



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 07:07 AM UTC

PDB ID : 8H34 / pdb_00008h34
EMDB ID : EMD-34450
Title : Cryo-EM Structure of the KBTBD2-Cul3-Rbx1 hexameric complex
Authors : Hu, Y.; Mao, Q.; Chen, Z.; Sun, L.
Deposited on : 2022-10-07
Resolution : 7.99 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

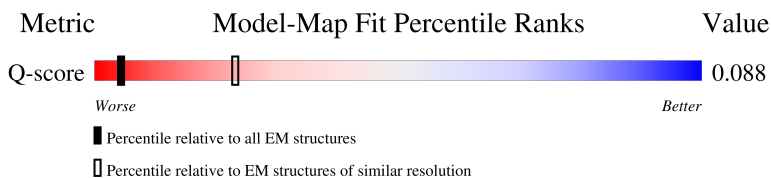
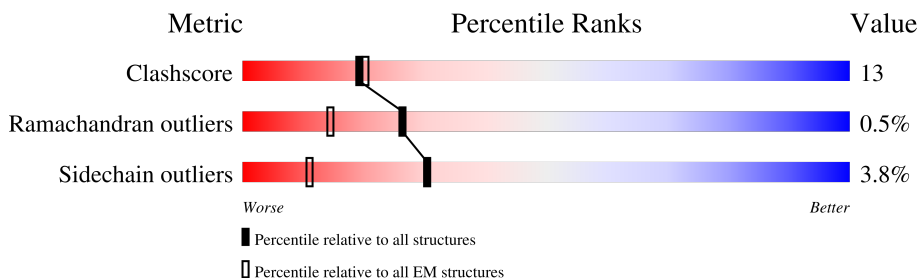
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.99 Å.

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



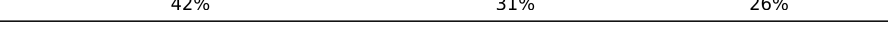
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	339 (7.50 - 8.47)

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	
2	A	623	
2	B	623	
2	G	623	
2	J	623	
2	N	623	
2	P	623	
3	D	121	
3	E	121	
3	K	121	
3	L	121	
3	Q	121	
3	R	121	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 65663 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	M	720	Total	C	N	O	S	0	0
			5718	3590	1008	1081	39		
1	O	720	Total	C	N	O	S	0	0
			5614	3517	999	1064	34		
1	C	720	Total	C	N	O	S	0	0
			5718	3582	1014	1083	39		
1	F	720	Total	C	N	O	S	0	0
			5782	3632	1017	1094	39		
1	I	720	Total	C	N	O	S	0	0
			5793	3638	1026	1091	38		
1	H	720	Total	C	N	O	S	0	0
			5789	3632	1026	1092	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	561	Total	C	N	O	S	0	0
			4437	2832	744	827	34		
2	N	563	Total	C	N	O	S	0	0
			4474	2854	751	834	35		
2	A	561	Total	C	N	O	S	0	0
			4504	2880	744	842	38		
2	B	563	Total	C	N	O	S	0	0
			4513	2885	749	842	37		
2	G	561	Total	C	N	O	S	0	0
			4437	2839	740	823	35		
2	J	563	Total	C	N	O	S	0	0
			4477	2860	744	837	36		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	89	Total	C	N	O	S	0	0
			737	466	135	127	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	89	Total	C	N	O	S	0	0
			737	466	135	127	9		
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
			737	466	135	127	9		
3	L	89	Total	C	N	O	S	0	0
			731	463	132	127	9		
3	K	89	Total	C	N	O	S	0	0
			714	453	128	124	9		

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-12	HIS	-	expression tag	UNP P62877
R	-11	HIS	-	expression tag	UNP P62877
R	-10	HIS	-	expression tag	UNP P62877
R	-9	HIS	-	expression tag	UNP P62877
R	-8	HIS	-	expression tag	UNP P62877
R	-7	HIS	-	expression tag	UNP P62877
R	-6	GLU	-	expression tag	UNP P62877
R	-5	ASN	-	expression tag	UNP P62877
R	-4	LEU	-	expression tag	UNP P62877
R	-3	TYR	-	expression tag	UNP P62877
R	-2	PHE	-	expression tag	UNP P62877
R	-1	GLN	-	expression tag	UNP P62877
R	0	GLY	-	expression tag	UNP P62877
Q	-12	HIS	-	expression tag	UNP P62877
Q	-11	HIS	-	expression tag	UNP P62877
Q	-10	HIS	-	expression tag	UNP P62877
Q	-9	HIS	-	expression tag	UNP P62877
Q	-8	HIS	-	expression tag	UNP P62877
Q	-7	HIS	-	expression tag	UNP P62877
Q	-6	GLU	-	expression tag	UNP P62877
Q	-5	ASN	-	expression tag	UNP P62877
Q	-4	LEU	-	expression tag	UNP P62877
Q	-3	TYR	-	expression tag	UNP P62877
Q	-2	PHE	-	expression tag	UNP P62877
Q	-1	GLN	-	expression tag	UNP P62877
Q	0	GLY	-	expression tag	UNP P62877
E	-12	HIS	-	expression tag	UNP P62877
E	-11	HIS	-	expression tag	UNP P62877
E	-10	HIS	-	expression tag	UNP P62877

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-9	HIS	-	expression tag	UNP P62877
E	-8	HIS	-	expression tag	UNP P62877
E	-7	HIS	-	expression tag	UNP P62877
E	-6	GLU	-	expression tag	UNP P62877
E	-5	ASN	-	expression tag	UNP P62877
E	-4	LEU	-	expression tag	UNP P62877
E	-3	TYR	-	expression tag	UNP P62877
E	-2	PHE	-	expression tag	UNP P62877
E	-1	GLN	-	expression tag	UNP P62877
E	0	GLY	-	expression tag	UNP P62877
D	-12	HIS	-	expression tag	UNP P62877
D	-11	HIS	-	expression tag	UNP P62877
D	-10	HIS	-	expression tag	UNP P62877
D	-9	HIS	-	expression tag	UNP P62877
D	-8	HIS	-	expression tag	UNP P62877
D	-7	HIS	-	expression tag	UNP P62877
D	-6	GLU	-	expression tag	UNP P62877
D	-5	ASN	-	expression tag	UNP P62877
D	-4	LEU	-	expression tag	UNP P62877
D	-3	TYR	-	expression tag	UNP P62877
D	-2	PHE	-	expression tag	UNP P62877
D	-1	GLN	-	expression tag	UNP P62877
D	0	GLY	-	expression tag	UNP P62877
L	-12	HIS	-	expression tag	UNP P62877
L	-11	HIS	-	expression tag	UNP P62877
L	-10	HIS	-	expression tag	UNP P62877
L	-9	HIS	-	expression tag	UNP P62877
L	-8	HIS	-	expression tag	UNP P62877
L	-7	HIS	-	expression tag	UNP P62877
L	-6	GLU	-	expression tag	UNP P62877
L	-5	ASN	-	expression tag	UNP P62877
L	-4	LEU	-	expression tag	UNP P62877
L	-3	TYR	-	expression tag	UNP P62877
L	-2	PHE	-	expression tag	UNP P62877
L	-1	GLN	-	expression tag	UNP P62877
L	0	GLY	-	expression tag	UNP P62877
K	-12	HIS	-	expression tag	UNP P62877
K	-11	HIS	-	expression tag	UNP P62877
K	-10	HIS	-	expression tag	UNP P62877
K	-9	HIS	-	expression tag	UNP P62877
K	-8	HIS	-	expression tag	UNP P62877
K	-7	HIS	-	expression tag	UNP P62877

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-6	GLU	-	expression tag	UNP P62877
K	-5	ASN	-	expression tag	UNP P62877
K	-4	LEU	-	expression tag	UNP P62877
K	-3	TYR	-	expression tag	UNP P62877
K	-2	PHE	-	expression tag	UNP P62877
K	-1	GLN	-	expression tag	UNP P62877
K	0	GLY	-	expression tag	UNP P62877

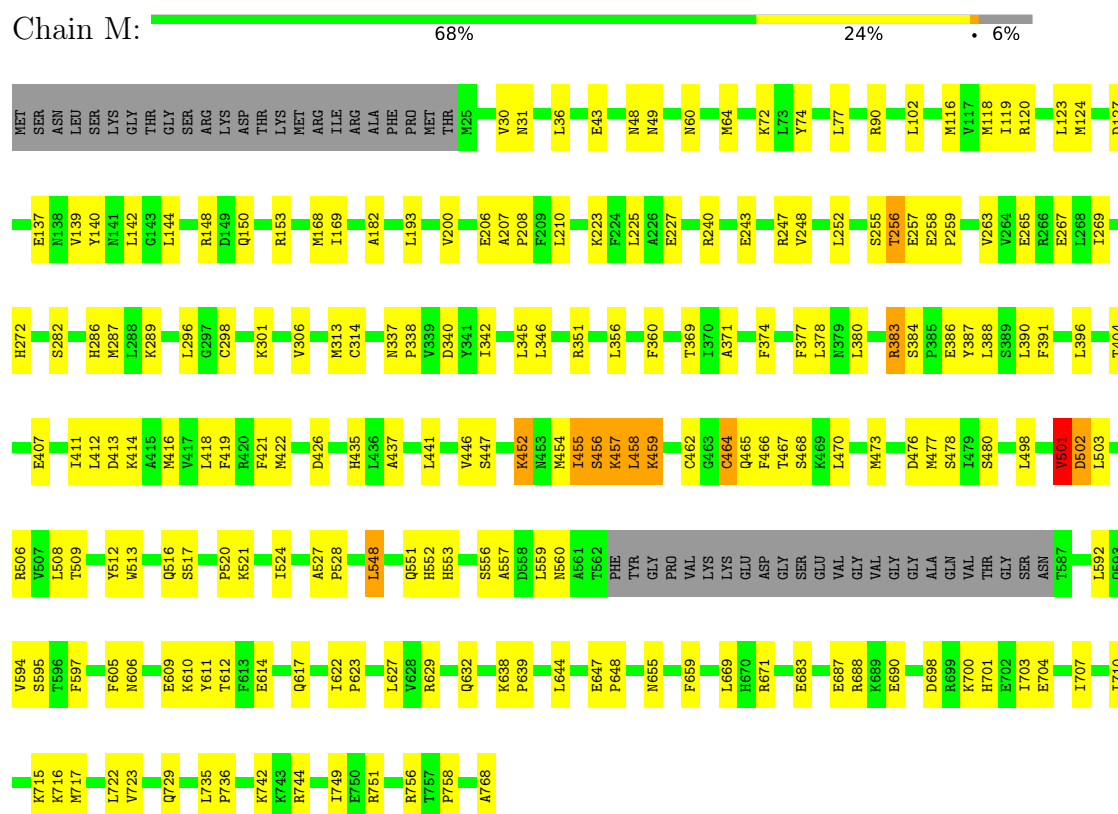
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

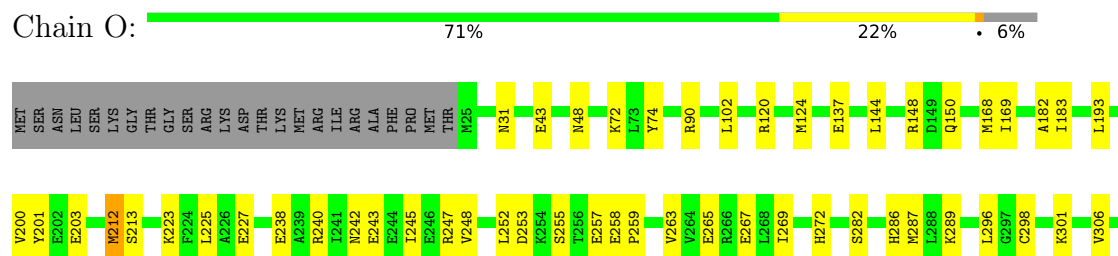
3 Residue-property plots

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.

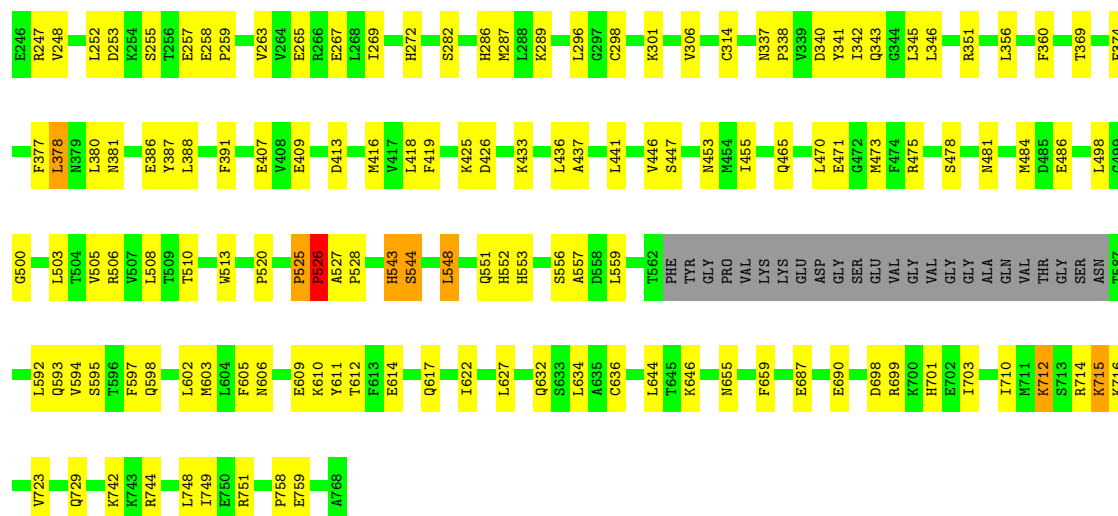
• Molecule 1: Cullin-3



• Molecule 1: Cullin-3

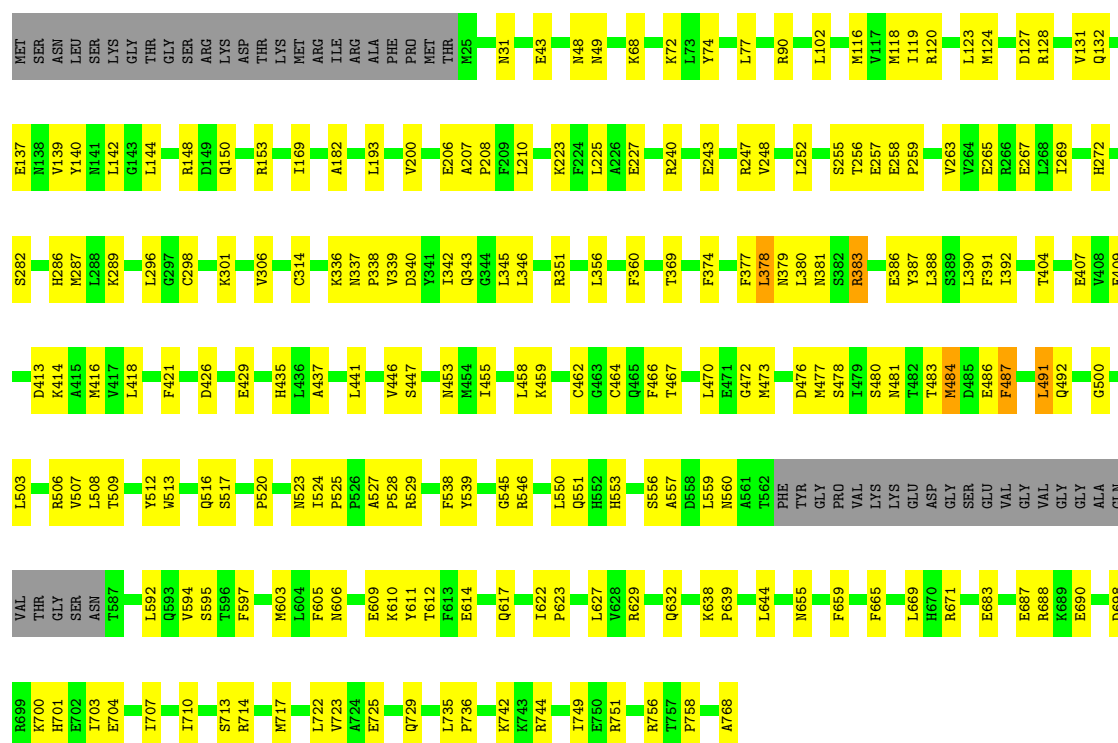






• Molecule 1: Cullin-3

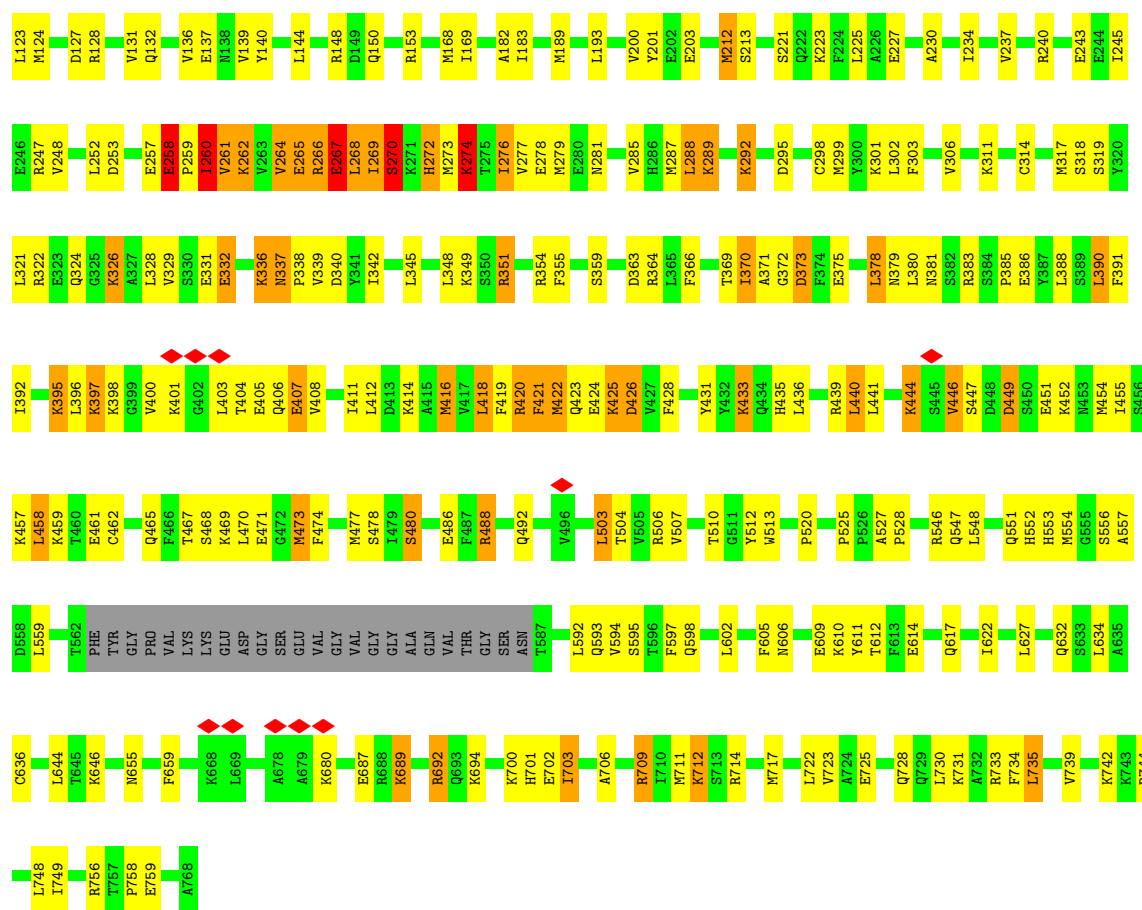
Chain I: 67% 26% • 6%



• Molecule 1: Cullin-3

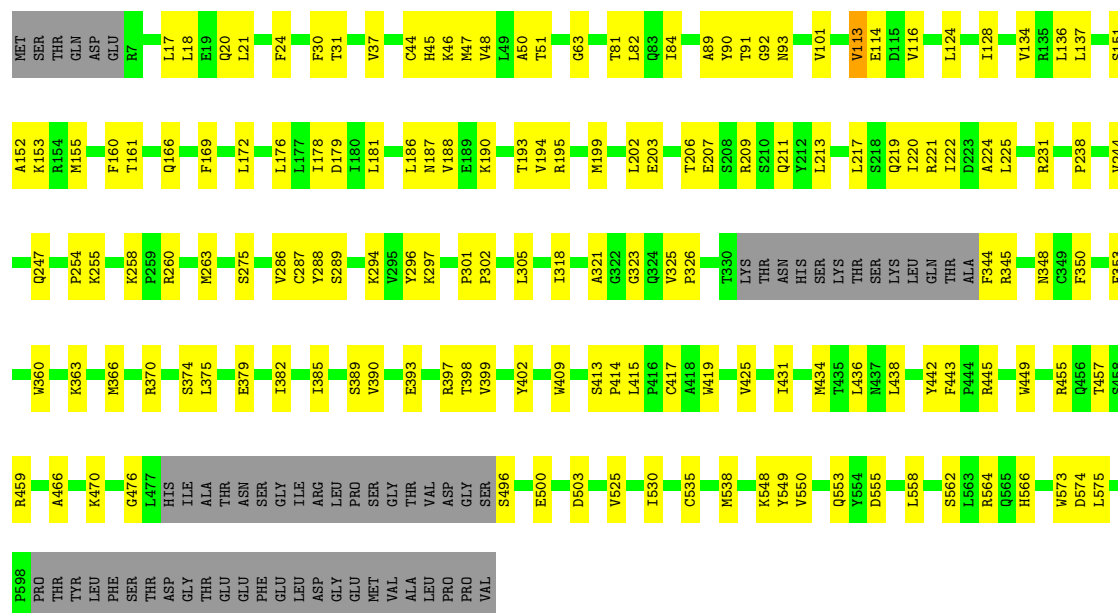
Chain H: 58% 29% 6% • 6%





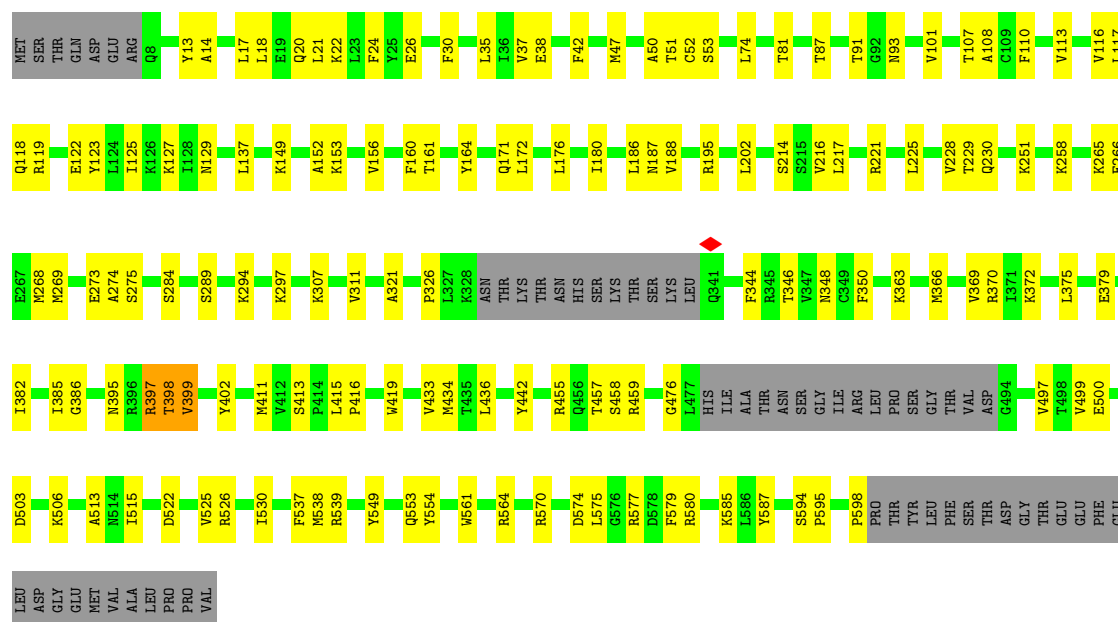
• Molecule 2: Kelch repeat and BTB domain-containing protein 2

Chain P:



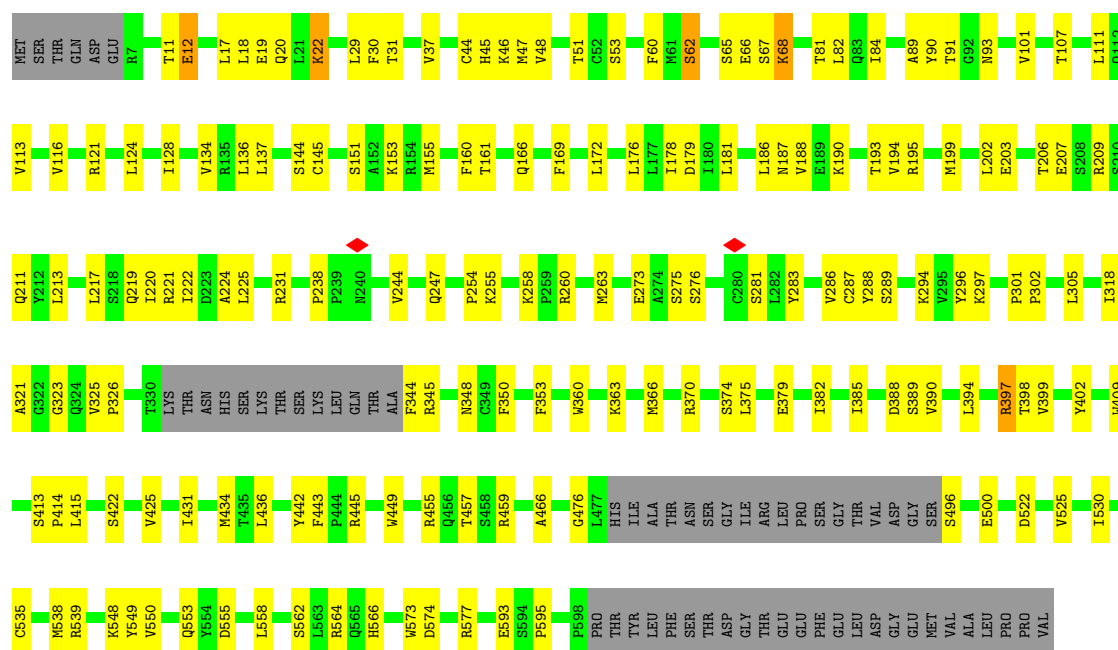
• Molecule 2: Kelch repeat and BTB domain-containing protein 2

Chain N: 



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

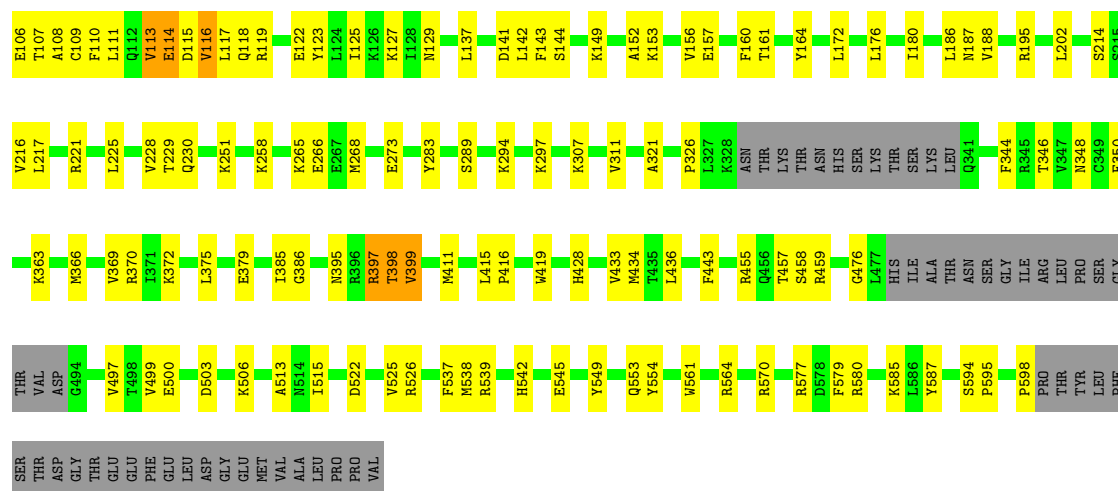
Chain A: 



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

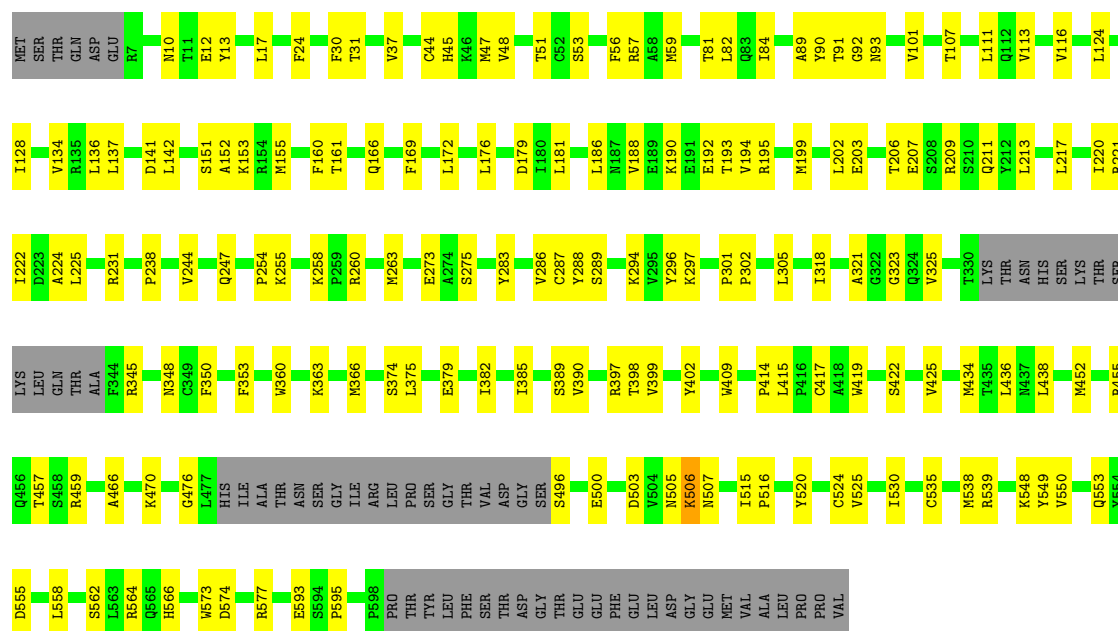
Chain B: 





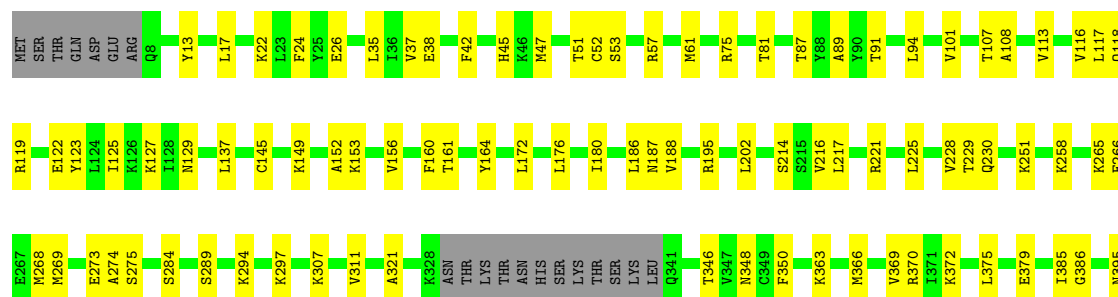
● Molecule 2: Kelch repeat and BTB domain-containing protein 2

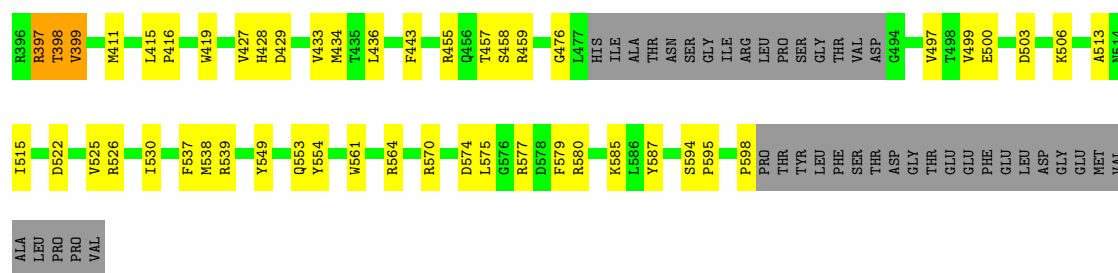
Chain G: 64% 26% 10%



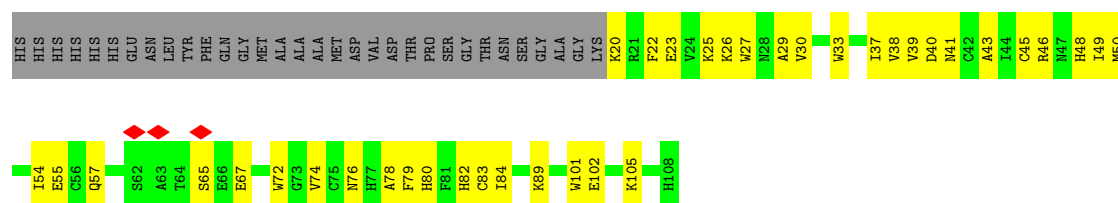
● Molecule 2: Kelch repeat and BTB domain-containing protein 2

Chain J: 68% 22% 10%

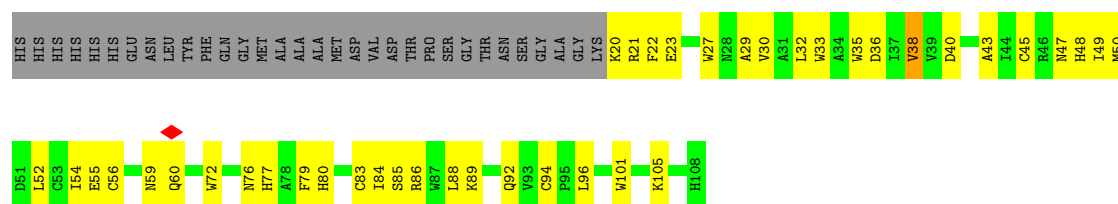




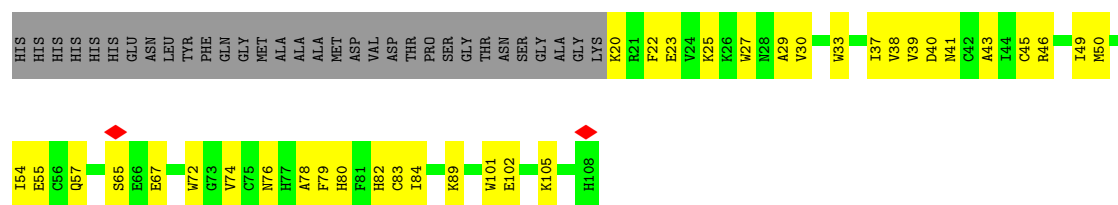
• Molecule 3: E3 ubiquitin-protein ligase RBX1



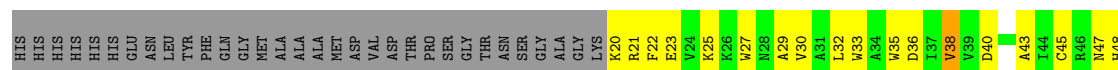
• Molecule 3: E3 ubiquitin-protein ligase RBX1



• Molecule 3: E3 ubiquitin-protein ligase RBX1

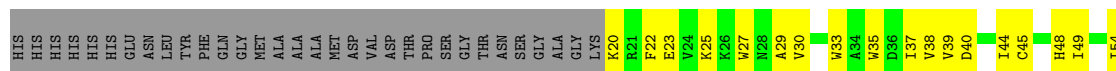


• Molecule 3: E3 ubiquitin-protein ligase RBX1

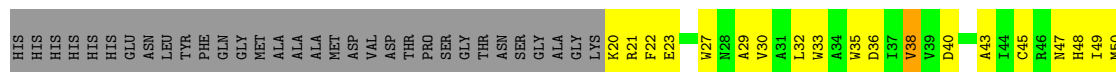




- Molecule 3: E3 ubiquitin-protein ligase RBX1



- Molecule 3: E3 ubiquitin-protein ligase RBX1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	51689	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	1.553	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 [i](#)

5.1 Standard geometry [i](#)

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	0.41	0/5801	0.54	3/7804 (0.0%)
1	F	0.34	1/5870 (0.0%)	0.51	3/7894 (0.0%)
1	H	0.66	4/5876 (0.1%)	0.87	4/7901 (0.1%)
1	I	0.23	0/5882	0.39	0/7908
1	M	0.39	0/5803	0.53	0/7808
1	O	0.40	1/5695 (0.0%)	0.52	0/7672
2	A	0.29	0/4611	0.43	0/6257
2	B	0.22	0/4618	0.36	0/6266
2	G	0.30	0/4539	0.43	0/6166
2	J	0.23	0/4580	0.37	0/6217
2	N	0.13	0/4577	0.31	0/6215
2	P	0.29	0/4537	0.42	0/6164
3	D	0.15	0/759	0.46	0/1029
3	E	0.16	0/755	0.49	1/1025 (0.1%)
3	K	0.15	0/736	0.46	0/1001
3	L	0.32	0/753	0.55	1/1022 (0.1%)
3	Q	0.15	0/759	0.46	0/1029
3	R	0.16	0/759	0.49	1/1029 (0.1%)
All	All	0.35	6/66910 (0.0%)	0.50	13/90407 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	525	PRO	C-O	-7.46	1.16	1.24
1	H	270	SER	C-O	6.77	1.31	1.24
1	H	274	LYS	C-O	6.71	1.32	1.24
1	O	525	PRO	C-O	-5.91	1.17	1.24
1	H	267	GLU	C-O	5.58	1.30	1.24
1	H	264	VAL	C-O	5.13	1.29	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	543	HIS	CA-C-O	-8.09	112.79	121.20
1	F	525	PRO	CB-CA-C	-5.98	103.63	110.92
1	C	463	GLY	CA-C-O	-5.93	117.83	122.52
1	H	272	HIS	CB-CA-C	5.85	120.15	110.90
1	H	380	LEU	CA-C-N	-5.22	115.79	123.00
1	H	380	LEU	C-N-CA	-5.22	115.79	123.00
1	C	525	PRO	CA-C-N	5.22	124.54	118.85
1	C	525	PRO	C-N-CA	5.22	124.54	118.85
1	F	543	HIS	N-CA-C	5.16	117.06	110.61
1	H	272	HIS	CA-C-O	-5.08	115.46	120.70
3	R	65	SER	CB-CA-C	-5.07	110.33	117.23
3	E	65	SER	CB-CA-C	-5.05	110.36	117.23
3	L	65	SER	CB-CA-C	-5.05	110.36	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	5718	0	5663	122	0
1	F	5782	0	5755	153	0
1	H	5789	0	5785	166	0
1	I	5793	0	5778	190	0
1	M	5718	0	5655	132	0
1	O	5614	0	5441	115	0
2	A	4504	0	4386	131	0
2	B	4513	0	4396	136	0
2	G	4437	0	4264	119	0
2	J	4477	0	4325	103	0
2	N	4474	0	4340	141	0
2	P	4437	0	4282	153	0
3	D	737	0	686	33	0
3	E	733	0	675	24	0
3	K	714	0	645	30	0
3	L	731	0	675	24	0
3	Q	737	0	686	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	737	0	686	25	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
All	All	65663	0	64123	1649	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 (1649) 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:F:338:PRO:HB3	1:F:387:TYR:CD1	1.50	1.45
1:I:345:LEU:CG	1:I:418:LEU:HD11	1.66	1.26
2:P:46:LYS:HB3	2:N:30:PHE:CE2	1.78	1.19
1:I:345:LEU:HG	1:I:418:LEU:CD1	1.74	1.16
2:B:144:SER:HB3	1:F:133:GLN:CD	1.69	1.16
1:H:234:ILE:HD11	1:H:298:CYS:O	1.46	1.13
2:J:75:ARG:HD2	1:H:59:ARG:HH12	1.01	1.11
1:H:234:ILE:CD1	1:H:299:MET:HA	1.82	1.10
1:O:346:LEU:CD1	1:O:418:LEU:HD13	1.82	1.08
1:O:342:ILE:CG1	1:O:387:TYR:HB3	1.82	1.07
1:O:346:LEU:HD13	1:O:418:LEU:HD13	1.24	1.07
1:O:342:ILE:HG12	1:O:387:TYR:HB3	1.37	1.06
1:H:237:VAL:HG11	1:H:302:LEU:HD21	1.30	1.06
2:G:30:PHE:CE1	2:J:61:MET:HB2	1.91	1.05
1:H:440:LEU:CD1	1:H:446:VAL:HG21	1.89	1.02
2:P:47:MET:HG2	2:N:21:LEU:HD22	1.37	1.01
1:F:338:PRO:CB	1:F:387:TYR:CD1	2.42	1.01
1:O:346:LEU:CD1	1:O:418:LEU:CD1	2.41	0.99
2:G:13:TYR:OH	2:J:52:CYS:HB3	1.61	0.99
2:J:75:ARG:HD2	1:H:59:ARG:NH1	1.79	0.97
1:I:345:LEU:HD23	1:I:418:LEU:HD21	1.44	0.97
1:M:345:LEU:HG	1:M:418:LEU:HD11	1.46	0.95
2:G:47:MET:HE3	2:J:45:HIS:CD2	2.01	0.95
1:H:237:VAL:CG1	1:H:302:LEU:HD21	1.96	0.95
1:O:342:ILE:CG1	1:O:387:TYR:CB	2.44	0.94
2:P:46:LYS:HB3	2:N:30:PHE:CD2	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:338:PRO:HB3	1:F:387:TYR:CG	2.03	0.94
1:I:346:LEU:HD11	1:I:414:LYS:HB3	1.48	0.94
2:P:46:LYS:HB3	2:N:30:PHE:HE2	1.25	0.94
1:H:234:ILE:HD11	1:H:298:CYS:C	1.92	0.93
1:I:336:LYS:HE3	1:I:387:TYR:CE2	2.04	0.91
2:P:17:LEU:HD22	2:N:18:LEU:HD13	1.50	0.91
1:I:346:LEU:HD11	1:I:414:LYS:C	1.96	0.91
1:O:346:LEU:HD13	1:O:418:LEU:CD1	1.98	0.90
1:F:338:PRO:HG3	1:F:387:TYR:CE1	2.06	0.90
1:H:234:ILE:HD12	1:H:299:MET:HA	1.52	0.90
2:P:89:ALA:HA	2:N:13:TYR:OH	1.71	0.89
1:I:339:VAL:HG23	1:I:391:PHE:CD1	2.08	0.89
2:P:18:LEU:HD13	2:N:17:LEU:HD23	1.55	0.89
1:I:336:LYS:HE3	1:I:387:TYR:HE2	1.37	0.88
1:O:346:LEU:HD12	1:O:418:LEU:HD12	1.53	0.88
1:I:346:LEU:HD21	1:I:414:LYS:HB2	1.53	0.88
1:H:440:LEU:HD13	1:H:446:VAL:HG21	1.56	0.87
2:A:29:LEU:HD21	2:B:61:MET:HE2	1.57	0.87
2:A:29:LEU:HG	2:B:61:MET:HG3	1.56	0.87
2:P:45:HIS:CD2	2:N:47:MET:SD	2.68	0.87
1:I:345:LEU:CD2	1:I:418:LEU:HD21	2.06	0.86
1:H:322:ARG:HH21	1:H:373:ASP:HA	1.42	0.85
2:B:141:ASP:O	1:F:68:LYS:HE3	1.77	0.85
1:I:346:LEU:CD1	1:I:414:LYS:HB3	2.07	0.85
2:P:47:MET:CG	2:N:21:LEU:HD22	2.06	0.85
1:O:342:ILE:HG13	1:O:387:TYR:CB	2.06	0.85
1:H:385:PRO:HB3	1:H:428:PHE:HB2	1.58	0.84
1:M:346:LEU:HD11	1:M:414:LYS:HB3	1.58	0.84
1:I:345:LEU:HG	1:I:418:LEU:HD11	0.88	0.84
1:I:346:LEU:CD1	1:I:414:LYS:O	2.24	0.84
1:H:266:ARG:HA	1:H:306:VAL:HG13	1.59	0.83
1:H:234:ILE:CD1	1:H:299:MET:CA	2.55	0.83
1:I:346:LEU:HD21	1:I:414:LYS:CB	2.08	0.83
1:I:480:SER:HB3	1:I:507:VAL:O	1.76	0.83
1:H:237:VAL:CG1	1:H:302:LEU:CD2	2.56	0.83
1:F:525:PRO:HA	1:F:603:MET:HE2	1.60	0.82
1:O:342:ILE:HG13	1:O:387:TYR:HB3	1.58	0.82
1:O:346:LEU:HD12	1:O:418:LEU:CD1	2.05	0.82
2:P:89:ALA:O	2:N:13:TYR:HE2	1.62	0.82
2:A:370:ARG:HG2	2:A:389:SER:HA	1.59	0.82
1:I:342:ILE:HG13	1:I:388:LEU:HA	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:342:ILE:HG13	1:F:387:TYR:C	2.03	0.82
2:P:89:ALA:O	2:N:13:TYR:CE2	2.33	0.81
2:P:47:MET:HG2	2:N:21:LEU:CD2	2.11	0.81
2:B:144:SER:HB3	1:F:133:GLN:NE2	1.95	0.81
1:F:124:MET:HA	1:F:127:ASP:HB2	1.62	0.81
2:P:30:PHE:CZ	2:N:50:ALA:CB	2.64	0.81
1:H:124:MET:HA	1:H:127:ASP:HB2	1.62	0.81
2:P:51:THR:OG1	2:N:20:GLN:CB	2.29	0.81
2:J:75:ARG:CD	1:H:59:ARG:HH12	1.89	0.81
1:H:440:LEU:CD1	1:H:446:VAL:CG2	2.58	0.80
1:I:124:MET:HA	1:I:127:ASP:HB2	1.62	0.80
1:M:124:MET:HA	1:M:127:ASP:HB2	1.62	0.79
1:C:124:MET:HA	1:C:127:ASP:HB2	1.62	0.79
1:M:378:LEU:HD21	1:M:422:MET:HE3	1.65	0.79
1:H:234:ILE:CD1	1:H:298:CYS:C	2.56	0.79
1:I:346:LEU:HD11	1:I:414:LYS:CB	2.13	0.78
1:I:346:LEU:CG	1:I:414:LYS:HB3	2.13	0.78
2:A:46:LYS:HB3	2:B:30:PHE:HE2	1.47	0.78
1:I:346:LEU:HD11	1:I:414:LYS:O	1.84	0.78
2:P:30:PHE:CZ	2:N:50:ALA:HB2	2.18	0.78
2:A:46:LYS:HB3	2:B:30:PHE:CE2	2.18	0.78
1:H:440:LEU:HD11	1:H:446:VAL:HG21	1.65	0.78
2:P:18:LEU:HD22	2:N:14:ALA:HA	1.64	0.77
1:O:346:LEU:HA	1:O:418:LEU:CD1	2.14	0.77
1:C:120:ARG:HG3	1:C:140:TYR:HB2	1.65	0.77
1:M:120:ARG:HG3	1:M:140:TYR:HB2	1.66	0.77
1:C:118:MET:HG2	2:A:62:SER:HB2	1.65	0.77
1:I:374:PHE:HB3	1:I:421:PHE:HB3	1.66	0.77
2:P:17:LEU:HD22	2:N:18:LEU:CD1	2.14	0.76
1:I:120:ARG:HG3	1:I:140:TYR:HB2	1.66	0.76
2:G:57:ARG:HH22	2:J:24:PHE:HZ	1.34	0.76
2:A:47:MET:HG2	2:B:21:LEU:HD22	1.68	0.75
1:H:269:ILE:HB	1:H:306:VAL:HG21	1.68	0.75
1:C:123:LEU:HB3	1:C:139:VAL:HG11	1.69	0.75
1:I:123:LEU:HB3	1:I:139:VAL:HG11	1.69	0.75
1:M:123:LEU:HB3	1:M:139:VAL:HG11	1.68	0.75
1:H:120:ARG:HG3	1:H:140:TYR:HB2	1.68	0.75
1:M:378:LEU:HD22	1:M:422:MET:HG2	1.67	0.75
1:I:346:LEU:CD1	1:I:414:LYS:C	2.61	0.74
1:F:338:PRO:CG	1:F:387:TYR:CE1	2.71	0.74
1:F:120:ARG:HG3	1:F:140:TYR:HB2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:374:PHE:HB3	1:I:421:PHE:CB	2.18	0.74
1:O:342:ILE:HG13	1:O:387:TYR:C	2.12	0.73
2:A:30:PHE:HE1	2:B:60:PHE:HB2	1.53	0.73
1:F:338:PRO:HB3	1:F:387:TYR:CE1	2.21	0.73
1:H:426:ASP:HB3	1:H:734:PHE:HB3	1.68	0.73
1:F:123:LEU:HB3	1:F:139:VAL:HG11	1.70	0.73
2:G:45:HIS:HD1	2:G:90:TYR:HH	1.37	0.73
1:O:342:ILE:HG12	1:O:387:TYR:CB	2.12	0.73
1:O:525:PRO:HA	1:O:603:MET:HE2	1.69	0.72
1:I:346:LEU:HD11	1:I:414:LYS:CA	2.20	0.72
2:P:397:ARG:HB2	2:P:415:LEU:HB2	1.71	0.72
2:G:397:ARG:HB2	2:G:415:LEU:HB2	1.71	0.72
1:H:480:SER:HB2	1:H:506:ARG:HB3	1.72	0.72
2:P:45:HIS:CD2	2:N:47:MET:HE3	2.25	0.71
2:B:143:PHE:HE1	1:F:66:LEU:HD13	1.56	0.71
1:C:40:ALA:HB1	1:C:52:LEU:HD21	1.72	0.71
1:I:346:LEU:HD13	1:I:414:LYS:O	1.89	0.71
1:I:516:GLN:HG2	1:I:517:SER:H	1.55	0.71
2:J:297:LYS:HZ1	2:J:595:PRO:HD3	1.56	0.71
1:H:123:LEU:HB3	1:H:139:VAL:HG11	1.70	0.71
1:M:516:GLN:HG2	1:M:517:SER:H	1.55	0.70
2:B:64:LEU:CD2	1:F:118:MET:HG2	2.20	0.70
1:I:206:GLU:O	1:I:210:LEU:N	2.20	0.69
1:I:458:LEU:HB3	1:I:467:THR:HG22	1.73	0.69
1:I:516:GLN:HG3	1:I:553:HIS:HB2	1.73	0.69
1:C:206:GLU:O	1:C:210:LEU:N	2.20	0.69
2:J:94:LEU:HD21	2:J:116:VAL:HG23	1.72	0.69
1:H:270:SER:HA	1:H:273:MET:SD	2.33	0.69
1:C:526:PRO:HA	1:C:529:ARG:HB2	1.74	0.69
2:B:144:SER:CB	1:F:133:GLN:CD	2.58	0.68
1:I:339:VAL:O	1:I:391:PHE:CD1	2.46	0.68
2:A:30:PHE:CE1	2:B:60:PHE:HB2	2.28	0.68
1:F:632:GLN:HG2	1:F:636:CYS:HB3	1.76	0.68
2:P:45:HIS:HD1	2:P:90:TYR:HH	1.40	0.68
2:P:390:VAL:HG12	2:P:393:GLU:HG3	1.74	0.68
3:R:33:TRP:O	3:R:76:ASN:ND2	2.27	0.68
1:H:440:LEU:HD11	1:H:446:VAL:CG2	2.21	0.68
2:B:443:PHE:CE2	1:I:713:SER:O	2.46	0.68
3:E:33:TRP:O	3:E:76:ASN:ND2	2.27	0.68
2:N:297:LYS:HZ1	2:N:595:PRO:HD3	1.58	0.68
2:G:92:GLY:HA2	2:J:13:TYR:CD2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:632:GLN:HG2	1:O:636:CYS:HB3	1.76	0.67
2:A:45:HIS:HD1	2:A:90:TYR:HH	1.40	0.67
2:J:22:LYS:NZ	2:J:26:GLU:OE2	2.27	0.67
1:M:206:GLU:O	1:M:210:LEU:N	2.20	0.67
2:N:22:LYS:NZ	2:N:26:GLU:OE2	2.27	0.67
1:M:516:GLN:HG3	1:M:553:HIS:HB2	1.74	0.67
2:P:45:HIS:CD2	2:N:47:MET:CE	2.77	0.67
2:B:22:LYS:NZ	2:B:26:GLU:OE2	2.27	0.67
1:H:378:LEU:HD22	1:H:422:MET:HB2	1.75	0.67
1:C:480:SER:HB2	1:C:506:ARG:HE	1.59	0.67
1:H:441:LEU:HG	1:H:513:TRP:CE3	2.30	0.67
2:G:161:THR:HB	2:G:188:VAL:HG13	1.77	0.67
2:P:89:ALA:CA	2:N:13:TYR:OH	2.41	0.67
1:I:487:PHE:HE1	1:I:491:LEU:HD12	1.58	0.67
1:M:412:LEU:HD21	1:M:454:MET:HE2	1.76	0.67
1:H:234:ILE:HD13	1:H:299:MET:N	2.09	0.67
1:H:292:LYS:HB3	1:H:295:ASP:HB2	1.77	0.67
1:H:441:LEU:HD22	1:H:554:MET:HG2	1.78	0.66
1:I:487:PHE:CE1	1:I:491:LEU:HD12	2.30	0.66
3:L:33:TRP:O	3:L:76:ASN:ND2	2.27	0.66
2:P:161:THR:HB	2:P:188:VAL:HG13	1.77	0.66
1:F:248:VAL:HG23	1:F:252:LEU:HD12	1.78	0.66
2:A:161:THR:HB	2:A:188:VAL:HG13	1.77	0.66
1:F:525:PRO:HB3	1:F:603:MET:HG3	1.77	0.66
2:G:141:ASP:O	1:I:68:LYS:HE3	1.96	0.66
1:I:339:VAL:CG2	1:I:391:PHE:CD1	2.79	0.66
1:H:248:VAL:HG23	1:H:252:LEU:HD12	1.78	0.66
2:N:187:ASN:ND2	2:N:587:TYR:OH	2.29	0.66
2:G:530:ILE:HD12	2:G:535:CYS:HB2	1.78	0.66
1:C:749:ILE:HD13	1:C:758:PRO:HD3	1.79	0.65
1:H:632:GLN:HG2	1:H:636:CYS:HB3	1.76	0.65
3:R:67:GLU:O	3:R:82:HIS:NE2	2.30	0.65
2:B:187:ASN:ND2	2:B:587:TYR:OH	2.29	0.65
1:M:749:ILE:HD13	1:M:758:PRO:HD3	1.79	0.65
2:B:54:SER:OG	1:F:128:ARG:NH2	2.29	0.65
1:I:669:LEU:HG	1:I:671:ARG:H	1.62	0.65
3:K:45:CYS:SG	3:K:80:HIS:HE1	2.20	0.65
2:P:47:MET:SD	2:N:21:LEU:HD22	2.37	0.65
3:E:72:TRP:HB2	3:E:105:LYS:HB3	1.79	0.65
1:I:749:ILE:HD13	1:I:758:PRO:HD3	1.78	0.65
2:A:530:ILE:HD12	2:A:535:CYS:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:187:ASN:ND2	2:J:587:TYR:OH	2.29	0.65
1:H:234:ILE:CD1	1:H:299:MET:N	2.60	0.65
1:H:439:ARG:HG3	1:H:440:LEU:H	1.62	0.65
2:P:207:GLU:HG3	2:P:238:PRO:HG3	1.79	0.65
2:A:207:GLU:HG3	2:A:238:PRO:HG3	1.79	0.65
2:B:144:SER:CB	1:F:133:GLN:NE2	2.59	0.65
3:R:72:TRP:HB2	3:R:105:LYS:HB3	1.79	0.65
1:C:669:LEU:HG	1:C:671:ARG:H	1.62	0.65
3:D:36:ASP:HB2	3:D:77:HIS:HE2	1.62	0.65
1:O:248:VAL:HG23	1:O:252:LEU:HD12	1.78	0.65
2:P:46:LYS:CB	2:N:30:PHE:CD2	2.77	0.65
3:Q:45:CYS:SG	3:Q:80:HIS:HE1	2.20	0.65
3:Q:36:ASP:HB2	3:Q:77:HIS:HE2	1.62	0.64
2:G:30:PHE:CZ	2:J:61:MET:HB2	2.32	0.64
3:L:72:TRP:HB2	3:L:105:LYS:HB3	1.79	0.64
2:B:66:GLU:OE2	1:F:54:PHE:HB3	1.97	0.64
1:O:342:ILE:CG1	1:O:387:TYR:HB2	2.26	0.64
3:E:67:GLU:O	3:E:82:HIS:NE2	2.29	0.64
1:O:342:ILE:HD11	1:O:387:TYR:HB2	1.80	0.64
3:D:45:CYS:SG	3:D:80:HIS:HE1	2.20	0.64
2:G:207:GLU:HG3	2:G:238:PRO:HG3	1.79	0.64
2:B:75:ARG:HD2	1:F:59:ARG:HH12	1.63	0.64
2:B:64:LEU:HD21	1:F:118:MET:HG2	1.79	0.63
1:I:342:ILE:HG21	1:I:388:LEU:HD12	1.80	0.63
3:K:36:ASP:HB2	3:K:77:HIS:HE2	1.62	0.63
2:P:530:ILE:HD12	2:P:535:CYS:HB2	1.79	0.63
3:L:67:GLU:O	3:L:82:HIS:NE2	2.29	0.63
2:A:222:ILE:HA	2:A:225:LEU:HB2	1.80	0.63
2:J:553:GLN:HB2	2:J:564:ARG:HB2	1.81	0.63
1:M:452:LYS:HA	1:M:455:ILE:HG23	1.81	0.63
1:M:473:MET:HG3	1:M:512:TYR:HB3	1.79	0.63
1:F:543:HIS:O	1:F:544:SER:C	2.41	0.63
2:P:222:ILE:HA	2:P:225:LEU:HB2	1.80	0.63
1:F:342:ILE:HG12	1:F:387:TYR:HB3	1.81	0.63
1:F:345:LEU:HG	1:F:418:LEU:HD11	1.81	0.63
2:G:222:ILE:HA	2:G:225:LEU:HB2	1.80	0.63
1:M:248:VAL:HG23	1:M:252:LEU:HD12	1.81	0.63
1:M:669:LEU:HG	1:M:671:ARG:H	1.62	0.63
2:N:214:SER:O	2:N:251:LYS:NZ	2.32	0.62
2:N:539:ARG:HH22	2:N:577:ARG:HD3	1.64	0.62
1:O:551:GLN:NE2	3:Q:30:VAL:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:VAL:HG23	1:C:252:LEU:HD12	1.81	0.62
2:B:553:GLN:HB2	2:B:564:ARG:HB2	1.81	0.62
1:O:282:SER:HA	1:O:286:HIS:HB3	1.80	0.62
1:M:342:ILE:HG13	1:M:387:TYR:O	1.99	0.62
1:M:378:LEU:CD2	1:M:422:MET:HG2	2.29	0.62
1:O:525:PRO:HB3	1:O:603:MET:HG3	1.81	0.62
2:N:553:GLN:HB2	2:N:564:ARG:HB2	1.81	0.62
1:F:551:GLN:NE2	3:D:30:VAL:O	2.32	0.62
1:I:480:SER:CB	1:I:507:VAL:O	2.48	0.62
2:P:30:PHE:CZ	2:N:50:ALA:HB1	2.34	0.62
2:B:539:ARG:HH22	2:B:577:ARG:HD3	1.64	0.62
1:M:90:ARG:NH2	1:M:150:GLN:OE1	2.33	0.62
2:N:370:ARG:NH1	2:N:386:GLY:O	2.33	0.62
1:F:282:SER:HA	1:F:286:HIS:HB3	1.80	0.62
1:M:314:CYS:HB3	1:M:369:THR:HG21	1.82	0.62
1:O:90:ARG:NH2	1:O:150:GLN:OE1	2.33	0.62
2:P:18:LEU:HD13	2:N:17:LEU:CD2	2.30	0.62
2:B:214:SER:O	2:B:251:LYS:NZ	2.32	0.62
1:H:234:ILE:HD13	1:H:299:MET:CA	2.29	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
2:P:45:HIS:HD2	2:N:47:MET:SD	2.21	0.61
1:H:314:CYS:HB3	1:H:369:THR:HG21	1.81	0.61
1:O:223:LYS:HE3	1:O:227:GLU:HG3	1.82	0.61
2:B:370:ARG:NH1	2:B:386:GLY:O	2.33	0.61
1:I:90:ARG:NH2	1:I:150:GLN:OE1	2.33	0.61
1:H:90:ARG:NH2	1:H:150:GLN:OE1	2.33	0.61
1:H:223:LYS:HE3	1:H:227:GLU:HG3	1.82	0.61
1:O:749:ILE:HD13	1:O:758:PRO:HD3	1.83	0.61
2:P:382:ILE:HB	2:P:402:TYR:HB3	1.82	0.61
1:C:314:CYS:HB3	1:C:369:THR:HG21	1.82	0.61
2:A:221:ARG:HH11	2:A:258:LYS:H	1.48	0.61
1:F:703:ILE:HD11	1:F:744:ARG:HD3	1.83	0.61
1:H:237:VAL:HG11	1:H:302:LEU:CD2	2.14	0.61
1:H:322:ARG:NH2	1:H:373:ASP:HA	2.13	0.61
1:F:749:ILE:HD13	1:F:758:PRO:HD3	1.83	0.61
1:I:314:CYS:HB3	1:I:369:THR:HG21	1.82	0.61
2:A:273:GLU:HA	2:A:283:TYR:HB3	1.81	0.61
2:G:535:CYS:SG	2:G:564:ARG:NH1	2.73	0.61
1:H:551:GLN:NE2	3:K:30:VAL:O	2.32	0.61
2:A:45:HIS:CD2	2:B:47:MET:SD	2.94	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:314:CYS:HB3	1:F:369:THR:HG21	1.82	0.61
2:A:382:ILE:HB	2:A:402:TYR:HB3	1.82	0.61
2:J:539:ARG:HH22	2:J:577:ARG:HD3	1.64	0.61
1:I:248:VAL:HG23	1:I:252:LEU:HD12	1.81	0.61
2:J:370:ARG:NH1	2:J:386:GLY:O	2.33	0.61
1:C:703:ILE:HD11	1:C:744:ARG:HD3	1.83	0.60
2:G:221:ARG:HH11	2:G:258:LYS:H	1.48	0.60
3:K:85:SER:HA	3:K:88:LEU:HD12	1.83	0.60
1:O:441:LEU:HD21	1:O:508:LEU:HD11	1.83	0.60
2:G:382:ILE:HB	2:G:402:TYR:HB3	1.82	0.60
1:I:77:LEU:HD22	1:I:123:LEU:HD22	1.83	0.60
1:I:703:ILE:HD11	1:I:744:ARG:HD3	1.83	0.60
1:O:703:ILE:HD11	1:O:744:ARG:HD3	1.83	0.60
1:C:90:ARG:NH2	1:C:150:GLN:OE1	2.33	0.60
1:C:540:LEU:O	1:C:541:ALA:C	2.45	0.60
2:B:64:LEU:HD21	1:F:118:MET:CG	2.30	0.60
1:F:441:LEU:HD21	1:F:508:LEU:HD11	1.84	0.60
2:G:273:GLU:HA	2:G:283:TYR:HB3	1.81	0.60
1:M:77:LEU:HD22	1:M:123:LEU:HD22	1.83	0.60
1:O:409:GLU:OE2	1:O:453:ASN:ND2	2.34	0.60
3:Q:85:SER:HA	3:Q:88:LEU:HD12	1.83	0.60
1:C:223:LYS:HE3	1:C:227:GLU:HG3	1.84	0.60
2:P:535:CYS:SG	2:P:564:ARG:NH1	2.73	0.60
1:H:120:ARG:O	1:H:124:MET:CB	2.50	0.60
1:M:223:LYS:HE3	1:M:227:GLU:HG3	1.84	0.60
1:O:314:CYS:HB3	1:O:369:THR:HG21	1.82	0.60
2:P:89:ALA:HA	2:N:13:TYR:CZ	2.37	0.60
2:A:535:CYS:SG	2:A:564:ARG:NH1	2.73	0.60
1:M:703:ILE:HD11	1:M:744:ARG:HD3	1.83	0.60
2:P:50:ALA:HB3	2:N:24:PHE:CE2	2.37	0.60
2:B:297:LYS:HZ1	2:B:595:PRO:HD3	1.65	0.60
1:H:749:ILE:HD13	1:H:758:PRO:HD3	1.83	0.60
2:A:434:MET:HE2	2:A:455:ARG:HE	1.67	0.60
2:P:113:VAL:HB	2:P:116:VAL:HG12	1.82	0.60
2:P:221:ARG:HH11	2:P:258:LYS:H	1.48	0.60
1:F:120:ARG:O	1:F:124:MET:CB	2.50	0.60
3:D:85:SER:HA	3:D:88:LEU:HD12	1.83	0.60
2:G:47:MET:CE	2:J:45:HIS:CD2	2.81	0.60
1:H:556:SER:HA	1:H:595:SER:HA	1.84	0.60
1:F:342:ILE:HG13	1:F:387:TYR:O	2.02	0.59
1:I:551:GLN:NE2	3:L:30:VAL:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:434:MET:HE2	2:G:455:ARG:HE	1.67	0.59
1:I:342:ILE:CG1	1:I:388:LEU:HA	2.30	0.59
1:M:644:LEU:HD11	1:M:659:PHE:HB3	1.84	0.59
1:O:506:ARG:HB2	3:Q:30:VAL:HG22	1.84	0.59
1:H:557:ALA:HB3	1:H:594:VAL:HG23	1.84	0.59
1:O:120:ARG:O	1:O:124:MET:CB	2.50	0.59
1:I:282:SER:HA	1:I:286:HIS:HB3	1.85	0.59
1:M:396:LEU:HD13	1:M:454:MET:HE3	1.82	0.59
2:A:289:SER:HG	2:A:294:LYS:H	1.50	0.59
1:F:223:LYS:HE3	1:F:227:GLU:HG3	1.82	0.59
1:F:409:GLU:OE2	1:F:453:ASN:ND2	2.34	0.59
2:G:128:ILE:HG23	2:G:136:LEU:HD21	1.84	0.59
1:C:30:VAL:HB	1:C:64:MET:HE1	1.84	0.59
1:C:77:LEU:HD22	1:C:123:LEU:HD22	1.83	0.59
1:C:282:SER:HA	1:C:286:HIS:HB3	1.85	0.59
2:P:51:THR:OG1	2:N:20:GLN:CG	2.51	0.59
2:P:434:MET:HE2	2:P:455:ARG:HE	1.67	0.59
1:C:551:GLN:NE2	3:E:30:VAL:O	2.35	0.59
2:B:214:SER:OG	2:B:251:LYS:NZ	2.33	0.59
1:F:356:LEU:HD12	1:F:360:PHE:HB2	1.84	0.59
2:G:57:ARG:NH2	2:J:24:PHE:HZ	2.00	0.59
1:I:342:ILE:HB	1:I:391:PHE:CG	2.38	0.59
1:F:506:ARG:HB2	3:D:30:VAL:HG22	1.84	0.59
1:I:223:LYS:HE3	1:I:227:GLU:HG3	1.84	0.59
1:F:556:SER:HA	1:F:595:SER:HA	1.84	0.59
2:J:225:LEU:O	2:J:230:GLN:NE2	2.36	0.59
1:I:525:PRO:HB2	1:I:528:PRO:HD2	1.84	0.59
1:M:768:ALA:HB1	3:R:89:LYS:HB3	1.85	0.58
2:P:555:ASP:HB3	2:P:558:LEU:HB2	1.85	0.58
2:N:153:LYS:HE3	2:N:180:ILE:HA	1.85	0.58
1:F:526:PRO:HD2	1:F:603:MET:SD	2.43	0.58
2:P:45:HIS:CG	2:N:47:MET:CE	2.86	0.58
2:A:128:ILE:HG23	2:A:136:LEU:HD21	1.84	0.58
2:B:225:LEU:O	2:B:230:GLN:NE2	2.36	0.58
2:B:350:PHE:HD2	2:B:363:LYS:HB2	1.68	0.58
2:B:443:PHE:HE2	1:I:713:SER:O	1.85	0.58
1:H:324:GLN:HG2	1:H:348:LEU:HD13	1.85	0.58
1:M:30:VAL:HB	1:M:64:MET:HE1	1.84	0.58
1:M:120:ARG:O	1:M:124:MET:CB	2.51	0.58
1:C:527:ALA:HB3	1:C:528:PRO:HD3	1.84	0.58
1:C:644:LEU:HD11	1:C:659:PHE:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:LEU:HD22	1:F:123:LEU:HD22	1.85	0.58
2:G:555:ASP:HB3	2:G:558:LEU:HB2	1.85	0.58
1:I:487:PHE:HA	1:I:538:PHE:CE2	2.38	0.58
2:N:225:LEU:O	2:N:230:GLN:NE2	2.36	0.58
2:J:161:THR:HG21	2:J:186:LEU:HB2	1.86	0.58
2:J:350:PHE:HD2	2:J:363:LYS:HB2	1.69	0.58
1:O:556:SER:HA	1:O:595:SER:HA	1.84	0.58
2:P:18:LEU:HD22	2:N:14:ALA:CA	2.33	0.58
2:P:286:VAL:HG11	2:P:573:TRP:HH2	1.69	0.58
2:N:350:PHE:HD2	2:N:363:LYS:HB2	1.69	0.58
1:M:551:GLN:NE2	3:R:30:VAL:O	2.35	0.58
2:P:128:ILE:HG23	2:P:136:LEU:HD21	1.84	0.58
1:C:683:GLU:HG3	1:C:688:ARG:HH21	1.69	0.58
2:A:555:ASP:HB3	2:A:558:LEU:HB2	1.85	0.58
2:G:385:ILE:HA	2:G:399:VAL:HG12	1.85	0.58
2:P:385:ILE:HA	2:P:399:VAL:HG12	1.85	0.58
2:N:214:SER:OG	2:N:251:LYS:NZ	2.33	0.58
2:A:459:ARG:HB3	2:A:476:GLY:HA3	1.86	0.58
2:A:525:VAL:HA	2:A:538:MET:HG2	1.86	0.58
1:I:120:ARG:O	1:I:124:MET:CB	2.52	0.58
1:I:644:LEU:HD11	1:I:659:PHE:HB3	1.84	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	1.68	0.58
1:M:622:ILE:HD12	1:M:623:PRO:HD2	1.85	0.58
1:M:698:ASP:HA	1:M:701:HIS:HD2	1.69	0.58
1:O:337:ASN:HB3	1:O:340:ASP:HB2	1.84	0.58
2:P:525:VAL:HA	2:P:538:MET:HG2	1.86	0.58
1:C:118:MET:HG2	2:A:62:SER:CB	2.34	0.58
2:J:214:SER:OG	2:J:251:LYS:NZ	2.33	0.58
1:F:557:ALA:HB3	1:F:594:VAL:HG23	1.84	0.58
1:M:282:SER:HA	1:M:286:HIS:HB3	1.85	0.58
1:O:356:LEU:HD12	1:O:360:PHE:HB2	1.84	0.58
2:N:161:THR:HG21	2:N:186:LEU:HB2	1.86	0.58
1:C:120:ARG:O	1:C:124:MET:CB	2.51	0.58
1:C:346:LEU:HD11	1:C:414:LYS:HB3	1.85	0.58
2:A:286:VAL:HG11	2:A:573:TRP:HH2	1.69	0.58
2:A:436:LEU:O	2:A:455:ARG:NH2	2.37	0.58
1:H:77:LEU:HD22	1:H:123:LEU:HD22	1.85	0.58
1:O:557:ALA:HB3	1:O:594:VAL:HG23	1.84	0.57
2:N:161:THR:HB	2:N:188:VAL:HG13	1.86	0.57
2:A:397:ARG:HB2	2:A:415:LEU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:436:LEU:O	2:G:455:ARG:NH2	2.37	0.57
1:M:683:GLU:HG3	1:M:688:ARG:HH21	1.69	0.57
2:P:374:SER:OG	2:P:385:ILE:O	2.21	0.57
2:N:52:CYS:SG	2:N:53:SER:N	2.77	0.57
1:C:441:LEU:HD21	1:C:508:LEU:HD11	1.86	0.57
1:C:768:ALA:HB1	3:E:89:LYS:HB3	1.85	0.57
2:A:385:ILE:HA	2:A:399:VAL:HG12	1.85	0.57
1:I:345:LEU:CD2	1:I:418:LEU:HD11	2.33	0.57
2:P:436:LEU:O	2:P:455:ARG:NH2	2.37	0.57
2:A:374:SER:OG	2:A:385:ILE:O	2.21	0.57
2:G:459:ARG:HB3	2:G:476:GLY:HA3	1.86	0.57
2:J:153:LYS:HE3	2:J:180:ILE:HA	1.85	0.57
1:M:356:LEU:HD12	1:M:360:PHE:HB2	1.86	0.57
1:C:440:LEU:HD13	1:C:477:MET:HG3	1.86	0.57
2:J:161:THR:HB	2:J:188:VAL:HG13	1.86	0.57
2:P:17:LEU:CD2	2:N:18:LEU:HD13	2.32	0.57
2:B:153:LYS:HE3	2:B:180:ILE:HA	1.85	0.57
1:F:127:ASP:O	1:F:131:VAL:HG22	2.04	0.57
1:I:441:LEU:HD21	1:I:508:LEU:HD11	1.86	0.57
1:C:356:LEU:HD12	1:C:360:PHE:HB2	1.86	0.57
1:C:622:ILE:HD12	1:C:623:PRO:HD2	1.86	0.57
1:F:338:PRO:CB	1:F:387:TYR:CE1	2.83	0.57
2:G:286:VAL:HG11	2:G:573:TRP:HH2	1.69	0.57
1:I:345:LEU:HD21	1:I:378:LEU:HD11	1.86	0.57
1:I:768:ALA:HB1	3:L:89:LYS:HB3	1.85	0.57
1:H:127:ASP:O	1:H:131:VAL:HG22	2.05	0.57
2:P:459:ARG:HB3	2:P:476:GLY:HA3	1.86	0.57
2:B:52:CYS:SG	2:B:53:SER:N	2.77	0.57
2:B:144:SER:OG	1:F:133:GLN:HG2	2.05	0.57
2:B:161:THR:HG21	2:B:186:LEU:HB2	1.86	0.57
2:J:52:CYS:SG	2:J:53:SER:N	2.77	0.57
2:J:160:PHE:O	2:J:164:TYR:N	2.38	0.57
1:I:476:ASP:OD2	1:I:509:THR:HB	2.04	0.57
2:P:455:ARG:NH1	2:P:500:GLU:OE2	2.38	0.57
2:A:30:PHE:CZ	2:B:50:ALA:HB2	2.40	0.57
2:A:455:ARG:NH1	2:A:500:GLU:OE2	2.38	0.57
2:B:75:ARG:HD2	1:F:59:ARG:NH1	2.20	0.57
1:F:144:LEU:HD12	1:F:193:LEU:HA	1.87	0.57
2:G:525:VAL:HA	2:G:538:MET:HG2	1.86	0.57
1:M:698:ASP:HA	1:M:701:HIS:CD2	2.40	0.57
2:N:455:ARG:NH1	2:N:500:GLU:OE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:455:ARG:NH1	2:B:500:GLU:OE2	2.38	0.57
1:F:43:GLU:OE2	1:F:48:ASN:ND2	2.33	0.57
1:I:622:ILE:HD12	1:I:623:PRO:HD2	1.86	0.57
1:I:698:ASP:HA	1:I:701:HIS:CD2	2.40	0.57
2:N:35:LEU:HB2	2:N:42:PHE:HB2	1.87	0.56
2:B:398:THR:HB	2:B:411:MET:HE1	1.87	0.56
2:B:434:MET:HE2	2:B:455:ARG:HE	1.69	0.56
1:I:478:SER:HA	1:I:481:ASN:HD21	1.69	0.56
1:I:483:THR:HG21	1:I:539:TYR:HE1	1.70	0.56
1:M:378:LEU:CD2	1:M:422:MET:HE3	2.35	0.56
2:N:434:MET:HE2	2:N:455:ARG:HE	1.69	0.56
2:J:459:ARG:HB3	2:J:476:GLY:HA3	1.88	0.56
1:M:557:ALA:HB3	1:M:594:VAL:HG23	1.87	0.56
1:O:144:LEU:HD12	1:O:193:LEU:HA	1.87	0.56
2:P:47:MET:HE2	2:N:21:LEU:HA	1.88	0.56
1:C:698:ASP:HA	1:C:701:HIS:HD2	1.69	0.56
2:A:153:LYS:NZ	2:A:179:ASP:OD1	2.38	0.56
2:G:455:ARG:NH1	2:G:500:GLU:OE2	2.38	0.56
2:J:434:MET:HE2	2:J:455:ARG:HE	1.68	0.56
2:J:455:ARG:NH1	2:J:500:GLU:OE2	2.38	0.56
1:I:356:LEU:HD12	1:I:360:PHE:HB2	1.87	0.56
1:H:225:LEU:HB3	1:H:272:HIS:CE1	2.40	0.56
1:O:343:GLN:OE1	1:O:391:PHE:CE1	2.59	0.56
2:N:436:LEU:O	2:N:455:ARG:NH2	2.39	0.56
1:C:698:ASP:HA	1:C:701:HIS:CD2	2.40	0.56
1:I:345:LEU:CB	1:I:418:LEU:HD11	2.36	0.56
1:H:273:MET:HA	1:H:303:PHE:HE2	1.70	0.56
1:H:234:ILE:HG13	1:H:302:LEU:HD22	1.87	0.56
1:M:441:LEU:HD21	1:M:508:LEU:HD11	1.86	0.56
2:A:254:PRO:O	2:A:255:LYS:HG2	2.06	0.56
1:I:127:ASP:O	1:I:131:VAL:HG22	2.06	0.56
2:P:153:LYS:NZ	2:P:179:ASP:OD1	2.38	0.56
2:J:35:LEU:HB2	2:J:42:PHE:HB2	1.87	0.56
1:H:230:ALA:HB2	1:H:276:ILE:HG12	1.87	0.56
2:P:254:PRO:O	2:P:255:LYS:HG2	2.06	0.56
2:J:436:LEU:O	2:J:455:ARG:NH2	2.39	0.56
1:M:560:ASN:HB2	3:R:25:LYS:HG2	1.88	0.56
2:N:459:ARG:HB3	2:N:476:GLY:HA3	1.88	0.56
1:I:404:THR:OG1	1:I:407:GLU:OE1	2.24	0.56
2:B:35:LEU:HB2	2:B:42:PHE:HB2	1.87	0.56
2:B:436:LEU:O	2:B:455:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:153:LYS:NZ	2:G:179:ASP:OD1	2.38	0.56
1:I:144:LEU:HD12	1:I:193:LEU:HA	1.88	0.56
1:H:237:VAL:CG1	1:H:302:LEU:HD22	2.36	0.56
2:P:370:ARG:HG2	2:P:389:SER:HA	1.87	0.55
2:N:137:LEU:HG	2:N:176:LEU:HD21	1.88	0.55
1:C:127:ASP:O	1:C:131:VAL:HG22	2.06	0.55
1:C:560:ASN:HB2	3:E:25:LYS:HG2	1.88	0.55
2:B:459:ARG:HB3	2:B:476:GLY:HA3	1.88	0.55
2:G:30:PHE:HE1	2:J:61:MET:HB2	1.66	0.55
2:G:91:THR:HG23	2:G:93:ASN:H	1.71	0.55
2:P:275:SER:OG	2:P:574:ASP:O	2.25	0.55
2:N:275:SER:OG	2:N:574:ASP:O	2.23	0.55
2:N:398:THR:HB	2:N:411:MET:HE1	1.88	0.55
1:F:346:LEU:HA	1:F:418:LEU:CD1	2.36	0.55
2:J:137:LEU:HG	2:J:176:LEU:HD21	1.88	0.55
2:J:275:SER:OG	2:J:574:ASP:O	2.23	0.55
1:I:557:ALA:HB3	1:I:594:VAL:HG23	1.87	0.55
1:H:43:GLU:OE2	1:H:48:ASN:ND2	2.33	0.55
2:P:476:GLY:O	2:P:496:SER:N	2.40	0.55
2:N:37:VAL:HG12	2:N:38:GLU:HG2	1.88	0.55
2:B:161:THR:HB	2:B:188:VAL:HG13	1.86	0.55
3:D:45:CYS:SG	3:D:47:ASN:ND2	2.79	0.55
2:G:254:PRO:O	2:G:255:LYS:HG2	2.06	0.55
3:K:45:CYS:SG	3:K:47:ASN:ND2	2.79	0.55
3:Q:45:CYS:SG	3:Q:47:ASN:ND2	2.79	0.55
1:C:144:LEU:HD12	1:C:193:LEU:HA	1.88	0.55
1:I:546:ARG:HH21	3:L:35:TRP:HE1	1.53	0.55
1:I:560:ASN:HB2	3:L:25:LYS:HG2	1.88	0.55
1:F:343:GLN:OE1	1:F:391:PHE:CE1	2.60	0.55
1:F:478:SER:HA	1:F:481:ASN:ND2	2.21	0.55
2:J:297:LYS:HB3	2:J:594:SER:HB2	1.89	0.55
2:P:91:THR:HG23	2:P:93:ASN:H	1.71	0.55
2:P:217:LEU:HG	2:P:225:LEU:HD21	1.89	0.55
2:A:217:LEU:HG	2:A:225:LEU:HD21	1.89	0.55
2:B:160:PHE:O	2:B:164:TYR:N	2.38	0.55
2:J:122:GLU:O	2:J:125:ILE:HG22	2.07	0.55
1:I:43:GLU:OE2	1:I:48:ASN:ND2	2.33	0.55
1:I:339:VAL:O	1:I:391:PHE:HD1	1.89	0.55
1:C:506:ARG:HB2	3:E:30:VAL:HG22	1.89	0.55
2:B:137:LEU:HG	2:B:176:LEU:HD21	1.88	0.55
1:I:546:ARG:HB3	3:L:35:TRP:HD1	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:459:LYS:HE3	1:M:464:CYS:HA	1.88	0.55
2:N:160:PHE:O	2:N:164:TYR:N	2.38	0.55
1:C:43:GLU:OE2	1:C:48:ASN:ND2	2.33	0.55
2:B:297:LYS:HB3	2:B:594:SER:HB2	1.89	0.55
1:M:342:ILE:HB	1:M:391:PHE:HB2	1.89	0.55
2:J:398:THR:HB	2:J:411:MET:HE1	1.88	0.55
1:I:346:LEU:CD2	1:I:414:LYS:CB	2.84	0.55
1:I:559:LEU:O	1:I:592:LEU:N	2.39	0.55
2:A:47:MET:HG2	2:B:21:LEU:CD2	2.36	0.55
2:N:122:GLU:O	2:N:125:ILE:HG22	2.07	0.54
1:C:557:ALA:HB3	1:C:594:VAL:HG23	1.87	0.54
2:A:476:GLY:O	2:A:496:SER:N	2.40	0.54
2:B:37:VAL:HG12	2:B:38:GLU:HG2	1.88	0.54
1:F:527:ALA:HB3	1:F:528:PRO:HD3	1.89	0.54
2:J:37:VAL:HG12	2:J:38:GLU:HG2	1.88	0.54
1:I:339:VAL:CG2	1:I:391:PHE:HD1	2.20	0.54
3:K:43:ALA:HB3	3:K:79:PHE:HE1	1.71	0.54
1:M:404:THR:OG1	1:M:407:GLU:OE1	2.24	0.54
2:A:51:THR:HG21	2:B:17:LEU:HD13	1.90	0.54
1:I:409:GLU:OE2	1:I:453:ASN:ND2	2.40	0.54
1:I:506:ARG:HB2	3:L:30:VAL:HG22	1.89	0.54
1:H:144:LEU:HD12	1:H:193:LEU:HA	1.87	0.54
1:M:102:LEU:HD11	1:M:182:ALA:HB1	1.90	0.54
1:M:383:ARG:HB3	1:M:688:ARG:HH12	1.72	0.54
2:P:24:PHE:CE2	2:N:51:THR:HG23	2.43	0.54
2:B:122:GLU:O	2:B:125:ILE:HG22	2.07	0.54
2:B:141:ASP:O	1:F:68:LYS:CE	2.53	0.54
1:F:759:GLU:OE1	1:F:759:GLU:N	2.37	0.54
2:P:414:PRO:O	2:P:449:TRP:NE1	2.41	0.54
1:M:144:LEU:HD12	1:M:193:LEU:HA	1.88	0.54
2:P:305:LEU:HD21	2:P:323:GLY:HA3	1.90	0.54
3:D:43:ALA:HB3	3:D:79:PHE:HE1	1.71	0.54
2:G:275:SER:OG	2:G:574:ASP:O	2.25	0.54
2:P:30:PHE:CE1	2:N:50:ALA:HB2	2.43	0.54
2:N:297:LYS:HB3	2:N:594:SER:HB2	1.89	0.54
1:I:102:LEU:HD11	1:I:182:ALA:HB1	1.90	0.54
1:H:703:ILE:HG22	1:H:730:LEU:HD13	1.90	0.54
1:H:717:MET:HB3	1:H:722:LEU:HG	1.89	0.54
1:M:735:LEU:HD13	1:M:736:PRO:HD2	1.90	0.54
1:C:559:LEU:O	1:C:592:LEU:N	2.39	0.54
2:A:522:ASP:OD1	2:A:522:ASP:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:186:LEU:HD13	2:G:194:VAL:HG11	1.90	0.54
2:G:455:ARG:NH1	2:G:457:THR:O	2.41	0.54
1:O:717:MET:HB3	1:O:722:LEU:HG	1.89	0.54
1:C:409:GLU:OE2	1:C:453:ASN:ND2	2.40	0.54
2:B:321:ALA:HB3	2:B:375:LEU:HD11	1.90	0.54
1:I:336:LYS:CE	1:I:387:TYR:HE2	2.13	0.54
1:H:644:LEU:HD11	1:H:659:PHE:HB3	1.90	0.54
2:P:455:ARG:NH1	2:P:457:THR:O	2.41	0.54
1:C:717:MET:HB3	1:C:722:LEU:HG	1.90	0.54
1:C:735:LEU:HD13	1:C:736:PRO:HD2	1.90	0.54
2:B:66:GLU:CD	1:F:54:PHE:HB3	2.33	0.54
1:F:644:LEU:HD11	1:F:659:PHE:HB3	1.90	0.54
2:G:548:LYS:NZ	2:G:549:TYR:O	2.41	0.54
1:I:383:ARG:HB2	1:I:688:ARG:HH12	1.72	0.54
1:I:520:PRO:HG3	1:I:553:HIS:CD2	2.43	0.54
1:H:326:LYS:HA	1:H:329:VAL:HG12	1.89	0.54
1:F:698:ASP:HA	1:F:701:HIS:CD2	2.43	0.54
2:G:289:SER:HG	2:G:294:LYS:H	1.55	0.54
2:G:476:GLY:O	2:G:496:SER:N	2.40	0.54
1:M:43:GLU:OE2	1:M:48:ASN:ND2	2.33	0.53
1:M:378:LEU:HD13	1:M:422:MET:HG2	1.90	0.53
1:M:506:ARG:HB2	3:R:30:VAL:HG22	1.89	0.53
1:O:43:GLU:OE2	1:O:48:ASN:ND2	2.33	0.53
3:Q:43:ALA:HB3	3:Q:79:PHE:HE1	1.71	0.53
2:A:47:MET:CG	2:B:21:LEU:HD22	2.38	0.53
2:A:414:PRO:O	2:A:449:TRP:NE1	2.41	0.53
2:J:321:ALA:HB3	2:J:375:LEU:HD11	1.90	0.53
1:I:717:MET:HB3	1:I:722:LEU:HG	1.90	0.53
1:M:338:PRO:HB3	1:M:387:TYR:CD1	2.44	0.53
2:N:273:GLU:OE2	2:N:307:LYS:N	2.41	0.53
2:N:321:ALA:HB3	2:N:375:LEU:HD11	1.90	0.53
2:N:415:LEU:HD23	2:N:416:PRO:HD2	1.91	0.53
2:A:548:LYS:NZ	2:A:549:TYR:O	2.41	0.53
1:I:339:VAL:CA	1:I:391:PHE:HD1	2.22	0.53
1:I:339:VAL:HA	1:I:391:PHE:HB2	1.90	0.53
1:M:717:MET:HB3	1:M:722:LEU:HG	1.90	0.53
2:G:217:LEU:HG	2:G:225:LEU:HD21	1.89	0.53
2:G:348:ASN:ND2	2:G:366:MET:O	2.42	0.53
2:J:273:GLU:OE2	2:J:307:LYS:N	2.41	0.53
1:C:612:THR:OG1	1:C:655:ASN:O	2.27	0.53
2:A:53:SER:OG	2:A:111:LEU:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:91:THR:HG23	2:A:93:ASN:H	1.71	0.53
3:E:46:ARG:O	3:E:46:ARG:NH1	2.42	0.53
1:I:472:GLY:C	1:I:512:TYR:CE1	2.87	0.53
1:I:735:LEU:HD13	1:I:736:PRO:HD2	1.90	0.53
1:M:371:ALA:CB	1:M:421:PHE:CE1	2.91	0.53
2:P:21:LEU:HD12	2:N:17:LEU:HD21	1.91	0.53
2:P:51:THR:OG1	2:N:20:GLN:HB2	2.05	0.53
1:C:397:LYS:HD2	1:C:398:LYS:HB2	1.90	0.53
1:H:329:VAL:HG22	1:H:381:ASN:HD22	1.73	0.53
1:C:698:ASP:OD1	1:C:701:HIS:NE2	2.41	0.53
2:A:348:ASN:ND2	2:A:366:MET:O	2.42	0.53
2:B:522:ASP:N	2:B:522:ASP:OD1	2.42	0.53
1:M:612:THR:OG1	1:M:655:ASN:O	2.27	0.53
2:P:186:LEU:HD13	2:P:194:VAL:HG11	1.90	0.53
2:B:273:GLU:OE2	2:B:307:LYS:N	2.41	0.53
2:G:305:LEU:HD21	2:G:323:GLY:HA3	1.90	0.53
2:G:374:SER:OG	2:G:385:ILE:O	2.21	0.53
1:M:698:ASP:OD1	1:M:701:HIS:NE2	2.41	0.53
1:O:546:ARG:HB2	3:Q:33:TRP:HB2	1.91	0.53
2:P:348:ASN:ND2	2:P:366:MET:O	2.41	0.53
3:R:46:ARG:O	3:R:46:ARG:NH1	2.42	0.53
2:A:455:ARG:NH1	2:A:457:THR:O	2.41	0.53
1:I:612:THR:OG1	1:I:655:ASN:O	2.27	0.53
1:H:700:LYS:O	1:H:703:ILE:HG12	2.09	0.53
1:M:710:ILE:HG21	1:M:729:GLN:HE22	1.74	0.53
1:O:342:ILE:HG21	1:O:388:LEU:HA	1.90	0.53
1:O:698:ASP:HA	1:O:701:HIS:CD2	2.43	0.53
2:P:46:LYS:CB	2:N:30:PHE:HD2	2.22	0.53
2:P:51:THR:OG1	2:N:20:GLN:HG3	2.09	0.53
1:C:499:GLY:O	1:C:531:ALA:HB2	2.09	0.53
2:G:47:MET:CE	2:J:45:HIS:CG	2.92	0.53
1:I:698:ASP:OD1	1:I:701:HIS:NE2	2.41	0.53
1:C:102:LEU:HD11	1:C:182:ALA:HB1	1.90	0.53
2:J:522:ASP:OD1	2:J:522:ASP:N	2.42	0.53
2:P:51:THR:OG1	2:N:20:GLN:HB3	2.08	0.52
2:P:431:ILE:HB	2:P:442:TYR:HB3	1.91	0.52
2:B:415:LEU:HD23	2:B:416:PRO:HD2	1.91	0.52
1:F:559:LEU:O	1:F:592:LEU:N	2.38	0.52
1:H:273:MET:HA	1:H:303:PHE:CE2	2.44	0.52
1:M:614:GLU:OE1	1:M:617:GLN:NE2	2.43	0.52
2:A:297:LYS:HZ1	2:A:595:PRO:HD3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:45:HIS:ND1	2:P:90:TYR:OH	2.32	0.52
2:P:47:MET:SD	2:N:21:LEU:HD13	2.49	0.52
2:P:301:PRO:HG3	2:P:360:TRP:CE2	2.45	0.52
2:A:186:LEU:HD13	2:A:194:VAL:HG11	1.90	0.52
2:A:431:ILE:HB	2:A:442:TYR:HB3	1.91	0.52
2:B:570:ARG:HA	2:B:598:PRO:HB3	1.90	0.52
1:F:343:GLN:OE1	1:F:391:PHE:CZ	2.62	0.52
1:M:556:SER:HA	1:M:595:SER:HA	1.91	0.52
2:N:274:ALA:N	2:N:284:SER:O	2.42	0.52
1:O:341:TYR:HD2	1:O:387:TYR:HD2	1.57	0.52
1:O:644:LEU:HD11	1:O:659:PHE:HB3	1.90	0.52
2:N:570:ARG:HA	2:N:598:PRO:HB3	1.90	0.52
1:C:437:ALA:HA	1:C:513:TRP:HZ3	1.74	0.52
2:G:275:SER:OG	2:G:573:TRP:NE1	2.43	0.52
2:G:301:PRO:HG3	2:G:360:TRP:CE2	2.45	0.52
1:I:710:ILE:HG21	1:I:729:GLN:HE22	1.73	0.52
1:M:437:ALA:HA	1:M:513:TRP:HZ3	1.74	0.52
2:P:30:PHE:CE2	2:N:50:ALA:CB	2.93	0.52
2:A:305:LEU:HD21	2:A:323:GLY:HA3	1.90	0.52
2:B:111:LEU:HB2	2:B:113:VAL:HG22	1.91	0.52
2:G:398:THR:HG22	2:G:414:PRO:HB3	1.91	0.52
2:J:570:ARG:HA	2:J:598:PRO:HB3	1.91	0.52
1:I:509:THR:HB	1:I:512:TYR:HD2	1.75	0.52
2:P:318:ILE:HB	2:P:353:PHE:HB3	1.92	0.52
1:C:133:GLN:CD	2:A:144:SER:HB3	2.34	0.52
2:A:318:ILE:HB	2:A:353:PHE:HB3	1.92	0.52
1:H:416:MET:HA	1:H:461:GLU:OE1	2.09	0.52
1:O:759:GLU:OE1	1:O:759:GLU:N	2.37	0.52
2:P:302:PRO:HG2	2:P:305:LEU:HB3	1.92	0.52
2:N:458:SER:O	2:N:459:ARG:NH1	2.41	0.52
1:I:346:LEU:HG	1:I:414:LYS:HB3	1.87	0.52
1:O:342:ILE:CD1	1:O:387:TYR:HB2	2.38	0.52
2:P:289:SER:HG	2:P:294:LYS:H	1.54	0.52
2:J:415:LEU:HD23	2:J:416:PRO:HD2	1.91	0.52
1:H:342:ILE:HB	1:H:391:PHE:HD2	1.74	0.52
2:N:522:ASP:N	2:N:522:ASP:OD1	2.42	0.52
1:I:546:ARG:HE	3:L:35:TRP:HE1	1.57	0.52
1:H:598:GLN:HG2	1:H:634:LEU:HG	1.92	0.52
1:M:509:THR:HB	1:M:512:TYR:HD2	1.75	0.51
2:P:275:SER:OG	2:P:573:TRP:NE1	2.43	0.51
2:P:548:LYS:NZ	2:P:549:TYR:O	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:614:GLU:OE1	1:C:617:GLN:NE2	2.43	0.51
2:A:195:ARG:HB2	2:A:224:ALA:HB1	1.93	0.51
2:G:53:SER:OG	2:G:111:LEU:O	2.27	0.51
1:H:759:GLU:OE1	1:H:759:GLU:N	2.37	0.51
2:A:275:SER:OG	2:A:573:TRP:NE1	2.43	0.51
2:A:301:PRO:HG3	2:A:360:TRP:CE2	2.45	0.51
2:P:30:PHE:CE2	2:N:50:ALA:HB1	2.45	0.51
2:J:348:ASN:ND2	2:J:366:MET:O	2.44	0.51
2:B:513:ALA:HB3	2:B:561:TRP:HZ3	1.76	0.51
2:G:209:ARG:O	2:G:213:LEU:N	2.43	0.51
1:M:638:LYS:HD3	1:M:639:PRO:HD2	1.93	0.51
2:P:398:THR:HG22	2:P:414:PRO:HB3	1.91	0.51
2:N:348:ASN:ND2	2:N:366:MET:O	2.43	0.51
2:A:209:ARG:O	2:A:213:LEU:N	2.43	0.51
1:I:556:SER:HA	1:I:595:SER:HA	1.91	0.51
1:I:638:LYS:HD3	1:I:639:PRO:HD2	1.93	0.51
3:R:20:LYS:HE3	3:R:23:GLU:HG2	1.92	0.51
3:R:40:ASP:OD2	3:R:41:ASN:ND2	2.44	0.51
1:C:116:MET:HA	1:C:119:ILE:HB	1.93	0.51
2:A:302:PRO:HG2	2:A:305:LEU:HB3	1.92	0.51
2:B:348:ASN:ND2	2:B:366:MET:O	2.44	0.51
1:F:337:ASN:ND2	1:F:340:ASP:OD1	2.44	0.51
1:H:388:LEU:HD22	1:H:418:LEU:HD22	1.91	0.51
1:M:116:MET:HA	1:M:119:ILE:HB	1.93	0.51
1:I:342:ILE:CD1	1:I:388:LEU:HA	2.41	0.51
1:C:509:THR:HB	1:C:512:TYR:HD2	1.75	0.51
1:C:638:LYS:HD3	1:C:639:PRO:HD2	1.93	0.51
1:C:710:ILE:HG21	1:C:729:GLN:HE22	1.74	0.51
1:F:698:ASP:HA	1:F:701:HIS:HD2	1.75	0.51
3:D:84:ILE:HG12	3:D:101:TRP:CE2	2.46	0.51
3:K:84:ILE:HG12	3:K:101:TRP:CE2	2.46	0.51
1:O:598:GLN:HG2	1:O:634:LEU:HG	1.92	0.51
2:G:47:MET:HE3	2:J:45:HIS:CG	2.43	0.51
2:G:297:LYS:HZ1	2:G:595:PRO:HD3	1.76	0.51
2:J:311:VAL:HB	2:J:375:LEU:HB3	1.93	0.51
1:H:473:MET:HG2	1:H:512:TYR:HB3	1.93	0.51
3:K:72:TRP:HB2	3:K:105:LYS:HB3	1.93	0.51
1:O:698:ASP:HA	1:O:701:HIS:HD2	1.75	0.51
2:P:195:ARG:HB2	2:P:224:ALA:HB1	1.93	0.51
2:N:513:ALA:HB3	2:N:561:TRP:HZ3	1.76	0.51
3:Q:84:ILE:HG12	3:Q:101:TRP:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:137:LEU:HG	2:A:176:LEU:HD21	1.93	0.51
2:B:289:SER:HG	2:B:294:LYS:H	1.58	0.51
1:I:437:ALA:HA	1:I:513:TRP:HZ3	1.74	0.51
1:H:527:ALA:HB3	1:H:528:PRO:HD3	1.93	0.51
1:C:556:SER:HA	1:C:595:SER:HA	1.91	0.50
1:F:598:GLN:HG2	1:F:634:LEU:HG	1.92	0.50
2:G:302:PRO:HG2	2:G:305:LEU:HB3	1.92	0.50
1:H:559:LEU:O	1:H:592:LEU:N	2.38	0.50
1:O:287:MET:HE3	1:O:296:LEU:HD22	1.93	0.50
1:C:287:MET:HE3	1:C:296:LEU:HD22	1.94	0.50
2:A:134:VAL:HG21	2:A:169:PHE:HA	1.93	0.50
2:A:275:SER:OG	2:A:574:ASP:O	2.25	0.50
2:J:274:ALA:N	2:J:284:SER:O	2.43	0.50
1:H:441:LEU:HD13	1:H:554:MET:HE3	1.92	0.50
3:L:20:LYS:HE3	3:L:23:GLU:HG2	1.92	0.50
1:O:717:MET:HE2	1:O:756:ARG:HD3	1.94	0.50
2:P:137:LEU:HG	2:P:176:LEU:HD21	1.93	0.50
1:F:287:MET:HE3	1:F:296:LEU:HD22	1.93	0.50
2:G:47:MET:HE3	2:J:45:HIS:NE2	2.25	0.50
2:G:134:VAL:HG21	2:G:169:PHE:HA	1.93	0.50
1:I:339:VAL:HA	1:I:391:PHE:HD1	1.76	0.50
1:I:484:MET:HA	1:I:487:PHE:HD2	1.77	0.50
1:M:559:LEU:O	1:M:592:LEU:N	2.39	0.50
3:Q:72:TRP:HB2	3:Q:105:LYS:HB3	1.93	0.50
1:F:710:ILE:HG21	1:F:729:GLN:HE22	1.77	0.50
3:E:20:LYS:HE3	3:E:23:GLU:HG2	1.92	0.50
3:E:40:ASP:OD2	3:E:41:ASN:ND2	2.44	0.50
2:J:228:VAL:O	2:J:229:THR:OG1	2.24	0.50
1:H:355:PHE:O	1:H:359:SER:HB3	2.11	0.50
2:P:348:ASN:HB2	2:P:366:MET:HB2	1.93	0.50
2:A:348:ASN:HB2	2:A:366:MET:HB2	1.93	0.50
1:I:49:ASN:HD22	1:I:118:MET:HE1	1.76	0.50
1:I:287:MET:HE3	1:I:296:LEU:HD22	1.94	0.50
1:I:374:PHE:CB	1:I:421:PHE:HB3	2.38	0.50
1:H:419:PHE:O	1:H:420:ARG:C	2.54	0.50
1:O:710:ILE:HG21	1:O:729:GLN:HE22	1.77	0.50
2:N:311:VAL:HB	2:N:375:LEU:HB3	1.93	0.50
2:B:311:VAL:HB	2:B:375:LEU:HB3	1.93	0.50
2:G:137:LEU:HG	2:G:176:LEU:HD21	1.93	0.50
1:H:612:THR:OG1	1:H:655:ASN:O	2.30	0.50
1:M:49:ASN:HD22	1:M:118:MET:HE1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:118:GLN:OE1	2:N:119:ARG:NH1	2.45	0.50
2:A:553:GLN:HB2	2:A:564:ARG:HB2	1.94	0.50
2:G:195:ARG:HB2	2:G:224:ALA:HB1	1.93	0.50
2:G:318:ILE:HB	2:G:353:PHE:HB3	1.92	0.50
1:I:480:SER:HB3	1:I:508:LEU:HD23	1.93	0.50
1:M:263:VAL:HG22	1:M:267:GLU:OE2	2.12	0.50
2:P:305:LEU:HD12	2:P:325:VAL:HB	1.94	0.50
2:B:202:LEU:HD11	2:B:216:VAL:HG11	1.94	0.50
1:F:612:THR:OG1	1:F:655:ASN:O	2.30	0.50
1:I:116:MET:HA	1:I:119:ILE:HB	1.93	0.50
1:I:614:GLU:OE1	1:I:617:GLN:NE2	2.43	0.50
1:H:120:ARG:O	1:H:124:MET:HB3	2.11	0.50
3:L:39:VAL:HA	3:L:49:ILE:HB	1.94	0.50
1:M:346:LEU:HD11	1:M:414:LYS:CB	2.38	0.50
2:P:134:VAL:HG21	2:P:169:PHE:HA	1.93	0.50
3:R:39:VAL:HA	3:R:49:ILE:HB	1.94	0.50
3:D:52:LEU:HD12	3:D:56:CYS:HB3	1.94	0.50
2:G:553:GLN:HB2	2:G:564:ARG:HB2	1.94	0.50
2:J:202:LEU:HD11	2:J:216:VAL:HG11	1.94	0.50
1:O:374:PHE:HA	1:O:377:PHE:CE1	2.47	0.49
2:B:157:GLU:O	2:B:161:THR:OG1	2.24	0.49
1:F:120:ARG:O	1:F:124:MET:HB3	2.12	0.49
2:P:209:ARG:O	2:P:213:LEU:N	2.43	0.49
2:N:289:SER:HG	2:N:294:LYS:H	1.58	0.49
1:C:49:ASN:HD22	1:C:118:MET:HE1	1.76	0.49
1:F:374:PHE:HA	1:F:377:PHE:CE1	2.47	0.49
2:J:118:GLN:OE1	2:J:119:ARG:NH1	2.45	0.49
1:I:343:GLN:HB2	1:I:391:PHE:CE1	2.47	0.49
1:O:612:THR:OG1	1:O:655:ASN:O	2.30	0.49
2:P:50:ALA:HB1	2:N:24:PHE:CZ	2.48	0.49
2:B:91:THR:HG23	2:B:93:ASN:H	1.77	0.49
2:G:348:ASN:HB2	2:G:366:MET:HB2	1.94	0.49
1:I:478:SER:HA	1:I:481:ASN:ND2	2.27	0.49
2:N:455:ARG:NH1	2:N:457:THR:O	2.46	0.49
1:H:269:ILE:O	1:H:273:MET:HG3	2.12	0.49
1:O:201:TYR:OH	1:O:253:ASP:OD1	2.30	0.49
2:N:113:VAL:HB	2:N:116:VAL:HG12	1.95	0.49
2:B:419:TRP:HZ3	2:B:433:VAL:HG13	1.77	0.49
2:B:455:ARG:NH1	2:B:457:THR:O	2.46	0.49
2:J:513:ALA:HB3	2:J:561:TRP:HZ3	1.76	0.49
1:I:263:VAL:HG22	1:I:267:GLU:OE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:751:ARG:NH2	3:R:55:GLU:OE1	2.46	0.49
1:C:263:VAL:HG22	1:C:267:GLU:OE2	2.12	0.49
3:D:72:TRP:HB2	3:D:105:LYS:HB3	1.93	0.49
2:J:455:ARG:NH1	2:J:457:THR:O	2.46	0.49
1:I:374:PHE:HB3	1:I:421:PHE:HB2	1.95	0.49
1:I:520:PRO:HG3	1:I:553:HIS:CG	2.48	0.49
2:P:263:MET:N	2:P:263:MET:SD	2.86	0.49
1:C:169:ILE:HD11	1:C:247:ARG:HD3	1.94	0.49
2:B:113:VAL:HB	2:B:116:VAL:HG13	1.95	0.49
2:P:47:MET:HE2	2:N:21:LEU:CA	2.41	0.49
2:N:91:THR:HG23	2:N:93:ASN:H	1.77	0.49
1:C:374:PHE:HA	1:C:377:PHE:CD1	2.48	0.49
2:J:113:VAL:HB	2:J:116:VAL:HG12	1.95	0.49
1:H:717:MET:HE2	1:H:756:ARG:HD3	1.94	0.49
3:L:54:ILE:HA	3:L:57:GLN:HE21	1.78	0.49
1:O:346:LEU:HA	1:O:418:LEU:HD12	1.92	0.49
2:N:385:ILE:HG13	2:N:399:VAL:HG21	1.95	0.49
2:B:428:HIS:HE1	1:I:714:ARG:CZ	2.26	0.49
1:F:407:GLU:OE1	1:F:407:GLU:N	2.35	0.49
1:I:751:ARG:NH2	3:L:55:GLU:OE1	2.46	0.49
1:M:169:ILE:HD11	1:M:247:ARG:HD3	1.94	0.49
1:M:371:ALA:HB1	1:M:421:PHE:CE1	2.47	0.49
1:M:374:PHE:HA	1:M:377:PHE:CD1	2.48	0.49
1:O:225:LEU:HB3	1:O:272:HIS:CE1	2.48	0.49
2:N:202:LEU:HD11	2:N:216:VAL:HG11	1.94	0.49
3:Q:52:LEU:HD12	3:Q:56:CYS:HB3	1.95	0.49
2:B:118:GLN:OE1	2:B:119:ARG:NH1	2.45	0.49
2:B:385:ILE:HG13	2:B:399:VAL:HG21	1.95	0.49
1:F:433:LYS:HA	1:F:436:LEU:HD12	1.95	0.49
1:F:481:ASN:HA	1:F:484:MET:HG3	1.94	0.49
2:G:92:GLY:CA	2:J:13:TYR:CD2	2.96	0.49
1:C:129:VAL:O	1:C:133:GLN:NE2	2.44	0.48
3:K:20:LYS:HE3	3:K:23:GLU:HG2	1.95	0.48
2:P:89:ALA:O	2:N:13:TYR:OH	2.30	0.48
2:B:195:ARG:HD3	2:B:229:THR:HG21	1.95	0.48
1:F:225:LEU:HB3	1:F:272:HIS:CE1	2.48	0.48
1:H:169:ILE:HD11	1:H:247:ARG:HD3	1.95	0.48
3:K:52:LEU:HD12	3:K:56:CYS:HB3	1.95	0.48
1:M:606:ASN:HD21	3:R:22:PHE:HD1	1.61	0.48
2:P:553:GLN:HB2	2:P:564:ARG:HB2	1.94	0.48
3:R:54:ILE:HA	3:R:57:GLN:HE21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:GLY:C	1:C:531:ALA:HB2	2.38	0.48
1:F:120:ARG:O	1:F:124:MET:HB2	2.13	0.48
1:I:472:GLY:O	1:I:512:TYR:CE1	2.65	0.48
1:O:346:LEU:CD1	1:O:418:LEU:HB2	2.44	0.48
2:P:397:ARG:HD2	2:P:417:CYS:HA	1.96	0.48
2:B:526:ARG:HB2	2:B:537:PHE:HB3	1.96	0.48
1:H:201:TYR:OH	1:H:253:ASP:OD1	2.30	0.48
1:H:692:ARG:HD3	1:H:692:ARG:HA	1.50	0.48
1:O:169:ILE:HD11	1:O:247:ARG:HD3	1.96	0.48
1:O:543:HIS:O	1:O:544:SER:C	2.56	0.48
3:E:39:VAL:HA	3:E:49:ILE:HB	1.94	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:H:120:ARG:O	1:H:124:MET:HB2	2.13	0.48
3:Q:20:LYS:HE3	3:Q:23:GLU:HG2	1.95	0.48
3:E:54:ILE:HA	3:E:57:GLN:HE21	1.78	0.48
2:G:263:MET:SD	2:G:263:MET:N	2.86	0.48
1:H:395:LYS:HE2	1:H:407:GLU:HG3	1.95	0.48
1:M:120:ARG:O	1:M:124:MET:HB2	2.14	0.48
2:N:419:TRP:HZ3	2:N:433:VAL:HG13	1.78	0.48
1:C:751:ARG:NH2	3:E:55:GLU:OE1	2.46	0.48
2:G:172:LEU:HD22	2:G:176:LEU:HD23	1.96	0.48
1:I:606:ASN:HD21	3:L:22:PHE:HD1	1.61	0.48
2:A:263:MET:SD	2:A:263:MET:N	2.86	0.48
2:G:305:LEU:HD12	2:G:325:VAL:HB	1.94	0.48
1:I:169:ILE:HD11	1:I:247:ARG:HD3	1.94	0.48
1:M:287:MET:HE3	1:M:296:LEU:HD22	1.94	0.48
2:A:321:ALA:HB3	2:A:375:LEU:HD11	1.96	0.48
1:F:201:TYR:OH	1:F:253:ASP:OD1	2.30	0.48
2:J:152:ALA:O	2:J:156:VAL:HB	2.14	0.48
1:I:74:TYR:OH	1:I:137:GLU:OE2	2.32	0.48
1:I:336:LYS:HE3	1:I:387:TYR:CZ	2.45	0.48
1:I:523:ASN:HB2	1:I:529:ARG:HH21	1.79	0.48
2:B:142:LEU:O	1:F:68:LYS:HE2	2.14	0.48
1:F:484:MET:HG2	1:F:505:VAL:O	2.14	0.48
2:G:397:ARG:HD2	2:G:417:CYS:HA	1.96	0.48
1:O:433:LYS:HA	1:O:436:LEU:HD12	1.95	0.47
2:P:45:HIS:CG	2:N:47:MET:SD	3.06	0.47
2:A:305:LEU:HD12	2:A:325:VAL:HB	1.94	0.47
1:F:687:GLU:O	1:F:690:GLU:HG3	2.15	0.47
2:G:321:ALA:HB3	2:G:375:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:289:LYS:O	1:O:351:ARG:NH2	2.48	0.47
2:N:265:LYS:HG3	2:N:585:LYS:HD3	1.96	0.47
2:B:152:ALA:O	2:B:156:VAL:HB	2.14	0.47
1:M:74:TYR:OH	1:M:137:GLU:OE2	2.32	0.47
2:N:526:ARG:HB2	2:N:537:PHE:HB3	1.96	0.47
1:F:437:ALA:HA	1:F:513:TRP:HZ3	1.78	0.47
3:D:20:LYS:HE3	3:D:23:GLU:HG2	1.95	0.47
2:G:199:MET:O	2:G:203:GLU:HG2	2.15	0.47
2:J:195:ARG:HD3	2:J:229:THR:HG21	1.96	0.47
1:I:714:ARG:NH1	1:I:725:GLU:OE2	2.47	0.47
1:H:36:LEU:HD11	1:H:60:ASN:ND2	2.30	0.47
1:C:74:TYR:OH	1:C:137:GLU:OE2	2.32	0.47
2:A:30:PHE:HE1	2:B:60:PHE:CB	2.26	0.47
2:A:47:MET:HE2	2:B:21:LEU:HD22	1.97	0.47
1:F:169:ILE:HD11	1:F:247:ARG:HD3	1.95	0.47
2:G:89:ALA:HA	2:J:13:TYR:OH	2.15	0.47
2:J:419:TRP:HZ3	2:J:433:VAL:HG13	1.78	0.47
1:I:374:PHE:HA	1:I:377:PHE:CD1	2.48	0.47
1:H:273:MET:CA	1:H:303:PHE:HE2	2.27	0.47
1:M:346:LEU:HD23	1:M:411:ILE:HD11	1.95	0.47
1:O:263:VAL:HG22	1:O:267:GLU:OE2	2.14	0.47
2:P:48:VAL:HG21	2:P:90:TYR:CZ	2.49	0.47
2:P:382:ILE:O	2:P:402:TYR:N	2.44	0.47
1:C:225:LEU:HB3	1:C:272:HIS:CE1	2.50	0.47
1:C:714:ARG:NH1	1:C:725:GLU:OE2	2.47	0.47
1:I:120:ARG:O	1:I:124:MET:HB3	2.14	0.47
1:M:225:LEU:HB3	1:M:272:HIS:CE1	2.50	0.47
1:M:687:GLU:O	1:M:690:GLU:HG3	2.14	0.47
2:N:149:LYS:HE2	2:N:149:LYS:HB2	1.75	0.47
3:Q:45:CYS:HB2	3:Q:54:ILE:HG23	1.96	0.47
1:C:255:SER:O	1:C:257:GLU:N	2.48	0.47
3:D:88:LEU:HD23	3:D:92:GLN:HG2	1.97	0.47
2:G:48:VAL:HG21	2:G:90:TYR:CZ	2.50	0.47
3:L:84:ILE:HD13	3:L:101:TRP:CE2	2.49	0.47
2:P:45:HIS:HB3	2:N:47:MET:SD	2.54	0.47
2:P:321:ALA:HB3	2:P:375:LEU:HD11	1.96	0.47
2:N:152:ALA:O	2:N:156:VAL:HB	2.14	0.47
1:C:398:LYS:HB3	1:C:400:VAL:HG12	1.96	0.47
1:C:606:ASN:HD21	3:E:22:PHE:HD1	1.61	0.47
1:C:687:GLU:O	1:C:690:GLU:HG3	2.14	0.47
1:F:374:PHE:O	1:F:378:LEU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:723:VAL:HG11	1:F:742:LYS:HZ3	1.79	0.47
3:E:43:ALA:HB3	3:E:79:PHE:HE1	1.80	0.47
3:E:84:ILE:HD13	3:E:101:TRP:CE2	2.49	0.47
2:J:265:LYS:HG3	2:J:585:LYS:HD3	1.96	0.47
1:I:476:ASP:OD2	1:I:512:TYR:CD2	2.67	0.47
1:H:237:VAL:HG13	1:H:302:LEU:CD2	2.43	0.47
1:M:120:ARG:O	1:M:124:MET:HB3	2.14	0.47
1:M:723:VAL:HG11	1:M:742:LYS:HZ3	1.80	0.47
2:P:199:MET:O	2:P:203:GLU:HG2	2.15	0.47
3:Q:88:LEU:HD23	3:Q:92:GLN:HG2	1.97	0.47
1:C:465:GLN:HE21	1:C:465:GLN:HB3	1.53	0.47
1:F:36:LEU:HD11	1:F:60:ASN:ND2	2.30	0.47
2:G:13:TYR:CE2	2:J:89:ALA:O	2.68	0.47
1:I:723:VAL:HG11	1:I:742:LYS:HZ3	1.80	0.47
2:A:48:VAL:HG21	2:A:90:TYR:CZ	2.49	0.47
2:A:172:LEU:HD22	2:A:176:LEU:HD23	1.96	0.47
1:I:687:GLU:O	1:I:690:GLU:HG3	2.14	0.47
1:H:714:ARG:NH1	1:H:725:GLU:OE2	2.48	0.47
1:O:687:GLU:O	1:O:690:GLU:HG3	2.15	0.47
1:O:714:ARG:NH1	1:O:725:GLU:OE2	2.48	0.47
2:N:195:ARG:HD3	2:N:229:THR:HG21	1.96	0.47
1:C:723:VAL:HG11	1:C:742:LYS:HZ3	1.79	0.47
2:A:382:ILE:O	2:A:402:TYR:N	2.44	0.47
2:B:149:LYS:HB2	2:B:149:LYS:HE2	1.75	0.47
1:F:49:ASN:HD22	1:F:118:MET:HE1	1.80	0.47
1:H:390:LEU:HD13	1:H:390:LEU:HA	1.76	0.47
1:H:425:LYS:HE3	1:H:425:LYS:HB3	1.45	0.47
1:C:120:ARG:O	1:C:124:MET:HB3	2.14	0.46
1:C:129:VAL:HG23	2:A:144:SER:HB2	1.97	0.46
2:A:350:PHE:HD2	2:A:363:LYS:HB2	1.80	0.46
1:F:263:VAL:HG22	1:F:267:GLU:OE2	2.14	0.46
1:F:289:LYS:O	1:F:351:ARG:NH2	2.48	0.46
1:F:342:ILE:HG21	1:F:388:LEU:HA	1.97	0.46
1:H:473:MET:HE3	1:H:473:MET:HB3	1.74	0.46
1:O:437:ALA:HA	1:O:513:TRP:HZ3	1.79	0.46
1:O:559:LEU:O	1:O:592:LEU:N	2.38	0.46
1:O:751:ARG:NH2	3:Q:55:GLU:OE1	2.48	0.46
2:P:89:ALA:O	2:N:13:TYR:CZ	2.66	0.46
2:P:425:VAL:HB	2:P:466:ALA:HB2	1.97	0.46
3:R:43:ALA:HB3	3:R:79:PHE:HE1	1.80	0.46
1:C:120:ARG:O	1:C:124:MET:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:199:MET:O	2:A:203:GLU:HG2	2.15	0.46
3:D:45:CYS:HB2	3:D:54:ILE:HG23	1.96	0.46
1:M:378:LEU:CD1	1:M:422:MET:HG2	2.45	0.46
1:M:614:GLU:HA	1:M:617:GLN:HG2	1.97	0.46
2:P:350:PHE:HD2	2:P:363:LYS:HB2	1.80	0.46
3:Q:47:ASN:HD21	3:Q:54:ILE:HG23	1.80	0.46
2:B:458:SER:O	2:B:459:ARG:NH1	2.42	0.46
1:F:751:ARG:NH2	3:D:55:GLU:OE1	2.48	0.46
2:G:382:ILE:O	2:G:402:TYR:N	2.44	0.46
2:J:202:LEU:HD21	2:J:216:VAL:HG11	1.97	0.46
1:I:255:SER:O	1:I:257:GLU:N	2.48	0.46
1:M:520:PRO:HG2	1:M:552:HIS:H	1.80	0.46
1:M:629:ARG:O	1:M:632:GLN:HG3	2.16	0.46
3:R:84:ILE:HD13	3:R:101:TRP:CE2	2.49	0.46
2:B:525:VAL:HA	2:B:538:MET:HG2	1.98	0.46
1:F:446:VAL:HG23	1:F:447:SER:H	1.79	0.46
1:F:465:GLN:N	1:F:465:GLN:OE1	2.49	0.46
1:F:471:GLU:HB3	1:F:475:ARG:HH21	1.80	0.46
2:G:425:VAL:HB	2:G:466:ALA:HB2	1.97	0.46
1:M:255:SER:O	1:M:257:GLU:N	2.48	0.46
2:B:144:SER:HB3	1:F:133:GLN:OE1	2.09	0.46
2:G:211:GLN:H	2:G:211:GLN:CD	2.24	0.46
2:G:325:VAL:O	2:G:345:ARG:N	2.49	0.46
1:I:342:ILE:HB	1:I:391:PHE:CB	2.45	0.46
2:N:202:LEU:HD21	2:N:216:VAL:HG11	1.97	0.46
2:G:181:LEU:HD21	2:G:220:ILE:HD12	1.98	0.46
1:I:509:THR:HB	1:I:512:TYR:CD2	2.51	0.46
1:I:546:ARG:HE	3:L:35:TRP:NE1	2.14	0.46
1:H:289:LYS:HB2	1:H:289:LYS:HE2	1.64	0.46
1:H:614:GLU:HA	1:H:617:GLN:HG2	1.98	0.46
3:L:45:CYS:HB2	3:L:54:ILE:HG23	1.98	0.46
1:O:471:GLU:HB3	1:O:475:ARG:HH21	1.80	0.46
2:P:172:LEU:HD22	2:P:176:LEU:HD23	1.96	0.46
2:A:388:ASP:O	2:A:389:SER:C	2.59	0.46
2:A:425:VAL:HB	2:A:466:ALA:HB2	1.97	0.46
2:B:265:LYS:HG3	2:B:585:LYS:HD3	1.96	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:O:622:ILE:HG21	1:O:627:LEU:HD22	1.98	0.46
1:C:55:GLU:H	2:A:66:GLU:HG3	1.80	0.46
1:C:509:THR:HB	1:C:512:TYR:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:629:ARG:O	1:C:632:GLN:HG3	2.16	0.46
1:F:553:HIS:HA	1:F:597:PHE:HE1	1.80	0.46
1:I:120:ARG:O	1:I:124:MET:HB2	2.14	0.46
1:I:225:LEU:HB3	1:I:272:HIS:CE1	2.50	0.46
1:I:629:ARG:O	1:I:632:GLN:HG3	2.16	0.46
1:H:74:TYR:OH	1:H:137:GLU:OE2	2.33	0.46
3:K:88:LEU:HD23	3:K:92:GLN:HG2	1.97	0.46
1:M:36:LEU:HD11	1:M:60:ASN:ND2	2.31	0.46
1:O:465:GLN:OE1	1:O:465:GLN:N	2.49	0.46
2:A:181:LEU:HD21	2:A:220:ILE:HD12	1.98	0.46
2:A:276:SER:OG	2:A:281:SER:O	2.33	0.46
2:A:402:TYR:HB2	2:A:409:TRP:CZ3	2.51	0.46
2:B:54:SER:CB	1:F:128:ARG:HH22	2.29	0.46
2:B:106:GLU:HG2	2:B:143:PHE:HE2	1.81	0.46
2:B:202:LEU:HD21	2:B:216:VAL:HG11	1.97	0.46
2:G:287:CYS:N	2:G:296:TYR:O	2.36	0.46
1:H:709:ARG:HE	1:H:709:ARG:HB3	1.48	0.46
1:O:614:GLU:HA	1:O:617:GLN:HG2	1.98	0.46
3:Q:33:TRP:HZ3	3:Q:35:TRP:CD1	2.34	0.46
1:C:36:LEU:HD11	1:C:60:ASN:ND2	2.31	0.46
2:G:402:TYR:HB2	2:G:409:TRP:CZ3	2.51	0.46
1:O:269:ILE:HB	1:O:306:VAL:HG21	1.97	0.45
1:O:723:VAL:HG11	1:O:742:LYS:HZ3	1.81	0.45
2:P:287:CYS:N	2:P:296:TYR:O	2.36	0.45
2:A:211:GLN:CD	2:A:211:GLN:H	2.24	0.45
1:F:74:TYR:OH	1:F:137:GLU:OE2	2.33	0.45
1:O:74:TYR:OH	1:O:137:GLU:OE2	2.33	0.45
1:O:212:MET:HE3	1:O:212:MET:HB3	1.63	0.45
2:A:379:GLU:O	2:A:379:GLU:HG3	2.16	0.45
3:E:80:HIS:HB2	3:E:83:CYS:SG	2.57	0.45
3:D:47:ASN:HD21	3:D:54:ILE:HG23	1.80	0.45
1:M:622:ILE:HG12	1:M:627:LEU:HB2	1.99	0.45
1:O:553:HIS:HA	1:O:597:PHE:CE1	2.52	0.45
2:P:181:LEU:HD21	2:P:220:ILE:HD12	1.98	0.45
2:P:379:GLU:HG3	2:P:379:GLU:O	2.16	0.45
2:B:153:LYS:HA	2:B:153:LYS:HD2	1.69	0.45
2:G:422:SER:OG	2:G:434:MET:O	2.27	0.45
2:J:458:SER:O	2:J:459:ARG:NH1	2.41	0.45
1:I:429:GLU:CD	1:I:466:PHE:HB3	2.41	0.45
1:I:446:VAL:HG23	1:I:447:SER:H	1.81	0.45
1:H:116:MET:HA	1:H:119:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:622:ILE:HG21	1:H:627:LEU:HD22	1.98	0.45
3:L:80:HIS:HB2	3:L:83:CYS:SG	2.57	0.45
1:M:446:VAL:HG23	1:M:447:SER:H	1.81	0.45
1:O:553:HIS:HA	1:O:597:PHE:HE1	1.80	0.45
2:P:402:TYR:HB2	2:P:409:TRP:CZ3	2.51	0.45
1:C:523:ASN:HD21	1:C:620:THR:HA	1.82	0.45
2:A:113:VAL:HB	2:A:116:VAL:HG12	1.98	0.45
2:A:244:VAL:O	2:A:247:GLN:HG3	2.16	0.45
2:A:353:PHE:HB2	2:A:360:TRP:CH2	2.52	0.45
1:F:342:ILE:HG13	1:F:388:LEU:N	2.30	0.45
3:D:33:TRP:HZ3	3:D:35:TRP:CD1	2.34	0.45
1:I:614:GLU:HA	1:I:617:GLN:HG2	1.97	0.45
1:I:622:ILE:HG12	1:I:627:LEU:HB2	1.98	0.45
1:H:548:LEU:HD23	3:K:33:TRP:HB3	1.97	0.45
2:P:51:THR:HA	2:N:20:GLN:OE1	2.16	0.45
2:N:275:SER:N	2:N:575:LEU:O	2.49	0.45
3:R:45:CYS:HB2	3:R:54:ILE:HG12	1.99	0.45
1:F:269:ILE:HB	1:F:306:VAL:HG21	1.97	0.45
2:G:350:PHE:HD2	2:G:363:LYS:HB2	1.80	0.45
1:H:407:GLU:HG2	1:H:408:VAL:N	2.31	0.45
1:H:553:HIS:HA	1:H:597:PHE:HE1	1.80	0.45
1:H:553:HIS:HA	1:H:597:PHE:CE1	2.52	0.45
3:K:33:TRP:HZ3	3:K:35:TRP:CD1	2.34	0.45
1:M:455:ILE:HG12	1:M:456:SER:N	2.24	0.45
2:N:366:MET:HE2	2:N:366:MET:HB3	1.84	0.45
2:N:525:VAL:HA	2:N:538:MET:HG2	1.97	0.45
1:C:269:ILE:HB	1:C:306:VAL:HG21	1.98	0.45
1:C:614:GLU:HA	1:C:617:GLN:HG2	1.97	0.45
2:B:74:LEU:HD11	2:B:110:PHE:HE2	1.82	0.45
1:F:346:LEU:HA	1:F:418:LEU:HD12	1.97	0.45
2:J:149:LYS:HB2	2:J:149:LYS:HE2	1.75	0.45
1:I:477:MET:HE3	1:I:513:TRP:CH2	2.51	0.45
1:O:527:ALA:HB3	1:O:528:PRO:HD3	1.99	0.45
2:G:51:THR:HG21	2:J:17:LEU:HD13	1.98	0.45
2:G:353:PHE:HB2	2:G:360:TRP:CH2	2.52	0.45
1:H:49:ASN:HD22	1:H:118:MET:HE1	1.80	0.45
1:H:342:ILE:HB	1:H:391:PHE:CD2	2.51	0.45
1:H:689:LYS:HD2	1:H:689:LYS:HA	1.56	0.45
1:M:390:LEU:HD22	1:M:435:HIS:NE2	2.32	0.45
2:A:68:LYS:HD2	2:A:68:LYS:HA	1.40	0.45
1:I:289:LYS:O	1:I:351:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:339:VAL:HA	1:I:391:PHE:CD1	2.52	0.45
1:H:260:ILE:O	1:H:261:VAL:C	2.59	0.45
1:H:488:ARG:HD2	1:H:488:ARG:HA	1.60	0.45
1:M:527:ALA:HB3	1:M:528:PRO:HD3	1.98	0.45
2:A:413:SER:HB3	2:A:442:TYR:HE1	1.82	0.45
2:B:58:ALA:HB1	1:F:121:ASP:HB3	1.99	0.45
1:H:273:MET:O	1:H:274:LYS:C	2.59	0.45
1:H:433:LYS:HA	1:H:436:LEU:HD12	1.99	0.45
1:M:412:LEU:CD2	1:M:454:MET:HE2	2.47	0.45
2:P:211:GLN:CD	2:P:211:GLN:H	2.24	0.45
2:P:244:VAL:O	2:P:247:GLN:HG3	2.16	0.45
3:Q:94:CYS:O	3:Q:96:LEU:N	2.50	0.45
1:F:553:HIS:HA	1:F:597:PHE:CE1	2.52	0.45
2:G:89:ALA:O	2:J:13:TYR:HE2	1.99	0.45
1:H:435:HIS:O	1:H:439:ARG:HG2	2.17	0.45
3:K:36:ASP:O	3:K:38:VAL:HG23	2.17	0.45
3:K:45:CYS:HB3	3:K:83:CYS:SG	2.57	0.45
1:M:386:GLU:OE1	1:M:386:GLU:N	2.46	0.44
1:M:502:ASP:HB2	3:R:26:LYS:HG2	1.99	0.44
2:P:225:LEU:HD23	2:P:225:LEU:HA	1.79	0.44
2:P:325:VAL:O	2:P:345:ARG:N	2.49	0.44
3:E:45:CYS:HB2	3:E:54:ILE:HG12	1.99	0.44
3:D:94:CYS:O	3:D:96:LEU:N	2.50	0.44
2:G:113:VAL:HB	2:G:116:VAL:HG12	1.98	0.44
1:I:207:ALA:HB3	1:I:208:PRO:HD3	2.00	0.44
1:H:525:PRO:HB2	1:H:528:PRO:HD2	1.99	0.44
2:P:301:PRO:HB2	2:P:302:PRO:HD3	1.99	0.44
2:N:221:ARG:NE	2:N:258:LYS:O	2.50	0.44
1:C:128:ARG:O	1:C:132:GLN:HB2	2.18	0.44
1:F:614:GLU:HA	1:F:617:GLN:HG2	1.98	0.44
1:F:712:LYS:HA	1:F:712:LYS:HD3	1.53	0.44
3:D:52:LEU:HD21	3:D:59:ASN:HB3	1.99	0.44
1:I:390:LEU:HD22	1:I:435:HIS:NE2	2.32	0.44
1:I:609:GLU:HG3	1:I:610:LYS:H	1.82	0.44
1:H:605:PHE:HE1	1:H:611:TYR:HB2	1.82	0.44
1:H:606:ASN:HD21	3:K:22:PHE:HD1	1.66	0.44
3:K:94:CYS:O	3:K:96:LEU:N	2.50	0.44
1:M:289:LYS:O	1:M:351:ARG:NH2	2.50	0.44
1:O:605:PHE:HE1	1:O:611:TYR:HB2	1.82	0.44
2:N:153:LYS:HD2	2:N:153:LYS:HA	1.69	0.44
2:A:121:ARG:HD3	2:A:145:CYS:SG	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:301:PRO:HB2	2:A:302:PRO:HD3	1.98	0.44
2:B:539:ARG:HH21	2:B:579:PHE:HE1	1.65	0.44
1:F:265:GLU:HB3	1:F:306:VAL:HG22	2.00	0.44
3:D:27:TRP:CE2	3:D:29:ALA:HB2	2.52	0.44
3:D:85:SER:O	3:D:89:LYS:NZ	2.50	0.44
2:J:275:SER:N	2:J:575:LEU:O	2.49	0.44
2:J:525:VAL:HA	2:J:538:MET:HG2	1.97	0.44
1:I:605:PHE:HE1	1:I:611:TYR:HB2	1.82	0.44
1:O:258:GLU:HB2	1:O:259:PRO:HD3	2.00	0.44
2:P:17:LEU:CD2	2:N:18:LEU:CD1	2.93	0.44
2:P:287:CYS:SG	2:P:288:TYR:N	2.90	0.44
1:C:622:ILE:HG12	1:C:627:LEU:HB2	1.99	0.44
2:A:12:GLU:H	2:A:12:GLU:HG3	1.52	0.44
1:F:168:MET:HE2	1:F:168:MET:HB3	1.90	0.44
1:F:714:ARG:HD2	1:F:714:ARG:HA	1.73	0.44
2:G:244:VAL:O	2:G:247:GLN:HG3	2.16	0.44
1:I:386:GLU:OE1	1:I:386:GLU:N	2.46	0.44
1:I:500:GLY:HA2	1:I:503:LEU:HD23	1.99	0.44
1:H:712:LYS:HA	1:H:712:LYS:HD3	1.65	0.44
3:K:40:ASP:HA	3:K:48:HIS:CE1	2.53	0.44
1:M:342:ILE:HG21	1:M:391:PHE:HB3	1.99	0.44
1:O:510:THR:HG22	3:Q:32:LEU:HG	2.00	0.44
2:P:353:PHE:HB2	2:P:360:TRP:CH2	2.52	0.44
2:P:413:SER:HB3	2:P:442:TYR:HE1	1.81	0.44
3:Q:27:TRP:CE2	3:Q:29:ALA:HB2	2.52	0.44
2:B:221:ARG:NE	2:B:258:LYS:O	2.50	0.44
3:D:40:ASP:HA	3:D:48:HIS:CE1	2.52	0.44
2:J:554:TYR:HA	2:J:561:TRP:HA	1.99	0.44
1:H:264:VAL:O	1:H:265:GLU:C	2.59	0.44
1:H:363:ASP:HB3	1:H:366:PHE:HD1	1.83	0.44
1:M:509:THR:HB	1:M:512:TYR:CD2	2.51	0.44
1:O:238:GLU:O	1:O:242:ASN:ND2	2.40	0.44
1:O:503:LEU:HA	1:O:503:LEU:HD22	1.72	0.44
3:R:80:HIS:HB2	3:R:83:CYS:SG	2.57	0.44
1:C:207:ALA:HB3	1:C:208:PRO:HD3	2.00	0.44
1:C:289:LYS:O	1:C:351:ARG:NH2	2.50	0.44
1:C:609:GLU:HG3	1:C:610:LYS:H	1.82	0.44
2:A:47:MET:SD	2:B:21:LEU:HD22	2.58	0.44
2:B:143:PHE:CE1	1:F:66:LEU:HD13	2.43	0.44
1:F:386:GLU:OE1	1:F:386:GLU:N	2.47	0.44
1:I:148:ARG:HH11	1:I:200:VAL:HG21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:269:ILE:HB	1:I:306:VAL:HG21	1.98	0.44
1:H:266:ARG:O	1:H:267:GLU:C	2.58	0.44
1:H:272:HIS:O	1:H:273:MET:C	2.60	0.44
3:K:52:LEU:HD21	3:K:59:ASN:HB3	1.99	0.44
2:N:539:ARG:HH21	2:N:579:PHE:HE1	1.65	0.44
3:R:46:ARG:HH11	3:R:46:ARG:C	2.26	0.44
3:Q:40:ASP:HA	3:Q:48:HIS:CE1	2.53	0.44
3:Q:52:LEU:HD21	3:Q:59:ASN:HB3	1.99	0.44
1:C:390:LEU:HD22	1:C:435:HIS:NE2	2.32	0.44
1:C:605:PHE:HE1	1:C:611:TYR:HB2	1.83	0.44
1:F:342:ILE:CG1	1:F:387:TYR:HB3	2.45	0.44
3:E:27:TRP:CE2	3:E:29:ALA:HB2	2.52	0.44
2:G:503:ASP:HB3	2:G:506:LYS:HB2	1.99	0.44
1:I:128:ARG:O	1:I:132:GLN:HB2	2.18	0.44
1:M:269:ILE:HB	1:M:306:VAL:HG21	1.98	0.44
1:M:553:HIS:HA	1:M:597:PHE:CE1	2.53	0.44
2:P:37:VAL:HG21	2:P:82:LEU:HD23	2.00	0.44
2:P:470:LYS:NZ	2:P:503:ASP:OD2	2.44	0.44
2:N:217:LEU:HD13	2:N:225:LEU:HD11	2.00	0.44
1:C:520:PRO:HG2	1:C:552:HIS:H	1.82	0.44
2:A:30:PHE:CE2	2:B:50:ALA:CB	3.01	0.44
2:A:287:CYS:N	2:A:296:TYR:O	2.36	0.44
2:B:379:GLU:HG3	2:B:379:GLU:O	2.18	0.44
1:F:31:ASN:OD1	1:F:72:LYS:NZ	2.51	0.44
1:F:605:PHE:HE1	1:F:611:TYR:HB2	1.82	0.44
2:G:101:VAL:HB	2:G:124:LEU:HD11	2.00	0.44
2:J:221:ARG:NE	2:J:258:LYS:O	2.50	0.44
1:O:346:LEU:CA	1:O:418:LEU:CD1	2.93	0.44
2:N:127:LYS:O	2:N:129:ASN:ND2	2.51	0.44
3:Q:36:ASP:O	3:Q:38:VAL:HG23	2.17	0.44
3:Q:85:SER:O	3:Q:89:LYS:NZ	2.50	0.44
2:A:60:PHE:HB2	2:B:30:PHE:CZ	2.53	0.44
2:A:221:ARG:NH2	2:A:260:ARG:HE	2.16	0.44
1:F:116:MET:HA	1:F:119:ILE:HB	1.99	0.44
1:F:245:ILE:HA	1:F:248:VAL:HG12	1.99	0.44
1:F:609:GLU:HG3	1:F:610:LYS:H	1.83	0.44
2:G:24:PHE:HZ	2:J:57:ARG:HH12	1.65	0.44
2:J:217:LEU:HD13	2:J:225:LEU:HD11	2.00	0.44
1:I:553:HIS:HA	1:I:597:PHE:CE1	2.53	0.44
1:H:31:ASN:OD1	1:H:72:LYS:NZ	2.51	0.44
1:H:723:VAL:HG11	1:H:742:LYS:HZ3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:27:TRP:CE2	3:L:29:ALA:HB2	2.53	0.44
3:K:27:TRP:CE2	3:K:29:ALA:HB2	2.52	0.44
1:O:311:LYS:HB3	1:O:311:LYS:HE3	1.89	0.43
2:N:554:TYR:HA	2:N:561:TRP:HA	1.99	0.43
3:R:27:TRP:CE2	3:R:29:ALA:HB2	2.53	0.43
1:C:148:ARG:HH11	1:C:200:VAL:HG21	1.83	0.43
3:E:46:ARG:HH11	3:E:46:ARG:C	2.26	0.43
2:G:17:LEU:HD12	2:J:51:THR:HG21	2.00	0.43
2:G:37:VAL:HG21	2:G:82:LEU:HD23	2.00	0.43
1:H:510:THR:HG22	3:K:32:LEU:HG	2.00	0.43
1:M:207:ALA:HB3	1:M:208:PRO:HD3	2.00	0.43
2:P:89:ALA:C	2:N:13:TYR:CE2	2.96	0.43
2:N:379:GLU:HG3	2:N:379:GLU:O	2.18	0.43
2:B:554:TYR:HA	2:B:561:TRP:HA	1.99	0.43
1:F:148:ARG:HH11	1:F:200:VAL:HG21	1.84	0.43
1:F:413:ASP:O	1:F:416:MET:HG3	2.19	0.43
2:G:47:MET:HB2	2:J:47:MET:SD	2.57	0.43
2:G:287:CYS:SG	2:G:288:TYR:N	2.90	0.43
1:I:525:PRO:HA	1:I:603:MET:HE2	1.99	0.43
1:H:102:LEU:HD22	1:H:182:ALA:HB1	2.01	0.43
3:K:59:ASN:ND2	3:K:60:GLN:OE1	2.51	0.43
3:K:86:ARG:O	3:K:89:LYS:HD2	2.18	0.43
1:M:148:ARG:HH11	1:M:200:VAL:HG21	1.83	0.43
1:M:337:ASN:ND2	1:M:340:ASP:OD1	2.51	0.43
1:M:609:GLU:HG3	1:M:610:LYS:H	1.82	0.43
1:O:245:ILE:HA	1:O:248:VAL:HG12	1.99	0.43
2:P:221:ARG:NH2	2:P:260:ARG:HE	2.16	0.43
3:R:43:ALA:HB3	3:R:79:PHE:CE1	2.54	0.43
3:Q:86:ARG:O	3:Q:89:LYS:HD2	2.18	0.43
2:A:287:CYS:SG	2:A:288:TYR:N	2.90	0.43
1:F:622:ILE:HG21	1:F:627:LEU:HD22	1.98	0.43
3:D:45:CYS:HB3	3:D:83:CYS:SG	2.57	0.43
2:J:153:LYS:HD2	2:J:153:LYS:HA	1.69	0.43
2:J:539:ARG:HH21	2:J:579:PHE:HE1	1.65	0.43
1:M:413:ASP:O	1:M:416:MET:HG3	2.19	0.43
1:O:31:ASN:OD1	1:O:72:LYS:NZ	2.51	0.43
1:C:337:ASN:ND2	1:C:340:ASP:OD1	2.52	0.43
2:B:217:LEU:HD13	2:B:225:LEU:HD11	2.00	0.43
1:F:525:PRO:O	1:F:526:PRO:C	2.61	0.43
1:F:593:GLN:HE21	1:F:593:GLN:HB3	1.68	0.43
1:F:609:GLU:OE2	3:D:21:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:36:ASP:O	3:D:38:VAL:HG23	2.17	0.43
3:D:86:ARG:O	3:D:89:LYS:HD2	2.18	0.43
1:M:458:LEU:HD13	1:M:458:LEU:HA	1.73	0.43
3:Q:45:CYS:HB3	3:Q:83:CYS:SG	2.57	0.43
1:C:553:HIS:HA	1:C:597:PHE:CE1	2.53	0.43
2:B:127:LYS:O	2:B:129:ASN:ND2	2.51	0.43
1:H:331:GLU:CD	1:H:336:LYS:HB3	2.44	0.43
1:M:553:HIS:HA	1:M:597:PHE:HE1	1.84	0.43
1:M:605:PHE:HE1	1:M:611:TYR:HB2	1.82	0.43
1:O:525:PRO:O	1:O:526:PRO:C	2.61	0.43
2:A:60:PHE:HB2	2:B:30:PHE:HZ	1.83	0.43
1:F:128:ARG:O	1:F:132:GLN:HB2	2.19	0.43
1:F:510:THR:HG22	3:D:32:LEU:HG	2.00	0.43
1:I:338:PRO:HB3	1:I:387:TYR:HA	2.00	0.43
1:I:527:ALA:HB3	1:I:528:PRO:HD3	2.00	0.43
1:H:425:LYS:HE2	1:H:733:ARG:HH21	1.83	0.43
2:A:190:LYS:HG3	2:A:193:THR:HG22	2.01	0.43
2:B:228:VAL:HG12	2:B:229:THR:H	1.84	0.43
1:F:258:GLU:HB2	1:F:259:PRO:HD3	2.00	0.43
3:D:59:ASN:ND2	3:D:60:GLN:OE1	2.51	0.43
2:J:127:LYS:HA	2:J:127:LYS:HD2	1.90	0.43
2:J:160:PHE:CE1	2:J:164:TYR:HA	2.54	0.43
2:J:172:LEU:HD22	2:J:176:LEU:HD23	2.01	0.43
1:I:455:ILE:HG22	1:I:470:LEU:HD21	1.99	0.43
3:L:74:VAL:HB	3:L:102:GLU:HB2	2.01	0.43
1:M:516:GLN:H	1:M:516:GLN:CD	2.24	0.43
1:O:148:ARG:HH11	1:O:200:VAL:HG21	1.84	0.43
1:O:265:GLU:HB3	1:O:306:VAL:HG22	2.00	0.43
3:Q:59:ASN:ND2	3:Q:60:GLN:OE1	2.51	0.43
1:C:413:ASP:O	1:C:416:MET:HG3	2.19	0.43
2:J:372:LYS:NZ	2:J:580:ARG:HE	2.17	0.43
2:J:379:GLU:O	2:J:379:GLU:HG3	2.18	0.43
1:I:346:LEU:CD2	1:I:414:LYS:HB3	2.47	0.43
1:H:609:GLU:HG3	1:H:610:LYS:H	1.83	0.43
3:L:40:ASP:HA	3:L:48:HIS:CE1	2.53	0.43
3:K:85:SER:O	3:K:89:LYS:NZ	2.50	0.43
1:O:606:ASN:HD21	3:Q:22:PHE:HD1	1.66	0.43
2:N:499:VAL:HG21	2:N:561:TRP:CZ2	2.53	0.43
3:R:74:VAL:HB	3:R:102:GLU:HB2	2.01	0.43
1:C:593:GLN:HE21	1:C:593:GLN:HB3	1.69	0.43
2:B:160:PHE:CE1	2:B:164:TYR:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:499:VAL:HG21	2:B:561:TRP:CZ2	2.54	0.43
2:G:142:LEU:O	1:I:68:LYS:HE2	2.19	0.43
1:I:337:ASN:ND2	1:I:340:ASP:OD1	2.52	0.43
1:I:524:ILE:HG22	1:I:528:PRO:HB2	2.00	0.43
1:H:128:ARG:O	1:H:132:GLN:HB2	2.19	0.43
1:H:245:ILE:HA	1:H:248:VAL:HG12	1.99	0.43
1:H:257:GLU:O	1:H:258:GLU:C	2.62	0.43
1:H:375:GLU:HG2	1:H:421:PHE:HB2	1.99	0.43
1:M:124:MET:HB3	1:M:124:MET:HE3	1.97	0.43
2:P:553:GLN:O	2:P:562:SER:N	2.51	0.43
2:N:160:PHE:CE1	2:N:164:TYR:HA	2.54	0.43
2:N:172:LEU:HD22	2:N:176:LEU:HD23	2.01	0.43
2:A:89:ALA:O	2:B:13:TYR:HE2	2.02	0.43
2:A:221:ARG:NH1	2:A:258:LYS:H	2.16	0.43
2:A:553:GLN:O	2:A:562:SER:N	2.51	0.43
1:F:478:SER:HA	1:F:481:ASN:HD21	1.81	0.43
2:G:190:LYS:HG3	2:G:193:THR:HG22	2.01	0.43
2:J:503:ASP:HB3	2:J:506:LYS:HB2	2.01	0.43
1:H:148:ARG:HH11	1:H:200:VAL:HG21	1.84	0.43
1:O:102:LEU:HD22	1:O:182:ALA:HB1	2.01	0.42
1:O:426:ASP:OD2	1:O:699:ARG:NH2	2.53	0.42
2:P:101:VAL:HB	2:P:124:LEU:HD11	2.00	0.42
1:C:455:ILE:HG22	1:C:470:LEU:HD21	2.00	0.42
2:A:45:HIS:ND1	2:A:90:TYR:OH	2.32	0.42
1:F:129:VAL:O	1:F:133:GLN:NE2	2.43	0.42
2:G:45:HIS:HB2	2:G:48:VAL:HG22	2.01	0.42
2:G:221:ARG:NH2	2:G:260:ARG:HE	2.16	0.42
2:G:553:GLN:O	2:G:562:SER:N	2.51	0.42
2:J:289:SER:HG	2:J:294:LYS:H	1.61	0.42
1:O:338:PRO:HG2	1:O:681:GLN:HB2	2.01	0.42
1:O:419:PHE:HZ	1:O:425:LYS:HG3	1.84	0.42
2:A:37:VAL:HG21	2:A:82:LEU:HD23	2.00	0.42
2:A:231:ARG:H	2:A:231:ARG:HD2	1.84	0.42
3:E:74:VAL:HB	3:E:102:GLU:HB2	2.01	0.42
2:G:47:MET:CB	2:J:47:MET:SD	3.07	0.42
2:J:127:LYS:O	2:J:129:ASN:ND2	2.51	0.42
2:J:499:VAL:HG21	2:J:561:TRP:CZ2	2.53	0.42
1:I:153:ARG:HH21	1:I:200:VAL:HG13	1.84	0.42
1:H:332:GLU:H	1:H:332:GLU:HG2	1.57	0.42
1:M:313:MET:HE2	1:M:313:MET:HB2	1.93	0.42
1:O:470:LEU:O	1:O:473:MET:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:286:VAL:HA	2:A:297:LYS:HA	2.02	0.42
2:A:394:LEU:H	2:G:520:TYR:H	1.68	0.42
1:F:131:VAL:HG12	1:F:136:VAL:HG23	2.02	0.42
1:F:212:MET:HB3	1:F:212:MET:HE3	1.63	0.42
1:F:240:ARG:O	1:F:243:GLU:HG3	2.19	0.42
1:F:426:ASP:OD2	1:F:699:ARG:NH2	2.53	0.42
1:F:606:ASN:HD21	3:D:22:PHE:HD1	1.66	0.42
1:I:717:MET:HE2	1:I:756:ARG:HD3	2.02	0.42
1:H:221:SER:HB3	1:H:268:LEU:HD13	2.00	0.42
1:M:298:CYS:HA	1:M:301:LYS:HG2	2.01	0.42
1:M:516:GLN:HG2	1:M:517:SER:N	2.30	0.42
1:O:477:MET:HB3	1:O:477:MET:HE3	1.62	0.42
2:B:81:THR:OG1	2:B:107:THR:HG21	2.20	0.42
1:F:102:LEU:HD22	1:F:182:ALA:HB1	2.01	0.42
1:H:168:MET:HE2	1:H:168:MET:HB3	1.90	0.42
1:H:706:ALA:HA	1:H:709:ARG:HH21	1.83	0.42
1:M:716:LYS:HG3	2:J:443:PHE:HE2	1.83	0.42
1:O:593:GLN:HE21	1:O:593:GLN:HB3	1.68	0.42
2:N:228:VAL:HG12	2:N:229:THR:H	1.84	0.42
2:N:503:ASP:HB3	2:N:506:LYS:HB2	2.01	0.42
2:A:45:HIS:HB2	2:A:48:VAL:HG22	2.01	0.42
2:A:151:SER:O	2:A:155:MET:HG2	2.20	0.42
2:B:172:LEU:HD22	2:B:176:LEU:HD23	2.01	0.42
2:G:141:ASP:O	1:I:68:LYS:CE	2.67	0.42
1:I:240:ARG:O	1:I:243:GLU:HG3	2.20	0.42
1:I:392:ILE:HD12	1:I:392:ILE:HA	1.95	0.42
1:I:553:HIS:HA	1:I:597:PHE:HE1	1.84	0.42
1:H:366:PHE:O	1:H:370:ILE:HG23	2.19	0.42
1:H:444:LYS:HA	1:H:444:LYS:HD3	1.66	0.42
1:H:503:LEU:HD22	1:H:503:LEU:HA	1.87	0.42
1:O:426:ASP:OD1	1:O:426:ASP:N	2.52	0.42
2:P:51:THR:CB	2:N:20:GLN:HB3	2.50	0.42
2:P:151:SER:O	2:P:155:MET:HG2	2.20	0.42
2:N:101:VAL:HG11	2:N:123:TYR:CD2	2.55	0.42
2:N:372:LYS:NZ	2:N:580:ARG:HE	2.17	0.42
3:Q:80:HIS:HB2	3:Q:83:CYS:SG	2.60	0.42
1:C:153:ARG:HH21	1:C:200:VAL:HG13	1.84	0.42
1:C:717:MET:HE2	1:C:756:ARG:HD3	2.02	0.42
2:A:31:THR:OG1	2:A:44:CYS:O	2.33	0.42
1:F:419:PHE:HZ	1:F:425:LYS:HG3	1.84	0.42
2:J:346:THR:HG22	2:J:369:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:426:ASP:OD1	1:I:426:ASP:N	2.52	0.42
1:H:703:ILE:HD11	1:H:744:ARG:HD3	2.01	0.42
3:K:49:ILE:HD12	3:K:49:ILE:HA	1.92	0.42
1:M:345:LEU:CG	1:M:418:LEU:HD11	2.34	0.42
1:O:609:GLU:OE2	3:Q:21:ARG:NH1	2.52	0.42
2:P:550:VAL:HG23	2:P:566:HIS:HA	2.02	0.42
2:N:395:ASN:O	2:N:395:ASN:ND2	2.53	0.42
3:R:37:ILE:HD12	3:R:78:ALA:HB3	2.02	0.42
1:C:345:LEU:HG	1:C:418:LEU:HD11	2.01	0.42
2:A:101:VAL:HB	2:A:124:LEU:HD11	2.00	0.42
2:A:202:LEU:HD13	2:A:213:LEU:HG	2.01	0.42
2:B:372:LYS:NZ	2:B:580:ARG:HE	2.17	0.42
1:F:470:LEU:O	1:F:473:MET:HG3	2.20	0.42
3:E:37:ILE:HD12	3:E:78:ALA:HB3	2.02	0.42
2:G:286:VAL:HA	2:G:297:LYS:HA	2.02	0.42
1:H:609:GLU:OE2	3:K:21:ARG:NH1	2.52	0.42
3:K:48:HIS:HB3	3:K:50:MET:O	2.20	0.42
1:M:74:TYR:CZ	1:M:142:LEU:HD22	2.54	0.42
2:B:114:GLU:HA	2:B:117:LEU:HB2	2.02	0.42
2:G:506:LYS:HA	2:G:506:LYS:HD3	1.88	0.42
1:I:342:ILE:CG2	1:I:388:LEU:HD12	2.49	0.42
1:I:472:GLY:C	1:I:512:TYR:HE1	2.28	0.42
1:H:336:LYS:HB3	1:H:336:LYS:HE2	1.71	0.42
1:H:458:LEU:HB3	1:H:467:THR:HG22	2.02	0.42
1:H:680:LYS:HE3	1:H:680:LYS:HB3	1.92	0.42
1:O:255:SER:O	1:O:257:GLU:N	2.53	0.42
2:P:221:ARG:NH1	2:P:258:LYS:H	2.16	0.42
2:N:171:GLN:H	2:N:171:GLN:HG2	1.69	0.42
1:C:276:ILE:HD12	1:C:276:ILE:HA	1.96	0.42
2:B:61:MET:HE3	2:B:61:MET:HB3	1.99	0.42
2:B:395:ASN:HB2	2:B:398:THR:HG23	2.02	0.42
1:F:255:SER:O	1:F:257:GLU:N	2.53	0.42
1:F:341:TYR:CD2	1:F:387:TYR:HD2	2.38	0.42
1:F:715:LYS:HE2	1:F:715:LYS:HB2	1.84	0.42
3:E:43:ALA:HB3	3:E:79:PHE:CE1	2.54	0.42
2:J:228:VAL:HG12	2:J:229:THR:H	1.84	0.42
1:H:269:ILE:CB	1:H:306:VAL:HG21	2.46	0.42
1:H:396:LEU:O	1:H:397:LYS:C	2.61	0.42
3:K:80:HIS:HB2	3:K:83:CYS:SG	2.60	0.42
1:M:153:ARG:HH21	1:M:200:VAL:HG13	1.85	0.42
1:O:609:GLU:HG3	1:O:610:LYS:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:31:THR:OG1	2:P:44:CYS:O	2.33	0.42
2:N:156:VAL:O	2:N:160:PHE:HB3	2.20	0.42
1:C:31:ASN:OD1	1:C:72:LYS:NZ	2.53	0.42
2:A:325:VAL:O	2:A:345:ARG:N	2.48	0.42
1:F:342:ILE:HD11	1:F:387:TYR:HB2	2.02	0.42
1:F:520:PRO:HG2	1:F:552:HIS:H	1.85	0.42
3:D:35:TRP:HD1	3:D:76:ASN:HB2	1.85	0.42
2:G:470:LYS:NZ	2:G:503:ASP:OD2	2.44	0.42
2:J:497:VAL:HB	2:J:515:ILE:H	1.85	0.42
1:I:339:VAL:C	1:I:391:PHE:HD1	2.28	0.42
1:I:458:LEU:HB3	1:I:467:THR:CG2	2.44	0.42
1:H:298:CYS:HA	1:H:301:LYS:HG2	2.01	0.42
1:H:337:ASN:HA	1:H:338:PRO:HD3	1.92	0.42
1:M:342:ILE:HG21	1:M:391:PHE:CB	2.50	0.41
1:O:240:ARG:O	1:O:243:GLU:HG3	2.19	0.41
2:P:47:MET:HE2	2:N:21:LEU:CB	2.50	0.41
2:P:160:PHE:HB2	2:P:166:GLN:HE22	1.85	0.41
2:P:190:LYS:HG3	2:P:193:THR:HG22	2.01	0.41
2:P:231:ARG:HD2	2:P:231:ARG:H	1.84	0.41
1:C:240:ARG:O	1:C:243:GLU:HG3	2.20	0.41
1:C:471:GLU:HB3	1:C:475:ARG:HH21	1.84	0.41
2:A:30:PHE:HZ	2:B:57:ARG:HA	1.84	0.41
2:A:160:PHE:HB2	2:A:166:GLN:HE22	1.85	0.41
2:B:395:ASN:O	2:B:395:ASN:ND2	2.52	0.41
1:F:426:ASP:OD1	1:F:426:ASP:N	2.53	0.41
2:G:202:LEU:HD13	2:G:213:LEU:HG	2.01	0.41
2:G:231:ARG:H	2:G:231:ARG:HD2	1.84	0.41
2:G:550:VAL:HG23	2:G:566:HIS:HA	2.02	0.41
2:J:269:MET:HE3	2:J:530:ILE:HD12	2.02	0.41
1:I:413:ASP:O	1:I:416:MET:HG3	2.19	0.41
1:I:516:GLN:H	1:I:516:GLN:CD	2.24	0.41
1:H:258:GLU:HB2	1:H:259:PRO:HD3	2.02	0.41
1:H:273:MET:O	1:H:277:VAL:HG22	2.20	0.41
1:H:734:PHE:HB2	1:H:735:LEU:H	1.61	0.41
1:O:413:ASP:O	1:O:416:MET:HG3	2.18	0.41
2:P:20:GLN:HB3	2:N:51:THR:HG22	2.03	0.41
2:P:81:THR:O	2:P:84:ILE:HG22	2.20	0.41
1:C:386:GLU:OE1	1:C:386:GLU:N	2.46	0.41
1:C:426:ASP:OD1	1:C:426:ASP:N	2.52	0.41
2:B:101:VAL:HG11	2:B:123:TYR:CD2	2.55	0.41
2:B:346:THR:HG22	2:B:369:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:238:GLU:O	1:F:242:ASN:ND2	2.41	0.41
2:J:81:THR:OG1	2:J:107:THR:HG21	2.20	0.41
1:I:74:TYR:CZ	1:I:142:LEU:HD22	2.54	0.41
1:H:559:LEU:HD22	1:H:602:LEU:HD13	2.02	0.41
3:L:37:ILE:HD12	3:L:78:ALA:HB3	2.02	0.41
1:M:388:LEU:HD21	1:M:419:PHE:HB2	2.03	0.41
1:M:717:MET:HE2	1:M:756:ARG:HD3	2.02	0.41
1:O:298:CYS:HA	1:O:301:LYS:HG2	2.01	0.41
2:P:137:LEU:HB2	2:P:152:ALA:HB1	2.03	0.41
2:P:443:PHE:HE1	2:P:445:ARG:HH21	1.69	0.41
2:N:497:VAL:HB	2:N:515:ILE:H	1.85	0.41
1:C:74:TYR:CZ	1:C:142:LEU:HD22	2.54	0.41
2:B:503:ASP:HB3	2:B:506:LYS:HB2	2.01	0.41
2:G:160:PHE:HB2	2:G:166:GLN:HE22	1.85	0.41
1:I:31:ASN:OD1	1:I:72:LYS:NZ	2.53	0.41
1:I:298:CYS:HA	1:I:301:LYS:HG2	2.01	0.41
1:H:212:MET:HE3	1:H:212:MET:HB3	1.63	0.41
3:K:35:TRP:HD1	3:K:76:ASN:HB2	1.85	0.41
1:M:426:ASP:OD1	1:M:426:ASP:N	2.52	0.41
2:P:45:HIS:HB2	2:P:48:VAL:HG22	2.01	0.41
2:N:269:MET:HE3	2:N:530:ILE:HD12	2.03	0.41
3:Q:48:HIS:HB3	3:Q:50:MET:O	2.20	0.41
1:C:388:LEU:HD21	1:C:419:PHE:HB2	2.03	0.41
2:A:51:THR:HG21	2:B:17:LEU:CD1	2.50	0.41
2:A:81:THR:O	2:A:84:ILE:HG22	2.20	0.41
2:B:108:ALA:HA	2:B:113:VAL:HG23	2.01	0.41
2:J:101:VAL:HG11	2:J:123:TYR:CD2	2.55	0.41
1:H:520:PRO:HG2	1:H:552:HIS:H	1.85	0.41
1:M:638:LYS:HG3	1:M:639:PRO:O	2.20	0.41
2:P:286:VAL:HA	2:P:297:LYS:HA	2.02	0.41
2:N:81:THR:OG1	2:N:107:THR:HG21	2.20	0.41
3:Q:35:TRP:HD1	3:Q:76:ASN:HB2	1.85	0.41
2:B:64:LEU:HD13	2:B:64:LEU:HA	1.92	0.41
1:F:337:ASN:HB3	1:F:340:ASP:HB2	2.03	0.41
3:D:48:HIS:HB3	3:D:50:MET:O	2.20	0.41
2:G:137:LEU:HB2	2:G:152:ALA:HB1	2.03	0.41
1:I:258:GLU:HB2	1:I:259:PRO:HD3	2.02	0.41
1:I:704:GLU:O	1:I:707:ILE:HG22	2.21	0.41
1:H:593:GLN:HE21	1:H:593:GLN:HB3	1.68	0.41
1:M:704:GLU:O	1:M:707:ILE:HG22	2.21	0.41
2:P:206:THR:O	2:P:207:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:81:THR:OG1	2:A:107:THR:HG21	2.21	0.41
2:B:64:LEU:CD2	1:F:118:MET:SD	3.09	0.41
1:F:298:CYS:HA	1:F:301:LYS:HG2	2.01	0.41
2:G:48:VAL:HA	2:G:51:THR:HG22	2.03	0.41
2:G:297:LYS:NZ	2:G:593:GLU:O	2.54	0.41
3:K:33:TRP:O	3:K:76:ASN:ND2	2.53	0.41
1:M:700:LYS:HG2	1:M:744:ARG:HD2	2.02	0.41
1:O:390:LEU:HD22	1:O:435:HIS:NE2	2.36	0.41
2:P:50:ALA:HB3	2:N:24:PHE:HE2	1.84	0.41
2:P:202:LEU:HD13	2:P:213:LEU:HG	2.01	0.41
2:P:326:PRO:HA	2:P:344:PHE:HA	2.03	0.41
2:P:549:TYR:OH	2:P:575:LEU:N	2.49	0.41
2:N:74:LEU:HD11	2:N:110:PHE:HE2	1.85	0.41
2:A:422:SER:OG	2:A:434:MET:O	2.27	0.41
2:B:542:HIS:HB2	2:B:545:GLU:HB2	2.02	0.41
1:F:500:GLY:HA2	1:F:503:LEU:HD23	2.03	0.41
2:G:56:PHE:HA	2:G:59:MET:HB3	2.03	0.41
2:J:395:ASN:C	2:J:397:ARG:H	2.29	0.41
1:I:476:ASP:OD2	1:I:509:THR:CB	2.68	0.41
1:H:240:ARG:O	1:H:243:GLU:HG3	2.19	0.41
1:O:341:TYR:CD2	1:O:387:TYR:HD2	2.36	0.41
1:O:346:LEU:CB	1:O:418:LEU:HD13	2.51	0.41
2:N:413:SER:HB3	2:N:442:TYR:HE1	1.86	0.41
1:C:298:CYS:HA	1:C:301:LYS:HG2	2.01	0.41
1:C:553:HIS:HA	1:C:597:PHE:HE1	1.84	0.41
2:A:48:VAL:HA	2:A:51:THR:HG22	2.03	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
1:F:168:MET:SD	1:F:183:ILE:HD11	2.61	0.41
1:F:559:LEU:HD22	1:F:602:LEU:HD13	2.02	0.41
3:D:80:HIS:HB2	3:D:83:CYS:SG	2.60	0.41
2:G:151:SER:O	2:G:155:MET:HG2	2.20	0.41
2:J:156:VAL:O	2:J:160:PHE:HB3	2.21	0.41
1:H:131:VAL:HG12	1:H:136:VAL:HG23	2.02	0.41
1:H:287:MET:HE2	1:H:287:MET:HB3	1.89	0.41
1:H:288:LEU:HD23	1:H:351:ARG:HH21	1.85	0.41
1:H:441:LEU:HG	1:H:513:TRP:HE3	1.79	0.41
1:M:240:ARG:O	1:M:243:GLU:HG3	2.20	0.41
1:M:258:GLU:HB2	1:M:259:PRO:HD3	2.02	0.41
1:M:501:VAL:HB	1:M:502:ASP:H	1.58	0.41
1:O:168:MET:SD	1:O:183:ILE:HD11	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:92:GLY:CA	2:N:13:TYR:CD2	3.03	0.41
2:N:395:ASN:C	2:N:397:ARG:H	2.28	0.41
3:Q:49:ILE:HD12	3:Q:49:ILE:HA	1.92	0.41
1:C:374:PHE:HA	1:C:377:PHE:HD1	1.86	0.41
1:C:634:LEU:HD23	1:C:634:LEU:HA	1.90	0.41
1:C:638:LYS:HG3	1:C:639:PRO:O	2.20	0.41
2:A:45:HIS:HB3	2:B:47:MET:SD	2.61	0.41
2:A:443:PHE:HE1	2:A:445:ARG:HH21	1.69	0.41
2:A:539:ARG:HH22	2:A:577:ARG:HD3	1.86	0.41
2:A:539:ARG:HD3	2:A:549:TYR:CZ	2.56	0.41
2:B:266:GLU:HB2	2:B:268:MET:HE3	2.03	0.41
3:E:50:MET:HE3	3:E:50:MET:HB3	1.97	0.41
3:D:25:LYS:HE2	3:D:25:LYS:HB2	1.88	0.41
3:D:33:TRP:O	3:D:76:ASN:ND2	2.53	0.41
2:G:206:THR:O	2:G:207:GLU:HB2	2.21	0.41
2:J:87:THR:O	2:J:91:THR:HG22	2.21	0.41
2:J:108:ALA:HB1	2:J:117:LEU:HG	2.03	0.41
1:I:374:PHE:HA	1:I:377:PHE:HD1	1.86	0.41
1:I:546:ARG:NH2	3:L:35:TRP:HE1	2.18	0.41
1:I:603:MET:HE3	1:I:603:MET:HB3	1.99	0.41
1:H:168:MET:SD	1:H:183:ILE:HD11	2.61	0.41
1:H:331:GLU:HG3	1:H:336:LYS:HB3	2.03	0.41
1:H:646:LYS:HE3	1:H:659:PHE:HE1	1.86	0.41
1:M:457:LYS:HA	1:M:457:LYS:HD2	1.82	0.41
1:M:548:LEU:HD22	1:M:548:LEU:HA	1.91	0.41
2:N:108:ALA:HB1	2:N:117:LEU:HG	2.03	0.41
1:C:248:VAL:O	1:C:256:THR:HG21	2.21	0.41
1:C:700:LYS:HG2	1:C:744:ARG:HD2	2.02	0.41
2:B:53:SER:HA	2:B:113:VAL:HG13	2.03	0.41
2:B:156:VAL:O	2:B:160:PHE:HB3	2.20	0.41
2:B:273:GLU:HA	2:B:283:TYR:HB3	2.02	0.41
2:B:326:PRO:HA	2:B:344:PHE:HA	2.03	0.41
2:G:81:THR:O	2:G:84:ILE:HG22	2.20	0.41
1:I:265:GLU:HB3	1:I:306:VAL:HG22	2.03	0.41
1:H:109:TRP:CD2	1:H:189:MET:HG3	2.56	0.41
1:M:31:ASN:OD1	1:M:72:LYS:NZ	2.53	0.40
1:M:508:LEU:HB3	1:M:513:TRP:CD1	2.56	0.40
1:O:559:LEU:HD22	1:O:602:LEU:HD13	2.02	0.40
1:O:719:HIS:CE1	1:O:761:ARG:HH12	2.39	0.40
2:P:48:VAL:HA	2:P:51:THR:HG22	2.02	0.40
2:P:50:ALA:CB	2:N:24:PHE:CZ	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:346:THR:HG22	2:N:369:VAL:HB	2.02	0.40
1:C:238:GLU:O	1:C:242:ASN:ND2	2.40	0.40
1:C:258:GLU:HB2	1:C:259:PRO:HD3	2.02	0.40
1:C:704:GLU:O	1:C:707:ILE:HG22	2.21	0.40
2:A:206:THR:O	2:A:207:GLU:HB2	2.21	0.40
1:F:97:LEU:O	1:F:160:HIS:NE2	2.49	0.40
1:F:455:ILE:HG22	1:F:470:LEU:HD22	2.04	0.40
2:J:266:GLU:HB2	2:J:268:MET:HE3	2.03	0.40
1:M:248:VAL:O	1:M:256:THR:HG21	2.21	0.40
1:M:265:GLU:HB3	1:M:306:VAL:HG22	2.03	0.40
1:O:646:LYS:HE3	1:O:659:PHE:HE1	1.86	0.40
1:O:647:GLU:HB2	1:O:648:PRO:HD3	2.03	0.40
2:P:45:HIS:CG	2:N:47:MET:HE3	2.53	0.40
2:P:178:ILE:HG23	2:P:219:GLN:HE21	1.86	0.40
2:N:266:GLU:HB2	2:N:268:MET:HE3	2.03	0.40
1:C:168:MET:SD	1:C:183:ILE:HD11	2.62	0.40
1:C:265:GLU:HB3	1:C:306:VAL:HG22	2.03	0.40
1:C:647:GLU:HB2	1:C:648:PRO:HD3	2.03	0.40
2:A:18:LEU:HD23	2:B:9:ILE:HG21	2.04	0.40
2:B:108:ALA:HB1	2:B:117:LEU:HG	2.03	0.40
2:G:81:THR:OG1	2:G:107:THR:HG21	2.21	0.40
2:G:539:ARG:HH22	2:G:577:ARG:HD3	1.86	0.40
1:I:248:VAL:O	1:I:256:THR:HG21	2.21	0.40
1:H:40:ALA:HB1	1:H:52:LEU:HD21	2.03	0.40
1:H:412:LEU:HD13	1:H:457:LYS:HG3	2.03	0.40
1:O:386:GLU:OE1	1:O:386:GLU:N	2.47	0.40
2:P:419:TRP:HZ2	2:P:438:LEU:HD23	1.87	0.40
2:N:87:THR:O	2:N:91:THR:HG22	2.21	0.40
2:N:382:ILE:HB	2:N:402:TYR:HB3	2.04	0.40
2:N:539:ARG:HD3	2:N:549:TYR:CZ	2.56	0.40
3:Q:33:TRP:O	3:Q:76:ASN:ND2	2.54	0.40
2:A:326:PRO:HA	2:A:344:PHE:HA	2.03	0.40
2:B:395:ASN:C	2:B:397:ARG:H	2.29	0.40
1:F:374:PHE:HA	1:F:377:PHE:CD1	2.56	0.40
2:G:539:ARG:HD3	2:G:549:TYR:CZ	2.57	0.40
1:I:473:MET:SD	1:I:512:TYR:HB3	2.61	0.40
1:I:508:LEU:HB3	1:I:513:TRP:CD1	2.56	0.40
1:H:371:ALA:O	1:H:372:GLY:C	2.64	0.40
1:M:168:MET:HE2	1:M:168:MET:HB3	1.90	0.40
1:O:392:ILE:HD12	1:O:392:ILE:HA	1.96	0.40
1:C:401:LYS:H	1:C:401:LYS:HG2	1.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:297:LYS:NZ	2:A:593:GLU:O	2.54	0.40
2:B:29:LEU:HB3	2:B:30:PHE:HD1	1.87	0.40
2:B:87:THR:O	2:B:91:THR:HG22	2.21	0.40
1:F:153:ARG:HH21	1:F:200:VAL:HG13	1.87	0.40
1:F:646:LYS:HE3	1:F:659:PHE:HE1	1.86	0.40
1:I:339:VAL:HA	1:I:391:PHE:CB	2.51	0.40
1:I:700:LYS:HG2	1:I:744:ARG:HD2	2.02	0.40
1:M:647:GLU:HB2	1:M:648:PRO:HD3	2.03	0.40
2:P:161:THR:HG21	2:P:187:ASN:H	1.87	0.40
2:N:326:PRO:HA	2:N:344:PHE:HA	2.03	0.40
3:R:48:HIS:HB3	3:R:50:MET:O	2.22	0.40
2:A:22:LYS:HD2	2:A:22:LYS:HA	1.74	0.40
2:A:161:THR:HG21	2:A:187:ASN:H	1.87	0.40
2:A:178:ILE:HG23	2:A:219:GLN:HE21	1.86	0.40
2:B:59:MET:HE3	2:B:66:GLU:HG2	2.03	0.40
2:B:539:ARG:HD3	2:B:549:TYR:CZ	2.56	0.40
1:F:548:LEU:HD22	1:F:548:LEU:HA	1.88	0.40
2:G:31:THR:OG1	2:G:44:CYS:O	2.33	0.40
2:G:190:LYS:HB2	2:G:192:GLU:OE1	2.22	0.40
2:G:419:TRP:HZ2	2:G:438:LEU:HD23	1.87	0.40
2:J:539:ARG:HD3	2:J:549:TYR:CZ	2.56	0.40
1:I:638:LYS:HG3	1:I:639:PRO:O	2.20	0.40
1:H:153:ARG:HH21	1:H:200:VAL:HG13	1.86	0.40
1:H:422:MET:HG3	1:H:423:GLN:O	2.21	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%)	650 (91%)	58 (8%)	8 (1%)	11 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	716/768 (93%)	654 (91%)	60 (8%)	2 (0%)	36	72
1	H	716/768 (93%)	619 (86%)	88 (12%)	9 (1%)	9	42
1	I	716/768 (93%)	658 (92%)	57 (8%)	1 (0%)	48	83
1	M	716/768 (93%)	653 (91%)	62 (9%)	1 (0%)	48	83
1	O	716/768 (93%)	651 (91%)	58 (8%)	7 (1%)	12	49
2	A	555/623 (89%)	520 (94%)	34 (6%)	1 (0%)	43	78
2	B	557/623 (89%)	534 (96%)	23 (4%)	0	100	100
2	G	555/623 (89%)	523 (94%)	30 (5%)	2 (0%)	30	67
2	J	557/623 (89%)	533 (96%)	24 (4%)	0	100	100
2	N	557/623 (89%)	535 (96%)	22 (4%)	0	100	100
2	P	555/623 (89%)	517 (93%)	37 (7%)	1 (0%)	43	78
3	D	87/121 (72%)	70 (80%)	16 (18%)	1 (1%)	11	46
3	E	87/121 (72%)	75 (86%)	11 (13%)	1 (1%)	11	46
3	K	87/121 (72%)	70 (80%)	16 (18%)	1 (1%)	11	46
3	L	87/121 (72%)	75 (86%)	11 (13%)	1 (1%)	11	46
3	Q	87/121 (72%)	70 (80%)	16 (18%)	1 (1%)	11	46
3	R	87/121 (72%)	75 (86%)	11 (13%)	1 (1%)	11	46
All	All	8154/9072 (90%)	7482 (92%)	634 (8%)	38 (0%)	26	63

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	544	SER
1	F	526	PRO
1	H	258	GLU
1	M	501	VAL
1	C	542	LYS
1	H	266	ARG
1	H	449	ASP
1	O	335	GLY
1	O	449	ASP
1	O	526	PRO
1	C	449	ASP
1	C	464	CYS
1	C	501	VAL
1	F	544	SER

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Mol	Chain	Res	Type
1	O	545	GLY
1	C	465	GLN
1	C	517	SER
1	C	540	LEU
1	C	545	GLY
1	H	262	LYS
1	H	416	MET
2	G	390	VAL
1	H	447	SER
1	O	338	PRO
1	O	501	VAL
2	P	63	GLY
3	Q	38	VAL
3	D	38	VAL
1	I	545	GLY
1	H	274	LYS
3	K	38	VAL
2	A	390	VAL
3	E	38	VAL
2	G	516	PRO
3	L	38	VAL
3	R	38	VAL
1	H	260	ILE
1	H	261	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	618/693 (89%)	586 (95%)	32 (5%)	21	42
1	F	632/693 (91%)	618 (98%)	14 (2%)	45	64
1	H	636/693 (92%)	525 (82%)	111 (18%)	2	9
1	I	634/693 (92%)	619 (98%)	15 (2%)	43	64
1	M	616/693 (89%)	587 (95%)	29 (5%)	23	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	583/693 (84%)	560 (96%)	23 (4%)	28	49
2	A	497/560 (89%)	485 (98%)	12 (2%)	43	64
2	B	495/560 (88%)	487 (98%)	8 (2%)	55	70
2	G	473/560 (84%)	464 (98%)	9 (2%)	50	67
2	J	484/560 (86%)	477 (99%)	7 (1%)	59	72
2	N	485/560 (87%)	482 (99%)	3 (1%)	78	83
2	P	476/560 (85%)	474 (100%)	2 (0%)	84	84
3	D	78/102 (76%)	78 (100%)	0	100	100
3	E	77/102 (76%)	77 (100%)	0	100	100
3	K	73/102 (72%)	73 (100%)	0	100	100
3	L	77/102 (76%)	76 (99%)	1 (1%)	61	74
3	Q	78/102 (76%)	78 (100%)	0	100	100
3	R	78/102 (76%)	78 (100%)	0	100	100
All	All	7090/8130 (87%)	6824 (96%)	266 (4%)	30	50

All (266) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	256	THR
1	M	380	LEU
1	M	383	ARG
1	M	384	SER
1	M	452	LYS
1	M	455	ILE
1	M	456	SER
1	M	457	LYS
1	M	458	LEU
1	M	459	LYS
1	M	462	CYS
1	M	464	CYS
1	M	465	GLN
1	M	466	PHE
1	M	467	THR
1	M	468	SER
1	M	470	LEU
1	M	476	ASP
1	M	477	MET

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Mol	Chain	Res	Type
1	M	478	SER
1	M	480	SER
1	M	498	LEU
1	M	501	VAL
1	M	502	ASP
1	M	503	LEU
1	M	521	LYS
1	M	524	ILE
1	M	548	LEU
1	M	715	LYS
1	O	203	GLU
1	O	212	MET
1	O	213	SER
1	O	329	VAL
1	O	332	GLU
1	O	336	LYS
1	O	380	LEU
1	O	477	MET
1	O	479	ILE
1	O	480	SER
1	O	485	ASP
1	O	486	GLU
1	O	501	VAL
1	O	502	ASP
1	O	503	LEU
1	O	504	THR
1	O	526	PRO
1	O	532	PHE
1	O	536	ARG
1	O	546	ARG
1	O	547	GLN
1	O	549	THR
1	O	748	LEU
2	P	113	VAL
2	P	114	GLU
2	N	397	ARG
2	N	398	THR
2	N	399	VAL
1	C	52	LEU
1	C	56	GLU
1	C	57	LEU
1	C	256	THR

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Mol	Chain	Res	Type
1	C	380	LEU
1	C	398	LYS
1	C	400	VAL
1	C	401	LYS
1	C	406	GLN
1	C	443	ASN
1	C	445	SER
1	C	446	VAL
1	C	447	SER
1	C	449	ASP
1	C	464	CYS
1	C	465	GLN
1	C	467	THR
1	C	468	SER
1	C	469	LYS
1	C	470	LEU
1	C	471	GLU
1	C	473	MET
1	C	478	SER
1	C	480	SER
1	C	483	THR
1	C	501	VAL
1	C	503	LEU
1	C	516	GLN
1	C	521	LYS
1	C	523	ASN
1	C	524	ILE
1	C	665	PHE
2	A	11	THR
2	A	12	GLU
2	A	17	LEU
2	A	19	GLU
2	A	20	GLN
2	A	22	LYS
2	A	62	SER
2	A	65	SER
2	A	67	SER
2	A	68	LYS
2	A	397	ARG
2	A	398	THR
2	B	109	CYS
2	B	113	VAL

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Mol	Chain	Res	Type
2	B	114	GLU
2	B	115	ASP
2	B	116	VAL
2	B	397	ARG
2	B	398	THR
2	B	399	VAL
1	F	203	GLU
1	F	212	MET
1	F	213	SER
1	F	378	LEU
1	F	380	LEU
1	F	381	ASN
1	F	486	GLU
1	F	498	LEU
1	F	526	PRO
1	F	548	LEU
1	F	712	LYS
1	F	715	LYS
1	F	716	LYS
1	F	748	LEU
2	G	10	ASN
2	G	12	GLU
2	G	389	SER
2	G	452	MET
2	G	505	ASN
2	G	506	LYS
2	G	507	ASN
2	G	515	ILE
2	G	524	CYS
2	J	145	CYS
2	J	397	ARG
2	J	398	THR
2	J	399	VAL
2	J	427	VAL
2	J	428	HIS
2	J	429	ASP
1	I	378	LEU
1	I	379	ASN
1	I	380	LEU
1	I	381	ASN
1	I	383	ARG
1	I	459	LYS

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Mol	Chain	Res	Type
1	I	462	CYS
1	I	464	CYS
1	I	484	MET
1	I	486	GLU
1	I	487	PHE
1	I	491	LEU
1	I	492	GLN
1	I	550	LEU
1	I	665	PHE
1	H	52	LEU
1	H	203	GLU
1	H	212	MET
1	H	213	SER
1	H	258	GLU
1	H	260	ILE
1	H	262	LYS
1	H	265	GLU
1	H	267	GLU
1	H	268	LEU
1	H	269	ILE
1	H	270	SER
1	H	274	LYS
1	H	276	ILE
1	H	278	GLU
1	H	279	MET
1	H	281	ASN
1	H	285	VAL
1	H	288	LEU
1	H	289	LYS
1	H	292	LYS
1	H	311	LYS
1	H	317	MET
1	H	318	SER
1	H	319	SER
1	H	321	LEU
1	H	326	LYS
1	H	328	LEU
1	H	332	GLU
1	H	336	LYS
1	H	337	ASN
1	H	339	VAL
1	H	340	ASP

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Mol	Chain	Res	Type
1	H	345	LEU
1	H	349	LYS
1	H	351	ARG
1	H	354	ARG
1	H	364	ARG
1	H	370	ILE
1	H	373	ASP
1	H	378	LEU
1	H	379	ASN
1	H	383	ARG
1	H	386	GLU
1	H	390	LEU
1	H	392	ILE
1	H	395	LYS
1	H	397	LYS
1	H	398	LYS
1	H	400	VAL
1	H	401	LYS
1	H	403	LEU
1	H	404	THR
1	H	405	GLU
1	H	406	GLN
1	H	407	GLU
1	H	411	ILE
1	H	414	LYS
1	H	418	LEU
1	H	420	ARG
1	H	421	PHE
1	H	422	MET
1	H	424	GLU
1	H	425	LYS
1	H	426	ASP
1	H	431	TYR
1	H	433	LYS
1	H	440	LEU
1	H	444	LYS
1	H	446	VAL
1	H	449	ASP
1	H	451	GLU
1	H	452	LYS
1	H	454	MET
1	H	455	ILE

Continued on next page...

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Mol	Chain	Res	Type
1	H	458	LEU
1	H	459	LYS
1	H	462	CYS
1	H	465	GLN
1	H	468	SER
1	H	469	LYS
1	H	470	LEU
1	H	471	GLU
1	H	473	MET
1	H	474	PHE
1	H	477	MET
1	H	478	SER
1	H	480	SER
1	H	486	GLU
1	H	488	ARG
1	H	492	GLN
1	H	503	LEU
1	H	504	THR
1	H	507	VAL
1	H	546	ARG
1	H	547	GLN
1	H	687	GLU
1	H	689	LYS
1	H	692	ARG
1	H	694	LYS
1	H	701	HIS
1	H	702	GLU
1	H	703	ILE
1	H	709	ARG
1	H	711	MET
1	H	712	LYS
1	H	728	GLN
1	H	731	LYS
1	H	735	LEU
1	H	739	VAL
1	H	748	LEU
3	L	44	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	87	ASN

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Mol	Chain	Res	Type
1	M	112	HIS
1	M	163	GLN
1	M	286	HIS
1	M	381	ASN
1	M	465	GLN
1	M	481	ASN
1	M	606	ASN
1	M	618	GLN
1	M	657	HIS
1	M	718	GLN
1	O	87	ASN
1	O	112	HIS
1	O	163	GLN
1	O	286	HIS
1	O	481	ASN
1	O	547	GLN
1	O	553	HIS
1	O	606	ASN
1	O	618	GLN
1	O	718	GLN
1	O	719	HIS
2	P	69	GLN
2	P	71	HIS
2	P	150	GLN
2	P	219	GLN
2	P	306	HIS
2	P	356	GLN
2	P	357	GLN
2	N	129	ASN
2	N	187	ASN
2	N	205	ASN
2	N	219	GLN
2	N	230	GLN
2	N	235	GLN
2	N	357	GLN
3	R	41	ASN
3	R	57	GLN
3	Q	47	ASN
3	Q	48	HIS
1	C	60	ASN
1	C	87	ASN
1	C	163	GLN

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Continued from previous page...

Mol	Chain	Res	Type
1	C	286	HIS
1	C	465	GLN
1	C	481	ASN
1	C	606	ASN
1	C	618	GLN
1	C	657	HIS
1	C	718	GLN
2	A	71	HIS
2	A	219	GLN
2	A	356	GLN
2	A	357	GLN
2	B	129	ASN
2	B	187	ASN
2	B	205	ASN
2	B	219	GLN
2	B	230	GLN
2	B	235	GLN
2	B	306	HIS
2	B	357	GLN
2	B	428	HIS
1	F	60	ASN
1	F	87	ASN
1	F	163	GLN
1	F	286	HIS
1	F	379	ASN
1	F	553	HIS
1	F	606	ASN
1	F	618	GLN
1	F	719	HIS
3	E	41	ASN
3	E	57	GLN
3	D	47	ASN
3	D	48	HIS
2	G	10	ASN
2	G	71	HIS
2	G	356	GLN
2	G	357	GLN
2	J	69	GLN
2	J	129	ASN
2	J	187	ASN
2	J	205	ASN
2	J	230	GLN

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Mol	Chain	Res	Type
2	J	235	GLN
2	J	357	GLN
2	J	428	HIS
1	I	87	ASN
1	I	163	GLN
1	I	286	HIS
1	I	381	ASN
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	60	ASN
1	H	87	ASN
1	H	163	GLN
1	H	286	HIS
1	H	290	ASN
1	H	324	GLN
1	H	379	ASN
1	H	381	ASN
1	H	547	GLN
1	H	553	HIS
1	H	606	ASN
1	H	618	GLN
1	H	701	HIS
1	H	718	GLN
1	H	719	HIS
1	H	728	GLN
3	L	48	HIS
3	L	57	GLN
3	K	47	ASN
3	K	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

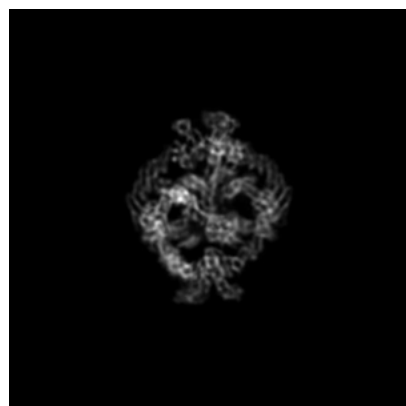
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34450. These allow visual inspection of the internal detail of the map and identification of artifacts.

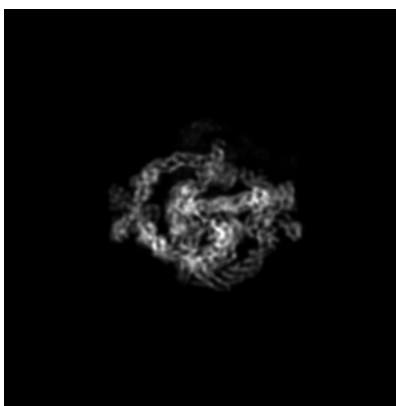
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

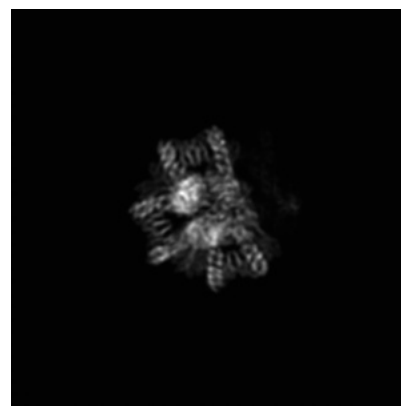
6.1.1 Primary map



X

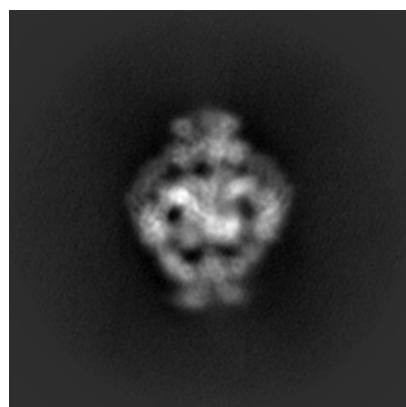


Y

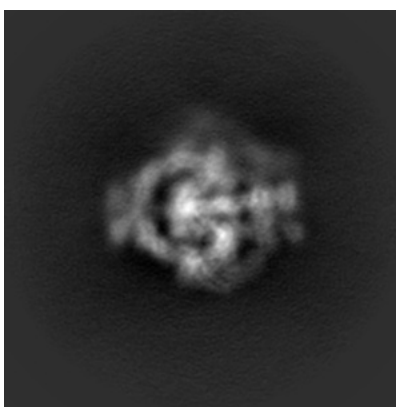


Z

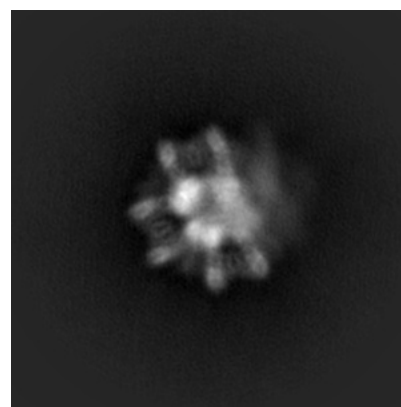
6.1.2 Raw map



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

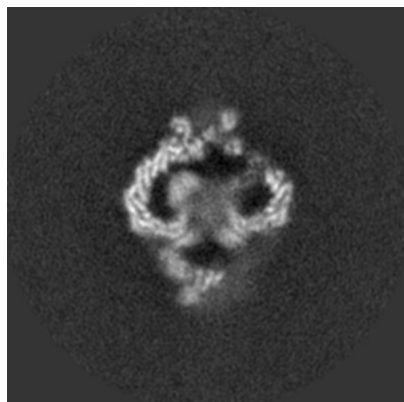


Y Index: 96

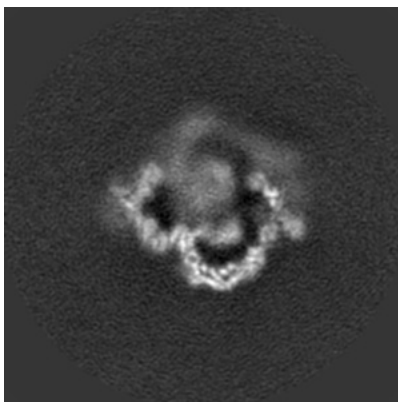


Z Index: 96

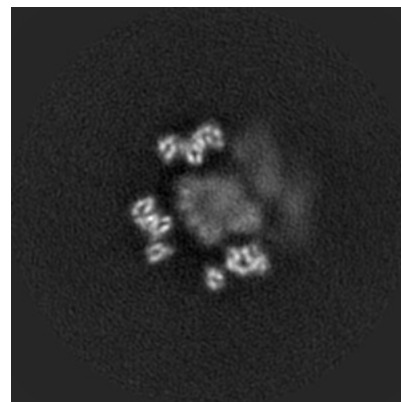
6.2.2 Raw map



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: 100

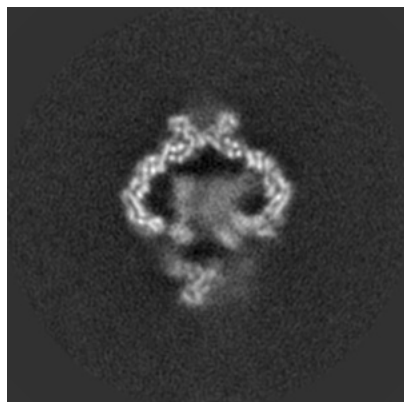


Y Index: 97

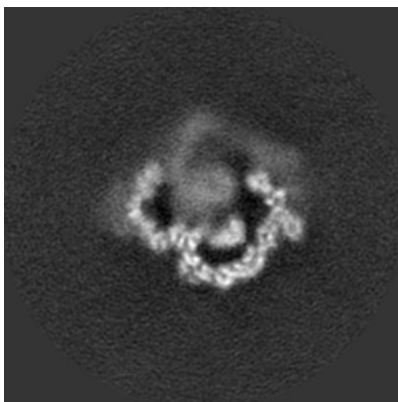


Z Index: 89

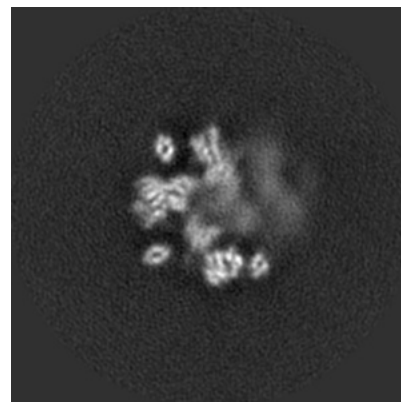
6.3.2 Raw map



X Index: 99



Y Index: 98

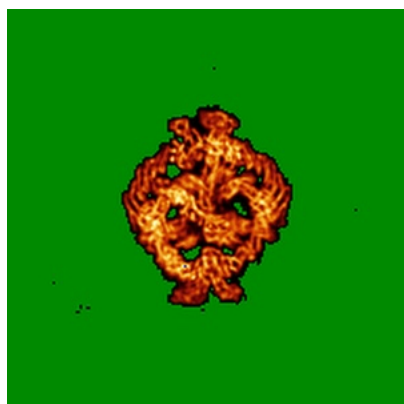


Z Index: 89

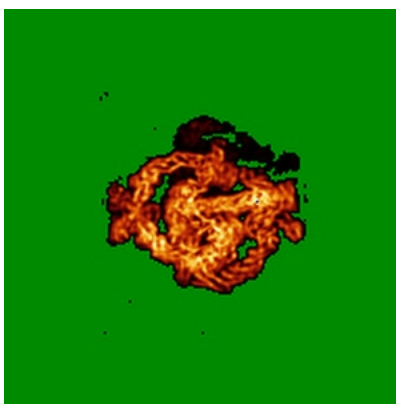
The images above show the largest variance slices of the map in three orthogonal directions.

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

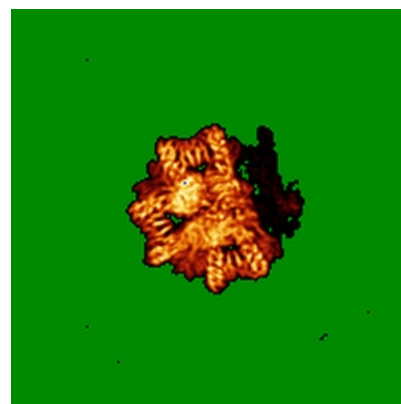
6.4.1 Primary map



X

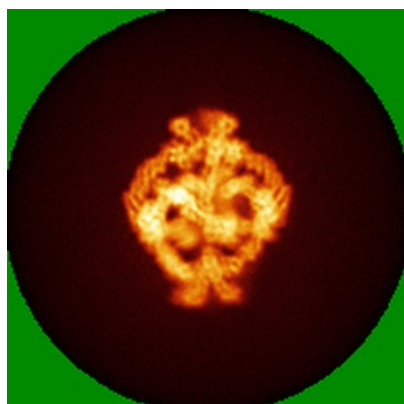


Y

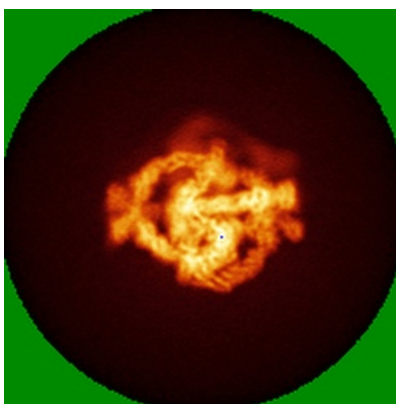


Z

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.

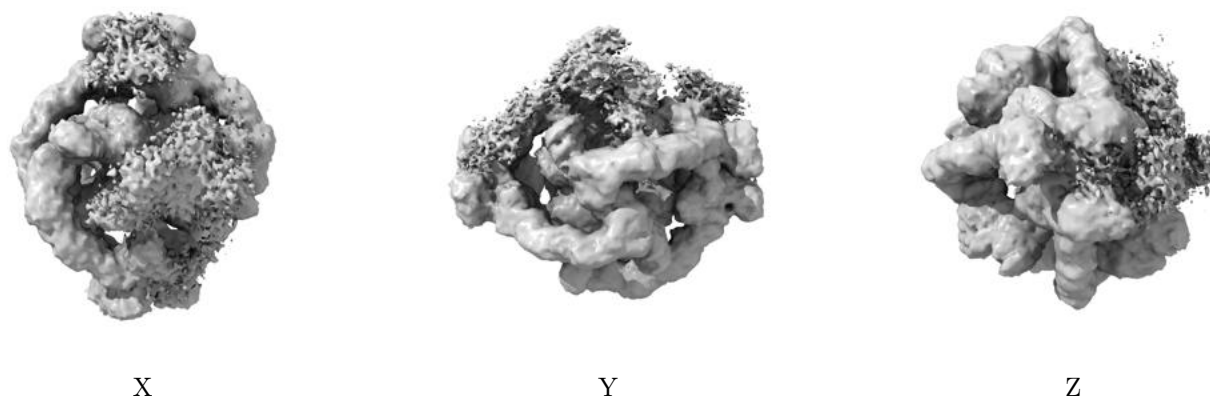
6.5 Orthogonal surface views [i](#)

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.

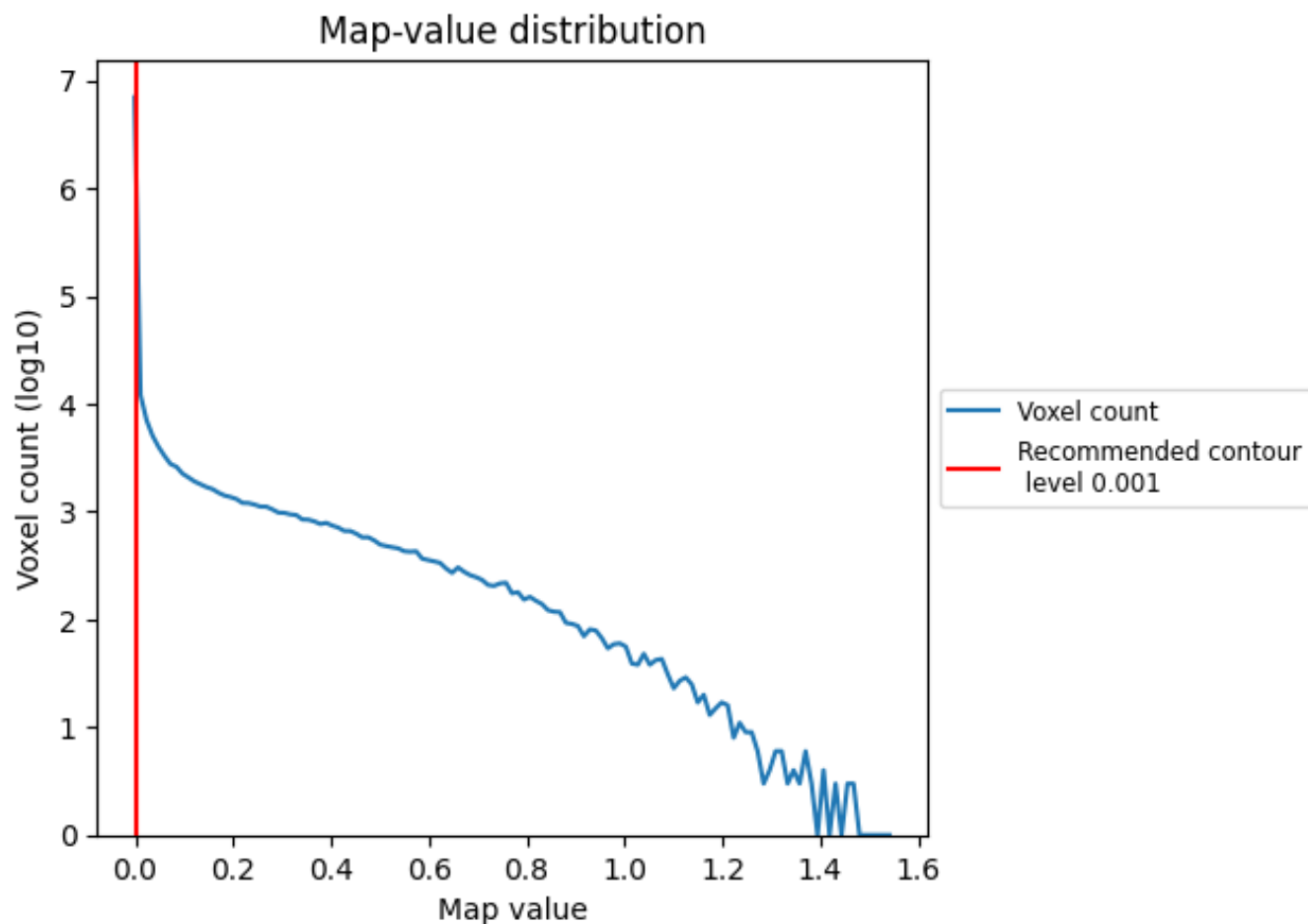
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

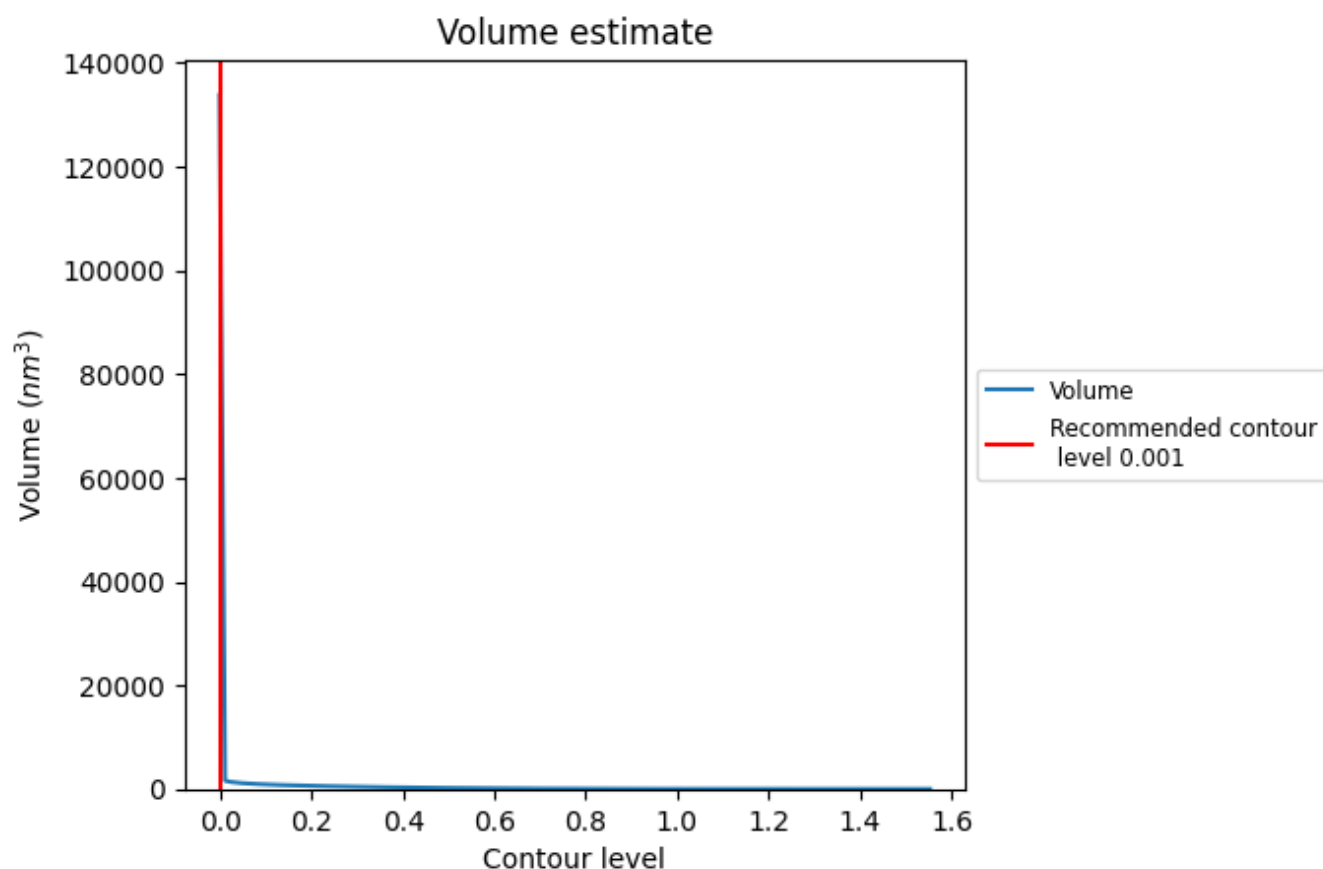
This section contains the results of statistical analysis of the map.

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.

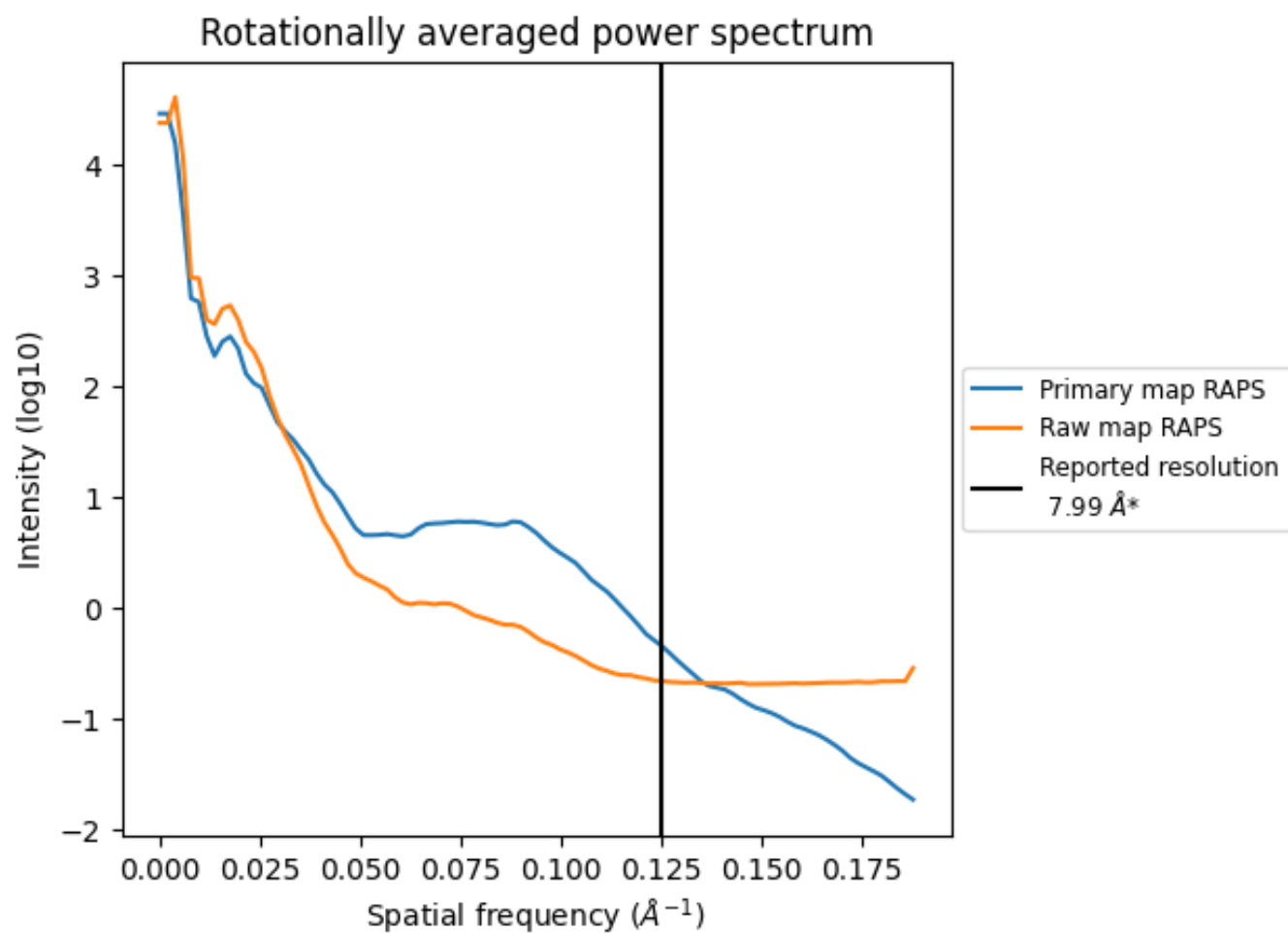
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 108238 nm^3 ; this corresponds to an approximate mass of 97774 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 ⓘ

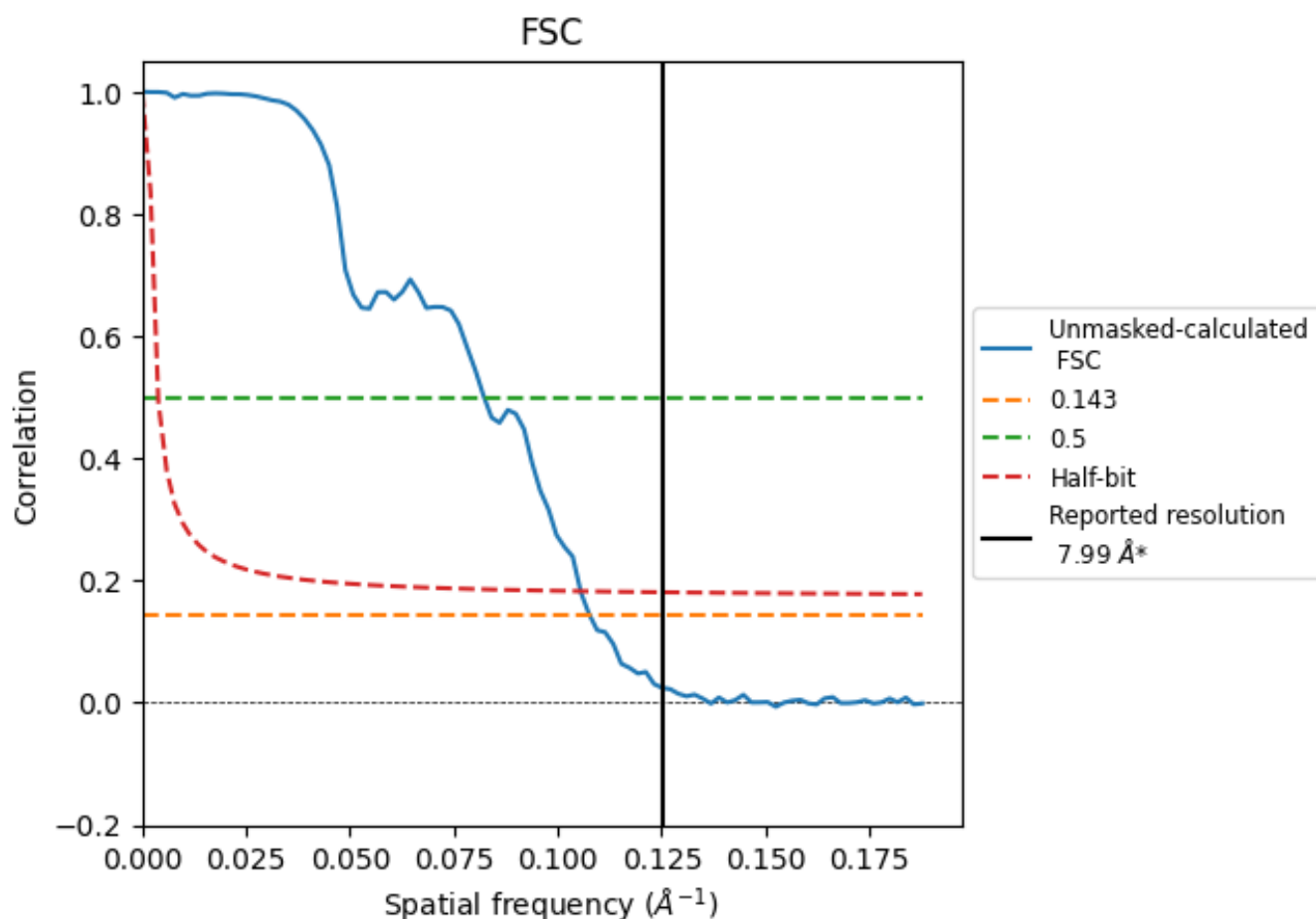


*Reported resolution corresponds to spatial frequency of 0.125 Å⁻¹

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 0.125 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

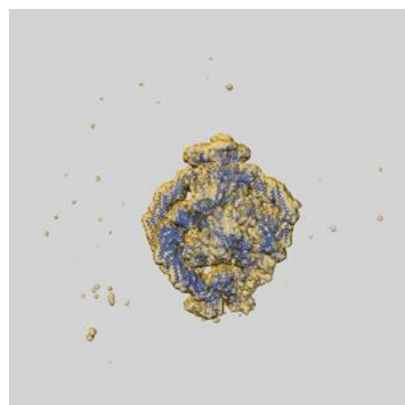
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.99	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.29	12.15	9.48

*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 9.29 differs from the reported value 7.99 by more than 10 %

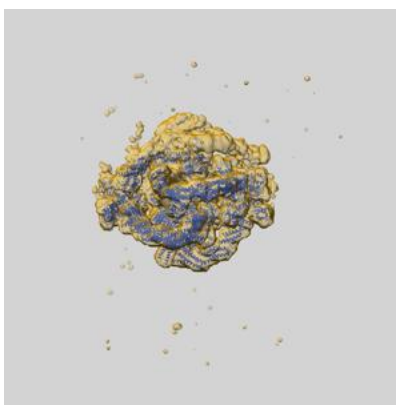
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34450 and PDB model 8H34. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

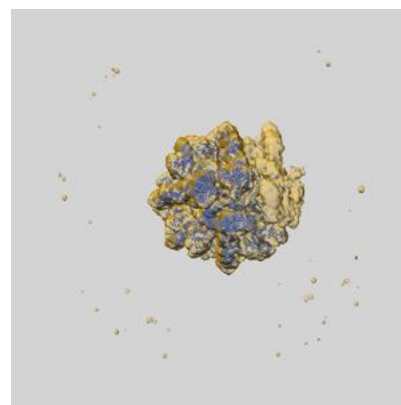
9.1 Map-model overlay [i](#)



X



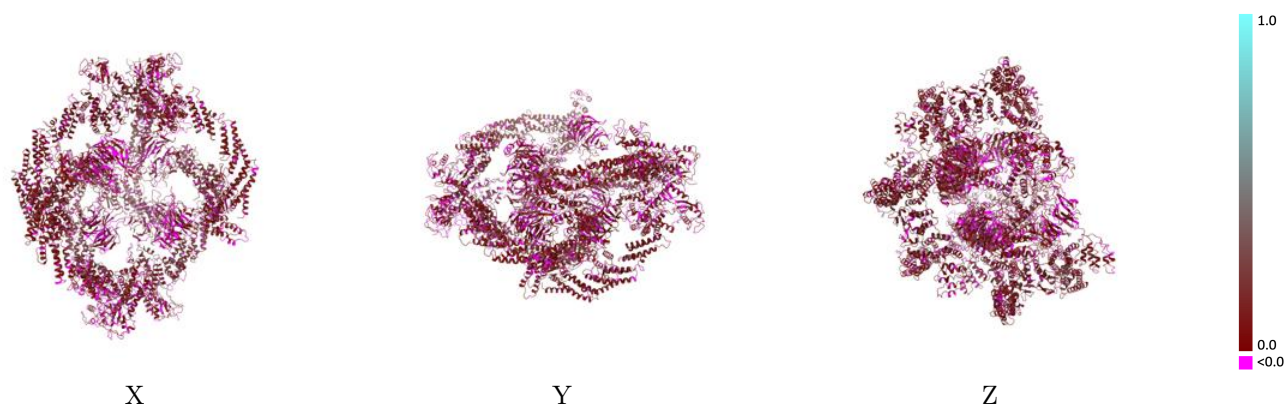
Y



Z

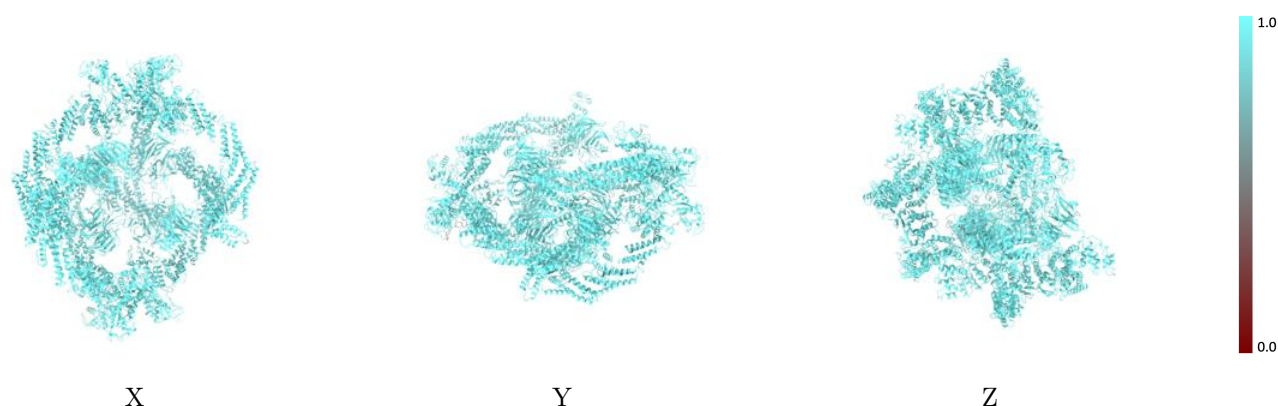
The images above show the 3D surface view of the map at the recommended contour level 0.001 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



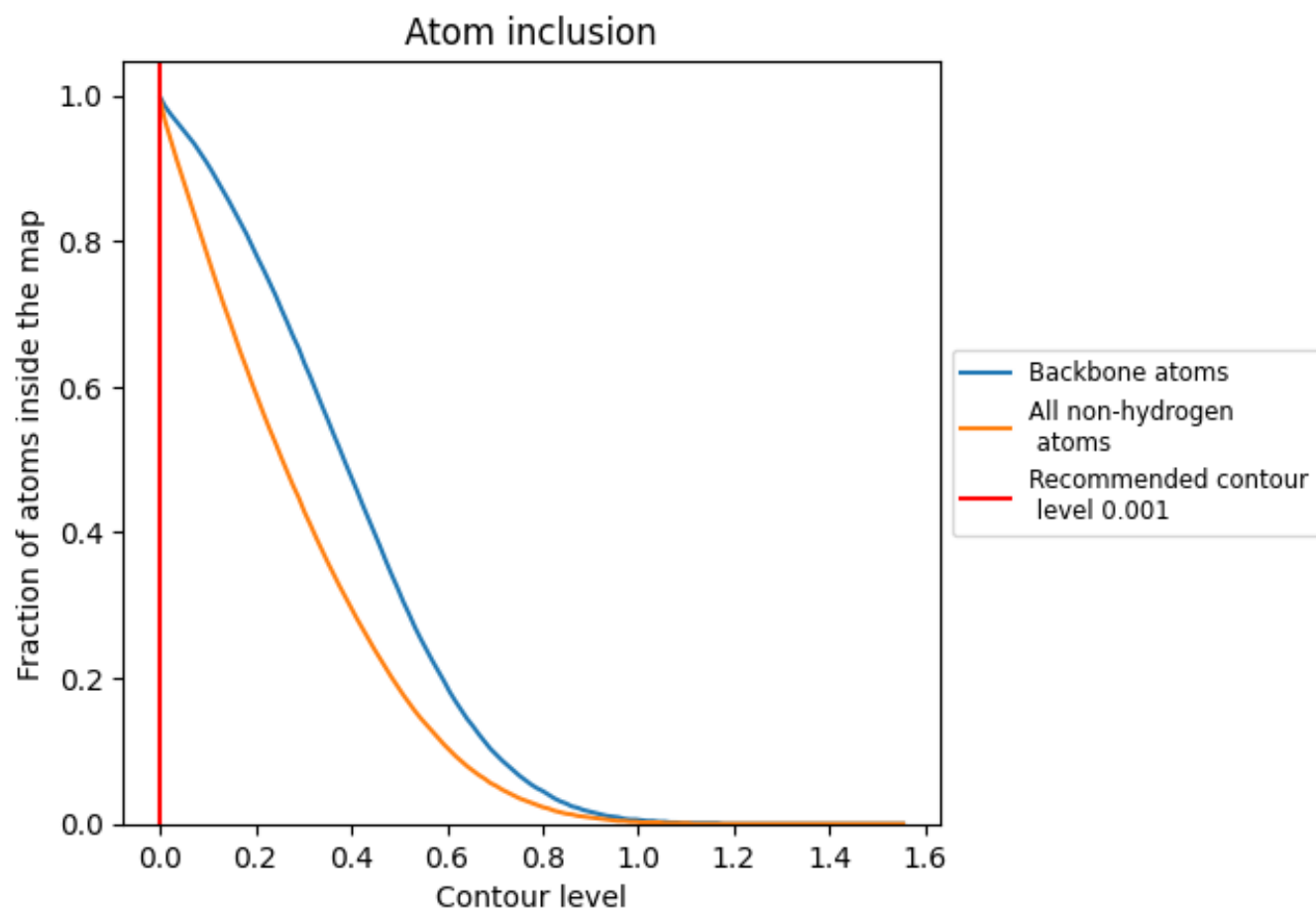
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.001).

9.4 Atom inclusion ⓘ



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	 0.9930	 0.0880
A	 0.9900	 0.0720
B	 0.9960	 0.0930
C	 0.9970	 0.1050
D	 0.9720	 0.0700
E	 0.9780	 0.0450
F	 0.9960	 0.0970
G	 0.9960	 0.0950
H	 0.9760	 0.0700
I	 0.9970	 0.0980
J	 0.9990	 0.0860
K	 0.9930	 0.0360
L	 0.9810	 0.0240
M	 0.9980	 0.1080
N	 0.9910	 0.0740
O	 0.9960	 0.1040
P	 0.9960	 0.0840
Q	 0.9750	 0.0460
R	 0.9520	 0.0540

