3:L:30:VAL:HG22	1.89	0.54
1:I:546:ARG:HB3	3:L:35:TRP:HD1	1.72	0.54
1:H:371:ALA:CB	1:H:421:PHE:CE1	2.91	0.54
2:P:92:GLY:CA	2:N:13:TYR:CB	2.85	0.54
2:N:122:GLU:O	2:N:125:ILE:HG22	2.07	0.54
1:M:409:GLU:OE2	1:M:453:ASN:ND2	2.40	0.54
1:O:717:MET:HB3	1:O:722:LEU:HG	1.89	0.54
1:T:506:ARG:HB2	3:W:30:VAL:HG22	1.89	0.54
1:C:735:LEU:HD13	1:C:736:PRO:HD2	1.90	0.54
1:I:520:PRO:HG3	1:I:553:HIS:CD2	2.43	0.54
1:I:698:ASP:OD1	1:I:701:HIS:NE2	2.41	0.54
1:I:717:MET:HB3	1:I:722:LEU:HG	1.90	0.54
1:M:735:LEU:HD13	1:M:736:PRO:HD2	1.90	0.54
1:O:374:PHE:CB	1:O:421:PHE:CB	2.81	0.54
1:T:345:LEU:HD22	1:T:377:PHE:CZ	2.41	0.54
1:T:371:ALA:HA	1:T:421:PHE:CD1	2.43	0.54
2:A:275:SER:OG	2:A:574:ASP:O	2.25	0.54
2:G:217:LEU:HG	2:G:225:LEU:HD21	1.89	0.54
2:G:476:GLY:O	2:G:496:SER:N	2.40	0.54
2:P:45:HIS:ND1	2:P:90:TYR:OH	2.32	0.54
2:P:217:LEU:HG	2:P:225:LEU:HD21	1.89	0.54
1:M:102:LEU:HD11	1:M:182:ALA:HB1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:520:PRO:HG3	1:T:553:HIS:CD2	2.43	0.54
2:S:305:LEU:HD21	2:S:323:GLY:HA3	1.90	0.54
2:J:37:VAL:HG12	2:J:38:GLU:HG2	1.88	0.54
2:P:305:LEU:HD21	2:P:323:GLY:HA3	1.90	0.54
2:P:548:LYS:NZ	2:P:549:TYR:O	2.41	0.54
2:N:297:LYS:HB3	2:N:594:SER:HB2	1.89	0.54
1:T:717:MET:HB3	1:T:722:LEU:HG	1.90	0.54
2:A:289:SER:HG	2:A:294:LYS:H	1.52	0.54
2:A:374:SER:OG	2:A:385:ILE:O	2.21	0.54
2:G:548:LYS:NZ	2:G:549:TYR:O	2.41	0.54
2:P:297:LYS:HZ1	2:P:595:PRO:HD3	1.72	0.54
1:O:644:LEU:HD11	1:O:659:PHE:HB3	1.90	0.54
2:S:348:ASN:ND2	2:S:366:MET:O	2.41	0.54
2:U:273:GLU:OE2	2:U:307:LYS:N	2.41	0.54
1:V:698:ASP:HA	1:V:701:HIS:CD2	2.43	0.54
1:C:698:ASP:OD1	1:C:701:HIS:NE2	2.41	0.54
2:G:414:PRO:O	2:G:449:TRP:NE1	2.41	0.54
2:P:186:LEU:HD13	2:P:194:VAL:HG11	1.90	0.54
2:S:548:LYS:NZ	2:S:549:TYR:O	2.41	0.54
1:V:436:LEU:CD1	1:V:470:LEU:CG	2.86	0.54
1:C:102:LEU:HD11	1:C:182:ALA:HB1	1.90	0.53
1:C:342:ILE:HG13	1:C:387:TYR:O	2.07	0.53
1:F:698:ASP:HA	1:F:701:HIS:CD2	2.43	0.53
2:A:186:LEU:HD13	2:A:194:VAL:HG11	1.90	0.53
2:A:348:ASN:ND2	2:A:366:MET:O	2.42	0.53
2:J:297:LYS:HB3	2:J:594:SER:HB2	1.89	0.53
2:P:17:LEU:CD2	2:N:18:LEU:CD1	2.80	0.53
2:P:348:ASN:ND2	2:P:366:MET:O	2.41	0.53
1:T:371:ALA:CB	1:T:421:PHE:HE1	2.21	0.53
1:T:735:LEU:HD13	1:T:736:PRO:HD2	1.90	0.53
1:C:473:MET:HE1	1:C:513:TRP:CD2	2.40	0.53
2:G:348:ASN:ND2	2:G:366:MET:O	2.42	0.53
2:J:415:LEU:HD23	2:J:416:PRO:HD2	1.91	0.53
1:H:698:ASP:HA	1:H:701:HIS:CD2	2.43	0.53
2:U:570:ARG:HA	2:U:598:PRO:HB3	1.90	0.53
2:A:548:LYS:NZ	2:A:549:TYR:O	2.41	0.53
2:J:321:ALA:HB3	2:J:375:LEU:HD11	1.90	0.53
2:J:570:ARG:HA	2:J:598:PRO:HB3	1.90	0.53
1:I:356:LEU:HA	1:I:360:PHE:HD2	1.73	0.53
1:H:644:LEU:HD11	1:H:659:PHE:HB3	1.90	0.53
2:P:46:LYS:HB3	2:N:30:PHE:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:289:SER:HG	2:P:294:LYS:H	1.55	0.53
1:O:698:ASP:HA	1:O:701:HIS:CD2	2.43	0.53
2:S:289:SER:HG	2:S:294:LYS:H	1.55	0.53
2:G:45:HIS:ND1	2:G:90:TYR:OH	2.32	0.53
2:N:273:GLU:OE2	2:N:307:LYS:N	2.41	0.53
1:O:356:LEU:HD11	1:O:363:ASP:N	2.24	0.53
1:T:710:ILE:HG21	1:T:729:GLN:HE22	1.74	0.53
2:U:297:LYS:HB3	2:U:594:SER:HB2	1.89	0.53
2:U:321:ALA:HB3	2:U:375:LEU:HD11	1.90	0.53
2:G:53:SER:OG	2:G:111:LEU:O	2.27	0.53
1:I:612:THR:OG1	1:I:655:ASN:O	2.27	0.53
2:N:570:ARG:HA	2:N:598:PRO:HB3	1.90	0.53
1:O:337:ASN:HB3	1:O:340:ASP:HB2	1.90	0.53
2:S:186:LEU:HD13	2:S:194:VAL:HG11	1.90	0.53
2:U:415:LEU:HD23	2:U:416:PRO:HD2	1.91	0.53
2:P:275:SER:OG	2:P:574:ASP:O	2.25	0.53
2:N:415:LEU:HD23	2:N:416:PRO:HD2	1.91	0.53
1:O:329:VAL:HB	1:O:341:TYR:CE1	2.44	0.53
1:T:612:THR:OG1	1:T:655:ASN:O	2.27	0.53
2:G:186:LEU:HD13	2:G:194:VAL:HG11	1.90	0.53
1:H:559:LEU:O	1:H:592:LEU:N	2.38	0.53
2:P:398:THR:HG22	2:P:414:PRO:HB3	1.91	0.53
1:O:759:GLU:OE1	1:O:759:GLU:N	2.37	0.53
1:T:102:LEU:HD11	1:T:182:ALA:HB1	1.90	0.53
2:A:305:LEU:HD21	2:A:323:GLY:HA3	1.90	0.53
2:A:398:THR:HG22	2:A:414:PRO:HB3	1.91	0.53
1:O:345:LEU:HD11	1:O:377:PHE:CE1	2.44	0.53
1:F:324:GLN:HG2	1:F:348:LEU:HD13	1.90	0.53
1:F:644:LEU:HD11	1:F:659:PHE:HB3	1.90	0.53
1:M:437:ALA:HA	1:M:513:TRP:HZ3	1.74	0.53
2:S:398:THR:HG22	2:S:414:PRO:HB3	1.91	0.53
2:A:92:GLY:HA3	2:B:13:TYR:CB	2.38	0.53
2:B:415:LEU:HD23	2:B:416:PRO:HD2	1.91	0.53
2:G:305:LEU:HD21	2:G:323:GLY:HA3	1.90	0.53
2:N:321:ALA:HB3	2:N:375:LEU:HD11	1.90	0.53
1:O:356:LEU:HD13	1:O:366:PHE:HB2	1.90	0.53
1:T:378:LEU:HD22	1:T:422:MET:CA	2.38	0.53
1:T:458:LEU:HB3	1:T:467:THR:HG22	1.91	0.53
2:S:275:SER:OG	2:S:574:ASP:O	2.25	0.53
2:S:431:ILE:HB	2:S:442:TYR:HB3	1.91	0.53
3:W:46:ARG:O	3:W:46:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:374:SER:OG	2:P:385:ILE:O	2.21	0.52
1:M:612:THR:OG1	1:M:655:ASN:O	2.27	0.52
1:T:546:ARG:HE	3:W:35:TRP:HE1	1.56	0.52
1:T:698:ASP:OD1	1:T:701:HIS:NE2	2.41	0.52
2:B:273:GLU:OE2	2:B:307:LYS:N	2.41	0.52
2:J:273:GLU:OE2	2:J:307:LYS:N	2.41	0.52
1:I:102:LEU:HD11	1:I:182:ALA:HB1	1.90	0.52
1:M:698:ASP:OD1	1:M:701:HIS:NE2	2.41	0.52
1:F:759:GLU:OE1	1:F:759:GLU:N	2.37	0.52
2:A:53:SER:OG	2:A:111:LEU:O	2.27	0.52
2:G:275:SER:OG	2:G:573:TRP:NE1	2.43	0.52
2:J:274:ALA:N	2:J:284:SER:O	2.42	0.52
1:T:378:LEU:CD2	1:T:422:MET:CE	2.75	0.52
1:F:356:LEU:HA	1:F:360:PHE:HB2	1.90	0.52
2:B:289:SER:HG	2:B:294:LYS:H	1.57	0.52
2:B:570:ARG:HA	2:B:598:PRO:HB3	1.90	0.52
2:G:398:THR:HG22	2:G:414:PRO:HB3	1.91	0.52
1:I:346:LEU:HD11	1:I:414:LYS:O	2.08	0.52
1:I:614:GLU:OE1	1:I:617:GLN:NE2	2.43	0.52
2:P:301:PRO:HG3	2:P:360:TRP:CE2	2.45	0.52
2:N:274:ALA:N	2:N:284:SER:O	2.42	0.52
1:C:710:ILE:HG21	1:C:729:GLN:HE22	1.73	0.52
1:F:483:THR:HA	1:F:486:GLU:HG2	1.91	0.52
2:A:318:ILE:HB	2:A:353:PHE:HB3	1.92	0.52
2:G:301:PRO:HG3	2:G:360:TRP:CE2	2.45	0.52
1:I:458:LEU:HB3	1:I:467:THR:HG22	1.91	0.52
1:H:481:ASN:HA	1:H:484:MET:HG3	1.92	0.52
2:P:53:SER:OG	2:P:111:LEU:O	2.27	0.52
1:M:458:LEU:HB3	1:M:467:THR:HG22	1.91	0.52
1:O:481:ASN:HA	1:O:484:MET:HG3	1.92	0.52
1:V:345:LEU:CG	1:V:418:LEU:HD11	2.28	0.52
1:C:383:ARG:HB3	1:C:688:ARG:HH12	1.74	0.52
1:C:612:THR:OG1	1:C:655:ASN:O	2.27	0.52
1:F:371:ALA:HA	1:F:421:PHE:CE1	2.44	0.52
1:I:300:TYR:CG	1:I:360:PHE:HA	2.45	0.52
2:N:144:SER:HB3	1:O:133:GLN:NE2	2.25	0.52
1:T:559:LEU:O	1:T:592:LEU:N	2.39	0.52
1:T:614:GLU:OE1	1:T:617:GLN:NE2	2.43	0.52
2:S:14:ALA:HB1	2:U:14:ALA:HB1	1.92	0.52
1:V:483:THR:HA	1:V:486:GLU:HG2	1.91	0.52
1:V:644:LEU:HD11	1:V:659:PHE:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:524:ILE:HB	1:F:529:ARG:HG3	1.92	0.52
2:A:275:SER:OG	2:A:573:TRP:NE1	2.43	0.52
3:L:46:ARG:NH1	3:L:46:ARG:O	2.42	0.52
2:P:275:SER:OG	2:P:573:TRP:NE1	2.43	0.52
1:M:556:SER:HA	1:M:595:SER:HA	1.91	0.52
1:V:481:ASN:HA	1:V:484:MET:HG3	1.92	0.52
1:C:473:MET:CE	1:C:513:TRP:CH2	2.93	0.52
1:F:314:CYS:HB3	1:F:369:THR:HG21	1.91	0.52
2:P:47:MET:SD	2:N:21:LEU:HD22	2.49	0.52
1:V:698:ASP:HA	1:V:701:HIS:HD2	1.75	0.52
1:C:614:GLU:OE1	1:C:617:GLN:NE2	2.43	0.52
1:I:437:ALA:HA	1:I:513:TRP:HZ3	1.74	0.52
1:H:507:VAL:HG23	1:H:535:PHE:CZ	2.32	0.52
1:C:509:THR:HB	1:C:512:TYR:HD2	1.75	0.51
1:C:536:ARG:HA	1:C:548:LEU:HD12	1.93	0.51
2:G:431:ILE:HB	2:G:442:TYR:HB3	1.91	0.51
2:N:348:ASN:ND2	2:N:366:MET:O	2.44	0.51
1:O:484:MET:HG2	1:O:505:VAL:O	2.10	0.51
2:S:275:SER:OG	2:S:573:TRP:NE1	2.43	0.51
2:S:301:PRO:HG3	2:S:360:TRP:CE2	2.45	0.51
3:W:20:LYS:HE3	3:W:23:GLU:HG2	1.92	0.51
1:C:559:LEU:O	1:C:592:LEU:N	2.39	0.51
1:F:481:ASN:HA	1:F:484:MET:HG3	1.92	0.51
1:I:43:GLU:OE2	1:I:48:ASN:ND2	2.33	0.51
1:M:509:THR:HB	1:M:512:TYR:HD2	1.75	0.51
1:T:300:TYR:HB2	1:T:360:PHE:CD1	2.41	0.51
1:T:509:THR:HB	1:T:512:TYR:HD2	1.75	0.51
1:C:437:ALA:HA	1:C:513:TRP:HZ3	1.74	0.51
1:F:484:MET:HG2	1:F:505:VAL:O	2.10	0.51
2:A:301:PRO:HG3	2:A:360:TRP:CE2	2.45	0.51
2:A:370:ARG:HG2	2:A:389:SER:HA	1.92	0.51
2:B:348:ASN:ND2	2:B:366:MET:O	2.44	0.51
3:E:46:ARG:NH1	3:E:46:ARG:O	2.42	0.51
1:I:556:SER:HA	1:I:595:SER:HA	1.91	0.51
1:H:407:GLU:OE1	1:H:407:GLU:N	2.35	0.51
2:P:61:MET:SD	2:N:29:LEU:HG	2.51	0.51
2:S:302:PRO:HG2	2:S:305:LEU:HB3	1.92	0.51
2:U:458:SER:O	2:U:459:ARG:NH1	2.42	0.51
1:V:598:GLN:HG2	1:V:634:LEU:HG	1.92	0.51
1:C:556:SER:HA	1:C:595:SER:HA	1.91	0.51
2:J:311:VAL:HB	2:J:375:LEU:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:614:GLU:OE1	1:M:617:GLN:NE2	2.43	0.51
3:Q:84:ILE:HG12	3:Q:101:TRP:CE2	2.46	0.51
2:G:195:ARG:HB2	2:G:224:ALA:HB1	1.93	0.51
1:H:483:THR:HA	1:H:486:GLU:HG2	1.91	0.51
1:H:535:PHE:HE2	3:K:31:ALA:CB	2.23	0.51
3:R:46:ARG:NH1	3:R:46:ARG:O	2.42	0.51
1:V:759:GLU:OE1	1:V:759:GLU:N	2.37	0.51
2:B:513:ALA:HB3	2:B:561:TRP:HZ3	1.76	0.51
3:K:84:ILE:HG12	3:K:101:TRP:CE2	2.46	0.51
2:P:302:PRO:HG2	2:P:305:LEU:HB3	1.92	0.51
1:M:638:LYS:HD3	1:M:639:PRO:HD2	1.93	0.51
1:O:342:ILE:HG23	1:O:418:LEU:HD13	1.91	0.51
1:T:437:ALA:HA	1:T:513:TRP:HZ3	1.74	0.51
2:S:18:LEU:HD13	2:U:17:LEU:HD23	1.92	0.51
2:S:318:ILE:HB	2:S:353:PHE:HB3	1.92	0.51
2:A:24:PHE:CE2	2:B:51:THR:CG2	2.94	0.51
2:J:289:SER:HG	2:J:294:LYS:H	1.59	0.51
1:O:598:GLN:HG2	1:O:634:LEU:HG	1.92	0.51
2:S:53:SER:OG	2:S:111:LEU:O	2.27	0.51
2:U:348:ASN:ND2	2:U:366:MET:O	2.44	0.51
1:F:345:LEU:HD21	1:F:377:PHE:HE2	1.75	0.51
1:F:363:ASP:HB3	1:F:366:PHE:HD1	1.76	0.51
1:F:598:GLN:HG2	1:F:634:LEU:HG	1.92	0.51
1:F:698:ASP:HA	1:F:701:HIS:HD2	1.75	0.51
2:A:134:VAL:HG21	2:A:169:PHE:HA	1.93	0.51
2:B:274:ALA:N	2:B:284:SER:O	2.42	0.51
1:H:287:MET:HE3	1:H:296:LEU:HD22	1.93	0.51
1:H:598:GLN:HG2	1:H:634:LEU:HG	1.92	0.51
1:O:345:LEU:HB3	1:O:418:LEU:HD11	1.93	0.51
1:O:524:ILE:HB	1:O:529:ARG:HG3	1.92	0.51
1:T:556:SER:HA	1:T:595:SER:HA	1.91	0.51
2:S:47:MET:HE3	2:U:45:HIS:CD2	2.46	0.51
2:U:513:ALA:HB3	2:U:561:TRP:HZ3	1.76	0.51
1:V:337:ASN:ND2	1:V:340:ASP:OD1	2.44	0.51
1:V:433:LYS:HD3	1:V:469:LYS:HZ1	1.74	0.51
1:I:509:THR:HB	1:I:512:TYR:HD2	1.75	0.51
1:H:484:MET:HG2	1:H:505:VAL:O	2.10	0.51
2:P:47:MET:HE2	2:N:21:LEU:CB	2.40	0.51
3:W:40:ASP:OD2	3:W:41:ASN:ND2	2.44	0.51
1:C:638:LYS:HD3	1:C:639:PRO:HD2	1.93	0.51
2:A:209:ARG:O	2:A:213:LEU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:84:ILE:HG12	3:D:101:TRP:CE2	2.46	0.51
2:G:302:PRO:HG2	2:G:305:LEU:HB3	1.92	0.51
1:I:116:MET:HA	1:I:119:ILE:HB	1.93	0.51
1:I:546:ARG:HE	3:L:35:TRP:HE1	1.57	0.51
1:I:710:ILE:HG21	1:I:729:GLN:HE22	1.74	0.51
1:H:337:ASN:ND2	1:H:340:ASP:OD1	2.44	0.51
1:H:698:ASP:HA	1:H:701:HIS:HD2	1.75	0.51
1:T:116:MET:HA	1:T:119:ILE:HB	1.93	0.51
1:C:116:MET:HA	1:C:119:ILE:HB	1.93	0.50
3:E:20:LYS:HE3	3:E:23:GLU:HG2	1.93	0.50
3:E:40:ASP:OD2	3:E:41:ASN:ND2	2.44	0.50
3:D:72:TRP:HB2	3:D:105:LYS:HB3	1.93	0.50
2:J:513:ALA:HB3	2:J:561:TRP:HZ3	1.76	0.50
2:P:318:ILE:HB	2:P:353:PHE:HB3	1.92	0.50
2:P:382:ILE:O	2:P:402:TYR:N	2.44	0.50
2:N:513:ALA:HB3	2:N:561:TRP:HZ3	1.76	0.50
1:O:287:MET:HE3	1:O:296:LEU:HD22	1.93	0.50
3:Q:72:TRP:HB2	3:Q:105:LYS:HB3	1.93	0.50
2:U:311:VAL:HB	2:U:375:LEU:HB3	1.93	0.50
1:F:58:TYR:CB	2:B:55:TYR:CE1	2.95	0.50
1:F:317:MET:CG	1:F:352:PHE:CZ	2.94	0.50
2:A:137:LEU:HG	2:A:176:LEU:HD21	1.93	0.50
2:G:318:ILE:HB	2:G:353:PHE:HB3	1.92	0.50
2:J:348:ASN:ND2	2:J:366:MET:O	2.44	0.50
1:O:710:ILE:HG21	1:O:729:GLN:HE22	1.77	0.50
1:F:612:THR:OG1	1:F:655:ASN:O	2.30	0.50
1:F:717:MET:HE2	1:F:756:ARG:HD3	1.94	0.50
3:L:20:LYS:HE3	3:L:23:GLU:HG2	1.92	0.50
2:J:91:THR:HG23	2:J:93:ASN:H	1.77	0.50
1:I:346:LEU:CG	1:I:414:LYS:HB3	2.41	0.50
1:I:638:LYS:HD3	1:I:639:PRO:HD2	1.93	0.50
2:P:92:GLY:HA2	2:N:13:TYR:CB	2.41	0.50
3:R:20:LYS:HE3	3:R:23:GLU:HG2	1.92	0.50
1:T:638:LYS:HD3	1:T:639:PRO:HD2	1.93	0.50
2:J:118:GLN:OE1	2:J:119:ARG:NH1	2.45	0.50
2:N:118:GLN:OE1	2:N:119:ARG:NH1	2.45	0.50
2:N:458:SER:O	2:N:459:ARG:NH1	2.42	0.50
1:M:116:MET:HA	1:M:119:ILE:HB	1.93	0.50
3:R:39:VAL:HA	3:R:49:ILE:HB	1.94	0.50
1:T:371:ALA:CB	1:T:421:PHE:CE1	2.95	0.50
2:S:137:LEU:HG	2:S:176:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:MET:HE3	1:C:296:LEU:HD22	1.94	0.50
1:F:317:MET:HG3	1:F:352:PHE:CZ	2.47	0.50
2:G:553:GLN:HB2	2:G:564:ARG:HB2	1.94	0.50
1:I:263:VAL:HG22	1:I:267:GLU:OE2	2.12	0.50
3:L:40:ASP:OD2	3:L:41:ASN:ND2	2.44	0.50
2:P:137:LEU:HG	2:P:176:LEU:HD21	1.93	0.50
1:T:287:MET:HE3	1:T:296:LEU:HD22	1.94	0.50
1:T:346:LEU:CD2	1:T:414:LYS:C	2.77	0.50
2:S:195:ARG:HB2	2:S:224:ALA:HB1	1.93	0.50
2:U:118:GLN:OE1	2:U:119:ARG:NH1	2.45	0.50
1:V:120:ARG:O	1:V:124:MET:HB3	2.11	0.50
3:X:84:ILE:HG12	3:X:101:TRP:CE2	2.46	0.50
1:C:49:ASN:HD22	1:C:118:MET:HE1	1.77	0.50
1:F:524:ILE:HG22	1:F:528:PRO:HB2	1.94	0.50
2:A:195:ARG:HB2	2:A:224:ALA:HB1	1.93	0.50
1:M:263:VAL:HG22	1:M:267:GLU:OE2	2.12	0.50
3:R:40:ASP:OD2	3:R:41:ASN:ND2	2.44	0.50
1:T:378:LEU:HD22	1:T:422:MET:HA	1.93	0.50
1:V:559:LEU:O	1:V:592:LEU:N	2.38	0.50
1:V:612:THR:OG1	1:V:655:ASN:O	2.30	0.50
2:G:137:LEU:HG	2:G:176:LEU:HD21	1.93	0.50
2:G:348:ASN:HB2	2:G:366:MET:HB2	1.93	0.50
1:H:374:PHE:HA	1:H:377:PHE:CE1	2.47	0.50
1:M:342:ILE:HG13	1:M:387:TYR:O	2.11	0.50
1:O:612:THR:OG1	1:O:655:ASN:O	2.30	0.50
1:T:478:SER:HA	1:T:481:ASN:ND2	2.27	0.50
2:S:134:VAL:HG21	2:S:169:PHE:HA	1.93	0.50
1:C:478:SER:HA	1:C:481:ASN:ND2	2.27	0.50
1:F:559:LEU:O	1:F:592:LEU:N	2.38	0.50
2:A:305:LEU:HD12	2:A:325:VAL:HB	1.94	0.50
2:B:91:THR:HG23	2:B:93:ASN:H	1.77	0.50
2:B:118:GLN:OE1	2:B:119:ARG:NH1	2.45	0.50
2:B:202:LEU:HD11	2:B:216:VAL:HG11	1.94	0.50
2:P:305:LEU:HD12	2:P:325:VAL:HB	1.94	0.50
2:N:311:VAL:HB	2:N:375:LEU:HB3	1.93	0.50
1:M:478:SER:HA	1:M:481:ASN:ND2	2.27	0.50
1:T:346:LEU:CB	1:T:418:LEU:HD12	2.42	0.50
2:S:382:ILE:O	2:S:402:TYR:N	2.44	0.50
3:X:72:TRP:HB2	3:X:105:LYS:HB3	1.93	0.50
1:C:263:VAL:HG22	1:C:267:GLU:OE2	2.12	0.49
1:F:491:LEU:HD11	1:F:500:GLY:HA3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:302:PRO:HG2	2:A:305:LEU:HB3	1.92	0.49
2:J:202:LEU:HD11	2:J:216:VAL:HG11	1.94	0.49
1:I:169:ILE:HD11	1:I:247:ARG:HD3	1.94	0.49
1:H:491:LEU:HD11	1:H:500:GLY:HA3	1.93	0.49
1:O:481:ASN:HA	1:O:484:MET:SD	2.52	0.49
1:T:356:LEU:HA	1:T:360:PHE:HB2	1.94	0.49
2:B:311:VAL:HB	2:B:375:LEU:HB3	1.93	0.49
2:G:55:TYR:CE1	1:I:54:PHE:HE2	2.30	0.49
1:I:287:MET:HE3	1:I:296:LEU:HD22	1.94	0.49
1:H:612:THR:OG1	1:H:655:ASN:O	2.30	0.49
2:P:134:VAL:HG21	2:P:169:PHE:HA	1.93	0.49
2:P:195:ARG:HB2	2:P:224:ALA:HB1	1.93	0.49
1:M:287:MET:HE3	1:M:296:LEU:HD22	1.94	0.49
3:Q:52:LEU:HD12	3:Q:56:CYS:HB3	1.94	0.49
1:T:263:VAL:HG22	1:T:267:GLU:OE2	2.12	0.49
1:V:481:ASN:HA	1:V:484:MET:SD	2.52	0.49
3:K:52:LEU:HD12	3:K:56:CYS:HB3	1.95	0.49
1:O:120:ARG:O	1:O:124:MET:HB3	2.11	0.49
1:T:169:ILE:HD11	1:T:247:ARG:HD3	1.94	0.49
2:S:553:GLN:HB2	2:S:564:ARG:HB2	1.94	0.49
3:E:39:VAL:HA	3:E:49:ILE:HB	1.94	0.49
1:O:717:MET:HE2	1:O:756:ARG:HD3	1.94	0.49
2:S:348:ASN:HB2	2:S:366:MET:HB2	1.93	0.49
2:A:382:ILE:O	2:A:402:TYR:N	2.44	0.49
2:J:455:ARG:NH1	2:J:457:THR:O	2.46	0.49
1:H:120:ARG:O	1:H:124:MET:HB2	2.13	0.49
1:H:433:LYS:HA	1:H:436:LEU:HD12	1.95	0.49
3:K:72:TRP:HB2	3:K:105:LYS:HB3	1.93	0.49
2:N:455:ARG:NH1	2:N:457:THR:O	2.46	0.49
1:O:300:TYR:HB2	1:O:360:PHE:HD1	1.77	0.49
1:O:345:LEU:HD23	1:O:418:LEU:HD11	1.94	0.49
1:O:524:ILE:HG22	1:O:528:PRO:HB2	1.94	0.49
2:U:419:TRP:HZ3	2:U:433:VAL:HG13	1.78	0.49
1:V:287:MET:HE3	1:V:296:LEU:HD22	1.93	0.49
1:C:371:ALA:HB1	1:C:421:PHE:CE1	2.48	0.49
3:D:38:VAL:HG12	3:D:41:ASN:H	1.77	0.49
1:I:520:PRO:HG3	1:I:553:HIS:CG	2.47	0.49
2:P:553:GLN:HB2	2:P:564:ARG:HB2	1.94	0.49
2:N:419:TRP:HZ3	2:N:433:VAL:HG13	1.78	0.49
1:O:328:LEU:CG	1:O:341:TYR:CD1	2.77	0.49
3:X:52:LEU:HD12	3:X:56:CYS:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:120:ARG:O	1:F:124:MET:HB3	2.11	0.49
1:F:481:ASN:HA	1:F:484:MET:SD	2.53	0.49
2:B:113:VAL:HB	2:B:116:VAL:HG12	1.95	0.49
2:B:385:ILE:HG13	2:B:399:VAL:HG21	1.95	0.49
2:B:455:ARG:NH1	2:B:457:THR:O	2.46	0.49
2:G:263:MET:N	2:G:263:MET:SD	2.86	0.49
1:I:49:ASN:HD22	1:I:118:MET:HE1	1.76	0.49
1:I:751:ARG:NH2	3:L:55:GLU:OE1	2.46	0.49
3:L:39:VAL:HA	3:L:49:ILE:HB	1.94	0.49
2:P:370:ARG:HG2	2:P:389:SER:HA	1.95	0.49
1:O:698:ASP:HA	1:O:701:HIS:HD2	1.75	0.49
2:A:553:GLN:HB2	2:A:564:ARG:HB2	1.94	0.49
2:G:134:VAL:HG21	2:G:169:PHE:HA	1.93	0.49
1:I:293:THR:HG22	1:I:355:PHE:HE1	1.76	0.49
1:I:383:ARG:HB2	1:I:688:ARG:HH12	1.78	0.49
2:P:209:ARG:O	2:P:213:LEU:N	2.43	0.49
2:N:385:ILE:HG13	2:N:399:VAL:HG21	1.95	0.49
2:N:395:ASN:HA	2:N:397:ARG:HD2	1.95	0.49
3:R:54:ILE:HA	3:R:57:GLN:HE21	1.78	0.49
1:V:374:PHE:HA	1:V:377:PHE:CE1	2.47	0.49
1:V:433:LYS:HA	1:V:436:LEU:HD12	1.95	0.49
1:C:169:ILE:HD11	1:C:247:ARG:HD3	1.94	0.49
1:C:371:ALA:CB	1:C:421:PHE:CE1	2.96	0.49
1:F:710:ILE:HG21	1:F:729:GLN:HE22	1.77	0.49
2:A:348:ASN:HB2	2:A:366:MET:HB2	1.94	0.49
2:J:144:SER:HB2	1:H:129:VAL:HB	1.95	0.49
1:I:559:LEU:O	1:I:592:LEU:N	2.38	0.49
3:L:54:ILE:HA	3:L:57:GLN:HE21	1.78	0.49
2:P:348:ASN:HB2	2:P:366:MET:HB2	1.94	0.49
2:N:91:THR:HG23	2:N:93:ASN:H	1.77	0.49
1:M:49:ASN:HD22	1:M:118:MET:HE1	1.76	0.49
1:M:169:ILE:HD11	1:M:247:ARG:HD3	1.94	0.49
1:V:120:ARG:O	1:V:124:MET:HB2	2.13	0.49
2:J:113:VAL:HB	2:J:116:VAL:HG12	1.94	0.49
1:H:120:ARG:O	1:H:124:MET:HB3	2.12	0.49
2:P:92:GLY:HA3	2:N:13:TYR:CB	2.42	0.49
1:O:225:LEU:HB3	1:O:272:HIS:CE1	2.48	0.49
2:U:113:VAL:HB	2:U:116:VAL:HG12	1.94	0.49
2:A:24:PHE:CE2	2:B:51:THR:HG23	2.48	0.48
3:D:20:LYS:HE3	3:D:23:GLU:HG2	1.95	0.48
2:G:209:ARG:O	2:G:213:LEU:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:202:LEU:HD11	2:N:216:VAL:HG11	1.94	0.48
1:M:751:ARG:NH2	3:R:55:GLU:OE1	2.46	0.48
1:O:433:LYS:HA	1:O:436:LEU:HD12	1.95	0.48
1:T:374:PHE:HA	1:T:377:PHE:CD1	2.48	0.48
1:T:520:PRO:HG3	1:T:553:HIS:CG	2.47	0.48
2:U:385:ILE:HG13	2:U:399:VAL:HG21	1.95	0.48
1:C:473:MET:CE	1:C:513:TRP:CE3	2.78	0.48
1:F:225:LEU:HB3	1:F:272:HIS:CE1	2.48	0.48
2:B:526:ARG:HB2	2:B:537:PHE:HB3	1.96	0.48
1:I:337:ASN:HB3	1:I:340:ASP:HB2	1.93	0.48
2:P:30:PHE:CE1	2:N:50:ALA:HB2	2.48	0.48
2:S:305:LEU:HD12	2:S:325:VAL:HB	1.94	0.48
1:V:225:LEU:HB3	1:V:272:HIS:CE1	2.48	0.48
3:W:39:VAL:HA	3:W:49:ILE:HB	1.94	0.48
2:B:419:TRP:HZ3	2:B:433:VAL:HG13	1.78	0.48
1:I:478:SER:HA	1:I:481:ASN:ND2	2.27	0.48
1:H:437:ALA:HA	1:H:513:TRP:HZ3	1.79	0.48
1:H:717:MET:HA	1:H:721:VAL:HB	1.95	0.48
1:H:723:VAL:HG11	1:H:742:LYS:HZ3	1.78	0.48
1:O:120:ARG:O	1:O:124:MET:HB2	2.13	0.48
1:O:169:ILE:HD11	1:O:247:ARG:HD3	1.95	0.48
1:T:751:ARG:NH2	3:W:55:GLU:OE1	2.46	0.48
1:C:133:GLN:NE2	2:A:144:SER:HB3	2.28	0.48
1:F:437:ALA:HA	1:F:513:TRP:HZ3	1.78	0.48
2:G:305:LEU:HD12	2:G:325:VAL:HB	1.94	0.48
2:N:526:ARG:HB2	2:N:537:PHE:HB3	1.96	0.48
2:U:455:ARG:NH1	2:U:457:THR:O	2.46	0.48
2:A:263:MET:SD	2:A:263:MET:N	2.86	0.48
2:B:195:ARG:HD3	2:B:229:THR:HG21	1.96	0.48
2:G:382:ILE:O	2:G:402:TYR:N	2.44	0.48
2:J:419:TRP:HZ3	2:J:433:VAL:HG13	1.78	0.48
1:I:74:TYR:OH	1:I:137:GLU:OE2	2.32	0.48
1:O:129:VAL:O	1:O:133:GLN:NE2	2.43	0.48
1:T:120:ARG:O	1:T:124:MET:HB2	2.14	0.48
2:U:202:LEU:HD11	2:U:216:VAL:HG11	1.93	0.48
3:W:54:ILE:HA	3:W:57:GLN:HE21	1.78	0.48
1:C:548:LEU:HD13	3:E:31:ALA:HB1	1.96	0.48
2:G:397:ARG:HD2	2:G:417:CYS:HA	1.96	0.48
1:I:714:ARG:NH1	1:I:725:GLU:OE2	2.47	0.48
1:H:481:ASN:HA	1:H:484:MET:SD	2.53	0.48
2:P:172:LEU:HD22	2:P:176:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:263:MET:N	2:P:263:MET:SD	2.86	0.48
2:P:321:ALA:HB3	2:P:375:LEU:HD11	1.96	0.48
1:M:129:VAL:O	1:M:133:GLN:NE2	2.44	0.48
2:S:263:MET:N	2:S:263:MET:SD	2.86	0.48
1:V:525:PRO:HA	1:V:603:MET:HE2	1.94	0.48
1:F:527:ALA:HB3	1:F:528:PRO:HD3	1.96	0.48
2:B:157:GLU:O	2:B:161:THR:OG1	2.23	0.48
2:J:385:ILE:HG13	2:J:399:VAL:HG21	1.95	0.48
2:J:526:ARG:HB2	2:J:537:PHE:HB3	1.96	0.48
1:I:723:VAL:HG11	1:I:742:LYS:HZ3	1.77	0.48
1:O:356:LEU:CD1	1:O:363:ASP:H	2.25	0.48
1:T:297:GLY:CA	1:T:359:SER:HB2	2.43	0.48
2:S:321:ALA:HB3	2:S:375:LEU:HD11	1.96	0.48
1:C:129:VAL:O	1:C:133:GLN:NE2	2.44	0.48
1:C:606:ASN:HD21	3:E:22:PHE:HD1	1.61	0.48
1:I:120:ARG:O	1:I:124:MET:HB2	2.14	0.48
1:O:527:ALA:HB3	1:O:528:PRO:HD3	1.96	0.48
1:V:263:VAL:HG22	1:V:267:GLU:OE2	2.14	0.48
1:V:437:ALA:HA	1:V:513:TRP:HZ3	1.78	0.48
1:V:446:VAL:HG23	1:V:447:SER:H	1.79	0.48
1:C:687:GLU:O	1:C:690:GLU:HG3	2.14	0.48
2:A:30:PHE:CE1	2:B:50:ALA:HB2	2.49	0.48
1:H:225:LEU:HB3	1:H:272:HIS:CE1	2.48	0.48
1:O:324:GLN:CG	1:O:348:LEU:HD21	2.43	0.48
1:T:606:ASN:HD21	3:W:22:PHE:HD1	1.61	0.48
2:U:152:ALA:O	2:U:156:VAL:HB	2.14	0.48
1:C:751:ARG:NH2	3:E:55:GLU:OE1	2.46	0.48
1:F:120:ARG:O	1:F:124:MET:HB2	2.13	0.48
1:F:169:ILE:HD11	1:F:247:ARG:HD3	1.95	0.48
2:G:321:ALA:HB3	2:G:375:LEU:HD11	1.96	0.48
1:H:201:TYR:OH	1:H:253:ASP:OD1	2.30	0.48
2:N:113:VAL:HB	2:N:116:VAL:HG12	1.95	0.48
1:T:714:ARG:NH1	1:T:725:GLU:OE2	2.47	0.48
1:F:723:VAL:HG11	1:F:742:LYS:HZ3	1.79	0.47
2:J:152:ALA:O	2:J:156:VAL:HB	2.14	0.47
1:I:328:LEU:HG	1:I:341:TYR:HD1	1.79	0.47
3:K:20:LYS:HE3	3:K:23:GLU:HG2	1.95	0.47
1:O:263:VAL:HG22	1:O:267:GLU:OE2	2.14	0.47
1:O:407:GLU:OE1	1:O:407:GLU:N	2.35	0.47
1:T:687:GLU:O	1:T:690:GLU:HG3	2.14	0.47
2:U:387:GLY:O	2:U:388:ASP:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:526:ARG:HB2	2:U:537:PHE:HB3	1.96	0.47
3:W:84:ILE:HD13	3:W:101:TRP:CE2	2.49	0.47
2:A:92:GLY:HA2	2:B:13:TYR:CB	2.44	0.47
2:B:152:ALA:O	2:B:156:VAL:HB	2.14	0.47
2:G:101:VAL:HB	2:G:124:LEU:HD11	1.96	0.47
1:I:687:GLU:O	1:I:690:GLU:HG3	2.14	0.47
1:M:338:PRO:HB3	1:M:387:TYR:CG	2.49	0.47
1:M:503:LEU:HD13	1:M:503:LEU:HA	1.77	0.47
1:V:371:ALA:HB1	1:V:421:PHE:HE1	1.78	0.47
1:C:374:PHE:HA	1:C:377:PHE:CD1	2.48	0.47
3:E:54:ILE:HA	3:E:57:GLN:HE21	1.78	0.47
2:G:18:LEU:HD13	2:J:17:LEU:HD23	1.95	0.47
1:H:446:VAL:HG23	1:H:447:SER:H	1.79	0.47
2:N:152:ALA:O	2:N:156:VAL:HB	2.14	0.47
1:T:383:ARG:HB2	1:T:688:ARG:HH12	1.78	0.47
2:U:195:ARG:HD3	2:U:229:THR:HG21	1.96	0.47
3:E:84:ILE:HD13	3:E:101:TRP:CE2	2.49	0.47
2:J:195:ARG:HD3	2:J:229:THR:HG21	1.96	0.47
2:J:228:VAL:O	2:J:229:THR:OG1	2.24	0.47
1:H:263:VAL:HG22	1:H:267:GLU:OE2	2.14	0.47
2:N:195:ARG:HD3	2:N:229:THR:HG21	1.96	0.47
1:O:201:TYR:OH	1:O:253:ASP:OD1	2.30	0.47
3:R:84:ILE:HD13	3:R:101:TRP:CE2	2.49	0.47
2:S:199:MET:O	2:S:203:GLU:HG2	2.15	0.47
3:X:20:LYS:HE3	3:X:23:GLU:HG2	1.95	0.47
1:C:120:ARG:O	1:C:124:MET:HB3	2.14	0.47
1:F:263:VAL:HG22	1:F:267:GLU:OE2	2.14	0.47
1:F:433:LYS:HA	1:F:436:LEU:HD12	1.95	0.47
2:A:172:LEU:HD22	2:A:176:LEU:HD23	1.96	0.47
1:I:255:SER:O	1:I:257:GLU:N	2.48	0.47
1:H:169:ILE:HD11	1:H:247:ARG:HD3	1.95	0.47
3:L:43:ALA:HB3	3:L:79:PHE:HE1	1.80	0.47
3:L:84:ILE:HD13	3:L:101:TRP:CE2	2.49	0.47
2:P:48:VAL:HG21	2:P:90:TYR:CZ	2.49	0.47
1:M:492:GLN:NE2	1:T:489:GLN:O	2.23	0.47
1:T:120:ARG:O	1:T:124:MET:HB3	2.14	0.47
1:T:356:LEU:HD13	1:T:366:PHE:CB	2.43	0.47
2:S:397:ARG:HD2	2:S:417:CYS:HA	1.96	0.47
2:U:91:THR:HG23	2:U:93:ASN:H	1.77	0.47
1:V:201:TYR:OH	1:V:253:ASP:OD1	2.30	0.47
1:C:74:TYR:OH	1:C:137:GLU:OE2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:321:ALA:HB3	2:A:375:LEU:HD11	1.96	0.47
1:I:300:TYR:HB2	1:I:360:PHE:CD1	2.49	0.47
3:K:45:CYS:HB2	3:K:54:ILE:HG23	1.96	0.47
2:N:265:LYS:HG3	2:N:585:LYS:HD3	1.96	0.47
1:M:74:TYR:OH	1:M:137:GLU:OE2	2.32	0.47
1:M:687:GLU:O	1:M:690:GLU:HG3	2.14	0.47
1:O:714:ARG:NH1	1:O:725:GLU:OE2	2.48	0.47
3:Q:20:LYS:HE3	3:Q:23:GLU:HG2	1.95	0.47
1:T:386:GLU:OE1	1:T:386:GLU:N	2.46	0.47
2:S:48:VAL:HG21	2:S:90:TYR:CZ	2.49	0.47
1:V:169:ILE:HD11	1:V:247:ARG:HD3	1.95	0.47
3:X:45:CYS:HB2	3:X:54:ILE:HG23	1.96	0.47
1:C:345:LEU:CG	1:C:418:LEU:HD11	2.30	0.47
1:C:346:LEU:HD11	1:C:414:LYS:CB	2.35	0.47
1:F:284:LEU:O	1:F:288:LEU:HB2	2.15	0.47
2:A:37:VAL:HG21	2:A:82:LEU:HD23	1.96	0.47
2:A:199:MET:O	2:A:203:GLU:HG2	2.15	0.47
2:A:350:PHE:HD2	2:A:363:LYS:HB2	1.80	0.47
2:G:14:ALA:HB1	2:J:14:ALA:HB1	1.97	0.47
2:G:48:VAL:HG21	2:G:90:TYR:CZ	2.49	0.47
2:G:172:LEU:HD22	2:G:176:LEU:HD23	1.96	0.47
1:I:225:LEU:HB3	1:I:272:HIS:CE1	2.50	0.47
1:I:523:ASN:HB2	1:I:529:ARG:HH21	1.79	0.47
1:H:548:LEU:HD22	1:H:548:LEU:HA	1.80	0.47
2:P:199:MET:O	2:P:203:GLU:HG2	2.15	0.47
1:M:255:SER:O	1:M:257:GLU:N	2.48	0.47
1:M:520:PRO:HG2	1:M:552:HIS:H	1.80	0.47
1:O:356:LEU:HA	1:O:360:PHE:CG	2.50	0.47
1:O:687:GLU:O	1:O:690:GLU:HG3	2.15	0.47
1:T:225:LEU:HB3	1:T:272:HIS:CE1	2.50	0.47
1:T:378:LEU:HD22	1:T:422:MET:HB3	1.92	0.47
1:T:378:LEU:HD11	1:T:422:MET:SD	2.55	0.47
2:S:172:LEU:HD22	2:S:176:LEU:HD23	1.96	0.47
1:V:687:GLU:O	1:V:690:GLU:HG3	2.15	0.47
1:V:723:VAL:HG11	1:V:742:LYS:HZ3	1.80	0.47
1:C:225:LEU:HB3	1:C:272:HIS:CE1	2.50	0.47
1:F:446:VAL:HG23	1:F:447:SER:H	1.79	0.47
2:A:78:ASP:O	2:A:82:LEU:HB2	2.15	0.47
2:J:153:LYS:HA	2:J:153:LYS:HD2	1.69	0.47
2:J:265:LYS:HG3	2:J:585:LYS:HD3	1.96	0.47
1:I:606:ASN:HD21	3:L:22:PHE:HD1	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:88:LEU:HD23	3:K:92:GLN:HG2	1.97	0.47
2:N:202:LEU:HD21	2:N:216:VAL:HG11	1.97	0.47
1:O:345:LEU:CD2	1:O:377:PHE:CZ	2.97	0.47
1:O:345:LEU:HD11	1:O:374:PHE:CZ	2.48	0.47
1:C:120:ARG:O	1:C:124:MET:HB2	2.14	0.47
1:F:74:TYR:OH	1:F:137:GLU:OE2	2.33	0.47
1:F:687:GLU:O	1:F:690:GLU:HG3	2.15	0.47
1:O:269:ILE:HB	1:O:306:VAL:HG21	1.97	0.47
1:O:548:LEU:HD23	3:Q:33:TRP:HB3	1.97	0.47
2:S:425:VAL:HB	2:S:466:ALA:HB2	1.97	0.47
2:U:202:LEU:HD21	2:U:216:VAL:HG11	1.97	0.47
1:F:494:THR:HG22	1:H:501:VAL:CB	2.45	0.47
3:D:88:LEU:HD23	3:D:92:GLN:HG2	1.97	0.47
2:J:202:LEU:HD21	2:J:216:VAL:HG11	1.97	0.47
1:H:49:ASN:HD22	1:H:118:MET:HE1	1.80	0.47
1:H:687:GLU:O	1:H:690:GLU:HG3	2.15	0.47
2:P:45:HIS:HB3	2:N:47:MET:SD	2.55	0.47
1:O:751:ARG:NH2	3:Q:55:GLU:OE1	2.48	0.47
3:Q:45:CYS:HB2	3:Q:54:ILE:HG23	1.96	0.47
1:T:74:TYR:OH	1:T:137:GLU:OE2	2.32	0.47
1:T:523:ASN:HB2	1:T:529:ARG:HH21	1.79	0.47
2:U:149:LYS:HB2	2:U:149:LYS:HE2	1.75	0.47
2:U:289:SER:HG	2:U:294:LYS:H	1.60	0.47
1:V:553:HIS:HA	1:V:597:PHE:HE1	1.80	0.47
1:V:751:ARG:NH2	3:X:55:GLU:OE1	2.48	0.47
1:M:606:ASN:HD21	3:R:22:PHE:HD1	1.61	0.46
1:O:356:LEU:HA	1:O:360:PHE:CD2	2.50	0.46
1:O:360:PHE:O	1:O:361:ASN:C	2.58	0.46
1:O:437:ALA:HA	1:O:513:TRP:HZ3	1.78	0.46
1:O:446:VAL:HG23	1:O:447:SER:H	1.79	0.46
1:O:553:HIS:HA	1:O:597:PHE:HE1	1.80	0.46
1:V:471:GLU:HB3	1:V:475:ARG:HH21	1.80	0.46
3:X:47:ASN:HD21	3:X:54:ILE:HG23	1.80	0.46
2:A:425:VAL:HB	2:A:466:ALA:HB2	1.97	0.46
2:B:525:VAL:HA	2:B:538:MET:HG2	1.97	0.46
2:P:425:VAL:HB	2:P:466:ALA:HB2	1.97	0.46
1:O:471:GLU:HB3	1:O:475:ARG:HH21	1.80	0.46
3:R:43:ALA:HB3	3:R:79:PHE:HE1	1.80	0.46
2:S:209:ARG:O	2:S:213:LEU:N	2.43	0.46
2:U:265:LYS:HG3	2:U:585:LYS:HD3	1.96	0.46
1:C:255:SER:O	1:C:257:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:74:TYR:OH	1:O:137:GLU:OE2	2.33	0.46
2:G:199:MET:O	2:G:203:GLU:HG2	2.15	0.46
2:G:275:SER:OG	2:G:574:ASP:O	2.25	0.46
2:J:525:VAL:HA	2:J:538:MET:HG2	1.97	0.46
1:I:386:GLU:OE1	1:I:386:GLU:N	2.46	0.46
1:H:346:LEU:HD11	1:H:414:LYS:CB	2.42	0.46
1:H:465:GLN:OE1	1:H:465:GLN:N	2.49	0.46
1:H:751:ARG:NH2	3:K:55:GLU:OE1	2.48	0.46
1:M:629:ARG:O	1:M:632:GLN:HG3	2.16	0.46
2:A:18:LEU:HD22	2:B:14:ALA:N	2.27	0.46
2:N:144:SER:HB3	1:O:133:GLN:CD	2.41	0.46
1:M:120:ARG:O	1:M:124:MET:HB3	2.14	0.46
2:S:325:VAL:O	2:S:345:ARG:N	2.49	0.46
1:V:374:PHE:O	1:V:378:LEU:HB2	2.15	0.46
1:C:374:PHE:O	1:C:378:LEU:HB2	2.15	0.46
1:F:465:GLN:OE1	1:F:465:GLN:N	2.49	0.46
1:F:471:GLU:HB3	1:F:475:ARG:HH21	1.80	0.46
1:F:751:ARG:NH2	3:D:55:GLU:OE1	2.48	0.46
2:B:228:VAL:O	2:B:229:THR:OG1	2.24	0.46
3:E:43:ALA:HB3	3:E:79:PHE:HE1	1.80	0.46
2:P:350:PHE:HD2	2:P:363:LYS:HB2	1.80	0.46
2:N:157:GLU:O	2:N:161:THR:OG1	2.23	0.46
1:O:300:TYR:HB2	1:O:360:PHE:CD1	2.50	0.46
1:O:345:LEU:HD22	1:O:377:PHE:HZ	1.80	0.46
3:Q:47:ASN:HD21	3:Q:54:ILE:HG23	1.80	0.46
1:T:255:SER:O	1:T:257:GLU:N	2.48	0.46
1:C:614:GLU:HA	1:C:617:GLN:HG2	1.98	0.46
1:F:548:LEU:HD23	3:D:33:TRP:HB3	1.97	0.46
1:F:714:ARG:NH1	1:F:725:GLU:OE2	2.48	0.46
2:B:265:LYS:HG3	2:B:585:LYS:HD3	1.96	0.46
2:G:8:GLN:HE22	2:J:22:LYS:HD2	1.80	0.46
1:O:465:GLN:N	1:O:465:GLN:OE1	2.49	0.46
1:T:546:ARG:HE	3:W:35:TRP:NE1	2.14	0.46
1:T:614:GLU:HA	1:T:617:GLN:HG2	1.98	0.46
3:W:43:ALA:HB3	3:W:79:PHE:HE1	1.80	0.46
1:C:523:ASN:HB2	1:C:620:THR:HG23	1.97	0.46
2:G:350:PHE:HD2	2:G:363:LYS:HB2	1.80	0.46
1:I:120:ARG:O	1:I:124:MET:HB3	2.14	0.46
1:I:629:ARG:O	1:I:632:GLN:HG3	2.16	0.46
2:P:24:PHE:CE2	2:N:51:THR:CG2	2.99	0.46
2:P:379:GLU:HG3	2:P:379:GLU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:723:VAL:HG11	1:O:742:LYS:HZ3	1.80	0.46
1:T:133:GLN:NE2	2:S:144:SER:HB3	2.31	0.46
3:X:88:LEU:HD23	3:X:92:GLN:HG2	1.97	0.46
1:F:269:ILE:HB	1:F:306:VAL:HG21	1.97	0.46
1:F:553:HIS:HA	1:F:597:PHE:HE1	1.80	0.46
2:G:181:LEU:HD21	2:G:220:ILE:HD12	1.98	0.46
2:G:211:GLN:H	2:G:211:GLN:CD	2.24	0.46
2:G:301:PRO:HB2	2:G:302:PRO:HD3	1.98	0.46
2:G:379:GLU:HG3	2:G:379:GLU:O	2.16	0.46
1:H:553:HIS:HA	1:H:597:PHE:HE1	1.80	0.46
2:P:301:PRO:HB2	2:P:302:PRO:HD3	1.98	0.46
2:N:275:SER:N	2:N:575:LEU:O	2.49	0.46
1:M:120:ARG:O	1:M:124:MET:HB2	2.14	0.46
3:Q:33:TRP:HZ3	3:Q:35:TRP:CD1	2.34	0.46
2:S:45:HIS:ND1	2:S:90:TYR:OH	2.32	0.46
2:S:287:CYS:N	2:S:296:TYR:O	2.36	0.46
1:V:238:GLU:O	1:V:242:ASN:ND2	2.40	0.46
1:C:509:THR:HB	1:C:512:TYR:CD2	2.51	0.46
2:B:106:GLU:HG2	2:B:143:PHE:HE2	1.81	0.46
2:G:425:VAL:HB	2:G:466:ALA:HB2	1.97	0.46
1:I:269:ILE:HB	1:I:306:VAL:HG21	1.98	0.46
1:I:446:VAL:HG23	1:I:447:SER:H	1.81	0.46
1:M:225:LEU:HB3	1:M:272:HIS:CE1	2.50	0.46
1:O:622:ILE:HG21	1:O:627:LEU:HD22	1.98	0.46
1:T:269:ILE:HB	1:T:306:VAL:HG21	1.98	0.46
1:C:629:ARG:O	1:C:632:GLN:HG3	2.16	0.45
1:H:289:LYS:O	1:H:351:ARG:NH2	2.48	0.45
1:H:386:GLU:OE1	1:H:386:GLU:N	2.47	0.45
1:O:356:LEU:O	1:O:360:PHE:C	2.59	0.45
1:T:336:LYS:H	1:T:336:LYS:HG3	1.55	0.45
1:F:288:LEU:HG	1:F:351:ARG:HH22	1.80	0.45
1:F:289:LYS:HA	1:F:351:ARG:HH12	1.81	0.45
1:F:386:GLU:OE1	1:F:386:GLU:N	2.47	0.45
2:A:325:VAL:O	2:A:345:ARG:N	2.49	0.45
2:G:325:VAL:O	2:G:345:ARG:N	2.49	0.45
2:G:402:TYR:HB2	2:G:409:TRP:CZ3	2.51	0.45
2:J:275:SER:N	2:J:575:LEU:O	2.49	0.45
2:J:539:ARG:HH21	2:J:579:PHE:HE1	1.65	0.45
1:I:546:ARG:HE	3:L:35:TRP:NE1	2.14	0.45
1:I:614:GLU:HA	1:I:617:GLN:HG2	1.97	0.45
1:H:471:GLU:HB3	1:H:475:ARG:HH21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:345:LEU:CD2	1:O:377:PHE:HZ	2.29	0.45
1:T:509:THR:HB	1:T:512:TYR:CD2	2.51	0.45
1:V:116:MET:HA	1:V:119:ILE:HB	1.99	0.45
1:V:546:ARG:HD3	1:V:546:ARG:HA	1.36	0.45
1:F:553:HIS:HA	1:F:597:PHE:CE1	2.52	0.45
2:A:244:VAL:O	2:A:247:GLN:HG3	2.16	0.45
2:B:202:LEU:HD21	2:B:216:VAL:HG11	1.97	0.45
1:I:371:ALA:HB2	1:I:421:PHE:HE1	1.80	0.45
3:K:47:ASN:HD21	3:K:54:ILE:HG23	1.80	0.45
2:P:181:LEU:HD21	2:P:220:ILE:HD12	1.98	0.45
2:N:221:ARG:NE	2:N:258:LYS:O	2.50	0.45
2:N:539:ARG:HH21	2:N:579:PHE:HE1	1.65	0.45
1:M:492:GLN:OE1	1:T:489:GLN:CB	2.64	0.45
2:S:211:GLN:CD	2:S:211:GLN:H	2.24	0.45
2:S:402:TYR:HB2	2:S:409:TRP:CZ3	2.51	0.45
1:V:269:ILE:HB	1:V:306:VAL:HG21	1.97	0.45
1:V:622:ILE:HG21	1:V:627:LEU:HD22	1.98	0.45
3:X:52:LEU:HD21	3:X:59:ASN:HB3	1.99	0.45
2:A:402:TYR:HB2	2:A:409:TRP:CZ3	2.51	0.45
2:J:221:ARG:NE	2:J:258:LYS:O	2.50	0.45
1:M:503:LEU:HD12	1:M:505:VAL:HG22	1.97	0.45
1:M:622:ILE:HG12	1:M:627:LEU:HB2	1.99	0.45
1:O:498:LEU:HA	1:O:498:LEU:HD13	1.76	0.45
1:T:300:TYR:CD2	1:T:360:PHE:HA	2.52	0.45
1:T:629:ARG:O	1:T:632:GLN:HG3	2.16	0.45
2:S:181:LEU:HD21	2:S:220:ILE:HD12	1.98	0.45
2:U:106:GLU:HG2	2:U:143:PHE:HE2	1.81	0.45
2:U:221:ARG:NE	2:U:258:LYS:O	2.50	0.45
1:V:553:HIS:HA	1:V:597:PHE:CE1	2.52	0.45
2:A:113:VAL:HB	2:A:116:VAL:HG12	1.98	0.45
2:A:353:PHE:HB2	2:A:360:TRP:CH2	2.52	0.45
2:G:244:VAL:O	2:G:247:GLN:HG3	2.16	0.45
2:G:287:CYS:N	2:G:296:TYR:O	2.36	0.45
2:J:458:SER:O	2:J:459:ARG:NH1	2.42	0.45
1:H:269:ILE:HB	1:H:306:VAL:HG21	1.97	0.45
1:H:605:PHE:HE1	1:H:611:TYR:HB2	1.82	0.45
3:L:80:HIS:HB2	3:L:83:CYS:SG	2.57	0.45
2:P:402:TYR:HB2	2:P:409:TRP:CZ3	2.51	0.45
2:N:525:VAL:HA	2:N:538:MET:HG2	1.97	0.45
1:M:509:THR:HB	1:M:512:TYR:CD2	2.51	0.45
1:O:300:TYR:CE2	1:O:360:PHE:C	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:346:LEU:HD11	1:O:414:LYS:HD2	1.98	0.45
3:R:80:HIS:HB2	3:R:83:CYS:SG	2.57	0.45
1:T:297:GLY:N	1:T:359:SER:HB2	2.30	0.45
2:S:301:PRO:HB2	2:S:302:PRO:HD3	1.99	0.45
2:S:350:PHE:HD2	2:S:363:LYS:HB2	1.80	0.45
2:U:539:ARG:HH21	2:U:579:PHE:HE1	1.65	0.45
1:C:269:ILE:HB	1:C:306:VAL:HG21	1.99	0.45
1:F:125:TYR:HD1	2:B:112:GLN:CG	2.30	0.45
1:F:614:GLU:HA	1:F:617:GLN:HG2	1.98	0.45
2:A:211:GLN:H	2:A:211:GLN:CD	2.24	0.45
3:K:52:LEU:HD21	3:K:59:ASN:HB3	1.99	0.45
2:P:121:ARG:HD3	2:P:145:CYS:SG	2.57	0.45
1:O:116:MET:HA	1:O:119:ILE:HB	1.99	0.45
1:O:328:LEU:CD1	1:O:341:TYR:HA	2.43	0.45
1:O:345:LEU:CD1	1:O:374:PHE:CZ	2.99	0.45
1:O:356:LEU:HD12	1:O:360:PHE:HB2	1.98	0.45
1:O:614:GLU:HA	1:O:617:GLN:HG2	1.98	0.45
1:T:129:VAL:O	1:T:133:GLN:NE2	2.44	0.45
2:S:379:GLU:O	2:S:379:GLU:HG3	2.16	0.45
2:U:371:ILE:HB	2:U:388:ASP:HB2	1.98	0.45
1:H:74:TYR:OH	1:H:137:GLU:OE2	2.33	0.45
2:P:225:LEU:HD23	2:P:225:LEU:HA	1.79	0.45
2:P:353:PHE:HB2	2:P:360:TRP:CH2	2.52	0.45
1:M:609:GLU:HG3	1:M:610:LYS:H	1.82	0.45
1:M:614:GLU:HA	1:M:617:GLN:HG2	1.98	0.45
1:O:478:SER:HA	1:O:481:ASN:HD21	1.81	0.45
1:T:609:GLU:HG3	1:T:610:LYS:H	1.82	0.45
2:S:244:VAL:O	2:S:247:GLN:HG3	2.16	0.45
2:S:353:PHE:HB2	2:S:360:TRP:CH2	2.52	0.45
3:W:45:CYS:HB2	3:W:54:ILE:HG12	1.99	0.45
1:C:516:GLN:HG2	1:C:517:SER:N	2.30	0.45
1:C:609:GLU:HG3	1:C:610:LYS:H	1.82	0.45
3:D:33:TRP:HZ3	3:D:35:TRP:CD1	2.34	0.45
1:O:245:ILE:HA	1:O:248:VAL:HG12	1.99	0.45
1:O:374:PHE:CB	1:O:421:PHE:HB3	2.46	0.45
1:V:74:TYR:OH	1:V:137:GLU:OE2	2.33	0.45
1:C:650:SER:OG	1:C:654:GLU:OE2	2.28	0.45
1:F:288:LEU:HD13	1:F:296:LEU:HD21	1.99	0.45
2:A:121:ARG:HD3	2:A:145:CYS:SG	2.57	0.45
2:A:379:GLU:HG3	2:A:379:GLU:O	2.16	0.45
2:B:275:SER:N	2:B:575:LEU:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:446:VAL:HG23	1:M:447:SER:H	1.81	0.45
1:M:516:GLN:H	1:M:516:GLN:CD	2.24	0.45
1:T:605:PHE:HE1	1:T:611:TYR:HB2	1.82	0.45
2:S:113:VAL:HB	2:S:116:VAL:HG12	1.98	0.45
2:S:287:CYS:SG	2:S:288:TYR:N	2.90	0.45
1:V:605:PHE:HE1	1:V:611:TYR:HB2	1.82	0.45
1:C:346:LEU:HD23	1:C:411:ILE:HD11	1.98	0.45
1:C:386:GLU:OE1	1:C:386:GLU:N	2.46	0.45
1:F:336:LYS:H	1:F:336:LYS:HG3	1.61	0.45
3:D:36:ASP:O	3:D:38:VAL:HG23	2.17	0.45
2:G:47:MET:CE	2:J:45:HIS:CG	2.99	0.45
2:G:113:VAL:HB	2:G:116:VAL:HG12	1.98	0.45
1:H:622:ILE:HG21	1:H:627:LEU:HD22	1.98	0.45
3:K:33:TRP:HZ3	3:K:35:TRP:CD1	2.34	0.45
1:M:390:LEU:HD22	1:M:435:HIS:NE2	2.32	0.45
1:V:478:SER:HA	1:V:481:ASN:HD21	1.81	0.45
1:F:265:GLU:HB3	1:F:306:VAL:HG22	1.99	0.44
1:F:605:PHE:HE1	1:F:611:TYR:HB2	1.82	0.44
2:B:458:SER:O	2:B:459:ARG:NH1	2.41	0.44
2:G:353:PHE:HB2	2:G:360:TRP:CH2	2.52	0.44
1:I:390:LEU:HD22	1:I:435:HIS:NE2	2.32	0.44
1:I:509:THR:HB	1:I:512:TYR:CD2	2.51	0.44
1:I:525:PRO:HA	1:I:603:MET:HE2	1.99	0.44
1:H:553:HIS:HA	1:H:597:PHE:CE1	2.52	0.44
2:P:287:CYS:SG	2:P:288:TYR:N	2.90	0.44
2:N:554:TYR:HA	2:N:561:TRP:HA	1.99	0.44
1:O:553:HIS:HA	1:O:597:PHE:CE1	2.52	0.44
3:R:27:TRP:CE2	3:R:29:ALA:HB2	2.53	0.44
1:T:446:VAL:HG23	1:T:447:SER:H	1.81	0.44
1:F:407:GLU:OE1	1:F:407:GLU:N	2.35	0.44
1:F:478:SER:HA	1:F:481:ASN:HD21	1.81	0.44
1:F:510:THR:HG22	3:D:32:LEU:HG	1.99	0.44
2:G:297:LYS:HZ1	2:G:595:PRO:HD3	1.83	0.44
2:J:106:GLU:HG2	2:J:143:PHE:HE2	1.81	0.44
2:J:217:LEU:HD13	2:J:225:LEU:HD11	2.00	0.44
3:L:45:CYS:HB2	3:L:54:ILE:HG12	1.99	0.44
2:P:244:VAL:O	2:P:247:GLN:HG3	2.16	0.44
3:Q:40:ASP:HA	3:Q:48:HIS:CE1	2.53	0.44
3:Q:45:CYS:HB3	3:Q:83:CYS:SG	2.57	0.44
1:T:346:LEU:CD2	1:T:414:LYS:O	2.65	0.44
2:S:121:ARG:HD3	2:S:145:CYS:SG	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:510:THR:HG22	3:X:32:LEU:HG	2.00	0.44
3:X:33:TRP:HZ3	3:X:35:TRP:CD1	2.34	0.44
1:C:342:ILE:HB	1:C:391:PHE:HB2	1.98	0.44
1:F:116:MET:HA	1:F:119:ILE:HB	1.99	0.44
2:A:19:GLU:HG2	2:B:9:ILE:HD13	2.00	0.44
2:B:539:ARG:HH21	2:B:579:PHE:HE1	1.65	0.44
3:D:27:TRP:CE2	3:D:29:ALA:HB2	2.53	0.44
3:D:85:SER:O	3:D:89:LYS:NZ	2.50	0.44
1:I:238:GLU:O	1:I:242:ASN:ND2	2.40	0.44
1:I:371:ALA:CA	1:I:421:PHE:CE1	2.97	0.44
1:I:605:PHE:HE1	1:I:611:TYR:HB2	1.83	0.44
3:L:27:TRP:CE2	3:L:29:ALA:HB2	2.53	0.44
3:K:27:TRP:CE2	3:K:29:ALA:HB2	2.53	0.44
3:K:94:CYS:O	3:K:96:LEU:N	2.50	0.44
2:P:113:VAL:HB	2:P:116:VAL:HG12	1.98	0.44
2:N:228:VAL:O	2:N:229:THR:OG1	2.24	0.44
1:M:605:PHE:HE1	1:M:611:TYR:HB2	1.83	0.44
2:U:217:LEU:HD13	2:U:225:LEU:HD11	2.00	0.44
2:U:525:VAL:HA	2:U:538:MET:HG2	1.97	0.44
3:W:80:HIS:HB2	3:W:83:CYS:SG	2.57	0.44
3:X:36:ASP:O	3:X:38:VAL:HG23	2.17	0.44
2:A:181:LEU:HD21	2:A:220:ILE:HD12	1.98	0.44
2:B:221:ARG:NE	2:B:258:LYS:O	2.50	0.44
3:E:80:HIS:HB2	3:E:83:CYS:SG	2.57	0.44
2:J:379:GLU:HG3	2:J:379:GLU:O	2.18	0.44
1:I:324:GLN:HG2	1:I:348:LEU:HD21	1.96	0.44
1:H:129:VAL:O	1:H:133:GLN:NE2	2.43	0.44
3:K:45:CYS:HB3	3:K:83:CYS:SG	2.57	0.44
2:N:379:GLU:O	2:N:379:GLU:HG3	2.18	0.44
1:T:390:LEU:HD22	1:T:435:HIS:NE2	2.32	0.44
2:U:228:VAL:O	2:U:229:THR:OG1	2.24	0.44
1:V:473:MET:HB2	1:V:513:TRP:CE2	2.52	0.44
3:W:27:TRP:CE2	3:W:29:ALA:HB2	2.53	0.44
1:C:523:ASN:HA	1:C:529:ARG:NH2	2.31	0.44
1:F:129:VAL:O	1:F:133:GLN:NE2	2.43	0.44
1:F:622:ILE:HG21	1:F:627:LEU:HD22	1.98	0.44
3:D:94:CYS:O	3:D:96:LEU:N	2.50	0.44
2:G:287:CYS:SG	2:G:288:TYR:N	2.90	0.44
1:I:128:ARG:O	1:I:132:GLN:HB2	2.18	0.44
1:I:207:ALA:HB3	1:I:208:PRO:HD3	1.99	0.44
1:H:265:GLU:HB3	1:H:306:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:478:SER:HA	1:H:481:ASN:HD21	1.81	0.44
3:K:36:ASP:O	3:K:38:VAL:HG23	2.17	0.44
2:P:144:SER:HB3	1:M:133:GLN:NE2	2.33	0.44
1:V:265:GLU:HB3	1:V:306:VAL:HG22	1.99	0.44
3:X:94:CYS:O	3:X:96:LEU:N	2.50	0.44
1:C:622:ILE:HG12	1:C:627:LEU:HB2	1.99	0.44
3:E:45:CYS:HB2	3:E:54:ILE:HG12	1.99	0.44
2:G:413:SER:HB3	2:G:442:TYR:HE1	1.81	0.44
2:P:325:VAL:O	2:P:345:ARG:N	2.49	0.44
3:Q:36:ASP:O	3:Q:38:VAL:HG23	2.17	0.44
3:Q:94:CYS:O	3:Q:96:LEU:N	2.50	0.44
2:U:127:LYS:O	2:U:129:ASN:ND2	2.51	0.44
3:X:85:SER:O	3:X:89:LYS:NZ	2.50	0.44
1:C:390:LEU:HD22	1:C:435:HIS:NE2	2.32	0.44
1:C:446:VAL:HG23	1:C:447:SER:H	1.81	0.44
1:C:553:HIS:HA	1:C:597:PHE:CE1	2.53	0.44
1:F:296:LEU:HD12	1:F:360:PHE:CZ	2.53	0.44
1:I:609:GLU:HG3	1:I:610:LYS:H	1.82	0.44
1:H:614:GLU:HA	1:H:617:GLN:HG2	1.98	0.44
1:M:128:ARG:O	1:M:132:GLN:HB2	2.18	0.44
1:M:207:ALA:HB3	1:M:208:PRO:HD3	2.00	0.44
1:O:345:LEU:HD11	1:O:374:PHE:CD2	2.51	0.44
1:O:371:ALA:HB2	1:O:421:PHE:CE1	2.51	0.44
1:T:346:LEU:CA	1:T:418:LEU:HD12	2.47	0.44
1:T:516:GLN:H	1:T:516:GLN:CD	2.24	0.44
2:S:413:SER:HB3	2:S:442:TYR:HE1	1.81	0.44
2:U:554:TYR:HA	2:U:561:TRP:HA	1.99	0.44
3:E:27:TRP:CE2	3:E:29:ALA:HB2	2.53	0.44
1:I:311:LYS:HE3	1:I:311:LYS:HB3	1.88	0.44
1:H:483:THR:HG21	1:H:507:VAL:HG21	2.00	0.44
1:H:520:PRO:HD2	1:H:551:GLN:HA	2.00	0.44
2:P:30:PHE:CE1	2:N:50:ALA:CB	3.01	0.44
1:V:31:ASN:OD1	1:V:72:LYS:NZ	2.51	0.44
1:V:386:GLU:OE1	1:V:386:GLU:N	2.47	0.44
2:A:301:PRO:HB2	2:A:302:PRO:HD3	1.99	0.44
2:J:366:MET:HE2	2:J:366:MET:HB3	1.84	0.44
2:J:554:TYR:HA	2:J:561:TRP:HA	1.99	0.44
1:H:31:ASN:OD1	1:H:72:LYS:NZ	2.51	0.44
1:H:116:MET:HA	1:H:119:ILE:HB	1.99	0.44
1:H:258:GLU:HB2	1:H:259:PRO:HD3	1.99	0.44
3:K:59:ASN:ND2	3:K:60:GLN:OE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:609:GLU:HG3	1:O:610:LYS:H	1.83	0.44
3:Q:27:TRP:CE2	3:Q:29:ALA:HB2	2.53	0.44
1:T:524:ILE:HG22	1:T:528:PRO:HB2	2.00	0.44
2:S:101:VAL:HB	2:S:124:LEU:HD11	2.00	0.44
2:U:499:VAL:HG21	2:U:561:TRP:CZ2	2.53	0.44
1:V:614:GLU:HA	1:V:617:GLN:HG2	1.98	0.44
3:X:45:CYS:HB3	3:X:83:CYS:SG	2.57	0.44
1:C:337:ASN:ND2	1:C:340:ASP:OD1	2.52	0.43
1:C:605:PHE:HE1	1:C:611:TYR:HB2	1.83	0.43
1:F:245:ILE:HA	1:F:248:VAL:HG12	1.99	0.43
1:F:321:LEU:HG	1:F:352:PHE:CE1	2.53	0.43
2:B:379:GLU:HG3	2:B:379:GLU:O	2.18	0.43
2:G:221:ARG:NH2	2:G:260:ARG:HE	2.16	0.43
2:G:553:GLN:O	2:G:562:SER:N	2.51	0.43
3:L:46:ARG:HH11	3:L:46:ARG:C	2.26	0.43
3:K:86:ARG:O	3:K:89:LYS:HD2	2.18	0.43
2:P:45:HIS:CD2	2:N:47:MET:SD	3.11	0.43
1:M:148:ARG:HH11	1:M:200:VAL:HG21	1.83	0.43
1:M:238:GLU:O	1:M:242:ASN:ND2	2.40	0.43
1:M:269:ILE:HB	1:M:306:VAL:HG21	1.98	0.43
1:O:413:ASP:O	1:O:416:MET:HG3	2.18	0.43
1:O:605:PHE:HE1	1:O:611:TYR:HB2	1.82	0.43
3:Q:52:LEU:HD21	3:Q:59:ASN:HB3	1.99	0.43
1:T:553:HIS:HA	1:T:597:PHE:CE1	2.53	0.43
2:S:225:LEU:HD23	2:S:225:LEU:HA	1.79	0.43
2:A:24:PHE:CE2	2:B:51:THR:HG22	2.53	0.43
2:G:31:THR:OG1	2:G:44:CYS:O	2.33	0.43
3:R:45:CYS:HB2	3:R:54:ILE:HG12	1.99	0.43
3:X:40:ASP:HA	3:X:48:HIS:CE1	2.53	0.43
1:F:201:TYR:OH	1:F:253:ASP:OD1	2.30	0.43
2:A:82:LEU:O	2:A:86:ILE:HG13	2.19	0.43
2:A:287:CYS:SG	2:A:288:TYR:N	2.90	0.43
2:B:554:TYR:HA	2:B:561:TRP:HA	1.99	0.43
1:I:129:VAL:O	1:I:133:GLN:NE2	2.44	0.43
3:K:40:ASP:HA	3:K:48:HIS:CE1	2.53	0.43
2:P:211:GLN:CD	2:P:211:GLN:H	2.24	0.43
2:N:499:VAL:HG21	2:N:561:TRP:CZ2	2.53	0.43
1:M:553:HIS:HA	1:M:597:PHE:CE1	2.53	0.43
1:O:609:GLU:OE2	3:Q:21:ARG:NH1	2.52	0.43
1:T:622:ILE:HG12	1:T:627:LEU:HB2	1.99	0.43
2:S:553:GLN:O	2:S:562:SER:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:413:ASP:O	1:V:416:MET:HG3	2.18	0.43
1:V:609:GLU:HG3	1:V:610:LYS:H	1.83	0.43
1:V:609:GLU:OE2	3:X:21:ARG:NH1	2.52	0.43
1:C:128:ARG:O	1:C:132:GLN:HB2	2.18	0.43
3:D:86:ARG:O	3:D:89:LYS:HD2	2.18	0.43
1:M:337:ASN:ND2	1:M:340:ASP:OD1	2.52	0.43
1:T:723:VAL:HG11	1:T:742:LYS:HZ3	1.83	0.43
1:V:258:GLU:HB2	1:V:259:PRO:HD3	2.00	0.43
1:C:520:PRO:HG2	1:C:552:HIS:H	1.82	0.43
1:F:320:TYR:CE2	1:F:351:ARG:NH2	2.86	0.43
2:B:395:ASN:HA	2:B:397:ARG:HD2	1.99	0.43
2:G:143:PHE:O	2:G:144:SER:C	2.61	0.43
1:I:622:ILE:HG12	1:I:627:LEU:HB2	1.99	0.43
2:N:372:LYS:NZ	2:N:580:ARG:HE	2.17	0.43
1:O:238:GLU:O	1:O:242:ASN:ND2	2.41	0.43
1:O:258:GLU:HB2	1:O:259:PRO:HD3	2.00	0.43
1:O:606:ASN:HD21	3:Q:22:PHE:HD1	1.66	0.43
1:T:413:ASP:O	1:T:416:MET:HG3	2.19	0.43
1:T:525:PRO:HA	1:T:603:MET:HE2	1.99	0.43
1:V:128:ARG:O	1:V:132:GLN:HB2	2.19	0.43
3:W:43:ALA:HB3	3:W:79:PHE:CE1	2.54	0.43
3:W:74:VAL:HB	3:W:102:GLU:HB2	2.01	0.43
3:X:27:TRP:CE2	3:X:29:ALA:HB2	2.53	0.43
1:C:413:ASP:O	1:C:416:MET:HG3	2.19	0.43
1:F:31:ASN:OD1	1:F:72:LYS:NZ	2.51	0.43
1:F:102:LEU:HD22	1:F:182:ALA:HB1	2.01	0.43
1:F:329:VAL:O	1:F:330:SER:C	2.61	0.43
1:F:413:ASP:O	1:F:416:MET:HG3	2.18	0.43
2:A:101:VAL:HB	2:A:124:LEU:HD11	2.00	0.43
2:J:395:ASN:C	2:J:397:ARG:H	2.26	0.43
1:I:500:GLY:HA2	1:I:503:LEU:HD23	1.99	0.43
3:L:43:ALA:HB3	3:L:79:PHE:CE1	2.54	0.43
2:N:228:VAL:HG12	2:N:229:THR:H	1.84	0.43
1:O:386:GLU:OE1	1:O:386:GLU:N	2.47	0.43
1:O:483:THR:HG21	1:O:507:VAL:HG21	2.00	0.43
1:O:501:VAL:HB	1:O:502:ASP:H	1.59	0.43
2:S:470:LYS:NZ	2:S:503:ASP:OD2	2.44	0.43
3:W:46:ARG:HH11	3:W:46:ARG:C	2.26	0.43
1:C:148:ARG:HH11	1:C:200:VAL:HG21	1.83	0.43
1:C:525:PRO:CA	1:C:603:MET:HE2	2.35	0.43
1:F:148:ARG:HH11	1:F:200:VAL:HG21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:LYS:O	2:B:129:ASN:ND2	2.51	0.43
2:B:153:LYS:HA	2:B:153:LYS:HD2	1.69	0.43
2:B:217:LEU:HD13	2:B:225:LEU:HD11	1.99	0.43
3:D:45:CYS:SG	3:D:47:ASN:HB2	2.59	0.43
2:G:102:GLU:HG3	2:G:135:ARG:HH12	1.83	0.43
1:I:524:ILE:HG22	1:I:528:PRO:HB2	2.00	0.43
1:I:553:HIS:HA	1:I:597:PHE:CE1	2.53	0.43
1:H:510:THR:HG22	3:K:32:LEU:HG	2.00	0.43
1:O:383:ARG:H	1:O:383:ARG:HG2	1.51	0.43
1:T:363:ASP:HB3	1:T:366:PHE:HD1	1.83	0.43
1:T:500:GLY:HA2	1:T:503:LEU:HD23	1.99	0.43
2:S:37:VAL:HG21	2:S:82:LEU:HD23	2.00	0.43
1:V:148:ARG:HH11	1:V:200:VAL:HG21	1.84	0.43
1:V:212:MET:HE3	1:V:212:MET:HB3	1.63	0.43
2:B:499:VAL:HG21	2:B:561:TRP:CZ2	2.53	0.43
2:J:372:LYS:NZ	2:J:580:ARG:HE	2.17	0.43
2:J:499:VAL:HG21	2:J:561:TRP:CZ2	2.53	0.43
1:I:148:ARG:HH11	1:I:200:VAL:HG21	1.83	0.43
1:I:413:ASP:O	1:I:416:MET:HG3	2.19	0.43
1:H:606:ASN:HD21	3:K:22:PHE:HD1	1.66	0.43
1:H:634:LEU:HD23	1:H:634:LEU:HA	1.84	0.43
2:P:190:LYS:HG3	2:P:193:THR:HG22	2.01	0.43
2:N:144:SER:HB2	1:O:129:VAL:HB	2.01	0.43
1:M:168:MET:HE2	1:M:168:MET:HB3	1.90	0.43
1:M:413:ASP:O	1:M:416:MET:HG3	2.19	0.43
1:M:757:THR:C	1:M:759:GLU:H	2.26	0.43
1:O:31:ASN:OD1	1:O:72:LYS:NZ	2.51	0.43
1:O:510:THR:HG22	3:Q:32:LEU:HG	2.00	0.43
1:T:128:ARG:O	1:T:132:GLN:HB2	2.18	0.43
1:V:102:LEU:HD22	1:V:182:ALA:HB1	2.01	0.43
1:F:258:GLU:HB2	1:F:259:PRO:HD3	2.00	0.43
1:F:609:GLU:OE2	3:D:21:ARG:NH1	2.52	0.43
3:E:43:ALA:HB3	3:E:79:PHE:CE1	2.54	0.43
2:N:127:LYS:O	2:N:129:ASN:ND2	2.51	0.43
2:N:503:ASP:HB3	2:N:506:LYS:HB2	2.01	0.43
1:O:102:LEU:HD22	1:O:182:ALA:HB1	2.01	0.43
1:O:265:GLU:HB3	1:O:306:VAL:HG22	2.00	0.43
3:R:46:ARG:HH11	3:R:46:ARG:C	2.26	0.43
1:T:207:ALA:HB3	1:T:208:PRO:HD3	2.00	0.43
1:T:356:LEU:HA	1:T:360:PHE:CD2	2.54	0.43
1:T:426:ASP:OD1	1:T:426:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:527:ALA:HB3	1:T:528:PRO:HD3	2.00	0.43
2:U:228:VAL:HG12	2:U:229:THR:H	1.84	0.43
3:X:59:ASN:ND2	3:X:60:GLN:OE1	2.51	0.43
1:C:207:ALA:HB3	1:C:208:PRO:HD3	2.00	0.43
1:C:298:CYS:HA	1:C:301:LYS:HG2	2.01	0.43
1:F:240:ARG:O	1:F:243:GLU:HG3	2.19	0.43
1:F:483:THR:HG21	1:F:507:VAL:HG21	2.00	0.43
2:A:221:ARG:NH2	2:A:260:ARG:HE	2.16	0.43
2:A:225:LEU:HD23	2:A:225:LEU:HA	1.79	0.43
2:B:160:PHE:CE1	2:B:164:TYR:HA	2.54	0.43
2:G:190:LYS:HG3	2:G:193:THR:HG22	2.01	0.43
2:J:127:LYS:O	2:J:129:ASN:ND2	2.51	0.43
1:I:339:VAL:HB	1:I:391:PHE:HD1	1.83	0.43
1:H:102:LEU:HD22	1:H:182:ALA:HB1	2.01	0.43
2:P:37:VAL:HG21	2:P:82:LEU:HD23	2.00	0.43
2:P:45:HIS:HB2	2:P:48:VAL:HG22	2.01	0.43
2:P:553:GLN:O	2:P:562:SER:N	2.51	0.43
2:N:172:LEU:HD22	2:N:176:LEU:HD23	2.01	0.43
1:O:329:VAL:CB	1:O:341:TYR:CE1	3.01	0.43
1:T:153:ARG:HH21	1:T:200:VAL:HG13	1.84	0.43
2:U:379:GLU:HG3	2:U:379:GLU:O	2.18	0.43
1:V:419:PHE:HZ	1:V:425:LYS:HG3	1.84	0.43
1:V:520:PRO:HD2	1:V:551:GLN:HA	2.01	0.43
1:V:540:LEU:HA	1:V:546:ARG:HB2	2.00	0.43
1:V:606:ASN:HD21	3:X:22:PHE:HD1	1.66	0.43
1:C:473:MET:HG2	1:C:512:TYR:HB3	2.01	0.42
1:C:634:LEU:HD23	1:C:634:LEU:HA	1.90	0.42
1:F:238:GLU:O	1:F:242:ASN:ND2	2.41	0.42
2:B:228:VAL:HG12	2:B:229:THR:H	1.84	0.42
3:E:74:VAL:HB	3:E:102:GLU:HB2	2.01	0.42
2:J:160:PHE:CE1	2:J:164:TYR:HA	2.54	0.42
2:J:171:GLN:H	2:J:171:GLN:HG2	1.69	0.42
1:H:168:MET:HE2	1:H:168:MET:HB3	1.90	0.42
1:H:240:ARG:O	1:H:243:GLU:HG3	2.19	0.42
1:H:413:ASP:O	1:H:416:MET:HG3	2.18	0.42
1:H:419:PHE:HZ	1:H:425:LYS:HG3	1.84	0.42
2:P:231:ARG:H	2:P:231:ARG:HD2	1.84	0.42
2:N:153:LYS:HD2	2:N:153:LYS:HA	1.69	0.42
1:M:553:HIS:HA	1:M:597:PHE:HE1	1.84	0.42
1:T:74:TYR:CZ	1:T:142:LEU:HD22	2.54	0.42
1:T:148:ARG:HH11	1:T:200:VAL:HG21	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:298:CYS:HA	1:T:301:LYS:HG2	2.01	0.42
1:T:313:MET:HE2	1:T:313:MET:HB2	1.93	0.42
2:S:221:ARG:NH2	2:S:260:ARG:HE	2.16	0.42
2:U:369:VAL:O	2:U:389:SER:HA	2.18	0.42
1:V:298:CYS:HA	1:V:301:LYS:HG2	2.01	0.42
1:F:606:ASN:HD21	3:D:22:PHE:HD1	1.66	0.42
2:A:231:ARG:H	2:A:231:ARG:HD2	1.84	0.42
1:H:482:THR:HA	1:H:485:ASP:OD2	2.20	0.42
2:P:101:VAL:HB	2:P:124:LEU:HD11	2.00	0.42
2:U:503:ASP:HB3	2:U:506:LYS:HB2	2.01	0.42
1:F:128:ARG:O	1:F:132:GLN:HB2	2.19	0.42
2:G:160:PHE:HB2	2:G:166:GLN:HE22	1.85	0.42
1:H:426:ASP:OD2	1:H:699:ARG:NH2	2.53	0.42
1:H:609:GLU:HG3	1:H:610:LYS:H	1.83	0.42
3:L:74:VAL:HB	3:L:102:GLU:HB2	2.01	0.42
3:K:85:SER:O	3:K:89:LYS:NZ	2.50	0.42
1:M:680:LYS:HE3	1:M:680:LYS:HB3	1.91	0.42
3:R:43:ALA:HB3	3:R:79:PHE:CE1	2.54	0.42
1:T:378:LEU:HD13	1:T:421:PHE:O	2.19	0.42
1:T:553:HIS:HA	1:T:597:PHE:HE1	1.84	0.42
1:V:470:LEU:O	1:V:473:MET:HG3	2.20	0.42
1:V:482:THR:HA	1:V:485:ASP:OD2	2.20	0.42
3:X:35:TRP:HD1	3:X:76:ASN:HB2	1.85	0.42
3:X:86:ARG:O	3:X:89:LYS:HD2	2.18	0.42
1:C:153:ARG:HH21	1:C:200:VAL:HG13	1.84	0.42
1:C:553:HIS:HA	1:C:597:PHE:HE1	1.84	0.42
2:A:19:GLU:CG	2:B:9:ILE:HD13	2.49	0.42
2:A:202:LEU:HD13	2:A:213:LEU:HG	2.01	0.42
2:A:287:CYS:N	2:A:296:TYR:O	2.36	0.42
2:A:553:GLN:O	2:A:562:SER:N	2.51	0.42
2:G:37:VAL:HG21	2:G:82:LEU:HD23	2.00	0.42
1:I:153:ARG:HH21	1:I:200:VAL:HG13	1.84	0.42
1:H:245:ILE:HA	1:H:248:VAL:HG12	1.99	0.42
2:N:217:LEU:HD13	2:N:225:LEU:HD11	2.00	0.42
1:O:148:ARG:HH11	1:O:200:VAL:HG21	1.84	0.42
1:O:419:PHE:HZ	1:O:425:LYS:HG3	1.84	0.42
2:S:47:MET:HE3	2:U:45:HIS:CE1	2.54	0.42
2:S:190:LYS:HG3	2:S:193:THR:HG22	2.01	0.42
2:U:160:PHE:CE1	2:U:164:TYR:HA	2.54	0.42
2:U:372:LYS:NZ	2:U:580:ARG:HE	2.17	0.42
1:V:245:ILE:HA	1:V:248:VAL:HG12	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:532:PHE:HB2	3:X:27:TRP:CH2	2.55	0.42
2:A:92:GLY:HA3	2:B:10:ASN:HB3	2.01	0.42
2:A:151:SER:O	2:A:155:MET:HG2	2.20	0.42
2:B:81:THR:OG1	2:B:107:THR:HG21	2.20	0.42
2:G:45:HIS:HB2	2:G:48:VAL:HG22	2.01	0.42
2:J:81:THR:OG1	2:J:107:THR:HG21	2.20	0.42
1:I:546:ARG:NH2	3:L:35:TRP:HE1	2.18	0.42
1:I:553:HIS:HA	1:I:597:PHE:HE1	1.84	0.42
1:H:148:ARG:HH11	1:H:200:VAL:HG21	1.84	0.42
3:R:25:LYS:HD3	3:R:25:LYS:HA	1.87	0.42
2:S:160:PHE:HB2	2:S:166:GLN:HE22	1.85	0.42
2:S:282:LEU:H	2:S:282:LEU:HG	1.66	0.42
1:V:426:ASP:OD1	1:V:426:ASP:N	2.52	0.42
1:C:523:ASN:HA	1:C:529:ARG:HH21	1.85	0.42
2:B:503:ASP:HB3	2:B:506:LYS:HB2	2.01	0.42
1:I:374:PHE:O	1:I:378:LEU:HB2	2.19	0.42
2:P:550:VAL:HG23	2:P:566:HIS:HA	2.02	0.42
2:N:101:VAL:HG11	2:N:123:TYR:CD2	2.55	0.42
1:O:124:MET:HB3	1:O:124:MET:HE3	1.98	0.42
1:T:258:GLU:HB2	1:T:259:PRO:HD3	2.02	0.42
1:V:240:ARG:O	1:V:243:GLU:HG3	2.19	0.42
1:C:238:GLU:O	1:C:242:ASN:ND2	2.40	0.42
2:J:149:LYS:HB2	2:J:149:LYS:HE2	1.75	0.42
2:J:228:VAL:HG12	2:J:229:THR:H	1.84	0.42
1:I:717:MET:HE2	1:I:756:ARG:HD3	2.02	0.42
1:H:484:MET:HE3	1:H:506:ARG:HG2	2.01	0.42
1:H:525:PRO:HB2	1:H:528:PRO:HD2	2.01	0.42
1:H:609:GLU:OE2	3:K:21:ARG:NH1	2.52	0.42
2:P:151:SER:O	2:P:155:MET:HG2	2.20	0.42
1:M:74:TYR:CZ	1:M:142:LEU:HD22	2.54	0.42
1:O:255:SER:O	1:O:257:GLU:N	2.53	0.42
1:O:426:ASP:OD2	1:O:699:ARG:NH2	2.53	0.42
3:R:74:VAL:HB	3:R:102:GLU:HB2	2.01	0.42
2:S:45:HIS:HB2	2:S:48:VAL:HG22	2.01	0.42
2:S:550:VAL:HG23	2:S:566:HIS:HA	2.02	0.42
1:C:74:TYR:CZ	1:C:142:LEU:HD22	2.54	0.42
1:F:426:ASP:OD2	1:F:699:ARG:NH2	2.53	0.42
1:F:470:LEU:O	1:F:473:MET:HG3	2.20	0.42
2:A:24:PHE:HE2	2:B:51:THR:HG23	1.85	0.42
2:B:372:LYS:NZ	2:B:580:ARG:HE	2.17	0.42
2:G:202:LEU:HD13	2:G:213:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:258:GLU:HB2	1:I:259:PRO:HD3	2.02	0.42
2:P:221:ARG:NH2	2:P:260:ARG:HE	2.16	0.42
2:N:160:PHE:CE1	2:N:164:TYR:HA	2.54	0.42
2:N:497:VAL:HB	2:N:515:ILE:H	1.85	0.42
1:M:153:ARG:HH21	1:M:200:VAL:HG13	1.84	0.42
1:O:128:ARG:O	1:O:132:GLN:HB2	2.19	0.42
1:T:482:THR:HA	1:T:485:ASP:OD2	2.20	0.42
2:S:151:SER:O	2:S:155:MET:HG2	2.20	0.42
2:B:172:LEU:HD22	2:B:176:LEU:HD23	2.01	0.42
2:J:542:HIS:HB2	2:J:545:GLU:HB2	2.02	0.42
1:H:128:ARG:O	1:H:132:GLN:HB2	2.19	0.42
1:H:131:VAL:HG12	1:H:136:VAL:HG23	2.02	0.42
1:H:255:SER:O	1:H:257:GLU:N	2.53	0.42
3:K:48:HIS:HB3	3:K:50:MET:O	2.20	0.42
2:N:81:THR:OG1	2:N:107:THR:HG21	2.20	0.42
1:M:473:MET:SD	1:M:512:TYR:HB3	2.60	0.42
1:M:482:THR:HA	1:M:485:ASP:OD2	2.20	0.42
1:M:532:PHE:HB2	3:R:27:TRP:CH2	2.55	0.42
1:T:378:LEU:CD2	1:T:422:MET:CB	2.80	0.42
2:U:101:VAL:HG11	2:U:123:TYR:CD2	2.55	0.42
2:U:172:LEU:HD22	2:U:176:LEU:HD23	2.01	0.42
1:V:255:SER:O	1:V:257:GLU:N	2.53	0.42
3:X:80:HIS:HB2	3:X:83:CYS:SG	2.60	0.42
1:C:258:GLU:HB2	1:C:259:PRO:HD3	2.02	0.42
1:F:318:SER:HB2	1:F:373:ASP:OD2	2.20	0.42
2:A:190:LYS:HG3	2:A:193:THR:HG22	2.01	0.42
3:E:46:ARG:HH11	3:E:46:ARG:C	2.26	0.42
2:G:121:ARG:HD3	2:G:145:CYS:SG	2.60	0.42
2:G:148:LEU:HD12	2:G:148:LEU:HA	1.92	0.42
2:G:221:ARG:NH1	2:G:258:LYS:H	2.16	0.42
2:J:497:VAL:HB	2:J:515:ILE:H	1.85	0.42
2:P:24:PHE:CE2	2:N:51:THR:HG23	2.55	0.42
1:M:240:ARG:O	1:M:243:GLU:HG3	2.20	0.42
1:O:298:CYS:HA	1:O:301:LYS:HG2	2.01	0.42
1:O:520:PRO:HG2	1:O:552:HIS:H	1.85	0.42
1:T:473:MET:SD	1:T:512:TYR:HB3	2.60	0.42
2:S:50:ALA:CB	2:U:30:PHE:CZ	3.03	0.42
2:S:286:VAL:HA	2:S:297:LYS:HA	2.02	0.42
2:U:81:THR:OG1	2:U:107:THR:HG21	2.20	0.42
1:V:131:VAL:HG12	1:V:136:VAL:HG23	2.02	0.42
1:V:426:ASP:OD2	1:V:699:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:37:ILE:HD12	3:W:78:ALA:HB3	2.02	0.42
1:F:58:TYR:CB	2:B:55:TYR:HE1	2.33	0.41
1:F:131:VAL:HG12	1:F:136:VAL:HG23	2.02	0.41
2:A:286:VAL:HA	2:A:297:LYS:HA	2.01	0.41
2:B:346:THR:HG22	2:B:369:VAL:HB	2.02	0.41
3:D:80:HIS:HB2	3:D:83:CYS:SG	2.60	0.41
2:J:101:VAL:HG11	2:J:123:TYR:CD2	2.55	0.41
2:J:172:LEU:HD22	2:J:176:LEU:HD23	2.01	0.41
1:I:74:TYR:CZ	1:I:142:LEU:HD22	2.54	0.41
1:I:240:ARG:O	1:I:243:GLU:HG3	2.20	0.41
1:I:473:MET:SD	1:I:512:TYR:HB3	2.60	0.41
1:I:484:MET:SD	1:I:504:THR:HA	2.60	0.41
1:I:516:GLN:H	1:I:516:GLN:CD	2.24	0.41
1:I:527:ALA:HB3	1:I:528:PRO:HD3	2.00	0.41
2:P:160:PHE:HB2	2:P:166:GLN:HE22	1.85	0.41
1:M:31:ASN:OD1	1:M:72:LYS:NZ	2.53	0.41
1:M:124:MET:HB3	1:M:124:MET:HE3	1.97	0.41
1:M:386:GLU:OE1	1:M:386:GLU:N	2.46	0.41
1:O:336:LYS:H	1:O:336:LYS:HG3	1.58	0.41
1:T:638:LYS:HG3	1:T:639:PRO:O	2.20	0.41
2:S:231:ARG:H	2:S:231:ARG:HD2	1.84	0.41
1:V:718:GLN:O	1:V:761:ARG:NH1	2.47	0.41
1:C:311:LYS:HE3	1:C:311:LYS:HB3	1.88	0.41
1:F:426:ASP:OD1	1:F:426:ASP:N	2.52	0.41
1:F:609:GLU:HG3	1:F:610:LYS:H	1.83	0.41
2:A:30:PHE:CE1	2:B:50:ALA:CB	3.02	0.41
3:D:33:TRP:O	3:D:76:ASN:ND2	2.53	0.41
3:D:36:ASP:HB2	3:D:77:HIS:NE2	2.33	0.41
2:G:231:ARG:H	2:G:231:ARG:HD2	1.84	0.41
2:P:286:VAL:HA	2:P:297:LYS:HA	2.02	0.41
1:M:638:LYS:HG3	1:M:639:PRO:O	2.20	0.41
1:O:345:LEU:HD11	1:O:377:PHE:HE1	1.84	0.41
3:Q:48:HIS:HB3	3:Q:50:MET:O	2.20	0.41
3:Q:59:ASN:ND2	3:Q:60:GLN:OE1	2.51	0.41
1:T:31:ASN:OD1	1:T:72:LYS:NZ	2.53	0.41
1:V:342:ILE:HG13	1:V:387:TYR:O	2.20	0.41
3:X:48:HIS:HB3	3:X:50:MET:O	2.20	0.41
1:C:700:LYS:HG2	1:C:744:ARG:HD2	2.02	0.41
1:F:55:GLU:HA	2:B:59:MET:HE1	2.02	0.41
1:F:125:TYR:CD1	2:B:112:GLN:NE2	2.83	0.41
1:F:298:CYS:HA	1:F:301:LYS:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:482:THR:HA	1:F:485:ASP:OD2	2.20	0.41
2:A:160:PHE:HB2	2:A:166:GLN:HE22	1.85	0.41
2:G:137:LEU:HB2	2:G:152:ALA:HB1	2.03	0.41
1:H:236:LYS:HE3	1:H:236:LYS:HB2	1.93	0.41
2:P:202:LEU:HD13	2:P:213:LEU:HG	2.01	0.41
2:P:549:TYR:OH	2:P:575:LEU:N	2.49	0.41
1:M:258:GLU:HB2	1:M:259:PRO:HD3	2.02	0.41
1:M:532:PHE:HB2	3:R:27:TRP:HH2	1.86	0.41
1:M:546:ARG:HA	3:R:33:TRP:HB2	2.02	0.41
1:O:131:VAL:HG12	1:O:136:VAL:HG23	2.02	0.41
1:O:313:MET:HE2	1:O:313:MET:HB2	1.93	0.41
1:O:634:LEU:HD23	1:O:634:LEU:HA	1.84	0.41
2:U:326:PRO:HA	2:U:344:PHE:HA	2.03	0.41
1:C:31:ASN:OD1	1:C:72:LYS:NZ	2.53	0.41
1:C:240:ARG:O	1:C:243:GLU:HG3	2.20	0.41
1:C:374:PHE:HA	1:C:377:PHE:HD1	1.86	0.41
1:F:255:SER:O	1:F:257:GLU:N	2.53	0.41
1:F:288:LEU:HD12	1:F:288:LEU:HA	1.90	0.41
2:B:101:VAL:HG11	2:B:123:TYR:CD2	2.55	0.41
2:G:48:VAL:HA	2:G:51:THR:HG22	2.03	0.41
2:G:151:SER:O	2:G:155:MET:HG2	2.20	0.41
2:G:550:VAL:HG23	2:G:566:HIS:HA	2.02	0.41
1:I:168:MET:HE2	1:I:168:MET:HB3	1.90	0.41
1:I:298:CYS:HA	1:I:301:LYS:HG2	2.01	0.41
1:I:356:LEU:HD21	1:I:367:LYS:HG2	2.01	0.41
1:I:680:LYS:HE3	1:I:680:LYS:HB3	1.91	0.41
1:H:212:MET:HE3	1:H:212:MET:HB3	1.63	0.41
3:K:33:TRP:O	3:K:76:ASN:ND2	2.54	0.41
1:M:298:CYS:HA	1:M:301:LYS:HG2	2.01	0.41
1:O:470:LEU:O	1:O:473:MET:HG3	2.20	0.41
1:O:482:THR:HA	1:O:485:ASP:OD2	2.20	0.41
1:T:346:LEU:HD21	1:T:414:LYS:CA	2.49	0.41
2:S:137:LEU:HB2	2:S:152:ALA:HB1	2.03	0.41
2:S:202:LEU:HD13	2:S:213:LEU:HG	2.01	0.41
2:S:443:PHE:HE1	2:S:445:ARG:HH21	1.69	0.41
2:U:269:MET:HE3	2:U:530:ILE:HD12	2.03	0.41
1:V:541:ALA:O	1:V:542:LYS:C	2.63	0.41
1:C:426:ASP:N	1:C:426:ASP:OD1	2.52	0.41
2:B:326:PRO:HA	2:B:344:PHE:HA	2.03	0.41
2:J:156:VAL:O	2:J:160:PHE:HB3	2.20	0.41
1:I:31:ASN:OD1	1:I:72:LYS:NZ	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:388:LEU:HD21	1:I:419:PHE:HB2	2.03	0.41
1:I:482:THR:HA	1:I:485:ASP:OD2	2.20	0.41
1:I:516:GLN:HG2	1:I:517:SER:N	2.30	0.41
1:H:337:ASN:HB3	1:H:340:ASP:HB2	2.03	0.41
3:R:37:ILE:HD12	3:R:78:ALA:HB3	2.02	0.41
1:T:133:GLN:OE1	2:S:144:SER:HB3	2.18	0.41
1:T:240:ARG:O	1:T:243:GLU:HG3	2.20	0.41
1:T:484:MET:SD	1:T:504:THR:HA	2.60	0.41
2:U:366:MET:HE2	2:U:366:MET:HB3	1.84	0.41
1:F:500:GLY:HA2	1:F:503:LEU:HD23	2.03	0.41
3:D:59:ASN:ND2	3:D:60:GLN:OE1	2.51	0.41
2:P:137:LEU:HB2	2:P:152:ALA:HB1	2.03	0.41
2:P:297:LYS:NZ	2:P:593:GLU:O	2.54	0.41
2:N:156:VAL:O	2:N:160:PHE:HB3	2.21	0.41
1:O:329:VAL:CG2	1:O:341:TYR:CZ	3.01	0.41
1:O:390:LEU:HD22	1:O:435:HIS:NE2	2.36	0.41
2:S:81:THR:OG1	2:S:107:THR:HG21	2.21	0.41
2:U:225:LEU:HD12	2:U:225:LEU:HA	1.94	0.41
2:U:497:VAL:HB	2:U:515:ILE:H	1.85	0.41
3:W:25:LYS:HA	3:W:25:LYS:HD3	1.87	0.41
1:C:625:ARG:H	1:C:625:ARG:HG2	1.75	0.41
1:F:287:MET:HE3	1:F:296:LEU:HD22	2.03	0.41
1:F:390:LEU:HD22	1:F:435:HIS:NE2	2.36	0.41
1:F:646:LYS:HE3	1:F:659:PHE:HE1	1.86	0.41
1:H:500:GLY:HA2	1:H:503:LEU:HD23	2.03	0.41
2:N:326:PRO:HA	2:N:344:PHE:HA	2.03	0.41
1:M:700:LYS:HG2	1:M:744:ARG:HD2	2.03	0.41
1:O:426:ASP:OD1	1:O:426:ASP:N	2.53	0.41
3:Q:80:HIS:HB2	3:Q:83:CYS:SG	2.60	0.41
1:T:133:GLN:NE2	2:S:144:SER:CB	2.83	0.41
2:U:156:VAL:O	2:U:160:PHE:HB3	2.20	0.41
1:V:476:ASP:OD2	1:V:509:THR:HG23	2.21	0.41
3:W:49:ILE:HD12	3:W:49:ILE:HA	1.98	0.41
1:F:593:GLN:HE21	1:F:593:GLN:HB3	1.68	0.41
1:F:680:LYS:HE3	1:F:680:LYS:HB3	1.91	0.41
2:A:297:LYS:NZ	2:A:593:GLU:O	2.54	0.41
2:A:550:VAL:HG23	2:A:566:HIS:HA	2.02	0.41
2:B:497:VAL:HB	2:B:515:ILE:H	1.85	0.41
3:E:37:ILE:HD12	3:E:78:ALA:HB3	2.02	0.41
2:G:57:ARG:HH22	2:J:24:PHE:HZ	1.69	0.41
2:G:539:ARG:HH22	2:G:577:ARG:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:539:ARG:HD3	2:J:549:TYR:CZ	2.56	0.41
1:H:168:MET:SD	1:H:183:ILE:HD11	2.61	0.41
1:O:240:ARG:O	1:O:243:GLU:HG3	2.19	0.41
2:S:206:THR:O	2:S:207:GLU:HB2	2.21	0.41
2:S:326:PRO:HA	2:S:344:PHE:HA	2.03	0.41
1:V:124:MET:HB3	1:V:124:MET:HE3	1.97	0.41
1:C:638:LYS:HG3	1:C:639:PRO:O	2.20	0.41
1:F:168:MET:SD	1:F:183:ILE:HD11	2.61	0.41
2:A:178:ILE:HG23	2:A:219:GLN:HE21	1.86	0.41
2:B:156:VAL:O	2:B:160:PHE:HB3	2.20	0.41
2:B:266:GLU:HB2	2:B:268:MET:HE3	2.03	0.41
3:D:35:TRP:HD1	3:D:76:ASN:HB2	1.85	0.41
2:G:56:PHE:HA	2:G:59:MET:HB3	2.03	0.41
2:G:286:VAL:HA	2:G:297:LYS:HA	2.02	0.41
2:J:258:LYS:HE2	2:J:258:LYS:HB2	1.97	0.41
1:I:324:GLN:CG	1:I:348:LEU:CD2	2.88	0.41
1:I:426:ASP:N	1:I:426:ASP:OD1	2.52	0.41
1:H:298:CYS:HA	1:H:301:LYS:HG2	2.01	0.41
1:H:390:LEU:HD22	1:H:435:HIS:NE2	2.36	0.41
1:H:470:LEU:O	1:H:473:MET:HG3	2.20	0.41
1:H:646:LYS:HE3	1:H:659:PHE:HE1	1.86	0.41
3:L:37:ILE:HD12	3:L:78:ALA:HB3	2.02	0.41
2:P:45:HIS:CB	2:N:47:MET:HE1	2.51	0.41
2:P:81:THR:O	2:P:84:ILE:HG22	2.20	0.41
2:P:81:THR:OG1	2:P:107:THR:HG21	2.21	0.41
2:N:269:MET:HE3	2:N:530:ILE:HD12	2.03	0.41
2:N:289:SER:HG	2:N:294:LYS:H	1.62	0.41
2:N:346:THR:HG22	2:N:369:VAL:HB	2.02	0.41
2:N:542:HIS:HB2	2:N:545:GLU:HB2	2.02	0.41
1:M:265:GLU:HB3	1:M:306:VAL:HG22	2.03	0.41
1:M:338:PRO:HG3	1:M:387:TYR:CE1	2.56	0.41
1:M:516:GLN:HG2	1:M:517:SER:N	2.30	0.41
1:O:212:MET:HE3	1:O:212:MET:HB3	1.63	0.41
1:O:371:ALA:HB2	1:O:421:PHE:HE1	1.78	0.41
1:O:484:MET:HE3	1:O:506:ARG:HG2	2.01	0.41
3:Q:35:TRP:HD1	3:Q:76:ASN:HB2	1.85	0.41
1:T:388:LEU:HD21	1:T:419:PHE:HB2	2.03	0.41
1:T:516:GLN:HG2	1:T:517:SER:N	2.30	0.41
1:T:631:LEU:HD12	1:T:631:LEU:HA	1.94	0.41
1:T:680:LYS:HE3	1:T:680:LYS:HB3	1.91	0.41
2:S:221:ARG:NH1	2:S:258:LYS:H	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:539:ARG:HH22	2:S:577:ARG:HD3	1.86	0.41
2:U:539:ARG:HD3	2:U:549:TYR:CZ	2.56	0.41
2:U:542:HIS:HB2	2:U:545:GLU:HB2	2.02	0.41
1:V:129:VAL:O	1:V:133:GLN:NE2	2.43	0.41
1:V:153:ARG:HH21	1:V:200:VAL:HG13	1.86	0.41
1:V:168:MET:HE2	1:V:168:MET:HB3	1.90	0.41
1:V:337:ASN:HB3	1:V:340:ASP:HB2	2.03	0.41
1:V:559:LEU:HD22	1:V:602:LEU:HD13	2.02	0.41
1:V:647:GLU:HB2	1:V:648:PRO:HD3	2.03	0.41
1:I:212:MET:HE3	1:I:212:MET:HB3	2.00	0.41
1:I:346:LEU:HD21	1:I:414:LYS:HB2	1.99	0.41
1:I:346:LEU:CD1	1:I:414:LYS:O	2.68	0.41
1:I:363:ASP:HB3	1:I:366:PHE:CD1	2.54	0.41
2:P:24:PHE:CE2	2:N:51:THR:HG22	2.56	0.41
1:M:765:THR:C	1:M:767:VAL:H	2.28	0.41
1:O:153:ARG:HH21	1:O:200:VAL:HG13	1.86	0.41
1:O:547:GLN:OE1	1:O:547:GLN:N	2.54	0.41
1:T:717:MET:HE2	1:T:756:ARG:HD3	2.02	0.41
2:S:297:LYS:NZ	2:S:593:GLU:O	2.54	0.41
1:V:390:LEU:HD22	1:V:435:HIS:NE2	2.36	0.41
3:X:33:TRP:O	3:X:76:ASN:ND2	2.54	0.41
1:F:484:MET:HE3	1:F:506:ARG:HG2	2.01	0.40
2:A:539:ARG:HH22	2:A:577:ARG:HD3	1.86	0.40
2:B:269:MET:HE3	2:B:530:ILE:HD12	2.02	0.40
2:B:542:HIS:HB2	2:B:545:GLU:HB2	2.02	0.40
2:J:87:THR:O	2:J:91:THR:HG22	2.21	0.40
2:J:269:MET:HE3	2:J:530:ILE:HD12	2.03	0.40
1:I:300:TYR:CD2	1:I:360:PHE:HA	2.57	0.40
1:I:625:ARG:H	1:I:625:ARG:HG2	1.75	0.40
1:I:700:LYS:HG2	1:I:744:ARG:HD2	2.02	0.40
1:H:311:LYS:HE3	1:H:311:LYS:HB3	1.89	0.40
1:H:559:LEU:HD22	1:H:602:LEU:HD13	2.02	0.40
3:K:35:TRP:HD1	3:K:76:ASN:HB2	1.85	0.40
2:P:178:ILE:HG23	2:P:219:GLN:HE21	1.86	0.40
2:P:206:THR:O	2:P:207:GLU:HB2	2.21	0.40
2:P:380:GLY:O	2:P:404:THR:OG1	2.34	0.40
1:M:704:GLU:O	1:M:707:ILE:HG22	2.21	0.40
1:O:455:ILE:HG22	1:O:470:LEU:HD22	2.04	0.40
3:Q:33:TRP:O	3:Q:76:ASN:ND2	2.53	0.40
1:T:248:VAL:O	1:T:256:THR:HG21	2.21	0.40
1:T:704:GLU:O	1:T:707:ILE:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:178:ILE:HG23	2:S:219:GLN:HE21	1.86	0.40
1:V:168:MET:SD	1:V:183:ILE:HD11	2.61	0.40
1:C:168:MET:SD	1:C:183:ILE:HD11	2.62	0.40
1:C:425:LYS:HE3	1:C:466:PHE:HE2	1.85	0.40
1:F:547:GLN:N	1:F:547:GLN:OE1	2.54	0.40
2:B:87:THR:O	2:B:91:THR:HG22	2.21	0.40
2:B:382:ILE:HB	2:B:402:TYR:HB3	2.04	0.40
2:B:539:ARG:HD3	2:B:549:TYR:CZ	2.56	0.40
2:J:382:ILE:HB	2:J:402:TYR:HB3	2.04	0.40
1:I:508:LEU:HB3	1:I:513:TRP:CD1	2.56	0.40
1:I:638:LYS:HG3	1:I:639:PRO:O	2.20	0.40
1:H:455:ILE:HG22	1:H:470:LEU:HD22	2.04	0.40
2:P:190:LYS:HB2	2:P:192:GLU:OE1	2.22	0.40
2:N:225:LEU:HD12	2:N:225:LEU:HA	1.94	0.40
1:M:508:LEU:HB3	1:M:513:TRP:CD1	2.56	0.40
1:O:168:MET:SD	1:O:183:ILE:HD11	2.61	0.40
1:O:559:LEU:HD22	1:O:602:LEU:HD13	2.02	0.40
1:T:374:PHE:HA	1:T:377:PHE:HD1	1.86	0.40
1:T:546:ARG:NH2	3:W:35:TRP:HE1	2.18	0.40
1:T:700:LYS:HG2	1:T:744:ARG:HD2	2.03	0.40
2:S:81:THR:O	2:S:84:ILE:HG22	2.20	0.40
2:U:258:LYS:HE2	2:U:258:LYS:HB2	1.97	0.40
2:U:346:THR:HG22	2:U:369:VAL:HB	2.02	0.40
1:V:614:GLU:OE1	1:V:617:GLN:NE2	2.54	0.40
1:C:647:GLU:HB2	1:C:648:PRO:HD3	2.04	0.40
1:F:419:PHE:HZ	1:F:425:LYS:HG3	1.84	0.40
1:F:559:LEU:HD22	1:F:602:LEU:HD13	2.02	0.40
1:F:647:GLU:HB2	1:F:648:PRO:HD3	2.03	0.40
2:B:413:SER:HB3	2:B:442:TYR:HE1	1.86	0.40
1:I:124:MET:HB3	1:I:124:MET:HE3	1.97	0.40
1:I:168:MET:SD	1:I:183:ILE:HD11	2.61	0.40
1:I:704:GLU:O	1:I:707:ILE:HG22	2.21	0.40
2:P:19:GLU:HG2	2:N:9:ILE:HD13	2.03	0.40
2:N:29:LEU:HB3	2:N:30:PHE:HD1	1.87	0.40
2:N:413:SER:HG	2:N:449:TRP:CD1	2.40	0.40
1:O:389:SER:O	1:O:392:ILE:HG22	2.21	0.40
1:T:508:LEU:HB3	1:T:513:TRP:CD1	2.56	0.40
2:S:320:ILE:HD13	2:S:320:ILE:HA	1.99	0.40
2:S:539:ARG:HD3	2:S:549:TYR:CZ	2.56	0.40
2:U:87:THR:O	2:U:91:THR:HG22	2.21	0.40
1:V:374:PHE:HA	1:V:377:PHE:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:326:PRO:HA	2:J:344:PHE:HA	2.03	0.40
3:L:48:HIS:HB3	3:L:50:MET:O	2.22	0.40
3:L:50:MET:HE3	3:L:50:MET:HB3	1.97	0.40
3:K:80:HIS:HB2	3:K:83:CYS:SG	2.60	0.40
2:P:326:PRO:HA	2:P:344:PHE:HA	2.03	0.40
1:O:341:TYR:HH	1:O:377:PHE:HE2	1.59	0.40
1:T:168:MET:HE2	1:T:168:MET:HB3	1.90	0.40
1:T:168:MET:SD	1:T:183:ILE:HD11	2.62	0.40
2:S:56:PHE:HA	2:S:59:MET:HB3	2.03	0.40
2:S:233:TRP:O	2:S:237:LEU:N	2.55	0.40
1:V:646:LYS:HE3	1:V:659:PHE:HE1	1.86	0.40
1:C:265:GLU:HB3	1:C:306:VAL:HG22	2.03	0.40
1:F:455:ILE:HG22	1:F:470:LEU:HD22	2.04	0.40
2:A:18:LEU:CD2	2:B:14:ALA:N	2.85	0.40
2:G:191:GLU:H	2:G:191:GLU:HG3	1.75	0.40
2:J:346:THR:HG22	2:J:369:VAL:HB	2.02	0.40
1:I:647:GLU:HB2	1:I:648:PRO:HD3	2.03	0.40
2:N:382:ILE:HB	2:N:402:TYR:HB3	2.04	0.40
1:M:388:LEU:HD21	1:M:419:PHE:HB2	2.03	0.40
1:M:609:GLU:OE2	3:R:21:ARG:NH1	2.55	0.40
2:S:371:ILE:N	2:S:387:GLY:O	2.52	0.40
1:V:389:SER:O	1:V:392:ILE:HG22	2.21	0.40
1:V:392:ILE:HD12	1:V:392:ILE:HA	1.96	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	C	716/768 (93%)	655 (92%)	61 (8%)	0	100	100
1	F	716/768 (93%)	655 (92%)	60 (8%)	1 (0%)	48	83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	716/768 (93%)	654 (91%)	61 (8%)	1 (0%)	48	83
1	I	716/768 (93%)	657 (92%)	58 (8%)	1 (0%)	48	83
1	M	716/768 (93%)	656 (92%)	60 (8%)	0	100	100
1	O	716/768 (93%)	650 (91%)	61 (8%)	5 (1%)	18	56
1	T	716/768 (93%)	656 (92%)	59 (8%)	1 (0%)	48	83
1	V	716/768 (93%)	647 (90%)	67 (9%)	2 (0%)	36	72
2	A	555/623 (89%)	521 (94%)	32 (6%)	2 (0%)	30	67
2	B	557/623 (89%)	532 (96%)	25 (4%)	0	100	100
2	G	555/623 (89%)	520 (94%)	34 (6%)	1 (0%)	43	78
2	J	557/623 (89%)	533 (96%)	24 (4%)	0	100	100
2	N	557/623 (89%)	534 (96%)	23 (4%)	0	100	100
2	P	555/623 (89%)	516 (93%)	39 (7%)	0	100	100
2	S	555/623 (89%)	520 (94%)	32 (6%)	3 (0%)	24	63
2	U	557/623 (89%)	531 (95%)	25 (4%)	1 (0%)	43	78
3	D	87/108 (81%)	67 (77%)	19 (22%)	1 (1%)	11	46
3	E	87/108 (81%)	75 (86%)	11 (13%)	1 (1%)	11	46
3	K	87/108 (81%)	70 (80%)	16 (18%)	1 (1%)	11	46
3	L	87/108 (81%)	75 (86%)	11 (13%)	1 (1%)	11	46
3	Q	87/108 (81%)	70 (80%)	16 (18%)	1 (1%)	11	46
3	R	87/108 (81%)	75 (86%)	11 (13%)	1 (1%)	11	46
3	W	87/108 (81%)	75 (86%)	11 (13%)	1 (1%)	11	46
3	X	87/108 (81%)	70 (80%)	16 (18%)	1 (1%)	11	46
All	All	10872/11992 (91%)	10014 (92%)	832 (8%)	26 (0%)	44	78

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S	279	PRO
2	S	515	ILE
1	O	501	VAL
2	U	388	ASP
2	G	144	SER
1	H	520	PRO
1	O	361	ASN

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Mol	Chain	Res	Type
1	V	520	PRO
1	F	330	SER
1	O	494	THR
1	T	335	GLY
1	O	336	LYS
1	O	362	ASN
1	V	496	VAL
3	D	38	VAL
1	I	335	GLY
3	K	38	VAL
3	Q	38	VAL
3	X	38	VAL
3	E	38	VAL
3	L	38	VAL
3	R	38	VAL
3	W	38	VAL
2	A	390	VAL
2	S	278	ASN
2	A	516	PRO

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	C	596/693 (86%)	579 (97%)	17 (3%)	37	58
1	F	636/693 (92%)	601 (94%)	35 (6%)	19	41
1	H	613/693 (88%)	604 (98%)	9 (2%)	57	72
1	I	626/693 (90%)	606 (97%)	20 (3%)	34	55
1	M	613/693 (88%)	594 (97%)	19 (3%)	35	56
1	O	621/693 (90%)	596 (96%)	25 (4%)	28	49
1	T	624/693 (90%)	609 (98%)	15 (2%)	43	64
1	V	595/693 (86%)	576 (97%)	19 (3%)	34	55
2	A	461/560 (82%)	456 (99%)	5 (1%)	65	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	464/560 (83%)	460 (99%)	4 (1%)	70	79
2	G	469/560 (84%)	464 (99%)	5 (1%)	65	76
2	J	460/560 (82%)	457 (99%)	3 (1%)	76	81
2	N	472/560 (84%)	463 (98%)	9 (2%)	50	67
2	P	462/560 (82%)	460 (100%)	2 (0%)	84	84
2	S	473/560 (84%)	472 (100%)	1 (0%)	87	87
2	U	463/560 (83%)	459 (99%)	4 (1%)	70	79
3	D	77/90 (86%)	71 (92%)	6 (8%)	11	32
3	E	77/90 (86%)	77 (100%)	0	100	100
3	K	76/90 (84%)	76 (100%)	0	100	100
3	L	68/90 (76%)	68 (100%)	0	100	100
3	Q	66/90 (73%)	66 (100%)	0	100	100
3	R	77/90 (86%)	77 (100%)	0	100	100
3	W	78/90 (87%)	78 (100%)	0	100	100
3	X	77/90 (86%)	77 (100%)	0	100	100
All	All	9244/10744 (86%)	9046 (98%)	198 (2%)	46	65

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	351	ARG
1	C	378	LEU
1	C	379	ASN
1	C	380	LEU
1	C	382	SER
1	C	383	ARG
1	C	384	SER
1	C	458	LEU
1	C	462	CYS
1	C	464	CYS
1	C	465	GLN
1	C	521	LYS
1	C	523	ASN
1	C	524	ILE
1	C	548	LEU
1	C	549	THR
1	C	665	PHE

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Mol	Chain	Res	Type
1	F	47	LYS
1	F	49	ASN
1	F	50	SER
1	F	52	LEU
1	F	68	LYS
1	F	203	GLU
1	F	212	MET
1	F	213	SER
1	F	288	LEU
1	F	289	LYS
1	F	328	LEU
1	F	329	VAL
1	F	332	GLU
1	F	336	LYS
1	F	339	VAL
1	F	345	LEU
1	F	349	LYS
1	F	351	ARG
1	F	354	ARG
1	F	356	LEU
1	F	357	LEU
1	F	359	SER
1	F	364	ARG
1	F	367	LYS
1	F	369	THR
1	F	370	ILE
1	F	373	ASP
1	F	375	GLU
1	F	378	LEU
1	F	379	ASN
1	F	380	LEU
1	F	381	ASN
1	F	383	ARG
1	F	384	SER
1	F	748	LEU
2	A	44	CYS
2	A	45	HIS
2	A	48	VAL
2	A	49	LEU
2	A	82	LEU
2	B	389	SER
2	B	397	ARG

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Mol	Chain	Res	Type
2	B	398	THR
2	B	399	VAL
3	D	42	CYS
3	D	44	ILE
3	D	47	ASN
3	D	49	ILE
3	D	50	MET
3	D	52	LEU
2	G	101	VAL
2	G	104	LEU
2	G	396	ARG
2	G	515	ILE
2	G	524	CYS
2	J	397	ARG
2	J	398	THR
2	J	399	VAL
1	I	68	LYS
1	I	256	THR
1	I	329	VAL
1	I	330	SER
1	I	332	GLU
1	I	336	LYS
1	I	339	VAL
1	I	341	TYR
1	I	351	ARG
1	I	357	LEU
1	I	358	GLU
1	I	359	SER
1	I	364	ARG
1	I	378	LEU
1	I	379	ASN
1	I	380	LEU
1	I	381	ASN
1	I	383	ARG
1	I	550	LEU
1	I	665	PHE
1	H	203	GLU
1	H	212	MET
1	H	213	SER
1	H	380	LEU
1	H	517	SER
1	H	521	LYS

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Mol	Chain	Res	Type
1	H	547	GLN
1	H	548	LEU
1	H	748	LEU
2	P	51	THR
2	P	52	CYS
2	N	141	ASP
2	N	281	SER
2	N	282	LEU
2	N	389	SER
2	N	395	ASN
2	N	396	ARG
2	N	397	ARG
2	N	398	THR
2	N	399	VAL
1	M	351	ARG
1	M	377	PHE
1	M	378	LEU
1	M	379	ASN
1	M	380	LEU
1	M	381	ASN
1	M	382	SER
1	M	503	LEU
1	M	504	THR
1	M	505	VAL
1	M	521	LYS
1	M	523	ASN
1	M	524	ILE
1	M	550	LEU
1	M	665	PHE
1	M	761	ARG
1	M	762	LYS
1	M	763	VAL
1	M	765	THR
1	O	68	LYS
1	O	203	GLU
1	O	212	MET
1	O	213	SER
1	O	317	MET
1	O	319	SER
1	O	330	SER
1	O	332	GLU
1	O	336	LYS

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Mol	Chain	Res	Type
1	O	339	VAL
1	O	348	LEU
1	O	351	ARG
1	O	353	ASP
1	O	354	ARG
1	O	357	LEU
1	O	359	SER
1	O	364	ARG
1	O	379	ASN
1	O	380	LEU
1	O	382	SER
1	O	383	ARG
1	O	384	SER
1	O	498	LEU
1	O	501	VAL
1	O	748	LEU
1	T	256	THR
1	T	326	LYS
1	T	328	LEU
1	T	330	SER
1	T	332	GLU
1	T	336	LYS
1	T	351	ARG
1	T	358	GLU
1	T	359	SER
1	T	362	ASN
1	T	364	ARG
1	T	380	LEU
1	T	381	ASN
1	T	383	ARG
1	T	665	PHE
2	S	282	LEU
2	U	275	SER
2	U	396	ARG
2	U	397	ARG
2	U	399	VAL
1	V	203	GLU
1	V	212	MET
1	V	213	SER
1	V	351	ARG
1	V	378	LEU
1	V	379	ASN

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Mol	Chain	Res	Type
1	V	380	LEU
1	V	381	ASN
1	V	384	SER
1	V	458	LEU
1	V	466	PHE
1	V	517	SER
1	V	521	LYS
1	V	524	ILE
1	V	546	ARG
1	V	547	GLN
1	V	548	LEU
1	V	549	THR
1	V	748	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	87	ASN
1	C	112	HIS
1	C	163	GLN
1	C	286	HIS
1	C	379	ASN
1	C	606	ASN
1	C	618	GLN
1	C	657	HIS
1	F	87	ASN
1	F	163	GLN
1	F	362	ASN
1	F	423	GLN
1	F	553	HIS
1	F	606	ASN
1	F	618	GLN
1	F	718	GLN
1	F	719	HIS
2	A	45	HIS
2	A	71	HIS
2	A	93	ASN
2	A	356	GLN
2	A	357	GLN
2	B	129	ASN
2	B	187	ASN
2	B	205	ASN

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Mol	Chain	Res	Type
2	B	219	GLN
2	B	230	GLN
2	B	235	GLN
2	B	357	GLN
3	E	41	ASN
3	E	57	GLN
3	D	47	ASN
3	D	48	HIS
2	G	8	GLN
2	G	306	HIS
2	G	356	GLN
2	G	357	GLN
2	J	129	ASN
2	J	187	ASN
2	J	205	ASN
2	J	219	GLN
2	J	230	GLN
2	J	235	GLN
2	J	357	GLN
1	I	87	ASN
1	I	163	GLN
1	I	286	HIS
1	I	423	GLN
1	I	465	GLN
1	I	523	ASN
1	I	552	HIS
1	I	606	ASN
1	I	618	GLN
1	I	657	HIS
1	I	718	GLN
1	H	87	ASN
1	H	163	GLN
1	H	286	HIS
1	H	381	ASN
1	H	553	HIS
1	H	606	ASN
1	H	618	GLN
3	L	41	ASN
3	L	48	HIS
3	L	57	GLN
3	K	47	ASN
3	K	48	HIS

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Mol	Chain	Res	Type
2	P	356	GLN
2	P	357	GLN
2	N	129	ASN
2	N	187	ASN
2	N	219	GLN
2	N	230	GLN
2	N	235	GLN
2	N	357	GLN
1	M	87	ASN
1	M	163	GLN
1	M	286	HIS
1	M	379	ASN
1	M	423	GLN
1	M	465	GLN
1	M	606	ASN
1	M	618	GLN
1	M	657	HIS
1	O	87	ASN
1	O	163	GLN
1	O	286	HIS
1	O	362	ASN
1	O	379	ASN
1	O	423	GLN
1	O	553	HIS
1	O	606	ASN
1	O	618	GLN
1	O	718	GLN
3	R	41	ASN
3	R	57	GLN
3	Q	47	ASN
3	Q	48	HIS
1	T	87	ASN
1	T	163	GLN
1	T	286	HIS
1	T	324	GLN
1	T	379	ASN
1	T	381	ASN
1	T	423	GLN
1	T	523	ASN
1	T	552	HIS
1	T	606	ASN
1	T	618	GLN

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Mol	Chain	Res	Type
1	T	657	HIS
1	T	718	GLN
2	S	8	GLN
2	S	356	GLN
2	S	357	GLN
2	U	129	ASN
2	U	187	ASN
2	U	205	ASN
2	U	219	GLN
2	U	230	GLN
2	U	235	GLN
2	U	357	GLN
1	V	87	ASN
1	V	163	GLN
1	V	286	HIS
1	V	379	ASN
1	V	423	GLN
1	V	553	HIS
1	V	606	ASN
1	V	618	GLN
3	W	41	ASN
3	W	57	GLN
3	X	28	ASN
3	X	47	ASN
3	X	48	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

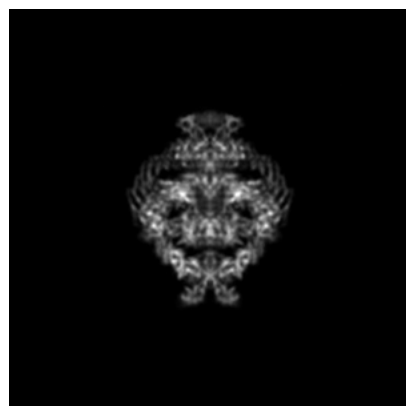
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34451. 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](#)

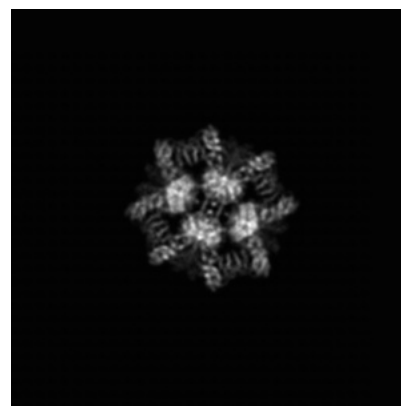
6.1.1 Primary map



X

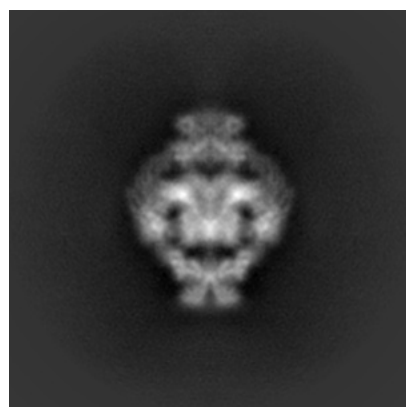


Y

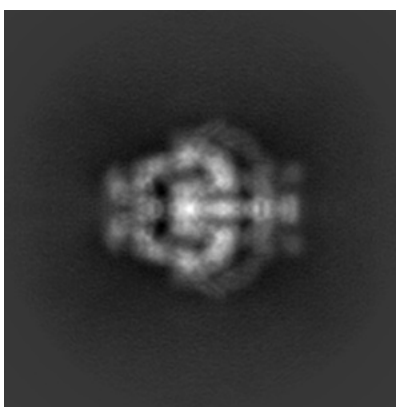


Z

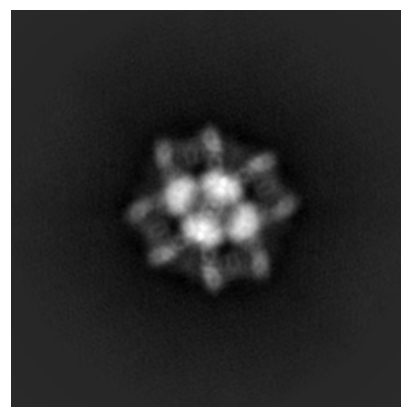
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

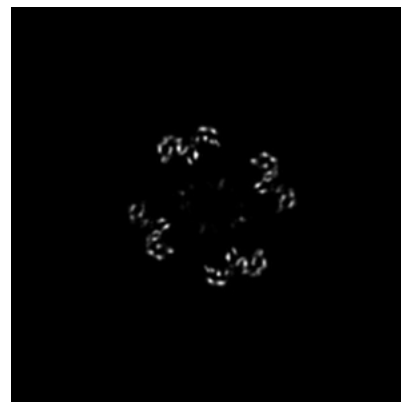
6.2.1 Primary map



X Index: 96

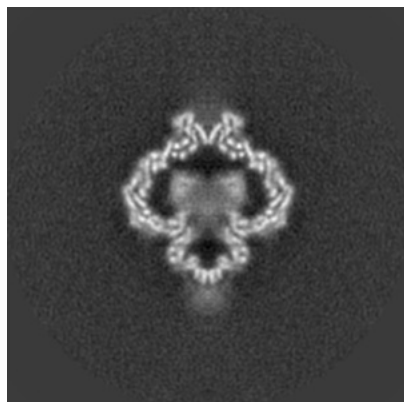


Y Index: 96

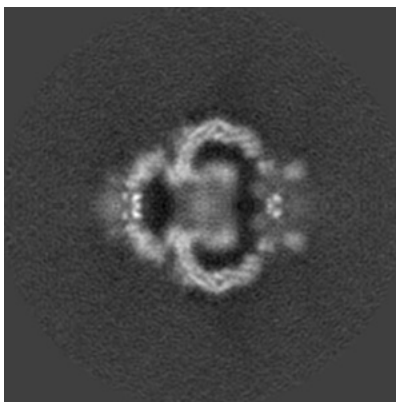


Z Index: 96

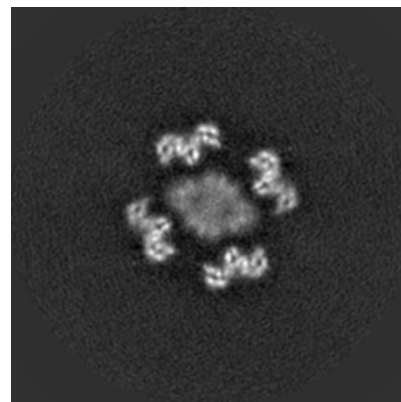
6.2.2 Raw map



X Index: 96



Y Index: 96



Z Index: 96

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: 96

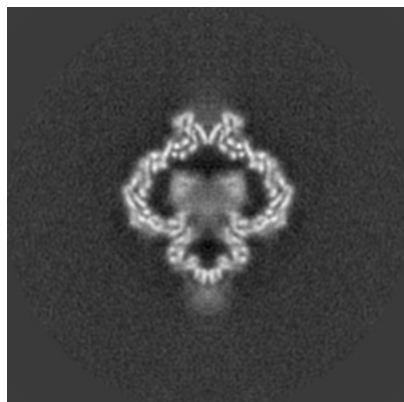


Y Index: 83

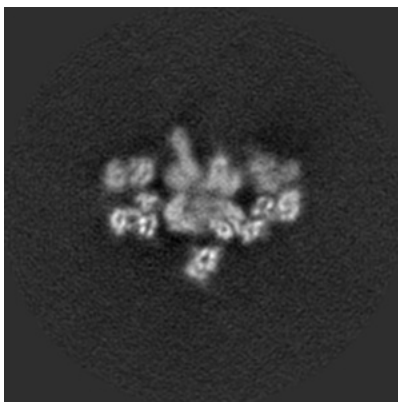


Z Index: 87

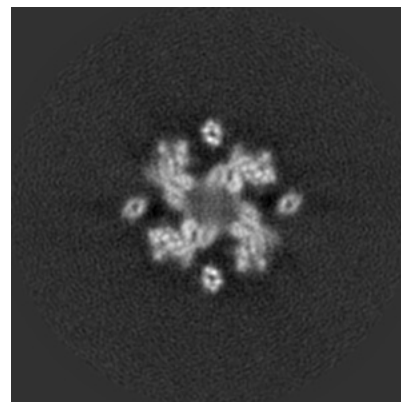
6.3.2 Raw map



X Index: 96



Y Index: 86

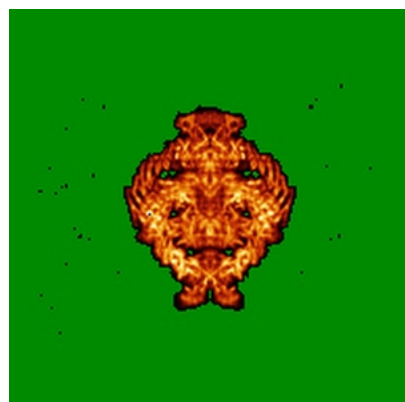


Z Index: 103

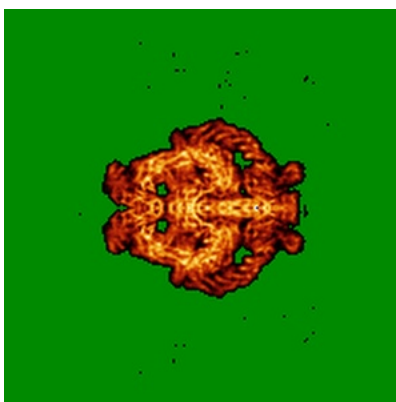
The images above show the largest variance slices of the map in three orthogonal directions.

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

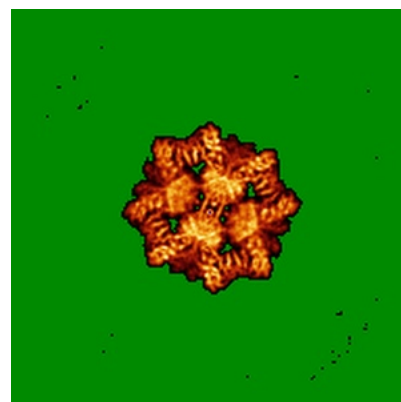
6.4.1 Primary map



X

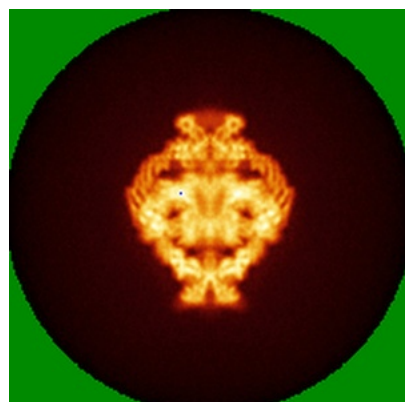


Y

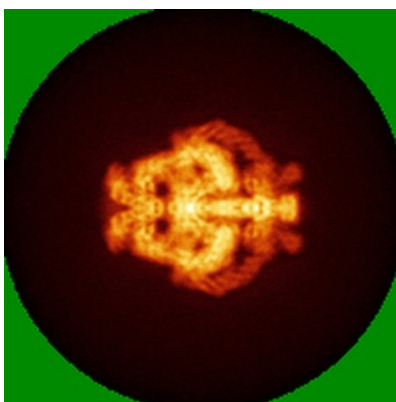


Z

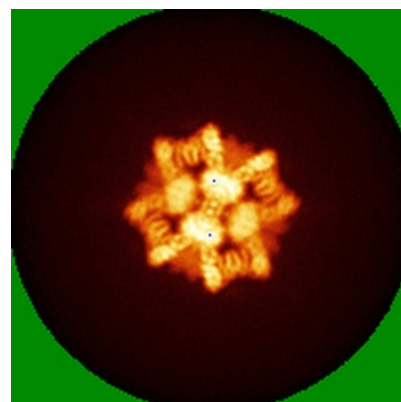
6.4.2 Raw map



X



Y

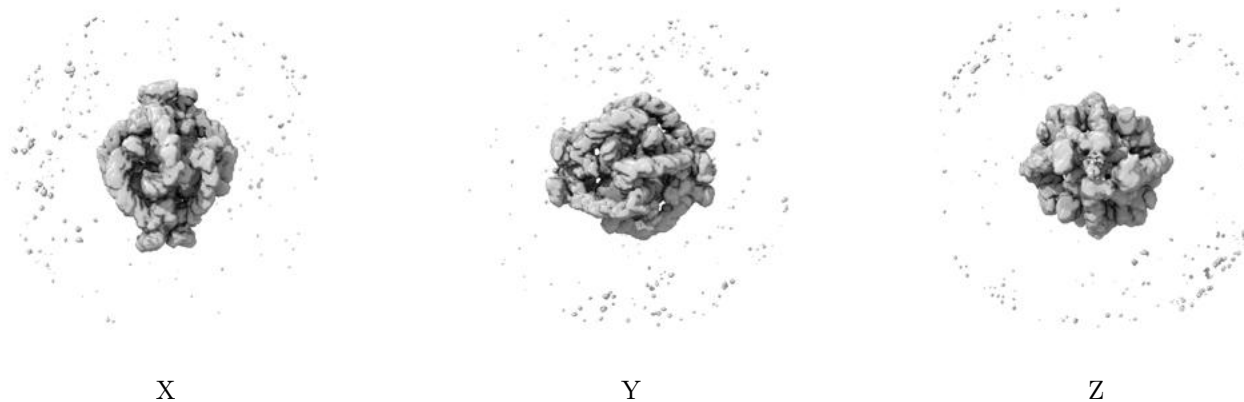


Z

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

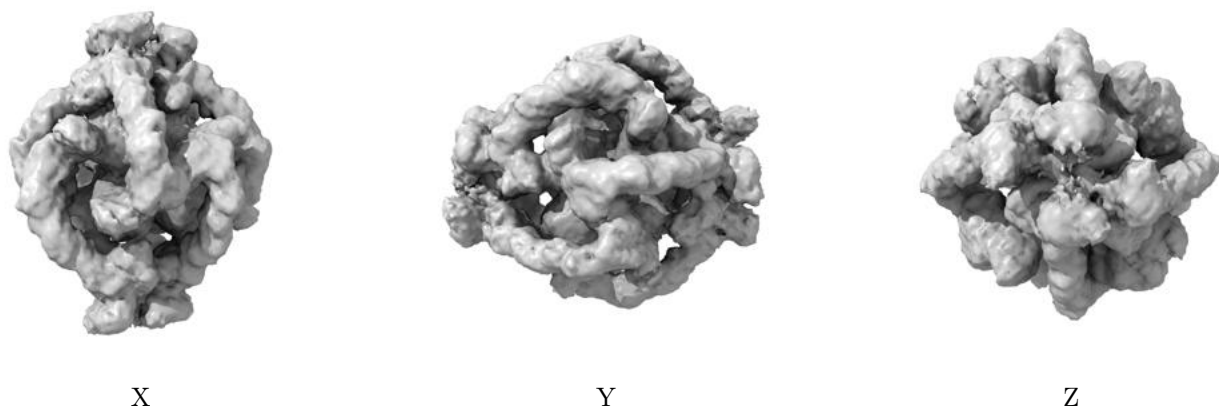
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.001. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

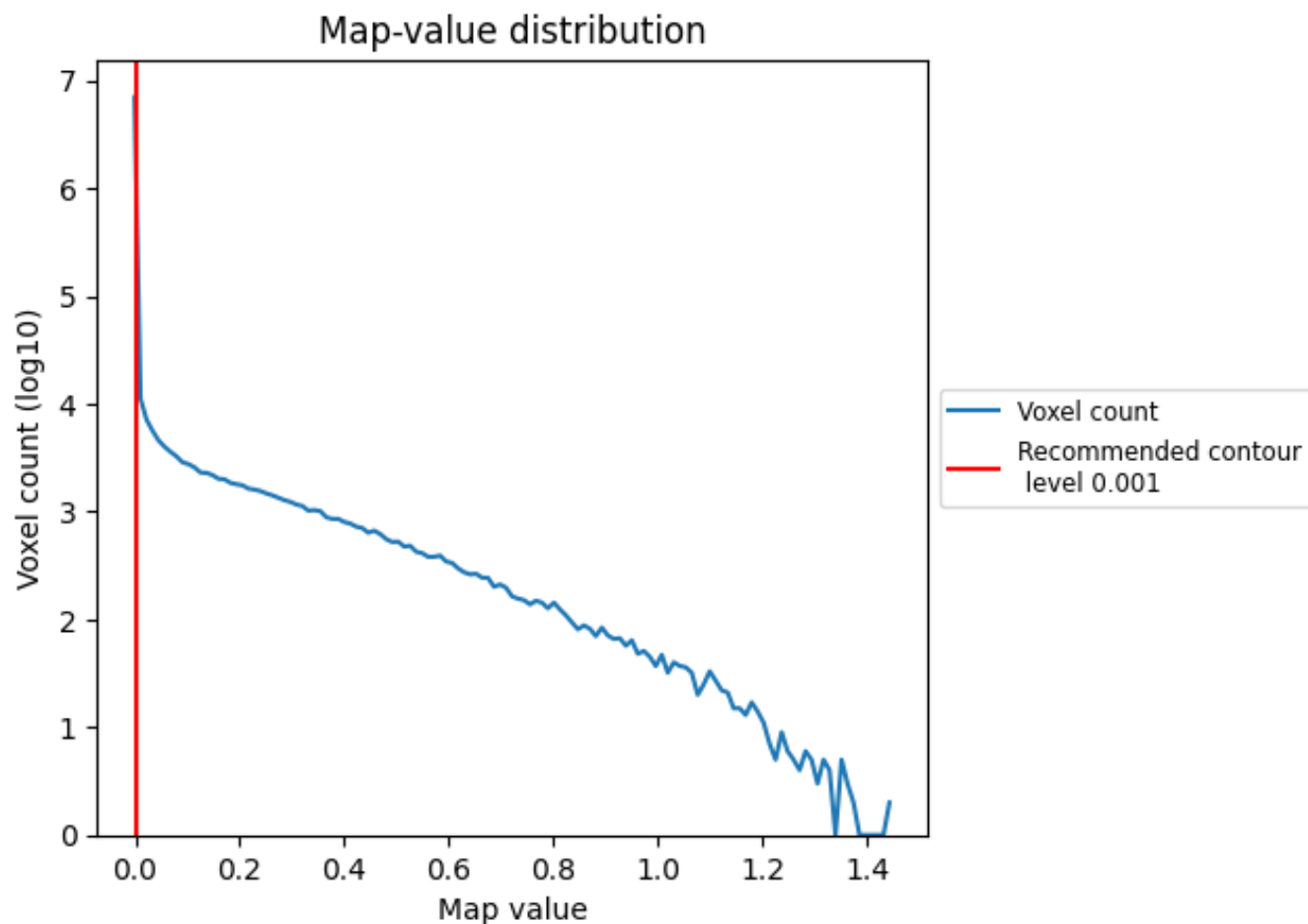
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

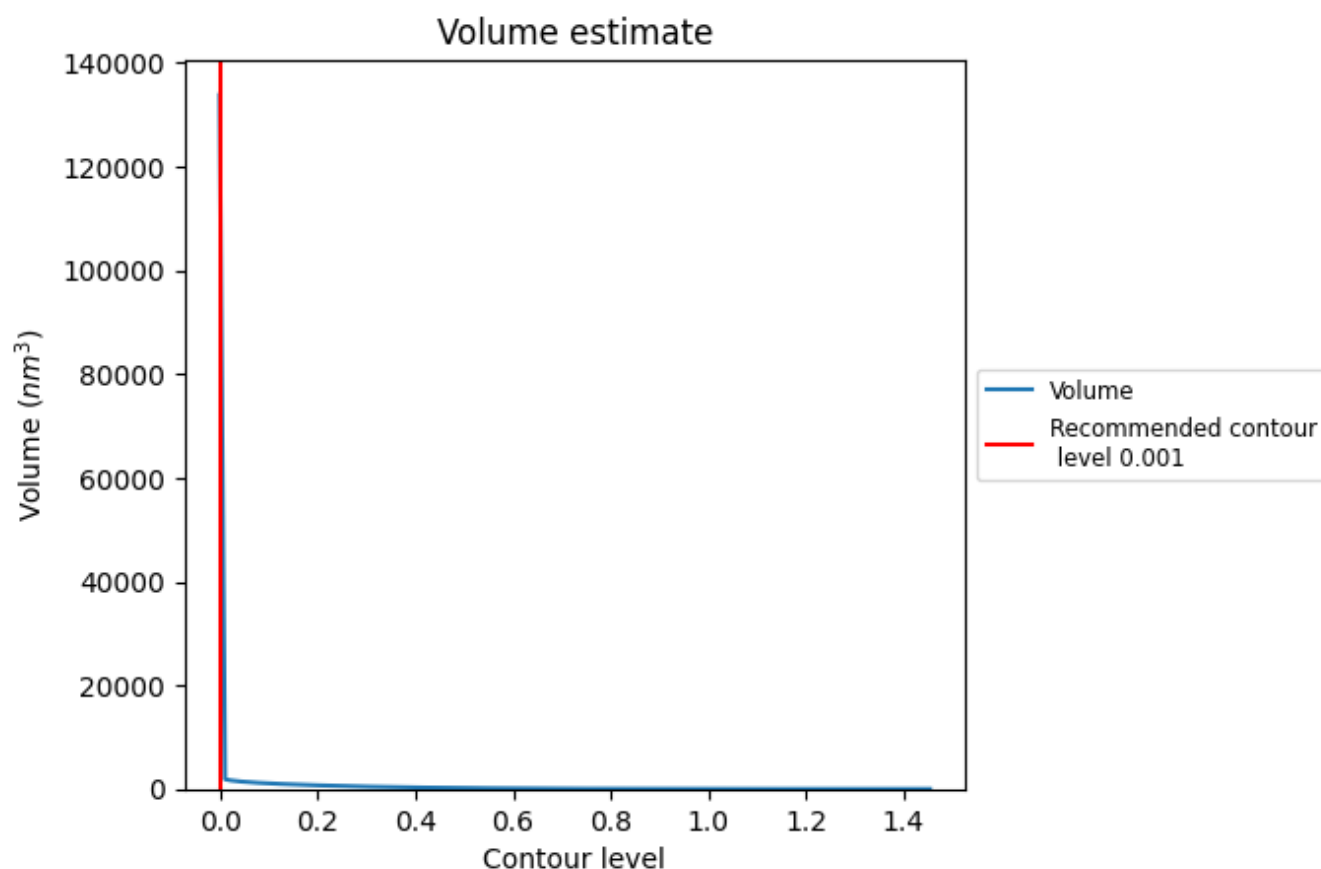
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

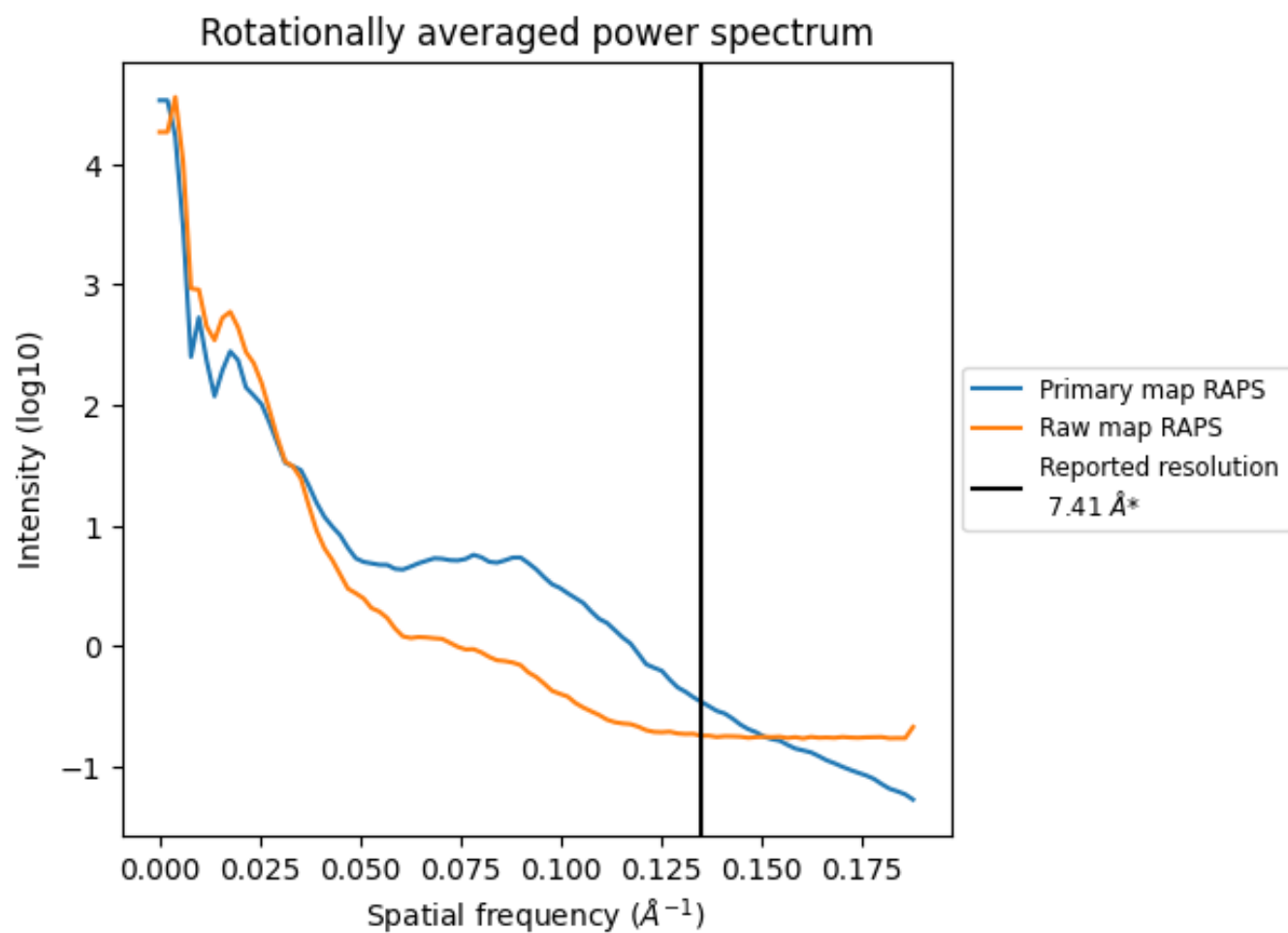
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 106431 nm^3 ; this corresponds to an approximate mass of 96142 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

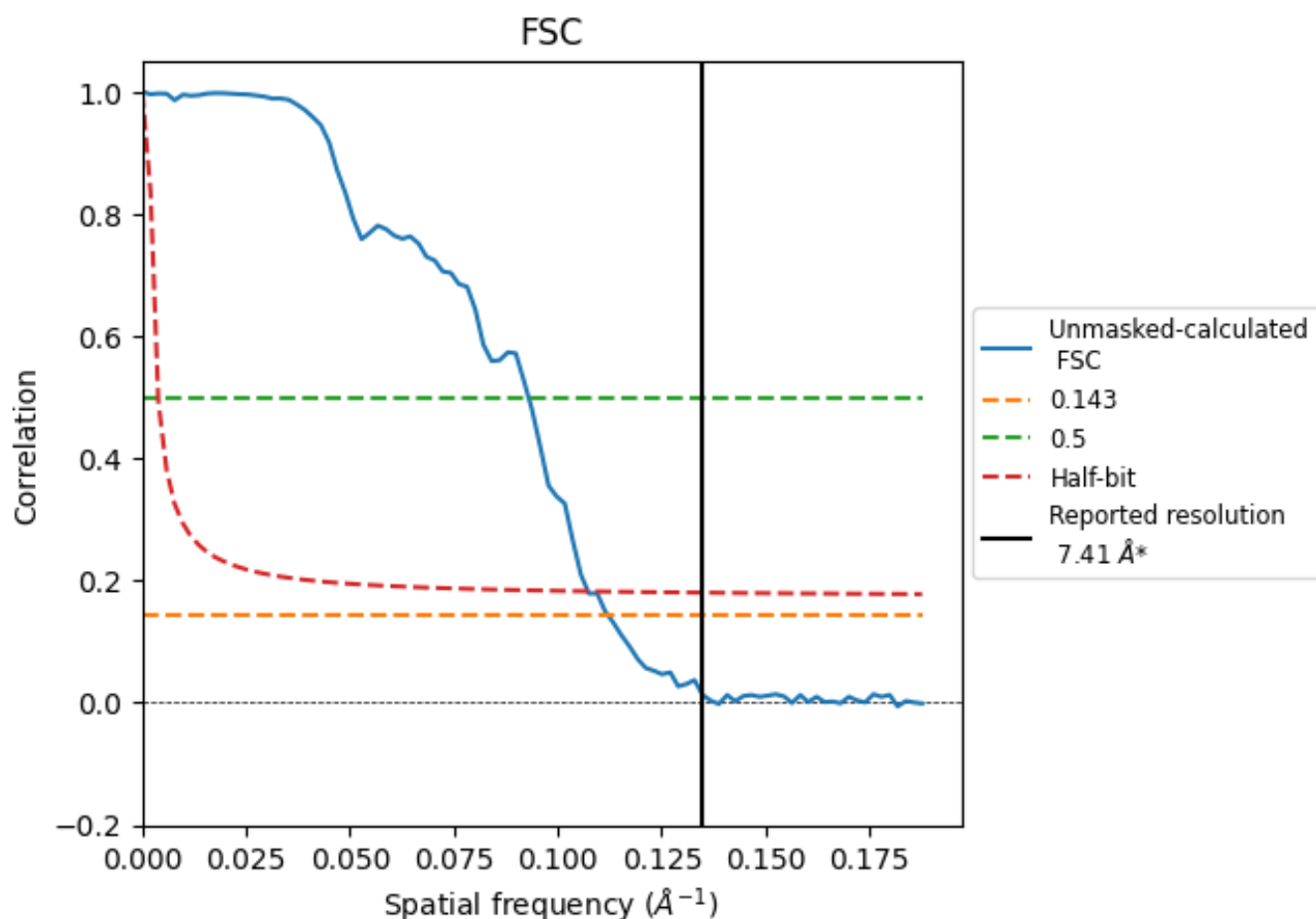


*Reported resolution corresponds to spatial frequency of 0.135 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.135 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

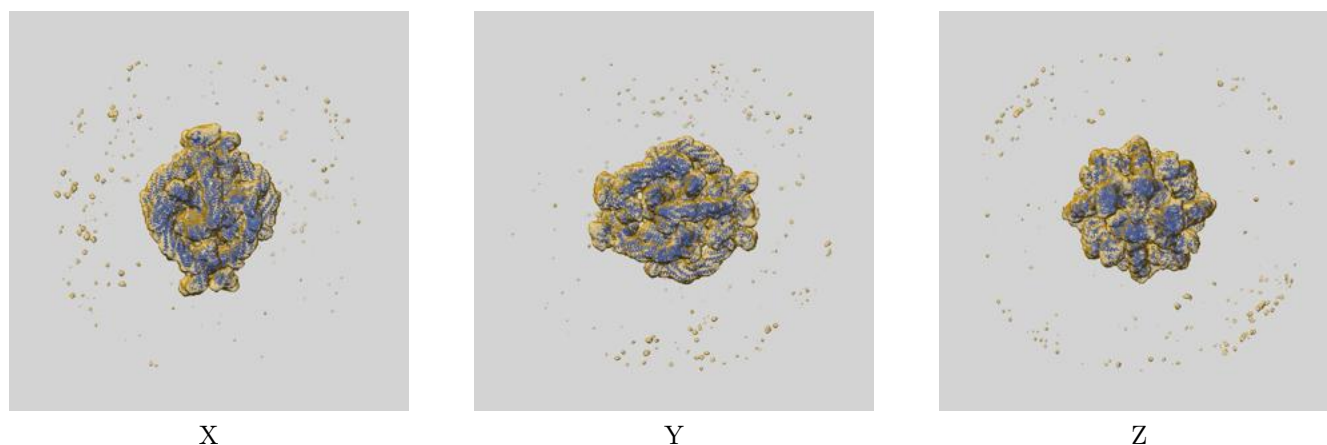
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.41	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.92	10.75	9.32

*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 8.92 differs from the reported value 7.41 by more than 10 %

9 Map-model fit [i](#)

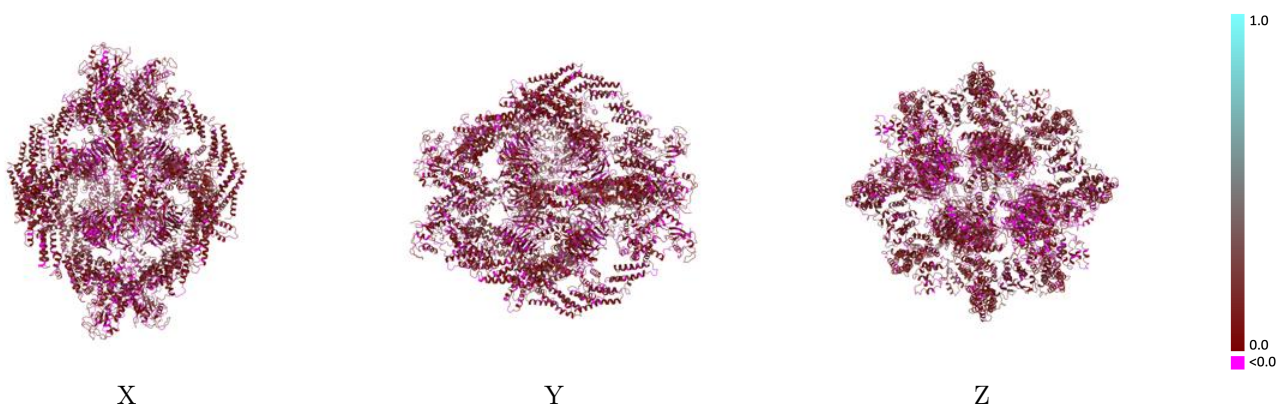
This section contains information regarding the fit between EMDB map EMD-34451 and PDB model 8H35. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.001 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](#)

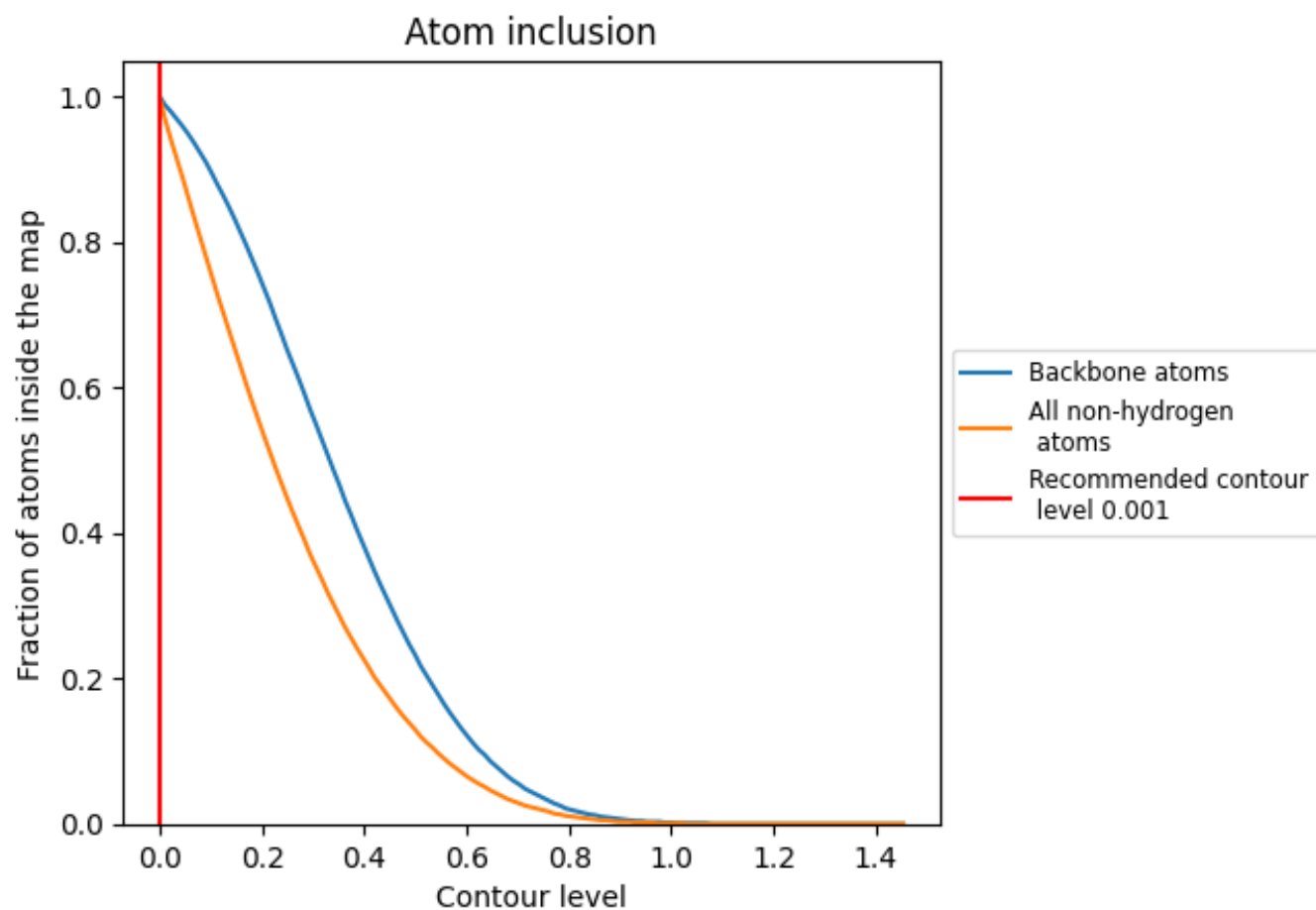


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.001) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9940	 0.0910
A	 0.9960	 0.1030
B	 0.9910	 0.0770
C	 0.9980	 0.1100
D	 0.9830	 0.0370
E	 0.9900	 0.0710
F	 0.9990	 0.0950
G	 0.9900	 0.0720
H	 0.9980	 0.1060
I	 0.9940	 0.0900
J	 0.9930	 0.0960
K	 0.9820	 0.0840
L	 0.9900	 0.0380
M	 0.9970	 0.1080
N	 0.9920	 0.0760
O	 0.9980	 0.0970
P	 0.9950	 0.1020
Q	 0.9900	 0.0380
R	 0.9790	 0.0640
S	 0.9890	 0.0690
T	 0.9940	 0.0910
U	 0.9930	 0.0930
V	 0.9970	 0.1050
W	 0.9860	 0.0380
X	 0.9430	 0.0710

