



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:29 AM UTC

PDB ID : 8H33 / pdb_00008h33
EMDB ID : EMD-34449
Title : Cryo-EM Structure of the KBTBD2-Cul3-Rbx1 tetrameric complex
Authors : Hu, Y.; Mao, Q.; Chen, Z.; Sun, L.
Deposited on : 2022-10-07
Resolution : 7.86 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

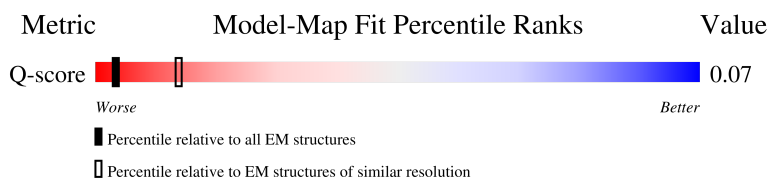
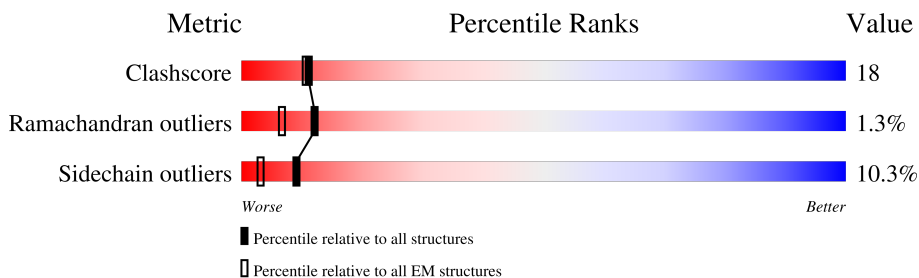
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.86 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.



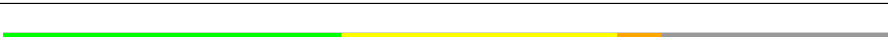
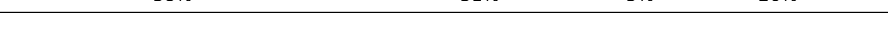
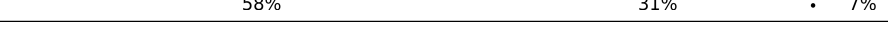
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	346 (7.39 - 8.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	623	
1	B	623	
1	G	623	
1	J	623	

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Mol	Chain	Length	Quality of chain
2	D	121	
2	E	121	
2	K	121	
2	L	121	
3	C	776	
3	F	776	
3	H	776	
3	I	776	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 43620 atoms, of which 72 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 Kelch repeat and BTB domain-containing protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	562	Total	C	H	N	O	S	0	0
			4473	2842	18	746	832	35		
1	B	557	Total	C	H	N	O	S	0	0
			4464	2839	18	737	834	36		
1	G	562	Total	C	H	N	O	S	0	0
			4438	2820	18	743	823	34		
1	J	555	Total	C	H	N	O	S	0	0
			4482	2855	18	740	832	37		

- Molecule 2 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	89	Total	C	N	O	S	0	0
			695	443	121	124	7		
2	K	89	Total	C	N	O	S	0	0
			737	466	135	127	9		
2	L	89	Total	C	N	O	S	0	0
			737	466	135	127	9		
2	E	89	Total	C	N	O	S	0	0
			737	466	135	127	9		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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
E	-12	HIS	-	expression tag	UNP P62877
E	-11	HIS	-	expression tag	UNP P62877
E	-10	HIS	-	expression tag	UNP P62877
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

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	GLY	-	expression tag	UNP P62877

- Molecule 3 is a protein called Cullin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	720	Total	C	N	O	S	0	0
			5651	3540	1003	1071	37		
3	H	720	Total	C	N	O	S	0	0
			5719	3589	1019	1073	38		
3	I	720	Total	C	N	O	S	0	0
			5722	3585	1013	1086	38		
3	C	720	Total	C	N	O	S	0	0
			5753	3613	1022	1081	37		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-7	TRP	-	expression tag	UNP Q13618
F	-6	SER	-	expression tag	UNP Q13618
F	-5	HIS	-	expression tag	UNP Q13618
F	-4	PRO	-	expression tag	UNP Q13618
F	-3	GLN	-	expression tag	UNP Q13618
F	-2	PHE	-	expression tag	UNP Q13618
F	-1	GLU	-	expression tag	UNP Q13618
F	0	LYS	-	expression tag	UNP Q13618
H	-7	TRP	-	expression tag	UNP Q13618
H	-6	SER	-	expression tag	UNP Q13618
H	-5	HIS	-	expression tag	UNP Q13618
H	-4	PRO	-	expression tag	UNP Q13618
H	-3	GLN	-	expression tag	UNP Q13618
H	-2	PHE	-	expression tag	UNP Q13618
H	-1	GLU	-	expression tag	UNP Q13618
H	0	LYS	-	expression tag	UNP Q13618
I	-7	TRP	-	expression tag	UNP Q13618
I	-6	SER	-	expression tag	UNP Q13618
I	-5	HIS	-	expression tag	UNP Q13618
I	-4	PRO	-	expression tag	UNP Q13618
I	-3	GLN	-	expression tag	UNP Q13618
I	-2	PHE	-	expression tag	UNP Q13618
I	-1	GLU	-	expression tag	UNP Q13618
I	0	LYS	-	expression tag	UNP Q13618
C	-7	TRP	-	expression tag	UNP Q13618

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	SER	-	expression tag	UNP Q13618
C	-5	HIS	-	expression tag	UNP Q13618
C	-4	PRO	-	expression tag	UNP Q13618
C	-3	GLN	-	expression tag	UNP Q13618
C	-2	PHE	-	expression tag	UNP Q13618
C	-1	GLU	-	expression tag	UNP Q13618
C	0	LYS	-	expression tag	UNP Q13618

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

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

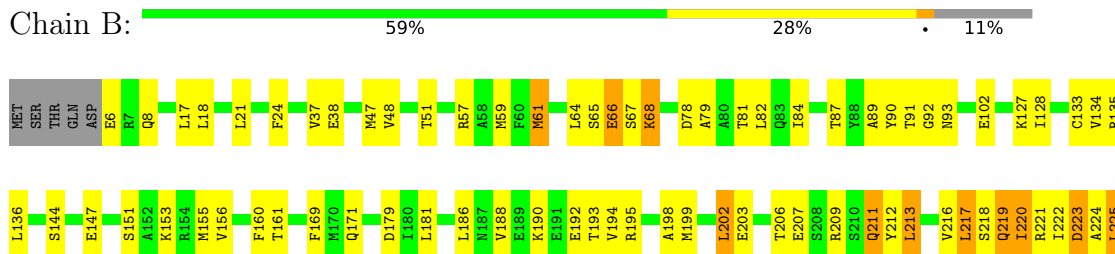
3 Residue-property plots

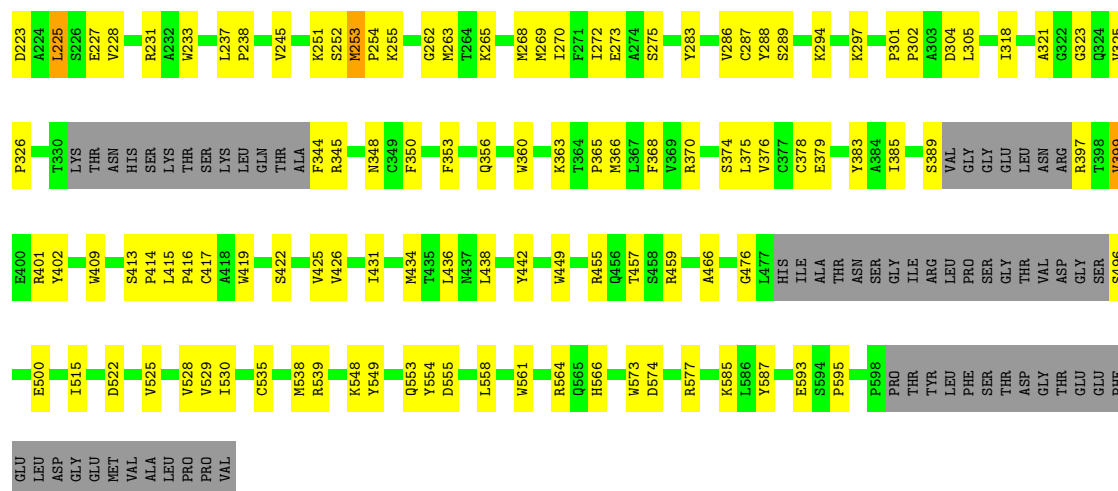
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Kelch repeat and BTB domain-containing protein 2



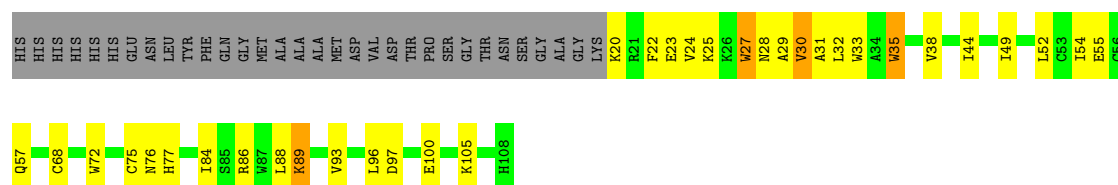
• Molecule 1: Kelch repeat and BTB domain-containing protein 2





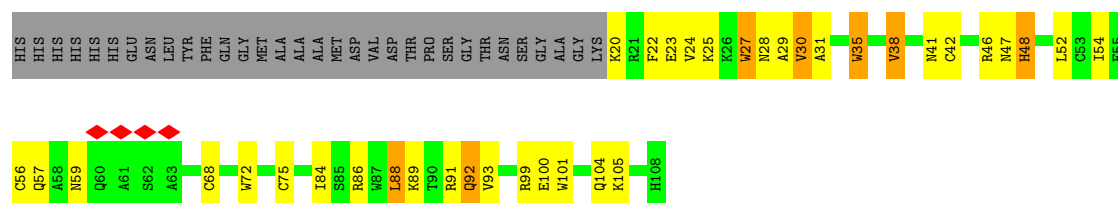
• Molecule 2: E3 ubiquitin-protein ligase RBX1

Chain D: 45% 25% 26%



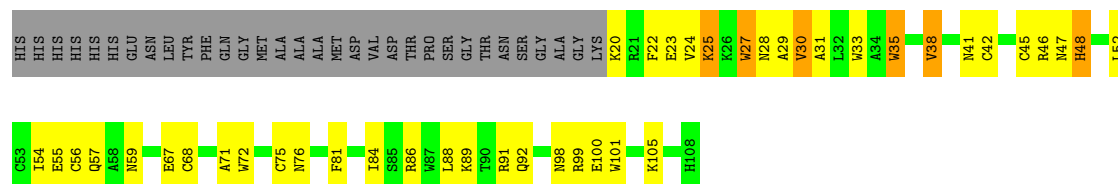
• Molecule 2: E3 ubiquitin-protein ligase RBX1

Chain K: 43% 25% 6% 26%



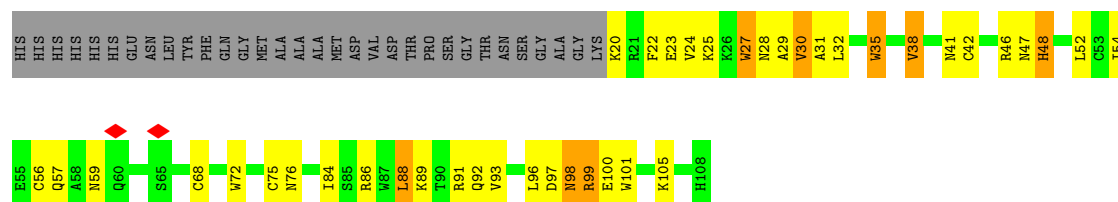
• Molecule 2: E3 ubiquitin-protein ligase RBX1

Chain L: 38% 31% 5% 26%



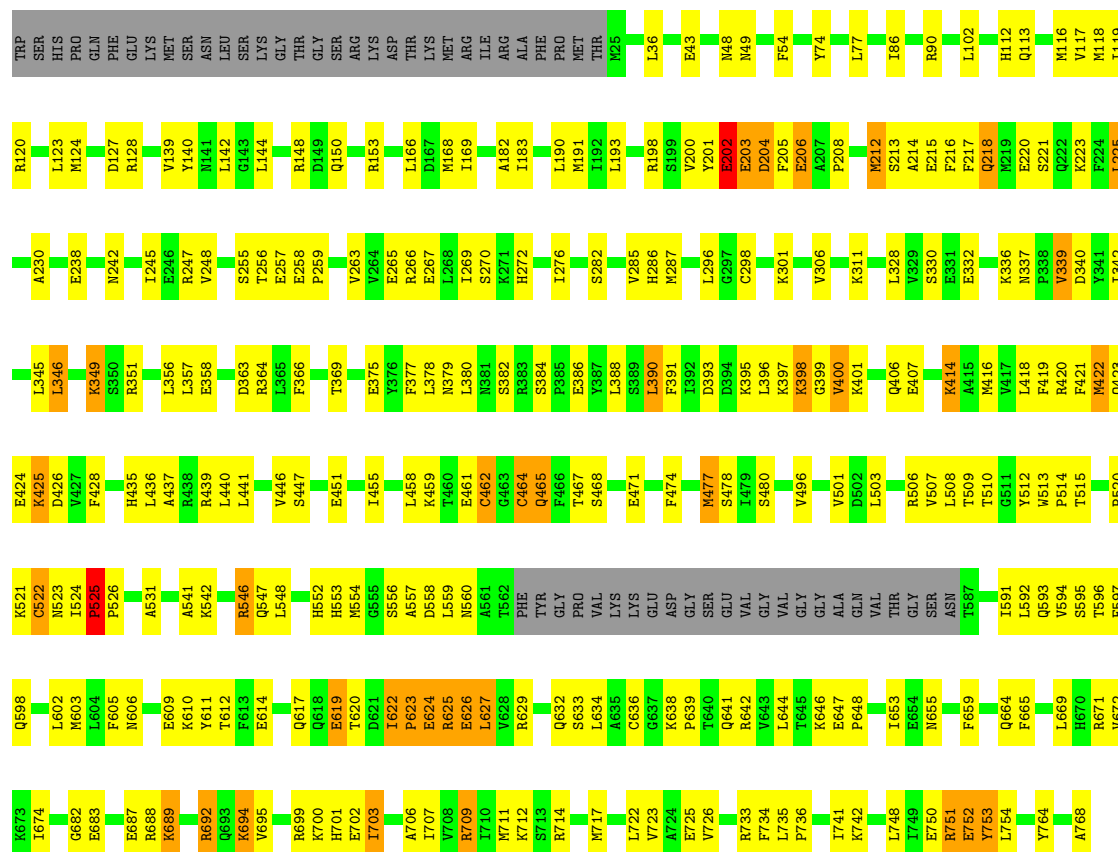
• Molecule 2: E3 ubiquitin-protein ligase RBX1

Chain E: 40% 27% 7% 26%



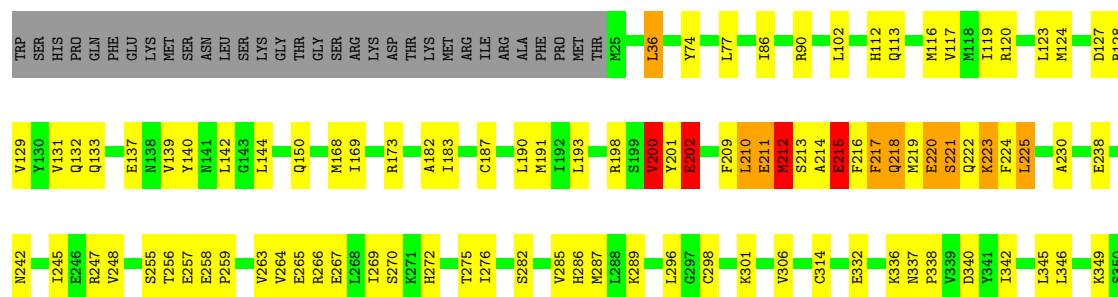
• Molecule 3: Cullin-3

Chain F: 57% 31% 5% 7%



• Molecule 3: Cullin-3

Chain H: 57% 31% 5% 7%





A768	E687	K610	E688	Y611	K542	R430	L345	E246	TRP
	R689	T612	K689	T612	H543	Q434	L346	R247	SER
	E690	F613	E691	S544	G435	Q435	R351	V248	HIS
	R692	E614	E692	G445	R546	L436	L356		GLN
	Q693	Q617	Q693	Q547	R546	R439			PHE
	K694	Q618	Q618		Q547	L440	F360	Y130	GLU
		E619	E619	H553	H553	L441		P259	LYS
	D697	T620	D697	M554	M554		T369		MET
	R699	D621	R699	S555	S555	V446		V263	ASN
	I622	I622	I622	A557	A557	S447	F374	V264	LEU
	K700	P623	K700	A557	A557		E375	E265	SER
	H701	E624	H701	D558	D558	E451	Y376	R266	LYS
	E702	R625	E702	L559	L559	K452	F377	E267	GLY
	I703	E626	I703	N560	N560	M453	L378	L268	THR
	E704	L627	E704	A561	A561	M454	N379	I269	GLY
	A705	V628	A705	T562	T562	I455	S270	K271	SER
	A706	R629	A706	PHE	PHE	S456	L380	G143	ARG
	I707		I707	TYR	TYR	K457	S382	H272	LYS
	V708	Q632	V708	GLY	GLY	K457	R383		ASP
	R709	S633	R709	PRO	PRO	K459	S384	I276	THR
	I710	L634	I710	VAL	VAL	K459	P385	Q150	LYS
	M711	A635	M711	LYS	LYS	F466	L388	S282	MET
	K712	G636	K712	LYS	LYS	T467	L388		ARG
	S713	G637	S713	GLU	GLU	S468	S389	V285	ILE
	R714	K638	R714	ASP	ASP	K469	L390	H286	ARG
		P639		GLY	GLY			M287	ALA
	M717	T640	M717	SER	SER	F474	D393	L288	PHE
		Q641		GLU	GLU		D394	K289	PRO
	L722	R642	L722	VAL	VAL	M477	K395	A182	MET
	V723	V643	V723	GLY	GLY			I183	THR
	A724	L644	A724	VAL	VAL	S480	K398	G297	K25
	E725	T645	E725	GLY	GLY		G399	C298	
	V726	K646	V726	GLY	GLY	L491	V400		L36
	E647	E647	E647	ALA	ALA		K401	K301	
	Q728	P648	Q728	GLN	GLN	L498	G402	V199	E43
	Q729		Q729	VAL	VAL		L403	V200	
	L730	I653	L730	THR	THR	R506	T404	Y201	K47
	K731	E654	K731	GLY	GLY	E607	E405	E202	
	A732	N655	A732	SER	SER		Q406	E203	
	R733	F659	R733	ASN	ASN				Y58
	F734		F734			T510	I411	A207	
	L735	Q664	L735	T587	T587	T510	L412	P208	
		F665				G511	L328		
	K742	Q664	K742	I591	I591	Y512	V329	L77	
	R743	F665	R743	L592	L592	M513	S330	E215	
	R744	L669	R744	Q593	Q593	F514	A415		I86
		H670		V594	V594	T515	M416	E332	
	L748	R671	L748	S595	S595	Q616	V417	G333	
	I749	V672	I749	R671	R671	S517	L418	F224	
	E750		E750	F597	F597		E419	A226	
	R751	A679	R751	Q698	Q698	K521	R420	E227	L102
	Y753	K680	Y753	L602	L602	C522	F421		H112
	L754	Q681	L754	M603	M603	I524	M422	A230	
		G682		L604	L604	P525	Q423		Q113
	T757	E683	T757	F605	F605	P526	E424	E238	
		S684		N606	N606		K425	Y341	M16
	V767	D685	V767	E609	E609	A527	F428	I342	
		P686				R529	E429	G344	
									R120

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50236	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	1.590	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.0001	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	A	0.50	0/4558	0.64	0/6191
1	B	0.51	0/4548	0.66	2/6172 (0.0%)
1	G	0.58	1/4521 (0.0%)	0.71	0/6146
1	J	0.51	0/4569	0.66	3/6201 (0.0%)
2	D	0.90	1/715 (0.1%)	1.09	1/973 (0.1%)
2	E	0.87	2/759 (0.3%)	1.01	1/1029 (0.1%)
2	K	0.82	1/759 (0.1%)	1.00	1/1029 (0.1%)
2	L	0.84	1/759 (0.1%)	1.01	1/1029 (0.1%)
3	C	0.58	0/5840	0.80	7/7853 (0.1%)
3	F	0.63	1/5728 (0.0%)	0.82	5/7706 (0.1%)
3	H	0.55	0/5806	0.76	10/7810 (0.1%)
3	I	0.64	0/5802	0.85	4/7804 (0.1%)
All	All	0.59	7/44364 (0.0%)	0.77	35/59943 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	96	LEU	C-N	7.00	1.43	1.33
1	G	223	ASP	C-O	6.27	1.31	1.24
2	K	30	VAL	CA-CB	-5.70	1.47	1.54
2	L	30	VAL	CA-CB	-5.69	1.47	1.54
2	D	30	VAL	CA-CB	-5.63	1.47	1.54
2	E	30	VAL	CA-CB	-5.62	1.47	1.54
3	F	202	GLU	C-O	-5.32	1.17	1.24

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	343	GLN	N-CA-C	-10.64	99.47	111.71
3	F	626	GLU	N-CA-C	-8.63	101.36	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	626	GLU	N-CA-C	-8.57	101.43	112.23
3	I	627	LEU	N-CA-C	-8.34	102.14	111.07
3	F	627	LEU	N-CA-C	-8.29	102.20	111.07
3	F	633	SER	N-CA-C	-6.63	104.08	111.71
3	I	633	SER	N-CA-C	-6.56	104.16	111.71
3	H	633	SER	N-CA-C	-6.54	104.19	111.71
3	C	633	SER	N-CA-C	-6.52	104.22	111.71
2	K	27	TRP	O-C-N	-6.48	116.00	123.33
2	D	27	TRP	O-C-N	-6.45	116.04	123.33
2	E	27	TRP	O-C-N	-6.42	116.08	123.33
3	H	210	LEU	N-CA-C	-6.39	103.83	111.69
2	L	27	TRP	O-C-N	-6.30	116.21	123.33
3	H	525	PRO	N-CA-C	6.02	118.04	110.70
1	B	279	PRO	N-CA-C	6.01	124.84	112.47
3	C	420	ARG	CB-CA-C	-5.82	101.13	110.79
3	C	377	PHE	CA-CB-CG	5.61	119.41	113.80
1	J	191	GLU	N-CA-C	-5.42	106.50	113.23
3	F	525	PRO	N-CA-C	5.41	117.31	110.70
3	H	211	GLU	N-CA-C	-5.35	105.53	111.36
3	H	221	SER	CA-C-N	-5.28	113.15	120.38
3	H	221	SER	C-N-CA	-5.28	113.15	120.38
3	C	730	LEU	N-CA-C	-5.27	108.11	114.75
3	H	217	PHE	CA-C-O	-5.24	115.50	120.90
3	H	383	ARG	N-CA-C	-5.24	106.14	112.54
3	I	46	ARG	N-CA-C	-5.21	107.09	112.93
3	H	225	LEU	N-CA-C	-5.19	105.05	111.33
1	J	162	ALA	N-CA-C	-5.17	106.78	114.64
1	B	203	GLU	N-CA-C	-5.13	107.40	113.97
3	C	456	SER	N-CA-C	-5.10	105.71	112.34
3	F	221	SER	N-CA-C	-5.07	105.44	110.97
1	J	211	GLN	N-CA-C	-5.07	105.41	112.45
3	C	491	LEU	N-CA-C	-5.06	105.95	111.82
3	H	212	MET	N-CA-C	-5.01	105.71	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4455	18	4288	148	0
1	B	4446	18	4306	173	0
1	G	4420	18	4240	153	0
1	J	4464	18	4343	149	0
2	D	695	0	608	43	0
2	E	737	0	686	57	0
2	K	737	0	686	52	0
2	L	737	0	686	58	0
3	C	5753	0	5709	201	0
3	F	5651	0	5542	208	0
3	H	5719	0	5634	233	0
3	I	5722	0	5664	194	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
All	All	43548	72	42392	1566	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 18.

All (1566) 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:G:47:MET:CE	1:J:21:LEU:HD22	1.45	1.44
2:K:24:VAL:C	2:K:25:LYS:HE2	1.43	1.43
2:D:24:VAL:C	2:D:25:LYS:HE2	1.43	1.42
2:L:24:VAL:C	2:L:25:LYS:HE2	1.43	1.40
2:E:24:VAL:C	2:E:25:LYS:HE2	1.43	1.40
3:I:665:PHE:HD1	3:I:665:PHE:O	1.07	1.31
3:F:665:PHE:HD1	3:F:665:PHE:O	1.07	1.29
3:H:665:PHE:HD1	3:H:665:PHE:O	1.07	1.29
3:C:730:LEU:HD13	3:C:733:ARG:NH2	1.43	1.29
3:C:665:PHE:HD1	3:C:665:PHE:O	1.07	1.27
3:I:665:PHE:O	3:I:665:PHE:CD1	1.89	1.25
3:C:665:PHE:O	3:C:665:PHE:CD1	1.89	1.25
3:F:665:PHE:O	3:F:665:PHE:CD1	1.89	1.25
3:H:665:PHE:O	3:H:665:PHE:CD1	1.89	1.25
1:G:47:MET:HE2	1:J:21:LEU:CD2	1.65	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:97:ASP:OD2	2:E:99:ARG:HG2	1.37	1.21
1:B:160:PHE:CE2	1:B:169:PHE:CE1	2.30	1.20
2:K:25:LYS:HE2	2:K:25:LYS:N	1.58	1.18
2:L:25:LYS:HE2	2:L:25:LYS:N	1.58	1.16
2:E:25:LYS:HE2	2:E:25:LYS:N	1.58	1.15
2:D:25:LYS:HE2	2:D:25:LYS:N	1.58	1.15
3:F:626:GLU:HA	3:F:629:ARG:HD2	1.25	1.13
3:I:626:GLU:HA	3:I:629:ARG:HD2	1.25	1.13
3:H:638:LYS:HD3	3:H:639:PRO:HD2	1.30	1.12
3:I:638:LYS:HD3	3:I:639:PRO:HD2	1.29	1.12
3:F:638:LYS:HD3	3:F:639:PRO:HD2	1.29	1.11
3:C:638:LYS:HD3	3:C:639:PRO:HD2	1.29	1.09
1:A:47:MET:HE2	1:B:21:LEU:HD22	1.29	1.08
3:I:455:ILE:HG22	3:I:470:LEU:HD21	1.34	1.08
3:H:346:LEU:HA	3:H:418:LEU:HD12	1.34	1.07
1:B:65:SER:HA	1:B:68:LYS:HZ1	1.19	1.07
3:H:455:ILE:HG22	3:H:470:LEU:HD21	1.34	1.06
1:B:65:SER:CA	1:B:68:LYS:HZ1	1.67	1.06
3:C:730:LEU:CD1	3:C:733:ARG:NH2	2.20	1.05
1:G:47:MET:HG2	1:J:21:LEU:CD2	1.87	1.04
3:H:470:LEU:HD11	3:H:474:PHE:CE2	1.93	1.04
3:I:470:LEU:HD11	3:I:474:PHE:CE2	1.93	1.03
1:G:47:MET:SD	1:J:21:LEU:HD22	1.97	1.03
2:K:28:ASN:OD1	2:K:28:ASN:O	1.76	1.02
2:L:24:VAL:C	2:L:25:LYS:CE	2.32	1.02
2:K:24:VAL:C	2:K:25:LYS:CE	2.32	1.02
1:G:47:MET:HG2	1:J:21:LEU:HD21	1.42	1.02
1:G:233:TRP:CH2	1:G:245:VAL:HA	1.95	1.02
2:D:24:VAL:C	2:D:25:LYS:CE	2.32	1.02
1:B:233:TRP:CH2	1:B:245:VAL:HA	1.95	1.02
2:L:28:ASN:OD1	2:L:28:ASN:O	1.76	1.02
2:E:24:VAL:C	2:E:25:LYS:CE	2.32	1.01
2:E:28:ASN:OD1	2:E:28:ASN:O	1.76	1.01
2:D:28:ASN:OD1	2:D:28:ASN:O	1.76	1.01
3:F:441:LEU:HB3	3:F:554:MET:SD	2.01	1.00
1:J:233:TRP:CH2	1:J:245:VAL:HA	1.95	1.00
3:H:560:ASN:HB2	2:K:25:LYS:HG2	1.43	1.00
3:I:560:ASN:HB2	2:L:25:LYS:HG2	1.43	1.00
2:D:25:LYS:HG2	3:F:560:ASN:HB2	1.43	0.99
1:A:21:LEU:HD22	1:B:47:MET:HE2	1.45	0.99
1:B:233:TRP:HH2	1:B:245:VAL:HA	1.26	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:233:TRP:HH2	1:J:245:VAL:HA	1.26	0.99
1:G:379:GLU:HG3	1:G:379:GLU:O	1.63	0.99
1:G:233:TRP:HH2	1:G:245:VAL:HA	1.26	0.98
1:B:233:TRP:HH2	1:B:245:VAL:CA	1.76	0.98
3:C:560:ASN:HB2	2:E:25:LYS:HG2	1.43	0.98
1:J:233:TRP:HH2	1:J:245:VAL:CA	1.76	0.97
1:B:379:GLU:HG3	1:B:379:GLU:O	1.63	0.97
1:G:233:TRP:HH2	1:G:245:VAL:CA	1.76	0.97
1:J:379:GLU:O	1:J:379:GLU:HG3	1.63	0.96
3:H:248:VAL:HG22	3:H:256:THR:HG23	1.46	0.96
3:I:263:VAL:HG22	3:I:267:GLU:OE2	1.66	0.96
1:A:190:LYS:HB2	1:A:192:GLU:OE2	1.65	0.96
1:B:65:SER:HA	1:B:68:LYS:NZ	1.81	0.96
1:B:160:PHE:CE2	1:B:169:PHE:CZ	2.53	0.96
3:I:524:ILE:HG12	3:I:525:PRO:HD2	1.46	0.96
2:L:23:GLU:O	2:L:25:LYS:HE3	1.65	0.96
2:E:23:GLU:O	2:E:25:LYS:HE3	1.65	0.95
1:J:233:TRP:CH2	1:J:245:VAL:HG22	2.02	0.95
3:C:451:GLU:HB3	3:C:474:PHE:CZ	2.02	0.95
3:F:263:VAL:HG22	3:F:267:GLU:OE2	1.65	0.95
2:K:23:GLU:O	2:K:25:LYS:HE3	1.65	0.95
3:C:263:VAL:HG22	3:C:267:GLU:OE2	1.66	0.95
1:B:190:LYS:HB2	1:B:192:GLU:OE2	1.65	0.95
3:F:248:VAL:HG22	3:F:256:THR:HG23	1.46	0.95
2:D:23:GLU:O	2:D:25:LYS:HE3	1.65	0.95
1:B:233:TRP:CH2	1:B:245:VAL:HG22	2.02	0.94
1:A:379:GLU:O	1:A:379:GLU:HG3	1.63	0.94
1:G:110:PHE:O	3:I:125:TYR:CE1	2.20	0.94
3:H:263:VAL:HG22	3:H:267:GLU:OE2	1.66	0.94
3:C:248:VAL:HG22	3:C:256:THR:HG23	1.46	0.94
1:G:233:TRP:CH2	1:G:245:VAL:HG22	2.02	0.93
3:C:730:LEU:HD13	3:C:733:ARG:CZ	1.97	0.92
1:A:370:ARG:HG2	1:A:389:SER:HA	1.51	0.91
3:H:225:LEU:HD11	3:H:275:THR:HG21	1.48	0.91
2:L:72:TRP:HB2	2:L:105:LYS:HB3	1.52	0.90
1:A:51:THR:HG21	1:B:17:LEU:CD1	2.01	0.90
3:I:455:ILE:HG22	3:I:470:LEU:CD2	2.01	0.90
3:I:524:ILE:HG12	3:I:525:PRO:CD	2.02	0.90
2:K:72:TRP:HB2	2:K:105:LYS:HB3	1.52	0.90
1:G:151:SER:O	1:G:155:MET:HG2	1.71	0.89
3:F:735:LEU:HD13	3:F:736:PRO:HD2	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:LEU:HD22	1:G:219:GLN:HB3	1.54	0.89
3:C:506:ARG:HB2	2:E:30:VAL:HG22	1.55	0.89
1:A:151:SER:O	1:A:155:MET:HG2	1.71	0.89
1:G:47:MET:CG	1:J:21:LEU:CD2	2.50	0.89
3:H:455:ILE:HG22	3:H:470:LEU:CD2	2.01	0.89
1:B:151:SER:O	1:B:155:MET:HG2	1.71	0.89
2:E:72:TRP:HB2	2:E:105:LYS:HB3	1.52	0.89
2:D:72:TRP:HB2	2:D:105:LYS:HB3	1.53	0.89
3:H:506:ARG:HB2	2:K:30:VAL:HG22	1.55	0.88
2:D:30:VAL:HG22	3:F:506:ARG:HB2	1.55	0.88
1:G:47:MET:HE2	1:J:21:LEU:HD22	0.90	0.88
3:H:735:LEU:HD13	3:H:736:PRO:HD2	1.54	0.87
1:B:233:TRP:NE1	1:B:237:LEU:HB3	1.89	0.87
3:I:506:ARG:HB2	2:L:30:VAL:HG22	1.55	0.87
2:E:97:ASP:OD2	2:E:99:ARG:CG	2.22	0.87
1:J:233:TRP:NE1	1:J:237:LEU:HB3	1.90	0.86
1:G:233:TRP:NE1	1:G:237:LEU:HB3	1.89	0.86
3:H:346:LEU:HD13	3:H:418:LEU:HB2	1.57	0.86
1:B:160:PHE:CE2	1:B:169:PHE:CD1	2.63	0.86
3:C:730:LEU:HD13	3:C:733:ARG:HH22	1.35	0.86
1:J:161:THR:HB	1:J:188:VAL:HG13	1.59	0.85
1:B:65:SER:CA	1:B:68:LYS:NZ	2.37	0.85
3:C:413:ASP:HA	3:C:457:LYS:HE2	1.58	0.85
1:A:161:THR:HB	1:A:188:VAL:HG13	1.59	0.85
3:I:198:ARG:HH21	3:I:202:GLU:HG3	1.40	0.85
1:B:160:PHE:CZ	1:B:169:PHE:CZ	2.65	0.84
3:H:346:LEU:HD11	3:H:414:LYS:O	1.75	0.84
1:B:161:THR:HB	1:B:188:VAL:HG13	1.59	0.84
3:C:248:VAL:HG22	3:C:256:THR:CG2	2.08	0.84
3:C:669:LEU:HG	3:C:671:ARG:H	1.43	0.83
3:F:669:LEU:HG	3:F:671:ARG:H	1.43	0.83
3:F:248:VAL:HG22	3:F:256:THR:CG2	2.08	0.83
3:I:127:ASP:O	3:I:131:VAL:HG22	1.79	0.83
2:K:41:ASN:HD21	2:K:46:ARG:CD	1.92	0.83
3:C:751:ARG:NH2	3:C:753:TYR:HD1	1.76	0.83
1:A:24:PHE:HZ	1:B:57:ARG:HH22	1.26	0.82
3:I:669:LEU:HG	3:I:671:ARG:H	1.43	0.82
3:C:127:ASP:O	3:C:131:VAL:HG22	1.79	0.82
3:H:248:VAL:HG22	3:H:256:THR:CG2	2.08	0.82
3:H:669:LEU:HG	3:H:671:ARG:H	1.42	0.82
2:L:41:ASN:HD21	2:L:46:ARG:CD	1.92	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:41:ASN:HD21	2:E:46:ARG:CD	1.92	0.81
1:G:21:LEU:HD22	1:J:47:MET:HE2	1.60	0.81
3:H:346:LEU:HB2	3:H:418:LEU:HD13	1.63	0.81
1:J:190:LYS:HG3	1:J:193:THR:HG22	1.61	0.81
3:H:127:ASP:O	3:H:131:VAL:HG22	1.79	0.81
3:H:346:LEU:CA	3:H:418:LEU:HD12	2.11	0.81
3:F:503:LEU:HD21	3:F:531:ALA:HB1	1.62	0.80
1:J:397:ARG:HD2	1:J:417:CYS:HA	1.63	0.80
1:B:262:GLY:O	1:B:265:LYS:HG2	1.82	0.80
1:J:262:GLY:O	1:J:265:LYS:HG2	1.82	0.80
3:H:346:LEU:HA	3:H:418:LEU:CD1	2.10	0.80
1:A:262:GLY:O	1:A:265:LYS:HG2	1.82	0.79
2:D:28:ASN:O	2:D:28:ASN:CG	2.25	0.79
1:B:64:LEU:O	1:B:68:LYS:CE	2.30	0.79
1:B:202:LEU:HD22	1:B:213:LEU:HA	1.65	0.79
1:B:160:PHE:HE2	1:B:169:PHE:CE1	1.95	0.79
1:G:262:GLY:O	1:G:265:LYS:HG2	1.82	0.79
3:H:225:LEU:HD11	3:H:275:THR:CG2	2.10	0.79
2:K:28:ASN:O	2:K:28:ASN:CG	2.25	0.79
1:A:17:LEU:CD1	1:B:51:THR:HG21	2.12	0.78
3:C:526:PRO:HA	3:C:529:ARG:HB2	1.65	0.78
1:A:181:LEU:HD22	1:A:219:GLN:HB3	1.65	0.78
1:B:160:PHE:HE2	1:B:169:PHE:CD1	2.02	0.78
3:H:346:LEU:CA	3:H:418:LEU:CD1	2.61	0.78
2:E:28:ASN:O	2:E:28:ASN:CG	2.25	0.78
1:G:390:VAL:HG12	1:G:393:GLU:HG3	1.66	0.78
1:J:397:ARG:HG3	1:J:415:LEU:O	1.84	0.78
3:H:526:PRO:HA	3:H:529:ARG:HB2	1.65	0.77
1:G:47:MET:SD	1:J:21:LEU:CD2	2.71	0.77
2:K:23:GLU:HB3	2:K:25:LYS:HZ1	1.48	0.77
3:F:541:ALA:HB2	3:H:501:VAL:O	1.84	0.77
3:C:751:ARG:HH21	3:C:753:TYR:HD1	1.33	0.77
3:F:440:LEU:HB2	3:F:513:TRP:CZ3	2.19	0.77
1:B:390:VAL:HG12	1:B:393:GLU:HG3	1.66	0.76
3:C:451:GLU:CB	3:C:474:PHE:CZ	2.67	0.76
1:A:51:THR:HG21	1:B:17:LEU:HD11	1.67	0.76
1:G:110:PHE:O	3:I:125:TYR:HE1	1.68	0.76
3:F:225:LEU:HB2	3:F:272:HIS:CE1	2.20	0.76
1:J:397:ARG:HD2	1:J:416:PRO:O	1.86	0.76
2:E:23:GLU:HB3	2:E:25:LYS:HZ1	1.49	0.75
3:F:120:ARG:HG3	3:F:140:TYR:HB2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:458:LEU:HB3	3:H:467:THR:HG22	1.69	0.75
3:I:437:ALA:HA	3:I:513:TRP:HZ3	1.51	0.75
3:F:754:LEU:HD11	3:F:764:TYR:HB3	1.68	0.75
1:B:65:SER:C	1:B:68:LYS:NZ	2.44	0.75
1:G:58:ALA:HB1	3:I:121:ASP:HB3	1.69	0.75
3:F:440:LEU:HB2	3:F:513:TRP:HZ3	1.51	0.75
2:K:46:ARG:CZ	2:K:46:ARG:O	2.35	0.74
3:I:509:THR:HB	3:I:512:TYR:HD2	1.51	0.74
3:C:480:SER:HB2	3:C:506:ARG:HE	1.52	0.74
3:H:124:MET:HA	3:H:127:ASP:HB2	1.70	0.74
2:L:46:ARG:O	2:L:46:ARG:CZ	2.35	0.74
3:F:509:THR:HB	3:F:512:TYR:HD2	1.53	0.74
3:C:124:MET:HA	3:C:127:ASP:HB2	1.70	0.74
3:H:480:SER:HB2	3:H:506:ARG:HE	1.52	0.74
1:J:397:ARG:HB2	1:J:415:LEU:HB2	1.69	0.74
3:F:441:LEU:HD13	3:F:554:MET:HE3	1.69	0.74
3:I:124:MET:HA	3:I:127:ASP:HB2	1.70	0.74
3:C:393:ASP:HA	3:C:439:ARG:HH21	1.52	0.74
3:H:120:ARG:HG3	3:H:140:TYR:HB2	1.68	0.74
3:C:416:MET:SD	3:C:457:LYS:HE3	2.28	0.74
2:E:46:ARG:CZ	2:E:46:ARG:O	2.35	0.74
3:C:451:GLU:HG2	3:C:474:PHE:HZ	1.53	0.74
3:I:470:LEU:HD11	3:I:474:PHE:HE2	1.51	0.74
3:I:120:ARG:HG3	3:I:140:TYR:HB2	1.68	0.73
1:J:397:ARG:HD2	1:J:417:CYS:CA	2.17	0.73
3:I:458:LEU:HB3	3:I:467:THR:HG22	1.69	0.73
1:A:181:LEU:HD21	1:A:220:ILE:HD13	1.70	0.73
1:G:47:MET:CE	1:J:21:LEU:CD2	2.40	0.73
3:F:124:MET:HA	3:F:127:ASP:HB2	1.70	0.73
2:L:28:ASN:O	2:L:28:ASN:CG	2.25	0.72
3:C:120:ARG:HG3	3:C:140:TYR:HB2	1.68	0.72
2:L:41:ASN:HD21	2:L:46:ARG:HD3	1.54	0.72
1:J:228:VAL:O	1:J:228:VAL:HG22	1.87	0.72
3:H:342:ILE:HG13	3:H:388:LEU:HA	1.71	0.72
3:C:245:ILE:HA	3:C:248:VAL:HG12	1.72	0.72
2:K:41:ASN:HD21	2:K:46:ARG:HD3	1.54	0.72
3:I:480:SER:HB2	3:I:506:ARG:HE	1.52	0.72
1:G:202:LEU:HD22	1:G:213:LEU:HA	1.71	0.72
1:G:273:GLU:HA	1:G:283:TYR:HB3	1.72	0.72
2:D:23:GLU:HB3	2:D:25:LYS:HZ1	1.55	0.72
3:H:470:LEU:HD11	3:H:474:PHE:HE2	1.51	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:47:MET:HE2	1:J:21:LEU:CG	2.20	0.71
3:F:245:ILE:HA	3:F:248:VAL:HG12	1.72	0.71
3:H:346:LEU:CD1	3:H:418:LEU:HB2	2.19	0.71
1:J:221:ARG:HA	1:J:255:LYS:HE2	1.72	0.71
3:C:638:LYS:HD3	3:C:639:PRO:CD	2.16	0.71
2:E:41:ASN:HD21	2:E:46:ARG:HD3	1.54	0.71
1:G:233:TRP:CD1	1:G:237:LEU:HB3	2.26	0.70
2:L:23:GLU:HB3	2:L:25:LYS:HZ1	1.56	0.70
2:L:24:VAL:O	2:L:25:LYS:HE2	1.91	0.70
1:B:233:TRP:CH2	1:B:245:VAL:CG2	2.74	0.70
1:J:233:TRP:CH2	1:J:245:VAL:CG2	2.74	0.70
3:H:389:SER:HB2	3:H:431:TYR:HB3	1.73	0.70
1:B:233:TRP:CD1	1:B:237:LEU:HB3	2.26	0.70
3:I:638:LYS:HD3	3:I:639:PRO:CD	2.16	0.70
2:E:24:VAL:O	2:E:25:LYS:HE2	1.91	0.70
3:H:245:ILE:HA	3:H:248:VAL:HG12	1.72	0.70
3:F:638:LYS:HD3	3:F:639:PRO:CD	2.16	0.69
1:B:379:GLU:O	1:B:379:GLU:CG	2.40	0.69
1:G:47:MET:CG	1:J:21:LEU:HD22	2.20	0.69
1:J:233:TRP:CD1	1:J:237:LEU:HB3	2.26	0.69
3:H:638:LYS:HD3	3:H:639:PRO:CD	2.16	0.69
3:H:425:LYS:NZ	3:H:462:CYS:SG	2.64	0.69
3:H:735:LEU:CD1	3:H:736:PRO:HD2	2.22	0.69
3:F:166:LEU:HD22	3:F:212:MET:HG3	1.73	0.69
3:F:735:LEU:CD1	3:F:736:PRO:HD2	2.22	0.69
3:H:123:LEU:HB3	3:H:139:VAL:HG11	1.75	0.69
3:C:198:ARG:HH21	3:C:202:GLU:HG3	1.57	0.69
3:I:425:LYS:NZ	3:I:462:CYS:SG	2.64	0.69
3:C:123:LEU:HB3	3:C:139:VAL:HG11	1.75	0.69
2:K:47:ASN:HD21	2:K:54:ILE:HG23	1.58	0.69
1:A:17:LEU:HD11	1:B:51:THR:HG21	1.75	0.68
3:C:751:ARG:NH2	3:C:753:TYR:CD1	2.59	0.68
3:I:470:LEU:HD12	3:I:470:LEU:O	1.94	0.68
3:I:665:PHE:HD1	3:I:665:PHE:C	1.98	0.68
1:G:233:TRP:CH2	1:G:245:VAL:CG2	2.74	0.68
2:K:24:VAL:O	2:K:25:LYS:HE2	1.91	0.68
3:I:123:LEU:HB3	3:I:139:VAL:HG11	1.75	0.68
3:H:470:LEU:HD12	3:H:470:LEU:O	1.94	0.68
2:L:47:ASN:HD21	2:L:54:ILE:HG23	1.58	0.68
1:G:91:THR:HG23	1:G:93:ASN:H	1.59	0.67
1:B:233:TRP:CH2	1:B:245:VAL:CA	2.64	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:220:ILE:HG23	1:G:224:ALA:HB2	1.76	0.67
1:B:91:THR:HG23	1:B:93:ASN:H	1.59	0.67
3:C:730:LEU:CD1	3:C:733:ARG:HH22	1.97	0.67
2:E:47:ASN:HD21	2:E:54:ILE:HG23	1.58	0.67
3:F:123:LEU:HB3	3:F:139:VAL:HG11	1.75	0.67
3:C:707:ILE:HB	3:C:726:VAL:HG21	1.76	0.67
1:G:378:CYS:HB2	1:G:426:VAL:HG21	1.77	0.67
1:A:379:GLU:O	1:A:379:GLU:CG	2.40	0.67
3:H:682:GLY:O	3:H:683:GLU:CD	2.38	0.67
2:K:23:GLU:HB3	2:K:25:LYS:NZ	2.10	0.67
1:B:378:CYS:HB2	1:B:426:VAL:HG21	1.77	0.67
2:D:23:GLU:HB3	2:D:25:LYS:NZ	2.10	0.67
3:C:682:GLY:O	3:C:683:GLU:CD	2.38	0.67
2:E:23:GLU:HB3	2:E:25:LYS:NZ	2.10	0.67
3:I:682:GLY:O	3:I:683:GLU:CD	2.38	0.66
2:L:23:GLU:HB3	2:L:25:LYS:NZ	2.10	0.66
1:A:19:GLU:OE2	1:B:8:GLN:NE2	2.28	0.66
1:J:378:CYS:HB2	1:J:426:VAL:HG21	1.77	0.66
3:I:446:VAL:HG23	3:I:447:SER:N	2.10	0.66
1:J:91:THR:HG23	1:J:93:ASN:H	1.59	0.66
3:F:455:ILE:HD12	3:F:471:GLU:HG2	1.78	0.66
2:L:25:LYS:N	2:L:25:LYS:CE	2.50	0.66
3:F:682:GLY:O	3:F:683:GLU:CD	2.38	0.66
3:I:90:ARG:NH2	3:I:150:GLN:OE1	2.29	0.66
1:G:190:LYS:HG3	1:G:193:THR:HG22	1.78	0.66
2:D:24:VAL:O	2:D:25:LYS:HE2	1.91	0.66
3:F:426:ASP:HB3	3:F:734:PHE:CD2	2.30	0.66
3:H:446:VAL:HG23	3:H:447:SER:N	2.10	0.66
1:B:65:SER:O	1:B:68:LYS:NZ	2.29	0.66
2:L:23:GLU:C	2:L:25:LYS:HE3	2.22	0.65
3:C:446:VAL:HG23	3:C:447:SER:N	2.10	0.65
3:C:451:GLU:CG	3:C:474:PHE:HZ	2.09	0.65
1:G:397:ARG:HB2	1:G:415:LEU:HB2	1.78	0.65
3:F:437:ALA:CB	3:F:514:PRO:CG	2.74	0.65
1:A:200:LEU:HA	1:A:203:GLU:HB2	1.78	0.65
2:K:23:GLU:C	2:K:25:LYS:HE3	2.22	0.65
2:L:72:TRP:HB2	2:L:105:LYS:CB	2.25	0.65
1:A:378:CYS:HB2	1:A:426:VAL:HG21	1.77	0.65
1:G:225:LEU:HD12	1:G:230:GLN:NE2	2.11	0.65
2:K:72:TRP:HB2	2:K:105:LYS:CB	2.25	0.65
1:G:436:LEU:O	1:G:455:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:90:ARG:NH2	3:C:150:GLN:OE1	2.29	0.65
1:J:436:LEU:O	1:J:455:ARG:NH2	2.30	0.65
3:C:374:PHE:HB3	3:C:421:PHE:CG	2.31	0.65
1:A:436:LEU:O	1:A:455:ARG:NH2	2.30	0.64
3:F:90:ARG:NH2	3:F:150:GLN:OE1	2.29	0.64
3:F:446:VAL:HG23	3:F:447:SER:N	2.10	0.64
1:B:436:LEU:O	1:B:455:ARG:NH2	2.30	0.64
2:D:23:GLU:C	2:D:25:LYS:HE3	2.22	0.64
3:H:90:ARG:NH2	3:H:150:GLN:OE1	2.29	0.64
3:I:509:THR:HB	3:I:512:TYR:CD2	2.33	0.64
2:E:23:GLU:C	2:E:25:LYS:HE3	2.22	0.64
3:I:180:ARG:HH22	3:I:250:HIS:HB3	1.63	0.64
3:I:546:ARG:HB2	2:L:33:TRP:HB2	1.77	0.64
3:I:559:LEU:HD22	3:I:602:LEU:HD23	1.80	0.64
3:I:508:LEU:HD13	3:I:513:TRP:CE2	2.32	0.64
3:C:556:SER:HA	3:C:595:SER:HA	1.80	0.64
1:B:64:LEU:O	1:B:68:LYS:NZ	2.31	0.63
2:D:25:LYS:N	2:D:25:LYS:CE	2.50	0.63
3:C:559:LEU:HD22	3:C:602:LEU:HD23	1.80	0.63
1:G:379:GLU:O	1:G:379:GLU:CG	2.40	0.63
1:J:397:ARG:HD2	1:J:416:PRO:C	2.23	0.63
3:I:198:ARG:O	3:I:202:GLU:HB3	1.99	0.63
3:C:451:GLU:CB	3:C:474:PHE:HZ	2.10	0.63
2:D:72:TRP:HB2	2:D:105:LYS:CB	2.25	0.63
3:F:440:LEU:HB3	3:F:513:TRP:HH2	1.64	0.63
3:I:522:CYS:HB3	3:I:622:ILE:HB	1.80	0.63
3:H:559:LEU:HD22	3:H:602:LEU:HD23	1.80	0.63
3:C:451:GLU:HB3	3:C:474:PHE:HZ	1.59	0.63
3:F:622:ILE:HG12	3:F:627:LEU:HD13	1.81	0.62
2:K:23:GLU:O	2:K:25:LYS:CE	2.46	0.62
1:G:47:MET:CG	1:J:21:LEU:HD21	2.21	0.62
3:F:556:SER:HA	3:F:595:SER:HA	1.80	0.62
3:H:346:LEU:CD1	3:H:414:LYS:O	2.48	0.62
2:L:41:ASN:ND2	2:L:46:ARG:CD	2.62	0.62
3:C:638:LYS:CG	3:C:642:ARG:HG2	2.30	0.62
1:A:19:GLU:CD	1:B:8:GLN:HE21	2.06	0.62
3:F:559:LEU:HD22	3:F:602:LEU:HD23	1.80	0.62
3:H:638:LYS:CG	3:H:642:ARG:HG2	2.30	0.62
1:J:233:TRP:CH2	1:J:245:VAL:CA	2.64	0.62
3:H:173:ARG:HH12	3:H:213:SER:HA	1.63	0.62
3:H:198:ARG:HH21	3:H:202:GLU:HG3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:556:SER:HA	3:H:595:SER:HA	1.80	0.62
2:E:23:GLU:O	2:E:25:LYS:CE	2.46	0.62
1:J:182:SER:HB3	1:J:219:GLN:HG3	1.82	0.62
3:F:248:VAL:CG2	3:F:256:THR:HG23	2.28	0.62
3:I:556:SER:HA	3:I:595:SER:HA	1.80	0.62
3:C:683:GLU:O	3:C:683:GLU:HG2	2.00	0.62
3:H:683:GLU:O	3:H:683:GLU:HG2	2.00	0.62
3:C:455:ILE:C	3:C:457:LYS:N	2.54	0.62
1:A:273:GLU:HA	1:A:283:TYR:HB3	1.82	0.61
3:F:426:ASP:HB3	3:F:734:PHE:HD2	1.65	0.61
2:E:72:TRP:HB2	2:E:105:LYS:CB	2.25	0.61
3:F:458:LEU:HB3	3:F:467:THR:HB	1.83	0.61
3:I:634:LEU:HB3	3:I:644:LEU:HD23	1.82	0.61
3:C:248:VAL:CG2	3:C:256:THR:HG23	2.28	0.61
3:C:509:THR:HB	3:C:512:TYR:HD2	1.64	0.61
3:C:560:ASN:HB2	2:E:25:LYS:CG	2.27	0.61
2:L:23:GLU:C	2:L:25:LYS:CE	2.74	0.61
3:F:598:GLN:HG2	3:F:634:LEU:HG	1.83	0.61
3:F:683:GLU:O	3:F:683:GLU:HG2	2.00	0.61
3:H:509:THR:HB	3:H:512:TYR:HD1	1.64	0.61
1:A:24:PHE:HZ	1:B:57:ARG:NH2	1.98	0.61
1:A:55:TYR:CE1	3:C:58:TYR:CB	2.84	0.61
3:H:560:ASN:HB2	2:K:25:LYS:CG	2.27	0.61
2:K:23:GLU:C	2:K:25:LYS:CE	2.74	0.61
2:K:41:ASN:ND2	2:K:46:ARG:CD	2.62	0.61
3:I:683:GLU:HG2	3:I:683:GLU:O	2.00	0.61
2:L:23:GLU:O	2:L:25:LYS:CE	2.46	0.61
1:B:273:GLU:HA	1:B:283:TYR:HB3	1.82	0.61
2:D:23:GLU:C	2:D:25:LYS:CE	2.74	0.61
3:F:638:LYS:CG	3:F:642:ARG:HG2	2.30	0.61
1:G:231:ARG:H	1:G:231:ARG:HD2	1.66	0.61
3:H:424:GLU:OE2	3:H:735:LEU:HD23	2.01	0.61
3:I:638:LYS:CG	3:I:642:ARG:HG2	2.30	0.61
3:H:220:GLU:HA	3:H:223:LYS:HB2	1.83	0.61
2:D:23:GLU:O	2:D:25:LYS:CE	2.46	0.61
2:K:25:LYS:HE2	2:K:25:LYS:CA	2.31	0.61
2:E:23:GLU:C	2:E:25:LYS:CE	2.73	0.61
1:A:127:LYS:HG3	1:A:127:LYS:O	2.01	0.60
1:B:231:ARG:H	1:B:231:ARG:HD2	1.66	0.60
3:I:598:GLN:HG2	3:I:634:LEU:HG	1.83	0.60
2:E:25:LYS:HE2	2:E:25:LYS:CA	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:HIS:CD2	1:J:47:MET:HE3	2.37	0.60
1:J:127:LYS:O	1:J:127:LYS:HG3	2.02	0.60
2:L:25:LYS:HE2	2:L:25:LYS:CA	2.32	0.60
1:G:186:LEU:HD13	1:G:194:VAL:HG11	1.83	0.60
3:H:598:GLN:HG2	3:H:634:LEU:HG	1.83	0.60
3:I:509:THR:HG23	2:L:76:ASN:ND2	2.17	0.60
1:J:231:ARG:H	1:J:231:ARG:HD2	1.66	0.60
3:F:634:LEU:HB3	3:F:644:LEU:HD23	1.82	0.60
3:H:346:LEU:HD13	3:H:418:LEU:CB	2.31	0.60
1:J:399:VAL:HG13	1:J:415:LEU:HD21	1.82	0.60
3:H:634:LEU:HB3	3:H:644:LEU:HD23	1.82	0.60
3:C:634:LEU:HB3	3:C:644:LEU:HD23	1.82	0.60
3:F:204:ASP:O	3:F:208:PRO:HD2	2.01	0.60
3:F:440:LEU:CB	3:F:513:TRP:CH2	2.85	0.60
3:I:385:PRO:HB3	3:I:428:PHE:HB2	1.83	0.60
3:C:451:GLU:HG2	3:C:474:PHE:CZ	2.36	0.60
1:J:273:GLU:HA	1:J:283:TYR:HB3	1.83	0.60
3:I:153:ARG:HH21	3:I:200:VAL:HG13	1.66	0.60
3:H:508:LEU:HD13	3:H:513:TRP:CE2	2.36	0.60
3:C:598:GLN:HG2	3:C:634:LEU:HG	1.83	0.60
1:A:153:LYS:HE3	1:A:179:ASP:OD1	2.02	0.60
3:F:437:ALA:HB2	3:F:514:PRO:CD	2.31	0.60
3:H:356:LEU:HD12	3:H:360:PHE:HB2	1.84	0.60
3:I:622:ILE:HG12	3:I:627:LEU:HD13	1.84	0.60
3:C:451:GLU:HB3	3:C:474:PHE:CE2	2.37	0.60
1:B:153:LYS:HE3	1:B:179:ASP:OD1	2.02	0.59
1:G:127:LYS:O	1:G:127:LYS:HG3	2.01	0.59
1:J:153:LYS:HE3	1:J:179:ASP:OD1	2.02	0.59
2:K:24:VAL:O	2:K:25:LYS:CE	2.49	0.59
2:E:41:ASN:ND2	2:E:46:ARG:CD	2.62	0.59
1:B:397:ARG:HB2	1:B:415:LEU:HB2	1.84	0.59
3:I:626:GLU:CA	3:I:629:ARG:HD2	2.18	0.59
1:A:434:MET:HE2	1:A:455:ARG:HE	1.67	0.59
1:G:47:MET:HE2	1:J:21:LEU:CB	2.33	0.59
2:E:25:LYS:N	2:E:25:LYS:CE	2.50	0.59
3:F:339:VAL:HA	3:F:391:PHE:HB2	1.84	0.59
1:A:57:ARG:HH22	1:B:24:PHE:HZ	1.49	0.59
3:F:217:PHE:HB2	3:F:267:GLU:OE1	2.03	0.59
3:H:641:GLN:HA	3:H:641:GLN:OE1	2.02	0.59
3:C:282:SER:HA	3:C:286:HIS:HB3	1.85	0.59
1:B:297:LYS:HZ1	1:B:595:PRO:HD3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:535:CYS:SG	1:G:564:ARG:NH1	2.76	0.59
2:K:25:LYS:N	2:K:25:LYS:CE	2.50	0.59
3:C:102:LEU:HD11	3:C:182:ALA:HB1	1.85	0.59
3:C:414:LYS:O	3:C:418:LEU:HG	2.03	0.59
3:H:346:LEU:HD11	3:H:414:LYS:C	2.28	0.59
3:I:641:GLN:OE1	3:I:641:GLN:HA	2.02	0.59
1:A:382:ILE:HB	1:A:402:TYR:HB3	1.85	0.59
1:G:127:LYS:O	1:G:127:LYS:CG	2.51	0.59
3:H:525:PRO:HB2	3:H:528:PRO:HG2	1.83	0.59
3:I:768:ALA:HB1	2:L:89:LYS:HB3	1.85	0.59
1:G:153:LYS:HE3	1:G:179:ASP:OD1	2.02	0.59
1:J:434:MET:HE2	1:J:455:ARG:HE	1.67	0.59
3:H:337:ASN:ND2	3:H:340:ASP:OD1	2.35	0.59
3:I:102:LEU:HD11	3:I:182:ALA:HB1	1.85	0.59
1:B:233:TRP:HE1	1:B:237:LEU:HB3	1.68	0.58
3:H:473:MET:SD	3:H:512:TYR:HB3	2.43	0.58
3:I:207:ALA:HB3	3:I:208:PRO:HD3	1.85	0.58
3:C:356:LEU:HD12	3:C:360:PHE:HB2	1.84	0.58
1:B:64:LEU:C	1:B:68:LYS:HZ1	2.10	0.58
3:F:446:VAL:CG2	3:F:447:SER:N	2.67	0.58
3:H:282:SER:HA	3:H:286:HIS:HB3	1.85	0.58
3:H:665:PHE:HD1	3:H:665:PHE:C	1.98	0.58
3:F:626:GLU:CA	3:F:629:ARG:HD2	2.18	0.58
3:H:389:SER:HB2	3:H:431:TYR:CB	2.34	0.58
3:H:446:VAL:CG2	3:H:447:SER:N	2.66	0.58
3:F:102:LEU:HD11	3:F:182:ALA:HB1	1.85	0.58
1:A:186:LEU:HD13	1:A:194:VAL:HG11	1.85	0.58
1:A:207:GLU:HG3	1:A:238:PRO:HG3	1.85	0.58
1:B:127:LYS:O	1:B:127:LYS:HG3	2.01	0.58
1:B:434:MET:HE2	1:B:455:ARG:HE	1.67	0.58
1:B:535:CYS:SG	1:B:564:ARG:NH1	2.76	0.58
1:J:535:CYS:SG	1:J:564:ARG:NH1	2.76	0.58
3:F:43:GLU:OE2	3:F:48:ASN:ND2	2.32	0.58
3:F:706:ALA:HA	3:F:709:ARG:HH21	1.68	0.58
3:I:560:ASN:HB2	2:L:25:LYS:CG	2.27	0.58
2:E:24:VAL:O	2:E:25:LYS:CE	2.49	0.58
2:D:25:LYS:CG	3:F:560:ASN:HB2	2.27	0.58
3:H:238:GLU:O	3:H:242:ASN:ND2	2.32	0.58
3:I:282:SER:HA	3:I:286:HIS:HB3	1.85	0.58
1:B:186:LEU:HD13	1:B:194:VAL:HG11	1.86	0.58
1:B:382:ILE:HB	1:B:402:TYR:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:127:LYS:O	1:J:127:LYS:CG	2.51	0.58
3:F:349:LYS:HE2	3:F:421:PHE:HE2	1.69	0.58
3:H:102:LEU:HD11	3:H:182:ALA:HB1	1.85	0.58
3:I:238:GLU:O	3:I:242:ASN:ND2	2.32	0.58
1:A:127:LYS:O	1:A:127:LYS:CG	2.51	0.58
1:A:535:CYS:SG	1:A:564:ARG:NH1	2.76	0.58
1:B:459:ARG:HB3	1:B:476:GLY:HA3	1.86	0.58
3:I:446:VAL:CG2	3:I:447:SER:N	2.67	0.58
1:B:127:LYS:O	1:B:127:LYS:CG	2.51	0.58
1:J:233:TRP:HE1	1:J:237:LEU:HB3	1.69	0.58
3:F:700:LYS:O	3:F:703:ILE:HG12	2.04	0.58
2:L:35:TRP:HD1	2:L:75:CYS:O	1.87	0.58
1:A:55:TYR:HE1	3:C:58:TYR:CB	2.17	0.57
1:G:459:ARG:HB3	1:G:476:GLY:HA3	1.86	0.57
3:F:441:LEU:HD21	3:F:508:LEU:CD1	2.34	0.57
2:L:46:ARG:O	2:L:46:ARG:NE	2.37	0.57
3:C:641:GLN:HA	3:C:641:GLN:OE1	2.02	0.57
2:D:77:HIS:CD2	2:D:96:LEU:CD1	2.87	0.57
2:K:46:ARG:O	2:K:46:ARG:NE	2.37	0.57
3:C:446:VAL:CG2	3:C:447:SER:N	2.66	0.57
2:D:35:TRP:HD1	2:D:75:CYS:O	1.86	0.57
2:L:38:VAL:HG12	2:L:41:ASN:N	2.18	0.57
3:C:509:THR:HG23	2:E:76:ASN:ND2	2.19	0.57
2:E:38:VAL:HG12	2:E:41:ASN:N	2.18	0.57
1:G:93:ASN:HD21	1:J:9:ILE:HG23	1.70	0.57
1:G:233:TRP:CZ3	1:G:245:VAL:HA	2.38	0.57
1:G:434:MET:HE2	1:G:455:ARG:HE	1.67	0.57
2:D:25:LYS:HE2	2:D:25:LYS:CA	2.32	0.57
2:L:24:VAL:O	2:L:25:LYS:CE	2.49	0.57
1:G:233:TRP:HE1	1:G:237:LEU:HB3	1.68	0.57
3:F:282:SER:HA	3:F:286:HIS:HB3	1.85	0.57
3:F:509:THR:HB	3:F:512:TYR:CD2	2.36	0.57
2:K:35:TRP:HD1	2:K:75:CYS:O	1.86	0.57
1:A:91:THR:HG23	1:A:93:ASN:H	1.69	0.57
3:F:440:LEU:HB3	3:F:513:TRP:CH2	2.39	0.57
3:H:346:LEU:CB	3:H:418:LEU:HD13	2.32	0.57
2:K:38:VAL:HG12	2:K:41:ASN:N	2.18	0.57
1:A:476:GLY:O	1:A:496:SER:N	2.38	0.57
3:F:337:ASN:HB3	3:F:340:ASP:HB2	1.85	0.57
3:F:641:GLN:HA	3:F:641:GLN:OE1	2.02	0.57
3:C:238:GLU:O	3:C:242:ASN:ND2	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:24:VAL:O	2:E:25:LYS:NZ	2.38	0.57
2:E:35:TRP:HD1	2:E:75:CYS:O	1.86	0.57
1:B:217:LEU:HG	1:B:225:LEU:HD11	1.86	0.57
3:F:446:VAL:CG2	3:F:447:SER:H	2.18	0.57
1:B:476:GLY:O	1:B:496:SER:N	2.38	0.57
1:J:297:LYS:HZ1	1:J:595:PRO:HD3	1.69	0.57
3:H:245:ILE:HA	3:H:248:VAL:CG1	2.35	0.57
3:H:638:LYS:HG2	3:H:642:ARG:HG2	1.87	0.57
2:K:24:VAL:O	2:K:25:LYS:NZ	2.38	0.57
3:C:289:LYS:O	3:C:351:ARG:NH2	2.38	0.57
3:C:455:ILE:C	3:C:457:LYS:H	2.12	0.57
3:C:638:LYS:HG2	3:C:642:ARG:HG2	1.87	0.57
1:A:459:ARG:HB3	1:A:476:GLY:HA3	1.86	0.56
1:B:181:LEU:HD21	1:B:220:ILE:HD13	1.86	0.56
1:J:233:TRP:CZ3	1:J:245:VAL:HA	2.38	0.56
3:I:625:ARG:H	3:I:625:ARG:HH21	1.51	0.56
3:I:638:LYS:HG2	3:I:642:ARG:HG2	1.87	0.56
3:C:446:VAL:CG2	3:C:447:SER:H	2.18	0.56
1:J:379:GLU:O	1:J:379:GLU:CG	2.40	0.56
3:F:437:ALA:CB	3:F:514:PRO:HG3	2.35	0.56
1:B:525:VAL:HA	1:B:538:MET:HG2	1.88	0.56
1:J:476:GLY:O	1:J:496:SER:N	2.38	0.56
3:F:202:GLU:O	3:F:203:GLU:C	2.46	0.56
3:F:638:LYS:HG2	3:F:642:ARG:HG2	1.87	0.56
3:H:289:LYS:O	3:H:351:ARG:NH2	2.38	0.56
3:I:612:THR:OG1	3:I:655:ASN:O	2.24	0.56
3:C:699:ARG:HE	3:C:734:PHE:HB2	1.70	0.56
1:G:286:VAL:HG11	1:G:573:TRP:HH2	1.71	0.56
3:F:612:THR:OG1	3:F:655:ASN:O	2.24	0.56
3:H:383:ARG:HD3	3:H:387:TYR:CZ	2.40	0.56
3:C:557:ALA:HB3	3:C:594:VAL:HG23	1.88	0.56
2:E:46:ARG:O	2:E:46:ARG:NE	2.37	0.56
1:B:305:LEU:HD21	1:B:323:GLY:HA3	1.88	0.56
1:J:228:VAL:O	1:J:228:VAL:CG2	2.54	0.56
2:D:24:VAL:O	2:D:25:LYS:CE	2.50	0.56
3:H:557:ALA:HB3	3:H:594:VAL:HG23	1.88	0.56
2:L:24:VAL:O	2:L:25:LYS:NZ	2.38	0.56
3:C:612:THR:OG1	3:C:655:ASN:O	2.24	0.56
1:G:525:VAL:HA	1:G:538:MET:HG2	1.88	0.56
1:J:166:GLN:HB2	1:J:169:PHE:HB3	1.88	0.56
2:D:24:VAL:O	2:D:25:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:PHE:O	1:A:237:LEU:HG	2.05	0.56
1:A:305:LEU:HD21	1:A:323:GLY:HA3	1.88	0.56
1:G:476:GLY:O	1:G:496:SER:N	2.38	0.56
1:J:459:ARG:HB3	1:J:476:GLY:HA3	1.86	0.56
3:H:612:THR:OG1	3:H:655:ASN:O	2.24	0.56
1:B:64:LEU:O	1:B:68:LYS:HE3	2.04	0.56
1:J:305:LEU:HD21	1:J:323:GLY:HA3	1.88	0.56
3:F:49:ASN:HD22	3:F:118:MET:HE1	1.69	0.56
3:H:221:SER:O	3:H:222:GLN:C	2.48	0.56
3:C:245:ILE:HA	3:C:248:VAL:CG1	2.35	0.56
3:F:245:ILE:HA	3:F:248:VAL:CG1	2.35	0.56
3:F:682:GLY:O	3:F:683:GLU:CG	2.54	0.56
3:H:437:ALA:HA	3:H:513:TRP:HZ3	1.71	0.56
3:C:415:ALA:HA	3:C:418:LEU:HD12	1.87	0.56
2:E:27:TRP:CZ2	2:E:29:ALA:HB2	2.40	0.56
2:D:76:ASN:ND2	3:F:509:THR:HG23	2.21	0.55
3:H:665:PHE:CD1	3:H:665:PHE:C	2.70	0.55
2:K:27:TRP:CZ2	2:K:29:ALA:HB2	2.40	0.55
2:L:27:TRP:CZ2	2:L:29:ALA:HB2	2.40	0.55
3:H:446:VAL:CG2	3:H:447:SER:H	2.18	0.55
3:C:144:LEU:HD12	3:C:193:LEU:HA	1.88	0.55
3:C:665:PHE:HD1	3:C:665:PHE:C	1.98	0.55
1:A:254:PRO:O	1:A:255:LYS:HG2	2.06	0.55
3:F:144:LEU:HD12	3:F:193:LEU:HA	1.88	0.55
3:H:473:MET:HG2	3:H:512:TYR:HB3	1.87	0.55
3:H:682:GLY:O	3:H:683:GLU:CG	2.54	0.55
3:I:446:VAL:CG2	3:I:447:SER:H	2.18	0.55
3:I:682:GLY:O	3:I:683:GLU:CG	2.54	0.55
2:L:47:ASN:HD21	2:L:54:ILE:CG2	2.18	0.55
3:C:129:VAL:O	3:C:133:GLN:NE2	2.34	0.55
1:B:286:VAL:HG11	1:B:573:TRP:HH2	1.71	0.55
1:J:198:ALA:O	1:J:202:LEU:HG	2.06	0.55
1:J:397:ARG:CD	1:J:416:PRO:O	2.55	0.55
3:I:559:LEU:CD2	3:I:602:LEU:HD23	2.36	0.55
3:C:525:PRO:HB2	3:C:528:PRO:HG2	1.87	0.55
3:C:682:GLY:O	3:C:683:GLU:CG	2.54	0.55
1:B:233:TRP:HH2	1:B:245:VAL:N	2.04	0.55
1:B:254:PRO:O	1:B:255:LYS:HG2	2.06	0.55
1:J:254:PRO:O	1:J:255:LYS:HG2	2.06	0.55
3:F:557:ALA:HB3	3:F:594:VAL:HG23	1.88	0.55
3:F:559:LEU:CD2	3:F:602:LEU:HD23	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:47:ASN:HD21	2:K:54:ILE:CG2	2.18	0.55
3:I:129:VAL:O	3:I:133:GLN:NE2	2.34	0.55
3:I:144:LEU:HD12	3:I:193:LEU:HA	1.88	0.55
1:B:233:TRP:CZ3	1:B:245:VAL:HA	2.38	0.55
1:J:286:VAL:HG11	1:J:573:TRP:HH2	1.71	0.55
2:K:38:VAL:HG12	2:K:41:ASN:H	1.72	0.55
1:B:195:ARG:HB2	1:B:224:ALA:HB1	1.89	0.55
3:H:710:ILE:HG21	3:H:729:GLN:HE22	1.71	0.55
1:G:233:TRP:HH2	1:G:245:VAL:N	2.04	0.55
1:J:233:TRP:HH2	1:J:245:VAL:N	2.04	0.55
2:D:27:TRP:CZ2	2:D:29:ALA:HB2	2.40	0.55
3:F:717:MET:HB3	3:F:722:LEU:HG	1.89	0.55
3:H:717:MET:HB3	3:H:722:LEU:HG	1.89	0.55
2:L:71:ALA:HB2	2:L:81:PHE:HA	1.88	0.55
3:C:717:MET:HB3	3:C:722:LEU:HG	1.89	0.55
1:A:22:LYS:HZ3	1:B:6:GLU:CD	2.15	0.55
1:J:207:GLU:HG3	1:J:238:PRO:HG3	1.88	0.55
3:H:314:CYS:HB3	3:H:369:THR:HG21	1.89	0.55
3:H:409:GLU:OE2	3:H:453:ASN:ND2	2.40	0.55
3:C:314:CYS:HB3	3:C:369:THR:HG21	1.89	0.55
1:A:53:SER:OG	1:A:111:LEU:O	2.25	0.55
1:G:305:LEU:HD21	1:G:323:GLY:HA3	1.88	0.55
3:H:559:LEU:CD2	3:H:602:LEU:HD23	2.36	0.55
3:I:314:CYS:HB3	3:I:369:THR:HG21	1.89	0.55
3:I:418:LEU:O	3:I:422:MET:HG3	2.06	0.55
3:C:559:LEU:CD2	3:C:602:LEU:HD23	2.36	0.55
1:J:525:VAL:HA	1:J:538:MET:HG2	1.88	0.54
1:G:555:ASP:HB3	1:G:558:LEU:HB2	1.90	0.54
1:J:275:SER:OG	1:J:574:ASP:O	2.25	0.54
3:F:342:ILE:HG13	3:F:388:LEU:HA	1.89	0.54
3:H:144:LEU:HD12	3:H:193:LEU:HA	1.88	0.54
3:C:338:PRO:HA	3:C:341:TYR:HD2	1.72	0.54
3:C:523:ASN:HD21	3:C:603:MET:HE1	1.73	0.54
3:C:641:GLN:OE1	3:C:664:GLN:HB3	2.08	0.54
1:J:53:SER:OG	1:J:111:LEU:O	2.25	0.54
3:H:491:LEU:C	3:H:493:ALA:H	2.15	0.54
3:I:751:ARG:NH2	2:L:55:GLU:HB3	2.22	0.54
2:E:84:ILE:HG12	2:E:101:TRP:CE2	2.43	0.54
1:A:525:VAL:HA	1:A:538:MET:HG2	1.88	0.54
3:H:641:GLN:OE1	3:H:664:GLN:HB3	2.08	0.54
2:E:47:ASN:HD21	2:E:54:ILE:CG2	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:ASP:HB3	1:B:558:LEU:HB2	1.90	0.54
3:H:768:ALA:HB1	2:K:89:LYS:HB3	1.90	0.54
3:I:557:ALA:HB3	3:I:594:VAL:HG23	1.88	0.54
3:F:638:LYS:HG3	3:F:639:PRO:O	2.08	0.54
3:H:466:PHE:HA	3:H:469:LYS:HG2	1.89	0.54
1:B:160:PHE:HE2	1:B:169:PHE:CG	2.25	0.54
3:H:622:ILE:HG12	3:H:627:LEU:HD13	1.89	0.54
3:I:466:PHE:HA	3:I:469:LYS:HG2	1.89	0.54
1:B:365:PRO:O	1:B:409:TRP:NE1	2.41	0.54
1:J:370:ARG:HG2	1:J:389:SER:HA	1.90	0.54
3:I:225:LEU:HB3	3:I:272:HIS:CE1	2.43	0.54
1:A:269:MET:HE1	1:A:528:VAL:HG11	1.88	0.54
3:H:638:LYS:HG3	3:H:639:PRO:O	2.08	0.54
2:K:23:GLU:CB	2:K:25:LYS:HZ1	2.18	0.54
3:I:638:LYS:HG3	3:I:639:PRO:O	2.08	0.54
3:I:641:GLN:OE1	3:I:664:GLN:HB3	2.08	0.54
2:L:38:VAL:HG12	2:L:41:ASN:H	1.72	0.54
1:A:51:THR:CG2	1:B:17:LEU:CD1	2.82	0.53
1:A:275:SER:OG	1:A:574:ASP:O	2.26	0.53
1:A:286:VAL:HG11	1:A:573:TRP:HH2	1.71	0.53
1:G:10:ASN:HB2	1:G:14:ALA:H	1.74	0.53
3:C:638:LYS:HG3	3:C:639:PRO:O	2.09	0.53
1:J:365:PRO:O	1:J:409:TRP:NE1	2.41	0.53
3:F:153:ARG:HH21	3:F:200:VAL:HG13	1.74	0.53
1:A:212:TYR:C	1:A:214:SER:H	2.16	0.53
1:G:161:THR:HB	1:G:188:VAL:HG13	1.90	0.53
2:D:93:VAL:HA	2:D:100:GLU:HA	1.91	0.53
3:F:440:LEU:CB	3:F:513:TRP:HH2	2.21	0.53
3:H:169:ILE:HD11	3:H:247:ARG:HD3	1.91	0.53
3:I:614:GLU:OE1	3:I:617:GLN:NE2	2.41	0.53
3:F:169:ILE:HD11	3:F:247:ARG:HD3	1.91	0.53
1:A:348:ASN:ND2	1:A:366:MET:O	2.42	0.53
1:G:370:ARG:HG2	1:G:389:SER:HA	1.90	0.53
3:F:625:ARG:H	3:F:625:ARG:HH21	1.55	0.53
3:H:214:ALA:HA	3:H:267:GLU:CD	2.34	0.53
2:L:41:ASN:ND2	2:L:46:ARG:HG2	2.24	0.53
1:G:365:PRO:O	1:G:409:TRP:NE1	2.41	0.53
3:F:614:GLU:OE1	3:F:617:GLN:NE2	2.41	0.53
3:H:393:ASP:HB2	3:H:435:HIS:NE2	2.24	0.53
3:I:166:LEU:HD11	3:I:208:PRO:HB3	1.90	0.53
3:C:614:GLU:OE1	3:C:617:GLN:NE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:41:ASN:ND2	2:E:46:ARG:HG2	2.24	0.53
1:J:289:SER:HG	1:J:294:LYS:H	1.55	0.53
2:D:77:HIS:CD2	2:D:96:LEU:HD12	2.44	0.53
1:A:13:TYR:OH	1:B:89:ALA:HA	2.08	0.53
3:F:287:MET:HE3	3:F:296:LEU:HD22	1.91	0.53
3:F:641:GLN:OE1	3:F:664:GLN:HB3	2.08	0.53
3:C:506:ARG:O	2:E:31:ALA:N	2.35	0.53
1:A:555:ASP:HB3	1:A:558:LEU:HB2	1.90	0.53
1:B:431:ILE:HB	1:B:442:TYR:HB3	1.91	0.53
1:G:263:MET:SD	1:G:263:MET:N	2.82	0.53
1:J:414:PRO:O	1:J:449:TRP:NE1	2.42	0.53
3:F:116:MET:HA	3:F:119:ILE:HB	1.91	0.53
3:H:248:VAL:CG2	3:H:256:THR:HG23	2.27	0.53
3:I:337:ASN:O	3:I:338:PRO:C	2.52	0.53
2:E:38:VAL:HG12	2:E:41:ASN:H	1.72	0.53
1:B:297:LYS:NZ	1:B:593:GLU:O	2.43	0.52
1:B:548:LYS:NZ	1:B:549:TYR:O	2.42	0.52
3:H:346:LEU:N	3:H:418:LEU:CD1	2.71	0.52
3:H:506:ARG:O	2:K:31:ALA:N	2.34	0.52
3:I:606:ASN:HD21	2:L:22:PHE:HD2	1.57	0.52
3:C:626:GLU:HA	3:C:629:ARG:HH11	1.74	0.52
1:A:263:MET:SD	1:A:263:MET:N	2.83	0.52
1:A:365:PRO:O	1:A:409:TRP:NE1	2.41	0.52
1:J:548:LYS:NZ	1:J:549:TYR:O	2.42	0.52
1:J:555:ASP:HB3	1:J:558:LEU:HB2	1.90	0.52
3:H:190:LEU:HB3	3:H:201:TYR:HB2	1.90	0.52
3:I:116:MET:HA	3:I:119:ILE:HB	1.90	0.52
2:L:47:ASN:ND2	2:L:54:ILE:HG23	2.24	0.52
1:G:414:PRO:O	1:G:449:TRP:NE1	2.42	0.52
1:G:548:LYS:NZ	1:G:549:TYR:O	2.42	0.52
1:J:263:MET:SD	1:J:263:MET:N	2.83	0.52
3:H:116:MET:HA	3:H:119:ILE:HB	1.90	0.52
1:A:548:LYS:NZ	1:A:549:TYR:O	2.42	0.52
1:B:553:GLN:HB2	1:B:564:ARG:HB2	1.91	0.52
1:G:348:ASN:ND2	1:G:366:MET:O	2.42	0.52
2:D:22:PHE:HD2	3:F:606:ASN:HD21	1.57	0.52
2:D:33:TRP:HB2	3:F:546:ARG:HB2	1.92	0.52
3:H:441:LEU:HD21	3:H:508:LEU:HD11	1.91	0.52
2:K:41:ASN:ND2	2:K:46:ARG:HG2	2.24	0.52
3:C:287:MET:HE3	3:C:296:LEU:HD22	1.92	0.52
3:C:509:THR:HB	3:C:512:TYR:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:228:VAL:HG23	1:J:231:ARG:HB2	1.91	0.52
3:H:606:ASN:HD21	2:K:22:PHE:HD1	1.57	0.52
3:H:614:GLU:OE1	3:H:617:GLN:NE2	2.41	0.52
3:H:708:VAL:HA	3:H:754:LEU:HD23	1.91	0.52
2:K:84:ILE:HG12	2:K:101:TRP:CE2	2.44	0.52
1:B:370:ARG:HG2	1:B:389:SER:HA	1.90	0.52
1:G:301:PRO:HG3	1:G:360:TRP:CE2	2.45	0.52
1:J:269:MET:HE1	1:J:528:VAL:HG11	1.91	0.52
3:F:541:ALA:HB2	3:H:502:ASP:HA	1.91	0.52
3:H:700:LYS:O	3:H:703:ILE:HG12	2.09	0.52
3:C:116:MET:HA	3:C:119:ILE:HB	1.91	0.52
1:J:348:ASN:ND2	1:J:366:MET:O	2.42	0.52
3:F:214:ALA:HA	3:F:267:GLU:CD	2.34	0.52
3:F:522:CYS:HB2	3:F:622:ILE:HB	1.92	0.52
3:H:509:THR:HB	3:H:512:TYR:CD1	2.44	0.52
3:I:102:LEU:CD1	3:I:182:ALA:HB1	2.40	0.52
3:C:169:ILE:HD11	3:C:247:ARG:HD3	1.91	0.52
3:I:169:ILE:HD11	3:I:247:ARG:HD3	1.91	0.52
1:B:522:ASP:N	1:B:522:ASP:OD1	2.43	0.52
1:G:233:TRP:CH2	1:G:245:VAL:CA	2.65	0.52
3:C:102:LEU:CD1	3:C:182:ALA:HB1	2.40	0.52
1:B:348:ASN:ND2	1:B:366:MET:O	2.42	0.51
1:G:269:MET:HE1	1:G:528:VAL:HG11	1.91	0.51
3:F:102:LEU:CD1	3:F:182:ALA:HB1	2.40	0.51
3:F:542:LYS:HA	3:H:488:ARG:CB	2.40	0.51
1:A:321:ALA:HB3	1:A:375:LEU:HD11	1.92	0.51
1:J:553:GLN:HB2	1:J:564:ARG:HB2	1.91	0.51
2:E:47:ASN:ND2	2:E:54:ILE:HG23	2.24	0.51
1:J:297:LYS:NZ	1:J:593:GLU:O	2.43	0.51
1:A:297:LYS:NZ	1:A:593:GLU:O	2.43	0.51
1:B:263:MET:SD	1:B:263:MET:N	2.82	0.51
1:B:374:SER:OG	1:B:385:ILE:O	2.28	0.51
1:J:301:PRO:HG3	1:J:360:TRP:CE2	2.45	0.51
3:H:102:LEU:CD1	3:H:182:ALA:HB1	2.40	0.51
3:H:129:VAL:O	3:H:133:GLN:NE2	2.34	0.51
1:A:553:GLN:HB2	1:A:564:ARG:HB2	1.91	0.51
1:B:301:PRO:HG3	1:B:360:TRP:CE2	2.45	0.51
1:G:297:LYS:NZ	1:G:593:GLU:O	2.42	0.51
1:G:553:GLN:HB2	1:G:564:ARG:HB2	1.91	0.51
3:H:287:MET:HE3	3:H:296:LEU:HD22	1.91	0.51
1:A:301:PRO:HG3	1:A:360:TRP:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:321:ALA:HB3	1:G:375:LEU:HD11	1.92	0.51
1:G:374:SER:OG	1:G:385:ILE:O	2.28	0.51
1:J:161:THR:HB	1:J:188:VAL:CG1	2.37	0.51
3:H:523:ASN:HD21	3:H:603:MET:HE1	1.75	0.51
3:I:287:MET:HE3	3:I:296:LEU:HD22	1.91	0.51
1:J:275:SER:OG	1:J:573:TRP:NE1	2.44	0.51
3:F:437:ALA:HB2	3:F:514:PRO:CG	2.41	0.51
3:H:215:GLU:O	3:H:216:PHE:C	2.54	0.51
3:I:413:ASP:O	3:I:416:MET:HG3	2.10	0.51
3:C:245:ILE:CA	3:C:248:VAL:HG12	2.41	0.51
1:A:22:LYS:HE3	1:B:8:GLN:HE22	1.76	0.51
1:A:237:LEU:HD13	1:A:241:ASP:HB2	1.93	0.51
1:B:275:SER:OG	1:B:573:TRP:NE1	2.44	0.51
1:B:321:ALA:HB3	1:B:375:LEU:HD11	1.92	0.51
3:F:258:GLU:HB2	3:F:259:PRO:HD3	1.93	0.51
3:F:477:MET:HE3	3:F:513:TRP:CZ2	2.46	0.51
3:I:437:ALA:HA	3:I:513:TRP:CZ3	2.38	0.51
3:C:699:ARG:O	3:C:703:ILE:HG12	2.10	0.51
3:C:706:ALA:HA	3:C:709:ARG:HH21	1.76	0.51
2:E:23:GLU:CB	2:E:25:LYS:HZ1	2.19	0.51
1:B:275:SER:OG	1:B:574:ASP:O	2.25	0.51
1:G:54:SER:CB	3:I:128:ARG:HH22	2.24	0.51
3:F:419:PHE:CD2	3:F:461:GLU:HG2	2.45	0.51
3:H:298:CYS:HA	3:H:301:LYS:HG2	1.93	0.51
3:H:388:LEU:HD22	3:H:422:MET:SD	2.51	0.51
3:H:596:THR:O	3:H:596:THR:HG22	2.11	0.51
3:C:298:CYS:HA	3:C:301:LYS:HG2	1.93	0.51
3:I:258:GLU:HB2	3:I:259:PRO:HD3	1.93	0.50
1:A:237:LEU:HB2	1:A:238:PRO:HD2	1.94	0.50
3:H:455:ILE:CG2	3:H:470:LEU:HD21	2.24	0.50
3:I:298:CYS:HA	3:I:301:LYS:HG2	1.93	0.50
3:H:522:CYS:HB2	3:H:622:ILE:HB	1.93	0.50
3:H:559:LEU:O	3:H:592:LEU:N	2.39	0.50
3:C:112:HIS:CE1	3:C:116:MET:HE3	2.46	0.50
3:C:606:ASN:HD21	2:E:22:PHE:HD2	1.57	0.50
3:C:596:THR:HG22	3:C:596:THR:O	2.12	0.50
1:A:275:SER:OG	1:A:573:TRP:NE1	2.44	0.50
1:J:321:ALA:HB3	1:J:375:LEU:HD11	1.92	0.50
3:F:238:GLU:O	3:F:242:ASN:ND2	2.32	0.50
3:F:596:THR:O	3:F:596:THR:HG22	2.12	0.50
3:H:112:HIS:CE1	3:H:116:MET:HE3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:626:GLU:HA	3:I:629:ARG:CD	2.18	0.50
2:E:20:LYS:HE3	2:E:23:GLU:HG2	1.93	0.50
3:F:496:VAL:HA	3:F:501:VAL:HA	1.94	0.50
3:I:446:VAL:HG23	3:I:447:SER:H	1.76	0.50
1:J:190:LYS:CG	1:J:193:THR:HG22	2.38	0.50
3:F:225:LEU:HB2	3:F:272:HIS:HE1	1.73	0.50
3:F:225:LEU:HD12	3:F:276:ILE:HD13	1.93	0.50
2:K:23:GLU:C	2:K:25:LYS:HZ1	2.20	0.50
1:A:374:SER:OG	1:A:385:ILE:O	2.28	0.50
2:D:31:ALA:N	3:F:506:ARG:O	2.34	0.50
2:D:77:HIS:CD2	2:D:96:LEU:HD13	2.47	0.50
3:F:112:HIS:CE1	3:F:116:MET:HE3	2.46	0.50
3:C:412:LEU:HD22	3:C:454:MET:HE1	1.94	0.50
1:A:522:ASP:OD1	1:A:522:ASP:N	2.43	0.50
1:B:181:LEU:HD22	1:B:219:GLN:HB3	1.92	0.50
1:J:33:ILE:HD11	1:J:72:VAL:HG22	1.93	0.50
3:F:213:SER:O	3:F:214:ALA:C	2.55	0.50
3:H:218:GLN:O	3:H:221:SER:HB3	2.12	0.50
3:H:706:ALA:HA	3:H:709:ARG:HH21	1.77	0.50
3:I:112:HIS:CE1	3:I:116:MET:HE3	2.46	0.50
2:E:23:GLU:C	2:E:25:LYS:HZ1	2.20	0.50
1:B:65:SER:N	1:B:68:LYS:HZ1	2.09	0.49
3:I:596:THR:HG22	3:I:596:THR:O	2.12	0.49
3:I:470:LEU:CD1	3:I:474:PHE:CE2	2.81	0.49
3:C:258:GLU:HB2	3:C:259:PRO:HD3	1.93	0.49
3:C:325:GLY:HA3	3:C:377:PHE:CD1	2.47	0.49
1:A:210:SER:HA	1:A:213:LEU:HB2	1.94	0.49
1:J:522:ASP:OD1	1:J:522:ASP:N	2.43	0.49
3:F:298:CYS:HA	3:F:301:LYS:HG2	1.93	0.49
3:H:213:SER:O	3:H:214:ALA:C	2.55	0.49
3:H:255:SER:O	3:H:257:GLU:N	2.46	0.49
2:L:20:LYS:HE3	2:L:23:GLU:HG2	1.93	0.49
1:A:8:GLN:NE2	1:B:18:LEU:HB3	2.28	0.49
1:G:289:SER:HG	1:G:294:LYS:H	1.58	0.49
3:I:717:MET:HB3	3:I:722:LEU:H	1.77	0.49
1:G:431:ILE:HB	1:G:442:TYR:HB3	1.95	0.49
3:I:697:ASP:HA	3:I:700:LYS:HD2	1.94	0.49
2:D:23:GLU:C	2:D:25:LYS:HZ1	2.20	0.49
2:K:20:LYS:HE3	2:K:23:GLU:HG2	1.94	0.49
3:F:255:SER:O	3:F:257:GLU:N	2.46	0.49
2:L:84:ILE:HG12	2:L:101:TRP:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:374:SER:OG	1:J:385:ILE:O	2.28	0.49
3:H:128:ARG:O	3:H:132:GLN:HB2	2.13	0.49
3:H:258:GLU:HB2	3:H:259:PRO:HD3	1.93	0.49
3:H:559:LEU:HD11	2:K:22:PHE:HB3	1.95	0.49
3:I:506:ARG:O	2:L:31:ALA:N	2.35	0.49
3:C:451:GLU:O	3:C:455:ILE:HG22	2.13	0.49
2:E:35:TRP:CD1	2:E:75:CYS:O	2.65	0.49
1:A:399:VAL:HG12	1:A:414:PRO:HA	1.95	0.49
1:J:37:VAL:HG21	1:J:82:LEU:HD23	1.95	0.49
2:D:20:LYS:HE3	2:D:23:GLU:HG2	1.93	0.49
3:C:560:ASN:CB	2:E:25:LYS:HG2	2.31	0.49
1:B:160:PHE:HE2	1:B:169:PHE:CE2	2.31	0.49
1:J:431:ILE:HB	1:J:442:TYR:HB3	1.95	0.49
2:K:35:TRP:CD1	2:K:75:CYS:O	2.65	0.49
3:I:477:MET:HE3	3:I:513:TRP:CH2	2.48	0.49
1:A:9:ILE:HG23	1:B:93:ASN:HD21	1.78	0.48
1:J:268:MET:HB3	1:J:287:CYS:SG	2.53	0.48
2:L:23:GLU:C	2:L:25:LYS:HZ1	2.20	0.48
3:C:559:LEU:HD11	2:E:22:PHE:HB3	1.95	0.48
1:A:161:THR:HB	1:A:188:VAL:CG1	2.37	0.48
3:F:217:PHE:O	3:F:218:GLN:C	2.56	0.48
3:I:477:MET:HE3	3:I:513:TRP:HH2	1.78	0.48
3:C:446:VAL:HG23	3:C:447:SER:H	1.76	0.48
1:A:431:ILE:HB	1:A:442:TYR:HB3	1.95	0.48
1:B:455:ARG:NH1	1:B:500:GLU:OE2	2.46	0.48
1:G:455:ARG:NH1	1:G:500:GLU:OE2	2.46	0.48
1:J:48:VAL:HG21	1:J:90:TYR:CZ	2.49	0.48
3:F:77:LEU:HD22	3:F:123:LEU:HD22	1.95	0.48
3:F:626:GLU:HA	3:F:629:ARG:CD	2.18	0.48
3:H:598:GLN:HB3	3:H:634:LEU:HD11	1.95	0.48
2:K:47:ASN:ND2	2:K:54:ILE:HG23	2.24	0.48
3:I:700:LYS:O	3:I:703:ILE:HG12	2.13	0.48
3:I:711:MET:HA	3:I:714:ARG:HB2	1.95	0.48
3:C:255:SER:O	3:C:257:GLU:N	2.46	0.48
1:G:399:VAL:HG13	1:G:415:LEU:HD21	1.94	0.48
1:G:455:ARG:NH1	1:G:457:THR:O	2.47	0.48
3:F:245:ILE:CA	3:F:248:VAL:HG12	2.41	0.48
3:I:128:ARG:O	3:I:132:GLN:HB2	2.13	0.48
3:I:629:ARG:O	3:I:632:GLN:HG3	2.14	0.48
3:I:706:ALA:HA	3:I:709:ARG:HH21	1.77	0.48
2:L:27:TRP:CE2	2:L:29:ALA:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:128:ARG:O	3:C:132:GLN:HB2	2.13	0.48
1:A:144:SER:CB	3:C:133:GLN:HG2	2.44	0.48
2:D:27:TRP:CE2	2:D:29:ALA:HB2	2.49	0.48
3:H:77:LEU:HD22	3:H:123:LEU:HD22	1.95	0.48
1:G:18:LEU:HB3	1:J:8:GLN:NE2	2.28	0.48
1:G:529:VAL:O	1:G:530:ILE:HG13	2.14	0.48
1:J:455:ARG:NH1	1:J:457:THR:O	2.47	0.48
2:D:35:TRP:CD1	2:D:75:CYS:O	2.65	0.48
3:F:598:GLN:HB3	3:F:634:LEU:HD11	1.95	0.48
3:F:703:ILE:HB	3:F:741:ILE:HD13	1.95	0.48
3:I:614:GLU:HA	3:I:617:GLN:HG2	1.96	0.48
2:L:35:TRP:CD1	2:L:75:CYS:O	2.65	0.48
1:G:13:TYR:C	1:G:13:TYR:CD2	2.92	0.48
1:J:397:ARG:CD	1:J:417:CYS:HA	2.40	0.48
1:J:455:ARG:NH1	1:J:500:GLU:OE2	2.46	0.48
2:D:89:LYS:HB3	3:F:768:ALA:HB1	1.96	0.48
3:F:198:ARG:O	3:F:202:GLU:HB3	2.14	0.48
3:F:629:ARG:O	3:F:632:GLN:HG3	2.14	0.48
3:H:191:MET:HE2	3:H:201:TYR:CD2	2.48	0.48
2:K:27:TRP:CE2	2:K:29:ALA:HB2	2.49	0.48
1:A:455:ARG:NH1	1:A:457:THR:O	2.47	0.48
1:J:413:SER:HB3	1:J:442:TYR:HE1	1.79	0.48
2:D:23:GLU:CB	2:D:25:LYS:HZ1	2.25	0.48
3:H:187:CYS:HB2	3:H:201:TYR:OH	2.14	0.48
3:H:614:GLU:HA	3:H:617:GLN:HG2	1.96	0.48
3:I:433:LYS:HB3	3:I:433:LYS:HE3	1.45	0.48
3:I:559:LEU:HD11	2:L:22:PHE:HB3	1.95	0.48
1:B:455:ARG:NH1	1:B:457:THR:O	2.47	0.48
1:G:318:ILE:HB	1:G:353:PHE:HB3	1.95	0.48
3:C:644:LEU:HD11	3:C:659:PHE:HB3	1.96	0.48
3:C:698:ASP:HA	3:C:701:HIS:CD2	2.48	0.48
1:A:368:PHE:HB3	1:A:389:SER:O	2.14	0.48
1:G:47:MET:HE2	1:J:21:LEU:HB3	1.94	0.48
1:G:48:VAL:HG21	1:G:90:TYR:CZ	2.49	0.48
1:G:413:SER:HB3	1:G:442:TYR:HE1	1.79	0.48
3:C:712:LYS:NZ	3:C:767:VAL:O	2.40	0.48
1:J:425:VAL:HB	1:J:466:ALA:HB2	1.96	0.47
1:J:529:VAL:O	1:J:530:ILE:HG13	2.14	0.47
3:F:393:ASP:HB2	3:F:435:HIS:CD2	2.49	0.47
3:F:559:LEU:O	3:F:592:LEU:N	2.39	0.47
3:F:644:LEU:HD11	3:F:659:PHE:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:458:LEU:HB3	3:H:467:THR:CG2	2.42	0.47
3:H:605:PHE:HE1	3:H:611:TYR:HB2	1.79	0.47
3:H:629:ARG:O	3:H:632:GLN:HG3	2.14	0.47
3:C:682:GLY:O	3:C:683:GLU:HG2	2.14	0.47
2:E:27:TRP:CE2	2:E:29:ALA:HB2	2.49	0.47
1:B:305:LEU:HB2	1:B:325:VAL:HB	1.96	0.47
1:G:37:VAL:HG13	1:G:77:VAL:HG23	1.96	0.47
1:G:47:MET:O	1:G:51:THR:HG23	2.15	0.47
3:F:614:GLU:HA	3:F:617:GLN:HG2	1.96	0.47
3:F:682:GLY:O	3:F:683:GLU:HG2	2.14	0.47
3:H:644:LEU:HD11	3:H:659:PHE:HB3	1.96	0.47
3:I:470:LEU:HD11	3:I:474:PHE:CD2	2.47	0.47
3:I:559:LEU:O	3:I:592:LEU:N	2.39	0.47
3:C:614:GLU:HA	3:C:617:GLN:HG2	1.96	0.47
3:C:629:ARG:O	3:C:632:GLN:HG3	2.14	0.47
1:A:289:SER:HG	1:A:294:LYS:H	1.58	0.47
3:F:420:ARG:HA	3:F:461:GLU:OE2	2.14	0.47
3:F:605:PHE:HE1	3:F:611:TYR:HB2	1.79	0.47
3:H:338:PRO:HB3	3:H:387:TYR:CG	2.48	0.47
3:I:689:LYS:HD2	3:I:689:LYS:HA	1.49	0.47
3:C:684:SER:O	3:C:688:ARG:HB2	2.14	0.47
1:G:305:LEU:HB2	1:G:325:VAL:HB	1.97	0.47
1:G:393:GLU:HB2	1:G:396:ARG:HA	1.95	0.47
1:J:305:LEU:HB2	1:J:325:VAL:HB	1.96	0.47
3:F:723:VAL:HG11	3:F:742:LYS:HZ3	1.79	0.47
3:H:346:LEU:CB	3:H:418:LEU:CD1	2.92	0.47
3:H:470:LEU:CD1	3:H:474:PHE:CE2	2.81	0.47
3:I:169:ILE:HG12	3:I:209:PHE:HE1	1.79	0.47
3:C:605:PHE:HE1	3:C:611:TYR:HB2	1.79	0.47
1:A:422:SER:OG	1:A:434:MET:O	2.24	0.47
1:A:425:VAL:HB	1:A:466:ALA:HB2	1.96	0.47
1:A:529:VAL:O	1:A:530:ILE:HG13	2.14	0.47
1:G:51:THR:HG21	1:J:17:LEU:HD12	1.96	0.47
1:G:304:ASP:OD1	1:G:304:ASP:N	2.47	0.47
3:H:191:MET:HE2	3:H:201:TYR:HD2	1.79	0.47
3:H:682:GLY:O	3:H:683:GLU:HG2	2.14	0.47
1:A:305:LEU:HB2	1:A:325:VAL:HB	1.96	0.47
1:A:455:ARG:NH1	1:A:500:GLU:OE2	2.46	0.47
1:G:350:PHE:HD2	1:G:363:LYS:HB2	1.80	0.47
3:H:712:LYS:NZ	3:H:767:VAL:O	2.40	0.47
3:I:47:LYS:HA	3:I:47:LYS:HD2	1.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:458:LEU:HB3	3:I:467:THR:CG2	2.41	0.47
3:C:345:LEU:HG	3:C:418:LEU:HD22	1.96	0.47
3:C:598:GLN:HB3	3:C:634:LEU:HD11	1.95	0.47
1:A:265:LYS:HD3	1:A:587:TYR:OH	2.15	0.47
1:A:318:ILE:HB	1:A:353:PHE:HB3	1.95	0.47
1:B:134:VAL:HG21	1:B:169:PHE:HA	1.96	0.47
1:B:160:PHE:CE2	1:B:169:PHE:CE2	3.02	0.47
1:B:304:ASP:OD1	1:B:304:ASP:N	2.47	0.47
1:B:530:ILE:HB	1:B:564:ARG:HH12	1.78	0.47
1:J:265:LYS:HD3	1:J:587:TYR:OH	2.15	0.47
1:J:318:ILE:HB	1:J:353:PHE:HB3	1.95	0.47
3:F:363:ASP:HB3	3:F:366:PHE:HD1	1.79	0.47
3:F:446:VAL:HG23	3:F:447:SER:H	1.76	0.47
3:F:609:GLU:HG3	3:F:610:LYS:H	1.80	0.47
3:I:77:LEU:HD22	3:I:123:LEU:HD22	1.95	0.47
3:I:339:VAL:HA	3:I:391:PHE:HD1	1.80	0.47
3:I:598:GLN:HB3	3:I:634:LEU:HD11	1.95	0.47
3:C:559:LEU:O	3:C:592:LEU:N	2.39	0.47
1:A:304:ASP:OD1	1:A:304:ASP:N	2.47	0.47
1:B:302:PRO:HG2	1:B:305:LEU:HB3	1.97	0.47
1:G:265:LYS:HD3	1:G:587:TYR:OH	2.15	0.47
3:I:102:LEU:HD12	3:I:102:LEU:C	2.40	0.47
3:I:682:GLY:O	3:I:683:GLU:HG2	2.14	0.47
1:A:195:ARG:HG3	1:A:224:ALA:HB1	1.97	0.47
1:B:390:VAL:CG1	1:B:393:GLU:HG3	2.43	0.47
1:G:227:GLU:HB3	1:G:228:VAL:H	1.63	0.47
2:D:22:PHE:HB3	3:F:559:LEU:HD11	1.95	0.47
3:F:398:LYS:HA	3:F:398:LYS:HD3	1.53	0.47
3:H:245:ILE:CA	3:H:248:VAL:HG12	2.41	0.47
3:I:609:GLU:HG3	3:I:610:LYS:H	1.80	0.47
3:C:374:PHE:O	3:C:421:PHE:HB3	2.15	0.47
1:A:144:SER:CB	3:C:129:VAL:HG23	2.45	0.47
1:A:326:PRO:HA	1:A:344:PHE:HA	1.97	0.47
1:B:425:VAL:HB	1:B:466:ALA:HB2	1.96	0.47
1:G:297:LYS:HZ1	1:G:595:PRO:HD3	1.77	0.47
1:J:326:PRO:HA	1:J:344:PHE:HA	1.98	0.47
3:C:477:MET:HE3	3:C:513:TRP:HH2	1.80	0.47
1:A:8:GLN:HE22	1:B:18:LEU:HB3	1.80	0.46
1:A:388:ASP:C	1:A:390:VAL:N	2.71	0.46
1:G:425:VAL:HB	1:G:466:ALA:HB2	1.96	0.46
1:J:202:LEU:HD22	1:J:213:LEU:HG	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:LEU:HD22	3:C:123:LEU:HD22	1.96	0.46
1:A:265:LYS:HE2	1:A:265:LYS:HA	1.98	0.46
1:B:265:LYS:HE2	1:B:265:LYS:HA	1.98	0.46
1:J:304:ASP:N	1:J:304:ASP:OD1	2.47	0.46
3:F:102:LEU:HD12	3:F:102:LEU:C	2.40	0.46
3:F:346:LEU:CD1	3:F:414:LYS:HB3	2.46	0.46
3:H:102:LEU:HD12	3:H:102:LEU:C	2.40	0.46
3:H:477:MET:HE3	3:H:513:TRP:CH2	2.50	0.46
3:C:623:PRO:HB2	3:C:624:GLU:H	1.63	0.46
1:B:161:THR:HB	1:B:188:VAL:CG1	2.37	0.46
1:B:171:GLN:HA	1:B:171:GLN:OE1	2.15	0.46
1:B:265:LYS:HD3	1:B:587:TYR:OH	2.15	0.46
3:H:336:LYS:HE3	3:H:387:TYR:CE2	2.50	0.46
3:C:102:LEU:HD12	3:C:102:LEU:C	2.40	0.46
3:C:525:PRO:HB2	3:C:528:PRO:HD2	1.96	0.46
3:C:692:ARG:HA	3:C:692:ARG:HD3	1.66	0.46
1:J:353:PHE:HB2	1:J:360:TRP:CH2	2.51	0.46
3:I:644:LEU:HD11	3:I:659:PHE:HB3	1.96	0.46
3:C:393:ASP:HA	3:C:439:ARG:NH2	2.25	0.46
3:C:395:LYS:HA	3:C:395:LYS:HD3	1.70	0.46
3:C:477:MET:HE3	3:C:513:TRP:CH2	2.50	0.46
1:B:318:ILE:HB	1:B:353:PHE:HB3	1.95	0.46
3:H:395:LYS:HA	3:H:395:LYS:HD3	1.59	0.46
3:I:605:PHE:HE1	3:I:611:TYR:HB2	1.79	0.46
3:C:646:LYS:HE3	3:C:659:PHE:HE1	1.80	0.46
3:H:429:GLU:HG2	3:H:466:PHE:HB3	1.98	0.46
3:I:509:THR:HG23	2:L:76:ASN:HD22	1.80	0.46
2:L:23:GLU:CB	2:L:25:LYS:HZ1	2.26	0.46
1:A:212:TYR:C	1:A:214:SER:N	2.74	0.46
1:G:326:PRO:HA	1:G:344:PHE:HA	1.97	0.46
3:F:646:LYS:HE3	3:F:659:PHE:HE1	1.80	0.46
3:H:224:PHE:O	3:H:225:LEU:C	2.59	0.46
1:B:422:SER:OG	1:B:434:MET:O	2.24	0.46
1:G:220:ILE:HG13	1:G:220:ILE:O	2.15	0.46
1:J:302:PRO:HG2	1:J:305:LEU:HB3	1.97	0.46
3:I:393:ASP:O	3:I:394:ASP:C	2.59	0.46
3:I:425:LYS:CE	3:I:462:CYS:SG	3.04	0.46
3:C:509:THR:C	2:E:32:LEU:HD11	2.41	0.46
3:C:516:GLN:HE21	3:C:516:GLN:HB3	1.48	0.46
1:A:51:THR:HG21	1:B:17:LEU:HD13	1.93	0.46
1:A:302:PRO:HG2	1:A:305:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:PRO:HB2	1:B:302:PRO:HD3	1.98	0.46
1:B:353:PHE:HB2	1:B:360:TRP:CH2	2.51	0.46
1:G:265:LYS:HA	1:G:265:LYS:HE2	1.98	0.46
1:G:353:PHE:HB2	1:G:360:TRP:CH2	2.51	0.46
3:F:198:ARG:HH21	3:F:202:GLU:HG3	1.80	0.46
3:F:503:LEU:HD21	3:F:531:ALA:CB	2.39	0.46
3:H:703:ILE:HB	3:H:741:ILE:HD13	1.97	0.46
3:I:520:PRO:HG2	3:I:552:HIS:H	1.80	0.46
3:I:646:LYS:HE3	3:I:659:PHE:HE1	1.80	0.46
3:C:455:ILE:HA	3:C:458:LEU:HB2	1.98	0.46
3:C:723:VAL:HA	3:C:726:VAL:HG12	1.98	0.46
1:J:350:PHE:HD2	1:J:363:LYS:HB2	1.80	0.46
3:I:438:ARG:HD2	3:I:438:ARG:HA	1.52	0.46
3:C:207:ALA:HB3	3:C:208:PRO:HD3	1.98	0.46
3:C:215:GLU:OE1	3:C:215:GLU:N	2.49	0.46
3:F:148:ARG:HH11	3:F:200:VAL:HG21	1.81	0.45
3:H:723:VAL:HA	3:H:726:VAL:HG12	1.98	0.45
3:C:346:LEU:HD11	3:C:414:LYS:CB	2.46	0.45
3:C:609:GLU:HG3	3:C:610:LYS:H	1.80	0.45
1:A:265:LYS:CD	1:A:587:TYR:CZ	3.00	0.45
1:A:297:LYS:HZ1	1:A:595:PRO:HD3	1.80	0.45
1:A:350:PHE:HD2	1:A:363:LYS:HB2	1.80	0.45
1:B:48:VAL:HG21	1:B:90:TYR:CZ	2.51	0.45
1:B:198:ALA:HB1	1:B:216:VAL:HG12	1.98	0.45
1:B:350:PHE:HD2	1:B:363:LYS:HB2	1.80	0.45
1:J:402:TYR:HB2	1:J:409:TRP:CZ3	2.51	0.45
1:A:146:GLU:HG2	3:C:133:GLN:OE1	2.16	0.45
1:B:66:GLU:HG2	3:F:54:PHE:HB3	1.98	0.45
1:G:222:ILE:HG12	1:G:257:PHE:CD1	2.51	0.45
1:J:265:LYS:HA	1:J:265:LYS:HE2	1.98	0.45
3:H:609:GLU:HG3	3:H:610:LYS:H	1.80	0.45
3:H:682:GLY:C	3:H:683:GLU:OE1	2.60	0.45
1:A:353:PHE:HB2	1:A:360:TRP:CH2	2.51	0.45
1:A:366:MET:HE2	1:A:368:PHE:H	1.82	0.45
1:B:265:LYS:HE2	1:B:585:LYS:HB3	1.99	0.45
3:H:425:LYS:CE	3:H:462:CYS:SG	3.04	0.45
3:I:560:ASN:CB	2:L:25:LYS:HG2	2.30	0.45
3:C:148:ARG:HH11	3:C:200:VAL:HG21	1.80	0.45
3:C:459:LYS:HZ1	3:C:468:SER:HA	1.82	0.45
3:C:748:LEU:HD13	3:C:748:LEU:HA	1.75	0.45
2:E:88:LEU:HD22	2:E:88:LEU:HA	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:MET:HE3	1:B:66:GLU:HB3	1.98	0.45
1:B:160:PHE:HE2	1:B:169:PHE:CZ	2.10	0.45
1:B:275:SER:O	1:B:276:SER:C	2.59	0.45
1:G:265:LYS:CD	1:G:587:TYR:CZ	3.00	0.45
1:G:301:PRO:HB2	1:G:302:PRO:HD3	1.99	0.45
3:H:560:ASN:CB	2:K:25:LYS:HG2	2.31	0.45
1:A:237:LEU:HB2	1:A:238:PRO:CD	2.46	0.45
1:B:57:ARG:O	1:B:61:MET:HB2	2.17	0.45
1:B:128:ILE:HG12	1:B:136:LEU:HD21	1.99	0.45
1:J:287:CYS:SG	1:J:288:TYR:N	2.90	0.45
3:H:200:VAL:O	3:H:201:TYR:C	2.58	0.45
3:H:749:ILE:HD13	3:H:758:PRO:HD3	1.98	0.45
3:C:682:GLY:C	3:C:683:GLU:OE1	2.60	0.45
1:A:37:VAL:HG21	1:A:82:LEU:HD23	1.99	0.45
1:B:156:VAL:O	1:B:160:PHE:HB3	2.17	0.45
1:B:231:ARG:HD2	1:B:231:ARG:N	2.32	0.45
1:B:289:SER:HG	1:B:294:LYS:H	1.59	0.45
1:J:265:LYS:CD	1:J:587:TYR:CZ	3.00	0.45
1:J:376:VAL:N	1:J:383:TYR:O	2.45	0.45
1:J:566:HIS:O	1:J:566:HIS:ND1	2.50	0.45
3:F:440:LEU:HB2	3:F:513:TRP:CH2	2.50	0.45
3:F:520:PRO:HG2	3:F:552:HIS:H	1.81	0.45
3:H:473:MET:CG	3:H:512:TYR:HB3	2.47	0.45
3:H:491:LEU:C	3:H:493:ALA:N	2.75	0.45
3:C:223:LYS:HE3	3:C:227:GLU:HG3	1.99	0.45
1:A:287:CYS:SG	1:A:288:TYR:N	2.90	0.45
1:A:566:HIS:O	1:A:566:HIS:ND1	2.50	0.45
1:B:84:ILE:HA	1:B:87:THR:HG22	1.99	0.45
1:B:269:MET:HE2	1:B:269:MET:HA	1.98	0.45
1:B:326:PRO:HA	1:B:344:PHE:HA	1.98	0.45
1:G:265:LYS:HE2	1:G:585:LYS:HB3	1.99	0.45
1:G:302:PRO:HG2	1:G:305:LEU:HB3	1.97	0.45
1:J:231:ARG:HD2	1:J:231:ARG:N	2.32	0.45
1:J:265:LYS:HE2	1:J:585:LYS:HB3	1.99	0.45
3:F:689:LYS:HD2	3:F:689:LYS:HA	1.41	0.45
3:I:703:ILE:HB	3:I:741:ILE:HD13	1.99	0.45
2:L:41:ASN:HD21	2:L:46:ARG:HD2	1.79	0.45
3:C:419:PHE:HE1	3:C:425:LYS:HB2	1.82	0.45
1:G:128:ILE:HG23	1:G:136:LEU:HD21	1.99	0.45
1:J:156:VAL:O	1:J:160:PHE:HB3	2.17	0.45
1:J:366:MET:HE2	1:J:368:PHE:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:425:LYS:HE2	3:F:425:LYS:HB3	1.37	0.45
3:F:682:GLY:C	3:F:683:GLU:OE1	2.60	0.45
3:F:714:ARG:NH1	3:F:725:GLU:OE2	2.50	0.45
3:H:338:PRO:HB3	3:H:387:TYR:HA	1.99	0.45
3:I:682:GLY:C	3:I:683:GLU:OE1	2.60	0.45
3:I:723:VAL:HA	3:I:726:VAL:HG12	1.98	0.45
3:C:436:LEU:HD23	3:C:439:ARG:HH11	1.82	0.45
1:B:128:ILE:HG23	1:B:136:LEU:HD21	1.99	0.45
1:B:366:MET:HE2	1:B:368:PHE:H	1.82	0.45
1:G:287:CYS:SG	1:G:288:TYR:N	2.90	0.45
1:J:539:ARG:HH22	1:J:577:ARG:HD3	1.82	0.45
3:F:230:ALA:HB2	3:F:276:ILE:HG13	1.99	0.45
3:F:694:LYS:HD2	3:F:694:LYS:HA	1.63	0.45
3:H:697:ASP:HA	3:H:700:LYS:HD2	1.98	0.45
3:I:714:ARG:HB3	3:I:715:LYS:H	1.61	0.45
3:C:455:ILE:HG12	3:C:459:LYS:HG2	1.98	0.45
1:B:265:LYS:CD	1:B:587:TYR:CZ	3.00	0.44
1:G:12:GLU:HA	1:G:15:VAL:CG2	2.47	0.44
1:G:255:LYS:HE2	1:G:255:LYS:HB2	1.70	0.44
2:D:25:LYS:HG2	3:F:560:ASN:CB	2.31	0.44
3:F:436:LEU:HD23	3:F:439:ARG:HH11	1.82	0.44
3:H:391:PHE:O	3:H:392:ILE:C	2.60	0.44
3:C:731:LYS:HD3	3:C:731:LYS:HA	1.49	0.44
1:A:376:VAL:N	1:A:383:TYR:O	2.45	0.44
3:F:440:LEU:CD1	3:F:513:TRP:CH2	3.00	0.44
3:H:190:LEU:C	3:H:201:TYR:HB2	2.42	0.44
3:I:592:LEU:HD23	3:I:672:VAL:HG13	1.99	0.44
3:C:376:TYR:O	3:C:379:ASN:HB2	2.17	0.44
3:C:665:PHE:CD1	3:C:665:PHE:C	2.69	0.44
3:C:714:ARG:NH1	3:C:725:GLU:OE2	2.50	0.44
2:E:98:ASN:HD22	2:E:98:ASN:HA	1.58	0.44
1:B:566:HIS:O	1:B:566:HIS:ND1	2.50	0.44
1:G:62:SER:HA	3:I:118:MET:HG2	2.00	0.44
1:G:78:ASP:OD1	1:G:79:ALA:N	2.51	0.44
1:G:366:MET:HE2	1:G:368:PHE:H	1.82	0.44
1:J:128:ILE:HG23	1:J:136:LEU:HD21	1.99	0.44
3:F:215:GLU:O	3:F:216:PHE:C	2.60	0.44
3:H:225:LEU:HB2	3:H:272:HIS:CE1	2.52	0.44
3:H:436:LEU:HD23	3:H:439:ARG:HH11	1.82	0.44
2:K:88:LEU:HD22	2:K:92:GLN:HA	1.98	0.44
3:I:396:LEU:HD23	3:I:439:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:ARG:HH22	1:B:577:ARG:HD3	1.83	0.44
1:G:397:ARG:O	1:G:414:PRO:HB2	2.18	0.44
1:J:128:ILE:HG12	1:J:136:LEU:HD21	1.99	0.44
1:J:301:PRO:HB2	1:J:302:PRO:HD3	1.99	0.44
3:I:204:ASP:O	3:I:208:PRO:HD2	2.17	0.44
3:I:230:ALA:HB2	3:I:276:ILE:HG13	1.99	0.44
3:I:346:LEU:HD12	3:I:346:LEU:HA	1.73	0.44
3:I:476:ASP:OD1	3:I:508:LEU:HD22	2.17	0.44
3:I:692:ARG:HD3	3:I:692:ARG:HA	1.62	0.44
1:A:301:PRO:HB2	1:A:302:PRO:HD3	1.99	0.44
1:B:282:LEU:HD23	1:B:282:LEU:HA	1.78	0.44
1:G:287:CYS:N	1:G:296:TYR:O	2.41	0.44
1:G:566:HIS:O	1:G:566:HIS:ND1	2.50	0.44
3:F:692:ARG:HD3	3:F:692:ARG:HA	1.50	0.44
3:I:707:ILE:HG12	3:I:726:VAL:HG21	2.00	0.44
3:C:265:GLU:HB3	3:C:306:VAL:HG22	2.00	0.44
3:C:632:GLN:HB2	3:C:636:CYS:HB3	2.00	0.44
1:A:265:LYS:HE2	1:A:585:LYS:HB3	1.99	0.44
1:A:539:ARG:HH22	1:A:577:ARG:HD3	1.82	0.44
1:B:78:ASP:OD1	1:B:79:ALA:N	2.51	0.44
3:F:592:LEU:HD23	3:F:672:VAL:HG13	1.99	0.44
3:H:230:ALA:HB2	3:H:276:ILE:HG13	1.99	0.44
3:H:476:ASP:OD1	3:H:508:LEU:HD22	2.17	0.44
1:A:128:ILE:HG23	1:A:136:LEU:HD21	1.99	0.44
1:J:211:GLN:H	1:J:211:GLN:HG3	1.56	0.44
3:H:113:GLN:O	3:H:117:VAL:HG23	2.18	0.44
3:H:653:ILE:N	3:H:653:ILE:HD13	2.33	0.44
3:H:689:LYS:HD2	3:H:689:LYS:HA	1.65	0.44
3:H:714:ARG:NH1	3:H:725:GLU:OE2	2.50	0.44
3:I:498:LEU:HD13	3:I:498:LEU:HA	1.74	0.44
3:I:634:LEU:HD23	3:I:634:LEU:HA	1.79	0.44
3:C:338:PRO:HA	3:C:341:TYR:CD2	2.52	0.44
3:C:653:ILE:N	3:C:653:ILE:HD13	2.33	0.44
1:A:78:ASP:OD1	1:A:79:ALA:N	2.51	0.44
1:B:211:GLN:H	1:B:211:GLN:HG3	1.37	0.44
1:B:287:CYS:SG	1:B:288:TYR:N	2.90	0.44
1:G:128:ILE:HG12	1:G:136:LEU:HD21	1.99	0.44
1:G:539:ARG:HH22	1:G:577:ARG:HD3	1.83	0.44
1:J:265:LYS:HD2	1:J:587:TYR:CZ	2.53	0.44
3:F:265:GLU:HB3	3:F:306:VAL:HG22	2.00	0.44
3:F:390:LEU:HD13	3:F:390:LEU:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:622:ILE:HG12	3:F:627:LEU:HB2	2.00	0.44
3:H:345:LEU:HG	3:H:418:LEU:HD11	2.00	0.44
3:H:509:THR:HG22	3:H:511:GLY:H	1.83	0.44
3:H:592:LEU:HD23	3:H:672:VAL:HG13	1.99	0.44
3:H:684:SER:O	3:H:688:ARG:HB2	2.17	0.44
3:C:230:ALA:HB2	3:C:276:ILE:HG13	1.99	0.44
1:B:37:VAL:HG21	1:B:82:LEU:HD23	1.99	0.44
1:B:265:LYS:HD2	1:B:587:TYR:CZ	2.53	0.44
3:H:632:GLN:HB2	3:H:636:CYS:HB3	2.00	0.44
3:I:731:LYS:HA	3:I:731:LYS:HD3	1.54	0.44
3:C:346:LEU:HD21	3:C:411:ILE:HA	2.00	0.44
2:E:47:ASN:O	2:E:48:HIS:HB2	2.18	0.44
1:A:128:ILE:HG12	1:A:136:LEU:HD21	1.99	0.43
1:A:415:LEU:H	1:A:415:LEU:HG	1.66	0.43
1:B:64:LEU:HB3	1:B:65:SER:H	1.61	0.43
1:G:58:ALA:HB1	3:I:121:ASP:CB	2.45	0.43
3:F:190:LEU:HB3	3:F:201:TYR:HB2	2.00	0.43
3:H:349:LYS:HE3	3:H:421:PHE:CE2	2.52	0.43
3:H:396:LEU:HD13	3:H:396:LEU:HA	1.81	0.43
3:H:646:LYS:HE3	3:H:659:PHE:HE1	1.80	0.43
3:I:337:ASN:OD1	3:I:339:VAL:HG13	2.17	0.43
3:I:751:ARG:HD2	3:I:751:ARG:HA	1.44	0.43
1:A:156:VAL:O	1:A:160:PHE:HB3	2.17	0.43
1:A:265:LYS:HD2	1:A:587:TYR:CZ	2.53	0.43
1:G:390:VAL:CG1	1:G:393:GLU:HG3	2.43	0.43
1:J:181:LEU:HD21	1:J:220:ILE:HD13	1.99	0.43
1:J:515:ILE:HG12	1:J:538:MET:HE1	2.00	0.43
3:F:113:GLN:O	3:F:117:VAL:HG23	2.18	0.43
3:F:425:LYS:N	3:F:733:ARG:O	2.50	0.43
3:F:464:CYS:O	3:F:465:GLN:C	2.61	0.43
3:F:653:ILE:N	3:F:653:ILE:HD13	2.33	0.43
3:F:751:ARG:HA	3:F:751:ARG:HD2	1.47	0.43
3:I:113:GLN:O	3:I:117:VAL:HG23	2.18	0.43
3:I:291:GLY:HA2	3:I:355:PHE:HZ	1.81	0.43
3:I:647:GLU:HB2	3:I:648:PRO:HD3	2.00	0.43
1:A:84:ILE:HA	1:A:87:THR:HG22	1.99	0.43
1:G:265:LYS:HD2	1:G:587:TYR:CZ	2.53	0.43
3:F:723:VAL:HA	3:F:726:VAL:HG12	1.98	0.43
3:F:752:GLU:HB2	3:F:753:TYR:H	1.52	0.43
3:H:707:ILE:HG12	3:H:726:VAL:HG21	2.00	0.43
3:C:86:ILE:HG23	3:C:90:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:153:ARG:HH21	3:C:200:VAL:HG13	1.83	0.43
3:C:225:LEU:HB3	3:C:272:HIS:CE1	2.53	0.43
3:C:592:LEU:HD23	3:C:672:VAL:HG13	1.99	0.43
1:A:22:LYS:NZ	1:B:6:GLU:OE1	2.51	0.43
3:H:86:ILE:HG23	3:H:90:ARG:HD2	2.00	0.43
3:H:470:LEU:HD11	3:H:474:PHE:CD2	2.47	0.43
3:I:86:ILE:HG23	3:I:90:ARG:HD2	2.00	0.43
3:I:212:MET:HE3	3:I:212:MET:HB3	1.62	0.43
3:C:508:LEU:HB3	3:C:513:TRP:CD1	2.54	0.43
3:C:526:PRO:O	3:C:529:ARG:HB2	2.18	0.43
3:C:527:ALA:HB3	3:C:528:PRO:HD3	2.00	0.43
1:A:133:CYS:SG	1:A:134:VAL:N	2.92	0.43
1:A:419:TRP:HZ2	1:A:438:LEU:HD23	1.84	0.43
1:B:160:PHE:HE2	1:B:169:PHE:CD2	2.37	0.43
1:J:133:CYS:SG	1:J:134:VAL:N	2.92	0.43
3:H:221:SER:HA	3:H:272:HIS:NE2	2.33	0.43
3:H:553:HIS:HA	3:H:597:PHE:CE1	2.53	0.43
3:I:414:LYS:HD3	3:I:414:LYS:HA	1.77	0.43
3:I:653:ILE:HD13	3:I:653:ILE:N	2.33	0.43
2:L:47:ASN:O	2:L:48:HIS:HB2	2.18	0.43
3:C:647:GLU:HB2	3:C:648:PRO:HD3	2.00	0.43
1:A:48:VAL:HA	1:A:51:THR:HG22	2.01	0.43
1:A:515:ILE:HG12	1:A:538:MET:HE1	2.00	0.43
3:F:441:LEU:CD1	3:F:554:MET:HE3	2.45	0.43
1:A:270:ILE:HD11	1:A:584:GLY:HA3	2.00	0.43
1:J:48:VAL:HA	1:J:51:THR:HG22	2.01	0.43
1:J:233:TRP:HH2	1:J:245:VAL:CG2	2.25	0.43
1:J:253:MET:HE2	1:J:253:MET:HB2	1.87	0.43
3:F:647:GLU:HB2	3:F:648:PRO:HD3	2.00	0.43
3:F:707:ILE:HB	3:F:726:VAL:HG21	1.99	0.43
3:I:202:GLU:O	3:I:203:GLU:C	2.61	0.43
3:C:113:GLN:O	3:C:117:VAL:HG23	2.18	0.43
3:C:248:VAL:O	3:C:256:THR:HG21	2.18	0.43
1:B:366:MET:HE1	1:B:370:ARG:HE	1.84	0.43
3:F:269:ILE:HB	3:F:306:VAL:HG21	2.01	0.43
3:F:425:LYS:NZ	3:F:462:CYS:HB2	2.33	0.43
3:H:446:VAL:HG23	3:H:447:SER:H	1.76	0.43
3:H:647:GLU:HB2	3:H:648:PRO:HD3	2.00	0.43
3:I:423:GLN:HG2	3:I:424:GLU:H	1.83	0.43
3:C:414:LYS:HA	3:C:417:VAL:HB	2.00	0.43
3:C:634:LEU:HD23	3:C:634:LEU:HA	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:MET:HB3	1:A:287:CYS:SG	2.58	0.43
1:B:193:THR:HG23	1:B:194:VAL:N	2.34	0.43
1:G:233:TRP:HH2	1:G:245:VAL:CG2	2.25	0.43
3:H:265:GLU:HB3	3:H:306:VAL:HG22	2.00	0.43
3:H:423:GLN:HG2	3:H:424:GLU:H	1.83	0.43
3:I:201:TYR:O	3:I:202:GLU:C	2.61	0.43
3:I:553:HIS:HA	3:I:597:PHE:CE1	2.53	0.43
3:I:717:MET:HA	3:I:721:VAL:HB	2.00	0.43
1:G:133:CYS:SG	1:G:134:VAL:N	2.91	0.43
3:F:86:ILE:HG23	3:F:90:ARG:HD2	2.00	0.43
3:H:511:GLY:O	3:H:512:TYR:C	2.61	0.43
3:I:488:ARG:HA	3:I:488:ARG:HD2	1.49	0.43
3:I:715:LYS:HB2	3:I:722:LEU:HD21	2.00	0.43
2:L:52:LEU:HD12	2:L:56:CYS:HB3	2.01	0.43
3:C:346:LEU:CD2	3:C:411:ILE:HA	2.49	0.43
3:C:553:HIS:HA	3:C:597:PHE:CE1	2.53	0.43
1:A:193:THR:HG23	1:A:194:VAL:N	2.33	0.42
1:A:366:MET:HE1	1:A:370:ARG:HE	1.84	0.42
1:B:133:CYS:SG	1:B:134:VAL:N	2.91	0.42
1:G:268:MET:HB3	1:G:287:CYS:SG	2.59	0.42
3:F:204:ASP:O	3:F:205:PHE:C	2.62	0.42
3:F:553:HIS:HA	3:F:597:PHE:CE1	2.53	0.42
3:H:74:TYR:OH	3:H:137:GLU:OE2	2.37	0.42
3:H:527:ALA:HB3	3:H:528:PRO:HD3	2.00	0.42
2:K:52:LEU:HD12	2:K:56:CYS:HB3	2.01	0.42
1:A:325:VAL:O	1:A:345:ARG:N	2.50	0.42
1:J:366:MET:HE1	1:J:370:ARG:HE	1.84	0.42
3:F:425:LYS:HA	3:F:428:PHE:HB3	2.00	0.42
3:H:269:ILE:HB	3:H:306:VAL:HG21	2.01	0.42
2:K:47:ASN:O	2:K:48:HIS:HB2	2.18	0.42
3:I:265:GLU:HB3	3:I:306:VAL:HG22	2.00	0.42
3:I:345:LEU:HD13	3:I:418:LEU:HD21	2.01	0.42
3:I:491:LEU:HD23	3:I:491:LEU:HA	1.79	0.42
3:I:714:ARG:HA	3:I:714:ARG:HD2	1.75	0.42
3:C:74:TYR:OH	3:C:137:GLU:OE2	2.37	0.42
3:C:691:THR:HA	3:C:694:LYS:HB2	2.01	0.42
1:A:376:VAL:O	1:A:383:TYR:N	2.38	0.42
1:B:286:VAL:HA	1:B:297:LYS:HA	2.01	0.42
3:F:191:MET:HE2	3:F:201:TYR:CD2	2.54	0.42
3:F:525:PRO:HA	3:F:603:MET:HE2	2.01	0.42
3:F:541:ALA:CB	3:H:501:VAL:O	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:217:PHE:CE2	3:H:264:VAL:HG22	2.54	0.42
3:H:509:THR:C	3:H:511:GLY:N	2.76	0.42
3:H:526:PRO:O	3:H:529:ARG:HB2	2.18	0.42
3:I:632:GLN:HB2	3:I:636:CYS:HB3	2.00	0.42
1:A:148:LEU:O	1:A:149:LYS:C	2.60	0.42
1:A:402:TYR:HB2	1:A:409:TRP:CZ3	2.55	0.42
1:B:325:VAL:O	1:B:345:ARG:N	2.50	0.42
1:B:470:LYS:NZ	1:B:503:ASP:OD2	2.47	0.42
1:G:515:ILE:HG12	1:G:538:MET:HE1	2.00	0.42
1:J:419:TRP:HZ2	1:J:438:LEU:HD23	1.84	0.42
3:F:632:GLN:HB2	3:F:636:CYS:HB3	2.00	0.42
3:H:248:VAL:O	3:H:256:THR:HG21	2.18	0.42
3:H:516:GLN:HE22	3:H:551:GLN:HG3	1.85	0.42
3:I:723:VAL:HG11	3:I:742:LYS:HZ3	1.84	0.42
3:C:269:ILE:HB	3:C:306:VAL:HG21	2.01	0.42
3:C:711:MET:HG3	3:C:722:LEU:HD13	1.99	0.42
3:F:285:VAL:CG2	3:F:286:HIS:N	2.83	0.42
1:A:276:SER:OG	1:A:281:SER:O	2.35	0.42
1:B:223:ASP:HB3	1:B:257:PHE:HE1	1.85	0.42
1:B:225:LEU:HD12	1:B:225:LEU:HA	1.82	0.42
1:B:402:TYR:HB2	1:B:409:TRP:CZ3	2.54	0.42
1:G:231:ARG:HD2	1:G:231:ARG:N	2.32	0.42
1:J:426:VAL:O	1:J:426:VAL:CG1	2.68	0.42
3:F:168:MET:HE2	3:F:168:MET:HB3	1.95	0.42
3:H:484:MET:SD	3:H:504:THR:HA	2.59	0.42
3:I:36:LEU:C	3:I:36:LEU:HD12	2.45	0.42
1:A:91:THR:HA	1:B:8:GLN:OE1	2.20	0.42
1:B:160:PHE:CD2	1:B:169:PHE:CD1	3.06	0.42
1:B:515:ILE:HG12	1:B:538:MET:HE1	2.00	0.42
1:B:554:TYR:HB2	1:B:561:TRP:CD1	2.55	0.42
1:J:397:ARG:HD2	1:J:417:CYS:N	2.33	0.42
3:F:248:VAL:O	3:F:256:THR:HG21	2.18	0.42
3:F:441:LEU:O	3:F:554:MET:SD	2.77	0.42
3:I:74:TYR:OH	3:I:137:GLU:OE2	2.37	0.42
3:I:470:LEU:CD1	3:I:474:PHE:CD2	3.03	0.42
3:C:385:PRO:HB3	3:C:428:PHE:HB2	2.02	0.42
2:E:52:LEU:HD12	2:E:56:CYS:HB3	2.01	0.42
1:A:143:PHE:O	1:A:144:SER:C	2.62	0.42
1:A:225:LEU:HD12	1:A:225:LEU:HA	1.68	0.42
1:A:554:TYR:HB2	1:A:561:TRP:CD1	2.55	0.42
1:G:325:VAL:O	1:G:345:ARG:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:366:MET:HE1	1:G:370:ARG:HE	1.84	0.42
1:G:376:VAL:N	1:G:383:TYR:O	2.45	0.42
3:F:451:GLU:HB3	3:F:474:PHE:CE2	2.55	0.42
3:F:638:LYS:HZ3	3:F:674:ILE:HG23	1.84	0.42
3:H:408:VAL:O	3:H:411:ILE:HG22	2.19	0.42
3:I:285:VAL:CG2	3:I:286:HIS:N	2.83	0.42
3:C:733:ARG:HD3	3:C:733:ARG:HA	1.82	0.42
1:A:225:LEU:HG	1:A:230:GLN:HE22	1.84	0.42
1:A:286:VAL:HA	1:A:297:LYS:HA	2.01	0.42
1:A:597:LYS:HA	1:A:598:PRO:HD2	1.91	0.42
1:G:280:CYS:HB3	1:G:281:SER:H	1.71	0.42
1:G:286:VAL:HA	1:G:297:LYS:HA	2.01	0.42
1:G:597:LYS:HA	1:G:598:PRO:HD2	1.91	0.42
1:J:217:LEU:HG	1:J:225:LEU:HD11	2.01	0.42
3:H:383:ARG:HE	3:H:383:ARG:HB2	1.33	0.42
3:H:509:THR:C	3:H:511:GLY:H	2.28	0.42
3:H:720:ASN:OD1	3:H:742:LYS:NZ	2.47	0.42
1:G:221:ARG:HB3	1:G:255:LYS:HE2	2.02	0.42
1:G:539:ARG:HD3	1:G:549:TYR:CZ	2.55	0.42
1:J:325:VAL:O	1:J:345:ARG:N	2.50	0.42
3:F:593:GLN:HE21	3:F:593:GLN:HB3	1.71	0.42
3:H:217:PHE:HB2	3:H:267:GLU:OE1	2.20	0.42
3:H:470:LEU:CD1	3:H:474:PHE:CD2	3.03	0.42
3:I:419:PHE:O	3:I:422:MET:HB2	2.20	0.42
3:I:470:LEU:HD12	3:I:470:LEU:C	2.44	0.42
2:E:25:LYS:CE	2:E:25:LYS:CA	2.96	0.42
1:A:388:ASP:C	1:A:390:VAL:H	2.26	0.41
1:B:102:GLU:HG3	1:B:135:ARG:HH12	1.85	0.41
1:G:41:GLU:H	1:G:41:GLU:HG2	1.42	0.41
1:G:195:ARG:HE	1:G:195:ARG:HB3	1.61	0.41
3:I:526:PRO:HA	3:I:529:ARG:CB	2.49	0.41
3:I:638:LYS:HZ3	3:I:674:ILE:HG23	1.85	0.41
2:L:23:GLU:CB	2:L:25:LYS:NZ	2.83	0.41
3:C:36:LEU:HD12	3:C:36:LEU:C	2.45	0.41
3:C:430:ARG:HE	3:C:434:GLN:HE21	1.67	0.41
3:C:452:LYS:O	3:C:455:ILE:HG23	2.19	0.41
1:A:539:ARG:HD3	1:A:549:TYR:CZ	2.55	0.41
1:B:48:VAL:HA	1:B:51:THR:HG22	2.01	0.41
1:G:102:GLU:HG3	1:G:135:ARG:HH12	1.85	0.41
1:G:269:MET:HE2	1:G:269:MET:HA	2.01	0.41
1:G:419:TRP:HZ2	1:G:438:LEU:HD23	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:87:THR:O	1:J:91:THR:HG22	2.20	0.41
3:F:214:ALA:O	3:F:215:GLU:C	2.63	0.41
3:F:400:VAL:CG1	3:F:401:LYS:N	2.83	0.41
3:H:285:VAL:CG2	3:H:286:HIS:N	2.83	0.41
3:I:455:ILE:CG2	3:I:470:LEU:HD21	2.24	0.41
3:I:500:GLY:HA2	3:I:503:LEU:HD23	2.01	0.41
3:C:406:GLN:H	3:C:406:GLN:HG3	1.38	0.41
1:G:554:TYR:HB2	1:G:561:TRP:CD1	2.55	0.41
1:J:539:ARG:HD3	1:J:549:TYR:CZ	2.55	0.41
3:F:285:VAL:HG23	3:F:286:HIS:N	2.35	0.41
3:F:508:LEU:HB3	3:F:513:TRP:CD1	2.55	0.41
3:H:124:MET:HE3	3:H:124:MET:HB3	1.99	0.41
3:I:269:ILE:HB	3:I:306:VAL:HG21	2.01	0.41
2:L:41:ASN:ND2	2:L:46:ARG:HD2	2.36	0.41
2:L:52:LEU:HD21	2:L:59:ASN:HA	2.03	0.41
3:C:700:LYS:HG2	3:C:744:ARG:HD2	2.02	0.41
2:D:84:ILE:HD12	2:D:84:ILE:HA	1.93	0.41
3:F:266:ARG:O	3:F:270:SER:HB2	2.21	0.41
3:F:422:MET:HE1	3:F:428:PHE:HB2	2.02	0.41
3:F:477:MET:HE3	3:F:513:TRP:CH2	2.56	0.41
3:F:709:ARG:HE	3:F:709:ARG:HB3	1.34	0.41
3:H:223:LYS:HB3	3:H:223:LYS:HE2	1.25	0.41
3:H:266:ARG:O	3:H:270:SER:HB2	2.21	0.41
3:I:285:VAL:HG23	3:I:286:HIS:N	2.35	0.41
3:C:112:HIS:HE1	3:C:116:MET:HE3	1.85	0.41
1:G:253:MET:HE2	1:G:253:MET:HB2	1.80	0.41
1:J:286:VAL:HA	1:J:297:LYS:HA	2.01	0.41
1:J:554:TYR:HB2	1:J:561:TRP:CD1	2.55	0.41
3:F:112:HIS:HE1	3:F:116:MET:HE3	1.85	0.41
3:H:212:MET:HB3	3:H:212:MET:HE3	1.43	0.41
3:H:374:PHE:O	3:H:378:LEU:HB2	2.20	0.41
3:H:625:ARG:H	3:H:625:ARG:HG2	1.50	0.41
3:I:221:SER:HB2	3:I:272:HIS:NE2	2.35	0.41
3:I:332:GLU:CD	3:I:332:GLU:H	2.29	0.41
3:C:266:ARG:O	3:C:270:SER:HB2	2.21	0.41
3:C:285:VAL:CG2	3:C:286:HIS:N	2.83	0.41
3:C:390:LEU:HD13	3:C:390:LEU:HA	1.75	0.41
2:E:52:LEU:HD21	2:E:59:ASN:HA	2.03	0.41
1:A:87:THR:O	1:A:91:THR:HG22	2.20	0.41
1:B:419:TRP:HZ2	1:B:438:LEU:HD23	1.84	0.41
3:F:36:LEU:HD12	3:F:36:LEU:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:74:TYR:CZ	3:F:142:LEU:HD22	2.56	0.41
2:L:41:ASN:ND2	2:L:46:ARG:CG	2.84	0.41
1:A:426:VAL:O	1:A:426:VAL:CG1	2.68	0.41
1:B:212:TYR:O	1:B:216:VAL:HG23	2.20	0.41
1:G:426:VAL:O	1:G:426:VAL:CG1	2.68	0.41
2:D:23:GLU:CB	2:D:25:LYS:NZ	2.83	0.41
3:F:349:LYS:HE2	3:F:421:PHE:CE2	2.53	0.41
3:F:558:ASP:OD1	3:F:671:ARG:NH2	2.54	0.41
3:H:36:LEU:HD12	3:H:36:LEU:C	2.45	0.41
3:H:74:TYR:CZ	3:H:142:LEU:HD22	2.56	0.41
3:H:218:GLN:O	3:H:222:GLN:HG2	2.21	0.41
3:H:285:VAL:HG23	3:H:286:HIS:N	2.35	0.41
3:I:266:ARG:O	3:I:270:SER:HB2	2.21	0.41
3:C:558:ASP:OD1	3:C:671:ARG:NH2	2.54	0.41
3:F:200:VAL:O	3:F:201:TYR:C	2.64	0.41
3:H:112:HIS:HE1	3:H:116:MET:HE3	1.85	0.41
3:H:480:SER:HB3	3:H:508:LEU:HD23	2.03	0.41
3:I:749:ILE:HD13	3:I:758:PRO:HD3	2.02	0.41
3:C:346:LEU:HD11	3:C:414:LYS:HB3	2.03	0.41
3:C:707:ILE:HG13	3:C:711:MET:HG2	2.02	0.41
1:A:102:GLU:HG3	1:A:135:ARG:HH12	1.85	0.41
1:A:185:ASN:CG	1:A:356:GLN:HE22	2.29	0.41
1:A:457:THR:HG22	1:A:459:ARG:HG2	2.02	0.41
1:B:87:THR:O	1:B:91:THR:HG22	2.21	0.41
1:B:426:VAL:O	1:B:426:VAL:CG1	2.68	0.41
1:G:185:ASN:CG	1:G:356:GLN:HE22	2.29	0.41
1:G:277:GLU:H	1:G:277:GLU:HG3	1.55	0.41
1:G:457:THR:HG22	1:G:459:ARG:HG2	2.02	0.41
1:J:185:ASN:CG	1:J:356:GLN:HE22	2.29	0.41
2:D:31:ALA:O	3:F:507:VAL:HA	2.21	0.41
3:F:346:LEU:HD12	3:F:346:LEU:HA	1.72	0.41
3:H:539:TYR:HE2	3:H:546:ARG:HB2	1.85	0.41
3:H:558:ASP:OD1	3:H:671:ARG:NH2	2.54	0.41
3:H:752:GLU:O	3:H:753:TYR:C	2.63	0.41
2:K:41:ASN:ND2	2:K:46:ARG:CG	2.84	0.41
3:I:112:HIS:HE1	3:I:116:MET:HE3	1.85	0.41
3:I:480:SER:HB3	3:I:508:LEU:HD23	2.03	0.41
3:C:524:ILE:HG22	3:C:529:ARG:HG3	2.02	0.41
2:E:41:ASN:ND2	2:E:46:ARG:CG	2.84	0.41
2:E:41:ASN:ND2	2:E:46:ARG:HD2	2.36	0.41
3:F:752:GLU:H	3:F:752:GLU:HG2	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:52:LEU:HD21	2:K:59:ASN:HA	2.02	0.41
3:I:204:ASP:O	3:I:205:PHE:C	2.64	0.41
3:C:285:VAL:HG23	3:C:286:HIS:N	2.35	0.41
3:C:619:GLU:H	3:C:619:GLU:HG3	1.64	0.41
3:C:638:LYS:HG3	3:C:642:ARG:HG2	2.03	0.41
1:A:91:THR:HG23	1:A:93:ASN:HB3	2.03	0.40
1:A:226:SER:HB2	1:A:228:VAL:HG23	2.03	0.40
1:B:81:THR:O	1:B:84:ILE:HG22	2.21	0.40
1:B:238:PRO:HA	1:B:239:PRO:HD3	1.98	0.40
1:B:397:ARG:O	1:B:414:PRO:HB2	2.21	0.40
1:G:45:HIS:CD2	1:J:47:MET:CE	3.04	0.40
1:G:82:LEU:HD12	1:G:82:LEU:HA	1.84	0.40
1:G:402:TYR:HB2	1:G:409:TRP:CZ3	2.57	0.40
1:J:102:GLU:HG3	1:J:135:ARG:HH12	1.85	0.40
1:J:221:ARG:HG2	1:J:255:LYS:HG3	2.03	0.40
1:J:422:SER:OG	1:J:434:MET:O	2.24	0.40
2:D:32:LEU:HD11	3:F:509:THR:C	2.46	0.40
3:F:168:MET:SD	3:F:183:ILE:HD11	2.62	0.40
3:H:709:ARG:HE	3:H:709:ARG:HB3	1.37	0.40
3:H:752:GLU:HB3	3:H:753:TYR:H	1.72	0.40
3:I:168:MET:HE2	3:I:168:MET:HB3	1.94	0.40
3:I:558:ASP:OD1	3:I:671:ARG:NH2	2.54	0.40
2:L:45:CYS:HB2	2:L:54:ILE:HG12	2.04	0.40
1:A:22:LYS:NZ	1:B:6:GLU:CD	2.78	0.40
1:B:282:LEU:HB3	1:B:283:TYR:CD2	2.56	0.40
1:B:457:THR:HG22	1:B:459:ARG:HG2	2.02	0.40
1:G:191:GLU:OE1	1:G:223:ASP:HB3	2.22	0.40
1:G:283:TYR:HB2	1:G:306:HIS:ND1	2.36	0.40
1:J:376:VAL:O	1:J:383:TYR:N	2.39	0.40
1:J:457:THR:HG22	1:J:459:ARG:HG2	2.02	0.40
3:F:619:GLU:H	3:F:619:GLU:HG3	1.68	0.40
3:H:332:GLU:CD	3:H:332:GLU:H	2.29	0.40
3:H:512:TYR:CD2	2:K:104:GLN:NE2	2.88	0.40
3:H:703:ILE:HD11	3:H:744:ARG:HD3	2.03	0.40
3:I:148:ARG:HH11	3:I:200:VAL:HG21	1.86	0.40
3:I:375:GLU:HA	3:I:421:PHE:O	2.21	0.40
3:I:638:LYS:HG2	3:I:642:ARG:HA	2.03	0.40
3:C:74:TYR:CZ	3:C:142:LEU:HD22	2.56	0.40
1:A:211:GLN:H	1:A:211:GLN:HG3	1.40	0.40
1:B:37:VAL:HG12	1:B:38:GLU:CD	2.46	0.40
1:B:265:LYS:HD3	1:B:587:TYR:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:434:MET:HE2	1:G:455:ARG:NE	2.36	0.40
1:J:269:MET:HA	1:J:269:MET:HE2	2.03	0.40
3:F:124:MET:O	3:F:128:ARG:HG2	2.22	0.40
3:F:560:ASN:HA	3:F:591:ILE:HG13	2.03	0.40
3:F:634:LEU:HD23	3:F:634:LEU:HA	1.78	0.40
3:H:411:ILE:HD12	3:H:411:ILE:HA	1.86	0.40
3:H:634:LEU:HA	3:H:634:LEU:HD23	1.78	0.40
3:I:74:TYR:CZ	3:I:142:LEU:HD22	2.56	0.40
3:I:249:MET:H	3:I:249:MET:HG3	1.77	0.40
3:I:717:MET:HG2	3:I:722:LEU:HD12	2.02	0.40
3:C:124:MET:O	3:C:128:ARG:HG2	2.21	0.40
3:C:168:MET:SD	3:C:183:ILE:HD11	2.62	0.40
3:C:723:VAL:HG11	3:C:742:LYS:HZ3	1.87	0.40
1:A:13:TYR:CE2	1:B:92:GLY:HA2	2.57	0.40
1:A:37:VAL:HG12	1:A:38:GLU:CD	2.46	0.40
1:B:539:ARG:HD3	1:B:549:TYR:CZ	2.55	0.40
1:G:13:TYR:O	1:G:14:ALA:C	2.61	0.40
1:G:198:ALA:HB1	1:G:216:VAL:HG11	2.03	0.40
1:J:190:LYS:HD3	1:J:192:GLU:HB2	2.02	0.40
3:F:311:LYS:HE3	3:F:311:LYS:HB3	1.90	0.40
3:F:416:MET:HE2	3:F:461:GLU:HB2	2.03	0.40
3:F:638:LYS:HG2	3:F:642:ARG:HA	2.03	0.40
3:H:638:LYS:HG2	3:H:642:ARG:HA	2.03	0.40
1:A:166:GLN:HB2	1:A:169:PHE:HB3	2.04	0.40
1:A:244:VAL:O	1:A:247:GLN:HG3	2.21	0.40
1:G:225:LEU:HD12	1:G:230:GLN:HE22	1.83	0.40
3:F:414:LYS:HA	3:F:414:LYS:HD3	1.43	0.40
3:H:168:MET:SD	3:H:183:ILE:HD11	2.62	0.40
3:H:606:ASN:HD21	2:K:22:PHE:HB2	1.87	0.40
3:I:393:ASP:HA	3:I:439:ARG:HH21	1.87	0.40
3:I:700:LYS:HG2	3:I:744:ARG:HD2	2.04	0.40
3:C:441:LEU:HD22	3:C:554:MET:HE3	2.02	0.40
3:C:560:ASN:HA	3:C:591:ILE:HG13	2.03	0.40
3:C:768:ALA:HB1	2:E:89:LYS:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	556/623 (89%)	509 (92%)	44 (8%)	3 (0%)	24	63
1	B	549/623 (88%)	506 (92%)	39 (7%)	4 (1%)	18	56
1	G	556/623 (89%)	495 (89%)	53 (10%)	8 (1%)	9	40
1	J	547/623 (88%)	495 (90%)	49 (9%)	3 (0%)	24	63
2	D	87/121 (72%)	61 (70%)	21 (24%)	5 (6%)	1	14
2	E	87/121 (72%)	59 (68%)	23 (26%)	5 (6%)	1	14
2	K	87/121 (72%)	60 (69%)	22 (25%)	5 (6%)	1	14
2	L	87/121 (72%)	62 (71%)	20 (23%)	5 (6%)	1	14
3	C	716/776 (92%)	629 (88%)	82 (12%)	5 (1%)	18	56
3	F	716/776 (92%)	610 (85%)	93 (13%)	13 (2%)	6	34
3	H	716/776 (92%)	615 (86%)	94 (13%)	7 (1%)	12	49
3	I	716/776 (92%)	620 (87%)	87 (12%)	9 (1%)	9	42
All	All	5420/6080 (89%)	4721 (87%)	627 (12%)	72 (1%)	12	42

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	390	VAL
1	B	279	PRO
1	G	221	ARG
2	D	68	CYS
3	F	400	VAL
3	F	464	CYS
3	F	465	GLN
3	F	526	PRO
3	F	623	PRO
3	H	200	VAL
2	K	68	CYS
3	I	200	VAL

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Mol	Chain	Res	Type
3	I	623	PRO
2	L	68	CYS
2	E	68	CYS
1	G	227	GLU
1	G	254	PRO
3	F	203	GLU
3	F	204	ASP
3	F	399	GLY
3	F	510	THR
3	I	510	THR
3	I	517	SER
3	C	330	SER
3	C	623	PRO
1	A	395	ASN
1	B	144	SER
1	J	252	SER
2	D	44	ILE
2	D	57	GLN
3	F	202	GLU
3	H	202	GLU
3	H	215	GLU
3	I	442	THR
3	I	624	GLU
2	L	57	GLN
3	C	510	THR
3	C	517	SER
1	B	252	SER
1	G	252	SER
1	G	256	PHE
1	G	276	SER
1	J	144	SER
1	J	207	GLU
2	D	35	TRP
2	D	38	VAL
3	F	624	GLU
3	H	400	VAL
3	H	753	TYR
2	K	35	TRP
2	K	38	VAL
2	K	57	GLN
3	I	204	ASP
2	L	35	TRP

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Mol	Chain	Res	Type
2	L	38	VAL
2	E	35	TRP
2	E	38	VAL
2	E	57	GLN
1	B	207	GLU
3	F	206	GLU
3	F	525	PRO
3	H	517	SER
2	K	48	HIS
3	I	199	SER
3	I	752	GLU
2	L	48	HIS
3	C	380	LEU
2	E	48	HIS
1	A	252	SER
1	G	220	ILE
3	H	686	PRO
1	G	253	MET

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	478/560 (85%)	443 (93%)	35 (7%)	13	34
1	B	485/560 (87%)	452 (93%)	33 (7%)	14	36
1	G	470/560 (84%)	427 (91%)	43 (9%)	9	27
1	J	491/560 (88%)	448 (91%)	43 (9%)	9	28
2	D	66/102 (65%)	58 (88%)	8 (12%)	5	17
2	E	78/102 (76%)	69 (88%)	9 (12%)	5	18
2	K	78/102 (76%)	70 (90%)	8 (10%)	7	23
2	L	78/102 (76%)	68 (87%)	10 (13%)	4	15
3	C	621/701 (89%)	545 (88%)	76 (12%)	5	17
3	F	597/701 (85%)	517 (87%)	80 (13%)	4	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	610/701 (87%)	558 (92%)	52 (8%)	10	29
3	I	617/701 (88%)	533 (86%)	84 (14%)	3	14
All	All	4669/5452 (86%)	4188 (90%)	481 (10%)	9	23

All (481) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	8	GLN
1	A	9	ILE
1	A	11	THR
1	A	91	THR
1	A	166	GLN
1	A	167	ASP
1	A	199	MET
1	A	203	GLU
1	A	206	THR
1	A	211	GLN
1	A	213	LEU
1	A	214	SER
1	A	217	LEU
1	A	219	GLN
1	A	220	ILE
1	A	221	ARG
1	A	222	ILE
1	A	225	LEU
1	A	226	SER
1	A	227	GLU
1	A	228	VAL
1	A	229	THR
1	A	230	GLN
1	A	231	ARG
1	A	251	LYS
1	A	253	MET
1	A	270	ILE
1	A	389	SER
1	A	397	ARG
1	A	398	THR
1	A	399	VAL
1	A	401	ARG
1	A	412	VAL

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Mol	Chain	Res	Type
1	A	415	LEU
1	B	61	MET
1	B	66	GLU
1	B	67	SER
1	B	68	LYS
1	B	147	GLU
1	B	199	MET
1	B	202	LEU
1	B	206	THR
1	B	209	ARG
1	B	211	GLN
1	B	213	LEU
1	B	217	LEU
1	B	218	SER
1	B	219	GLN
1	B	220	ILE
1	B	221	ARG
1	B	222	ILE
1	B	223	ASP
1	B	225	LEU
1	B	226	SER
1	B	227	GLU
1	B	253	MET
1	B	270	ILE
1	B	272	ILE
1	B	278	ASN
1	B	279	PRO
1	B	280	CYS
1	B	397	ARG
1	B	399	VAL
1	B	401	ARG
1	B	439	MET
1	B	450	VAL
1	B	530	ILE
1	G	8	GLN
1	G	11	THR
1	G	34	VAL
1	G	40	THR
1	G	41	GLU
1	G	71	HIS
1	G	74	LEU
1	G	75	ARG

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Mol	Chain	Res	Type
1	G	84	ILE
1	G	160	PHE
1	G	167	ASP
1	G	171	GLN
1	G	172	LEU
1	G	173	SER
1	G	192	GLU
1	G	193	THR
1	G	194	VAL
1	G	195	ARG
1	G	199	MET
1	G	200	LEU
1	G	203	GLU
1	G	206	THR
1	G	209	ARG
1	G	210	SER
1	G	211	GLN
1	G	213	LEU
1	G	218	SER
1	G	219	GLN
1	G	221	ARG
1	G	222	ILE
1	G	223	ASP
1	G	225	LEU
1	G	227	GLU
1	G	253	MET
1	G	255	LYS
1	G	270	ILE
1	G	277	GLU
1	G	280	CYS
1	G	282	LEU
1	G	396	ARG
1	G	397	ARG
1	G	399	VAL
1	G	401	ARG
1	J	8	GLN
1	J	11	THR
1	J	57	ARG
1	J	59	MET
1	J	71	HIS
1	J	74	LEU
1	J	75	ARG

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Mol	Chain	Res	Type
1	J	82	LEU
1	J	146	GLU
1	J	167	ASP
1	J	169	PHE
1	J	171	GLN
1	J	172	LEU
1	J	173	SER
1	J	191	GLU
1	J	193	THR
1	J	194	VAL
1	J	195	ARG
1	J	196	GLU
1	J	200	LEU
1	J	201	TRP
1	J	204	TYR
1	J	205	ASN
1	J	206	THR
1	J	208	SER
1	J	210	SER
1	J	211	GLN
1	J	213	LEU
1	J	214	SER
1	J	217	LEU
1	J	218	SER
1	J	220	ILE
1	J	221	ARG
1	J	222	ILE
1	J	223	ASP
1	J	225	LEU
1	J	227	GLU
1	J	251	LYS
1	J	253	MET
1	J	270	ILE
1	J	272	ILE
1	J	399	VAL
1	J	401	ARG
2	D	49	ILE
2	D	52	LEU
2	D	54	ILE
2	D	55	GLU
2	D	86	ARG
2	D	88	LEU

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Mol	Chain	Res	Type
2	D	89	LYS
2	D	97	ASP
3	F	202	GLU
3	F	206	GLU
3	F	212	MET
3	F	218	GLN
3	F	220	GLU
3	F	223	LYS
3	F	225	LEU
3	F	328	LEU
3	F	330	SER
3	F	332	GLU
3	F	336	LYS
3	F	339	VAL
3	F	345	LEU
3	F	346	LEU
3	F	349	LYS
3	F	351	ARG
3	F	356	LEU
3	F	357	LEU
3	F	358	GLU
3	F	364	ARG
3	F	369	THR
3	F	375	GLU
3	F	377	PHE
3	F	378	LEU
3	F	379	ASN
3	F	380	LEU
3	F	382	SER
3	F	384	SER
3	F	386	GLU
3	F	390	LEU
3	F	395	LYS
3	F	396	LEU
3	F	397	LYS
3	F	398	LYS
3	F	406	GLN
3	F	407	GLU
3	F	414	LYS
3	F	418	LEU
3	F	422	MET
3	F	423	GLN

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Mol	Chain	Res	Type
3	F	424	GLU
3	F	425	LYS
3	F	459	LYS
3	F	462	CYS
3	F	468	SER
3	F	477	MET
3	F	478	SER
3	F	480	SER
3	F	515	THR
3	F	521	LYS
3	F	522	CYS
3	F	523	ASN
3	F	524	ILE
3	F	546	ARG
3	F	547	GLN
3	F	548	LEU
3	F	619	GLU
3	F	620	THR
3	F	622	ILE
3	F	623	PRO
3	F	624	GLU
3	F	625	ARG
3	F	687	GLU
3	F	688	ARG
3	F	689	LYS
3	F	692	ARG
3	F	694	LYS
3	F	695	VAL
3	F	699	ARG
3	F	701	HIS
3	F	702	GLU
3	F	703	ILE
3	F	709	ARG
3	F	711	MET
3	F	712	LYS
3	F	748	LEU
3	F	750	GLU
3	F	751	ARG
3	F	752	GLU
3	F	753	TYR
3	H	36	LEU
3	H	200	VAL

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Mol	Chain	Res	Type
3	H	202	GLU
3	H	209	PHE
3	H	210	LEU
3	H	211	GLU
3	H	212	MET
3	H	215	GLU
3	H	218	GLN
3	H	219	MET
3	H	220	GLU
3	H	223	LYS
3	H	377	PHE
3	H	378	LEU
3	H	380	LEU
3	H	381	ASN
3	H	383	ARG
3	H	386	GLU
3	H	389	SER
3	H	390	LEU
3	H	394	ASP
3	H	395	LYS
3	H	396	LEU
3	H	515	THR
3	H	521	LYS
3	H	522	CYS
3	H	523	ASN
3	H	524	ILE
3	H	542	LYS
3	H	547	GLN
3	H	549	THR
3	H	620	THR
3	H	622	ILE
3	H	625	ARG
3	H	687	GLU
3	H	688	ARG
3	H	689	LYS
3	H	691	THR
3	H	694	LYS
3	H	695	VAL
3	H	698	ASP
3	H	701	HIS
3	H	702	GLU
3	H	703	ILE

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Mol	Chain	Res	Type
3	H	707	ILE
3	H	709	ARG
3	H	748	LEU
3	H	750	GLU
3	H	752	GLU
3	H	754	LEU
3	H	756	ARG
3	H	757	THR
2	K	42	CYS
2	K	86	ARG
2	K	88	LEU
2	K	91	ARG
2	K	92	GLN
2	K	93	VAL
2	K	99	ARG
2	K	100	GLU
3	I	47	LYS
3	I	72	LYS
3	I	97	LEU
3	I	202	GLU
3	I	206	GLU
3	I	210	LEU
3	I	212	MET
3	I	213	SER
3	I	219	MET
3	I	220	GLU
3	I	223	LYS
3	I	225	LEU
3	I	248	VAL
3	I	249	MET
3	I	254	LYS
3	I	255	SER
3	I	257	GLU
3	I	339	VAL
3	I	342	ILE
3	I	345	LEU
3	I	346	LEU
3	I	349	LYS
3	I	356	LEU
3	I	357	LEU
3	I	378	LEU
3	I	379	ASN

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Mol	Chain	Res	Type
3	I	380	LEU
3	I	381	ASN
3	I	383	ARG
3	I	384	SER
3	I	390	LEU
3	I	395	LYS
3	I	398	LYS
3	I	400	VAL
3	I	407	GLU
3	I	414	LYS
3	I	417	VAL
3	I	418	LEU
3	I	427	VAL
3	I	433	LYS
3	I	436	LEU
3	I	438	ARG
3	I	486	GLU
3	I	488	ARG
3	I	491	LEU
3	I	496	VAL
3	I	497	SER
3	I	498	LEU
3	I	515	THR
3	I	516	GLN
3	I	519	THR
3	I	521	LYS
3	I	546	ARG
3	I	547	GLN
3	I	619	GLU
3	I	622	ILE
3	I	623	PRO
3	I	624	GLU
3	I	625	ARG
3	I	687	GLU
3	I	688	ARG
3	I	689	LYS
3	I	691	THR
3	I	692	ARG
3	I	694	LYS
3	I	695	VAL
3	I	701	HIS
3	I	702	GLU

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Mol	Chain	Res	Type
3	I	703	ILE
3	I	707	ILE
3	I	709	ARG
3	I	712	LYS
3	I	714	ARG
3	I	715	LYS
3	I	716	LYS
3	I	717	MET
3	I	731	LYS
3	I	735	LEU
3	I	748	LEU
3	I	750	GLU
3	I	751	ARG
3	I	753	TYR
3	I	754	LEU
3	I	756	ARG
2	L	25	LYS
2	L	42	CYS
2	L	67	GLU
2	L	86	ARG
2	L	88	LEU
2	L	91	ARG
2	L	92	GLN
2	L	98	ASN
2	L	99	ARG
2	L	100	GLU
3	C	43	GLU
3	C	47	LYS
3	C	203	GLU
3	C	328	LEU
3	C	330	SER
3	C	332	GLU
3	C	334	GLU
3	C	336	LYS
3	C	340	ASP
3	C	341	TYR
3	C	378	LEU
3	C	382	SER
3	C	383	ARG
3	C	388	LEU
3	C	390	LEU
3	C	395	LYS

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Mol	Chain	Res	Type
3	C	398	LYS
3	C	400	VAL
3	C	401	LYS
3	C	403	LEU
3	C	404	THR
3	C	405	GLU
3	C	406	GLN
3	C	411	ILE
3	C	417	VAL
3	C	419	PHE
3	C	422	MET
3	C	423	GLN
3	C	425	LYS
3	C	454	MET
3	C	455	ILE
3	C	456	SER
3	C	466	PHE
3	C	469	LYS
3	C	498	LEU
3	C	515	THR
3	C	516	GLN
3	C	521	LYS
3	C	522	CYS
3	C	523	ASN
3	C	524	ILE
3	C	542	LYS
3	C	544	SER
3	C	546	ARG
3	C	547	GLN
3	C	619	GLU
3	C	620	THR
3	C	621	ASP
3	C	622	ILE
3	C	625	ARG
3	C	626	GLU
3	C	627	LEU
3	C	687	GLU
3	C	688	ARG
3	C	689	LYS
3	C	691	THR
3	C	692	ARG
3	C	694	LYS

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Mol	Chain	Res	Type
3	C	697	ASP
3	C	703	ILE
3	C	704	GLU
3	C	709	ARG
3	C	710	ILE
3	C	711	MET
3	C	728	GLN
3	C	729	GLN
3	C	731	LYS
3	C	733	ARG
3	C	735	LEU
3	C	748	LEU
3	C	750	GLU
3	C	751	ARG
3	C	752	GLU
3	C	753	TYR
3	C	754	LEU
3	C	757	THR
2	E	42	CYS
2	E	86	ARG
2	E	88	LEU
2	E	91	ARG
2	E	92	GLN
2	E	93	VAL
2	E	98	ASN
2	E	99	ARG
2	E	100	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	150	GLN
1	A	158	HIS
1	A	166	GLN
1	A	211	GLN
1	A	219	GLN
1	A	230	GLN
1	A	329	ASN
1	A	356	GLN
1	A	357	GLN
1	B	8	GLN

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Mol	Chain	Res	Type
1	B	69	GLN
1	B	71	HIS
1	B	93	ASN
1	B	150	GLN
1	B	158	HIS
1	B	166	GLN
1	B	329	ASN
1	B	356	GLN
1	B	357	GLN
1	G	8	GLN
1	G	150	GLN
1	G	158	HIS
1	G	219	GLN
1	G	230	GLN
1	G	329	ASN
1	G	356	GLN
1	G	357	GLN
1	J	8	GLN
1	J	73	HIS
1	J	93	ASN
1	J	150	GLN
1	J	158	HIS
1	J	219	GLN
1	J	230	GLN
1	J	329	ASN
1	J	356	GLN
1	J	357	GLN
2	D	28	ASN
2	D	41	ASN
2	D	104	GLN
3	F	49	ASN
3	F	112	HIS
3	F	163	GLN
3	F	218	GLN
3	F	222	GLN
3	F	286	HIS
3	F	435	HIS
3	F	465	GLN
3	F	481	ASN
3	F	547	GLN
3	F	606	ASN
3	F	618	GLN

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Mol	Chain	Res	Type
3	F	657	HIS
3	F	718	GLN
3	H	112	HIS
3	H	163	GLN
3	H	222	GLN
3	H	286	HIS
3	H	381	ASN
3	H	423	GLN
3	H	465	GLN
3	H	481	ASN
3	H	523	ASN
3	H	606	ASN
3	H	618	GLN
3	H	657	HIS
3	H	718	GLN
3	H	729	GLN
2	K	41	ASN
2	K	47	ASN
2	K	48	HIS
3	I	112	HIS
3	I	163	GLN
3	I	286	HIS
3	I	434	GLN
3	I	465	GLN
3	I	481	ASN
3	I	606	ASN
3	I	618	GLN
3	I	657	HIS
2	L	28	ASN
2	L	41	ASN
2	L	47	ASN
2	L	48	HIS
2	L	104	GLN
3	C	112	HIS
3	C	163	GLN
3	C	286	HIS
3	C	337	ASN
3	C	379	ASN
3	C	434	GLN
3	C	481	ASN
3	C	523	ASN
3	C	547	GLN

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Mol	Chain	Res	Type
3	C	606	ASN
3	C	618	GLN
3	C	657	HIS
3	C	718	GLN
3	C	728	GLN
2	E	28	ASN
2	E	41	ASN
2	E	47	ASN
2	E	48	HIS
2	E	98	ASN
2	E	104	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

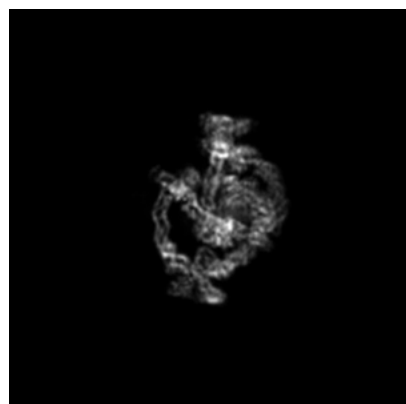
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34449. These allow visual inspection of the internal detail of the map and identification of artifacts.

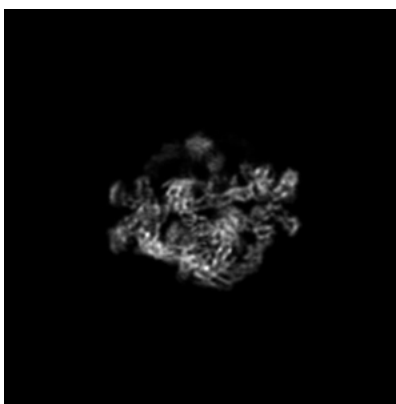
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

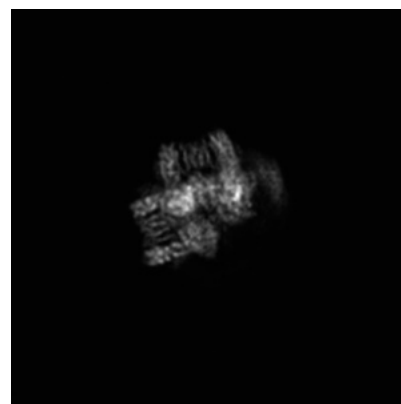
6.1.1 Primary map



X

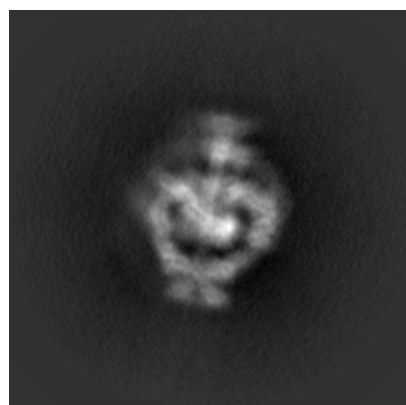


Y

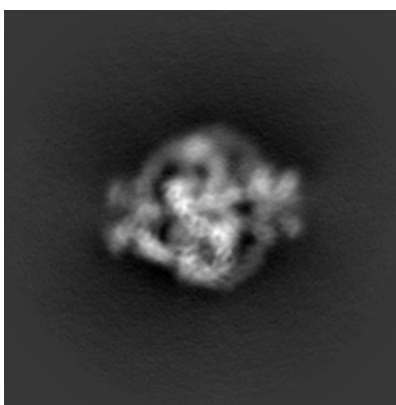


Z

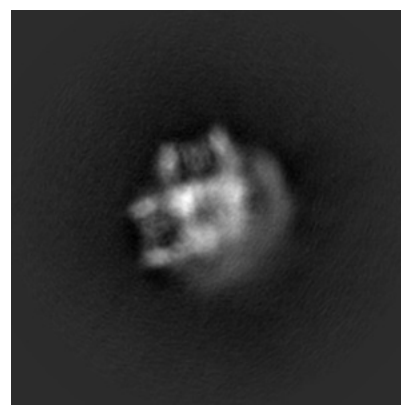
6.1.2 Raw map



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

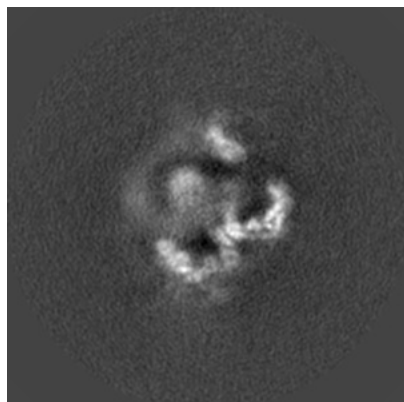


Y Index: 96

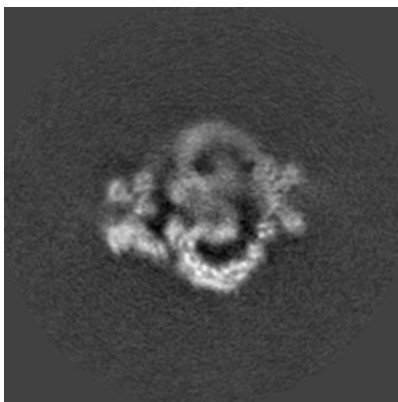


Z Index: 96

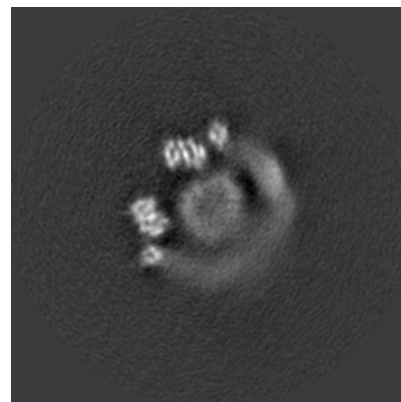
6.2.2 Raw map



X Index: 96



Y Index: 96



Z Index: 96

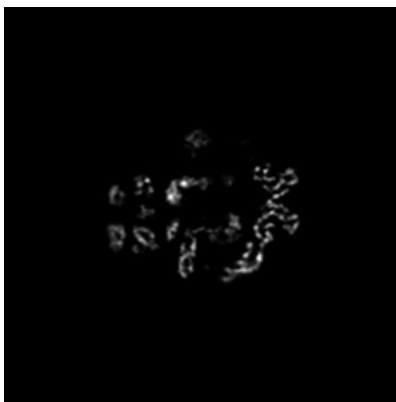
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 86

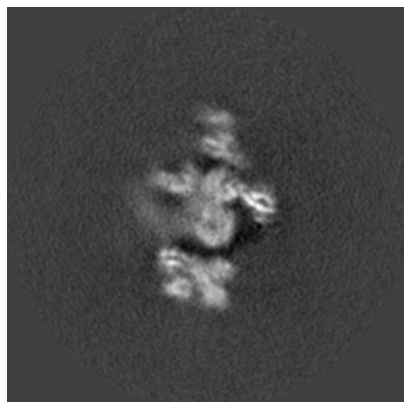


Y Index: 100

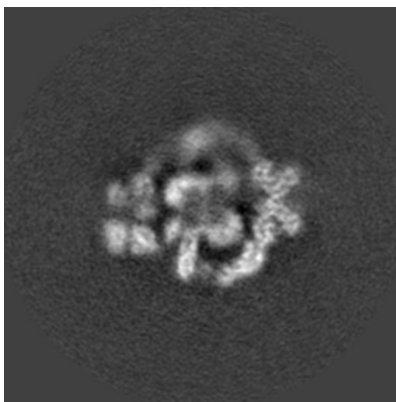


Z Index: 86

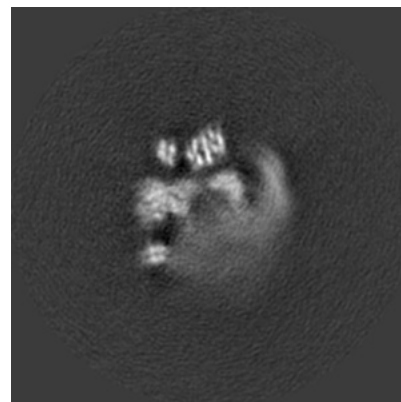
6.3.2 Raw map



X Index: 84



Y Index: 100

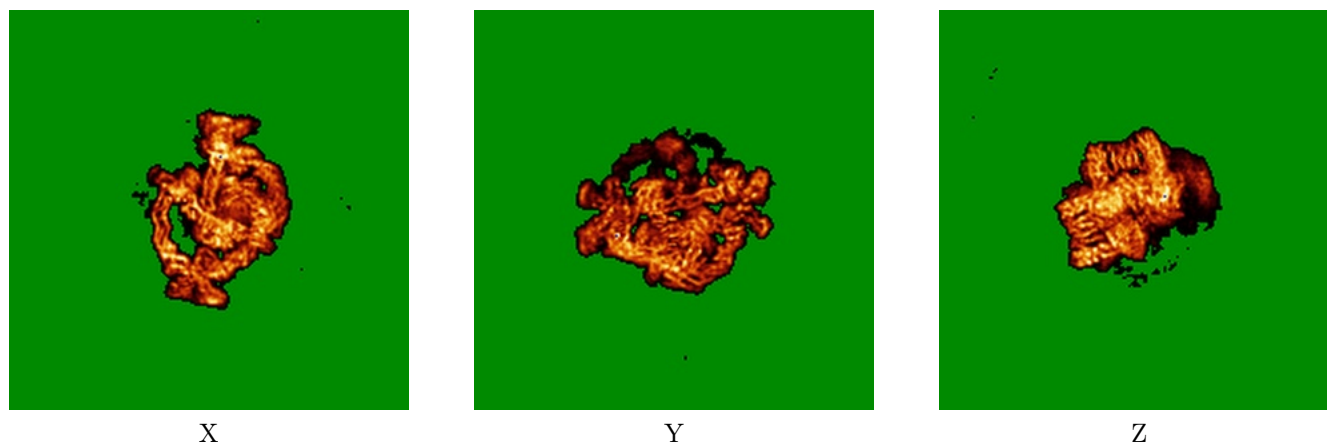


Z Index: 89

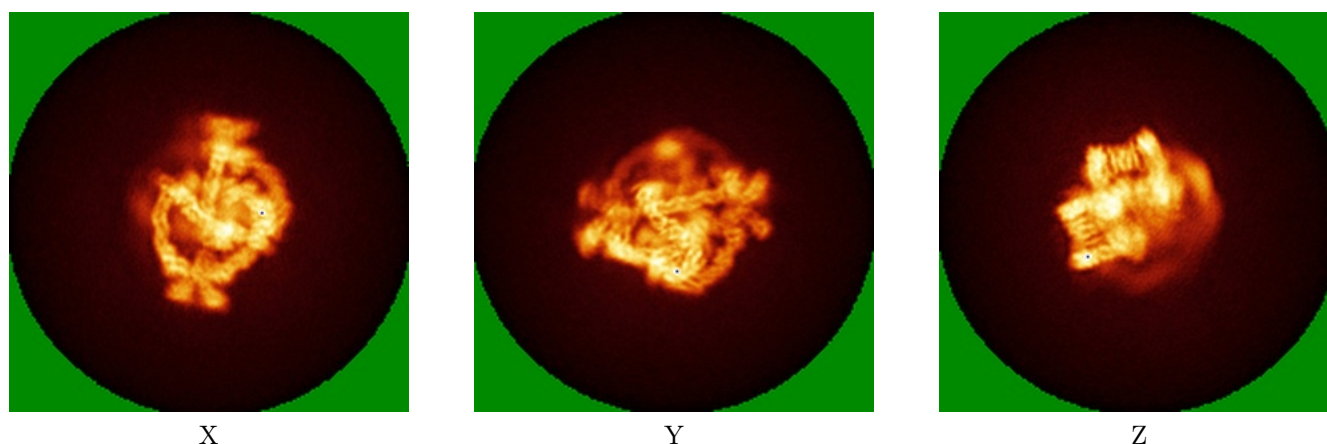
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

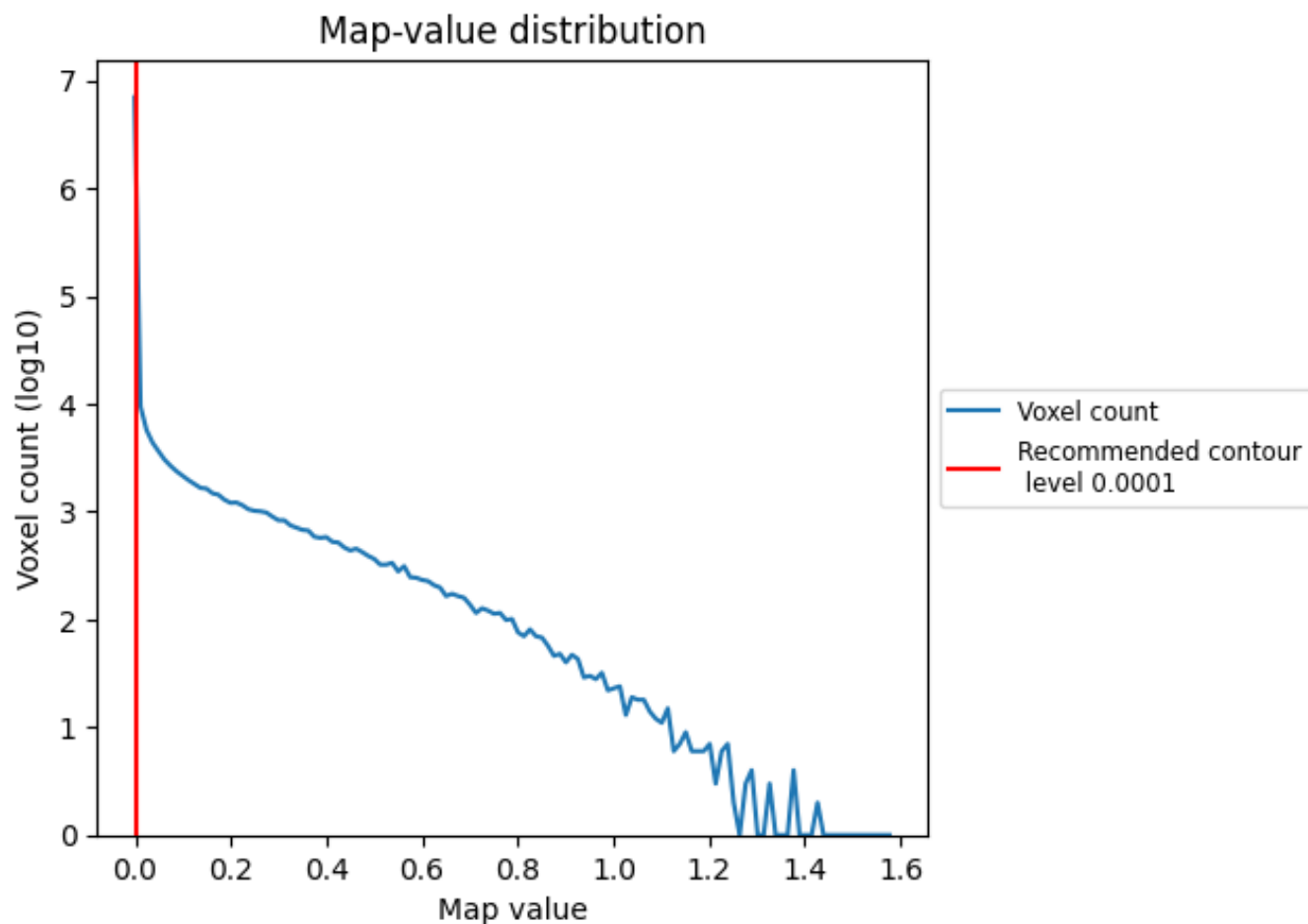
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

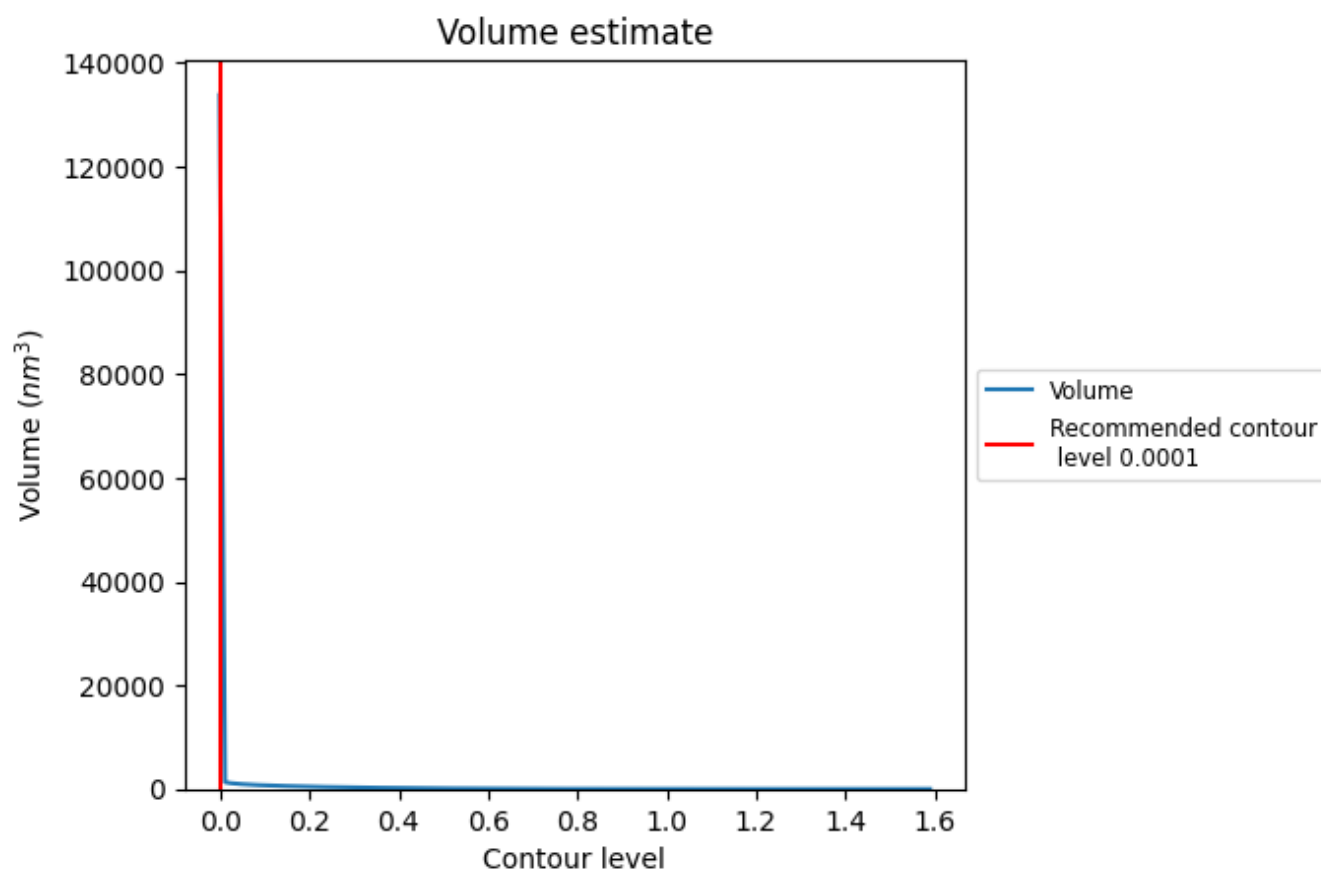
This section contains the results of statistical analysis of the map.

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.

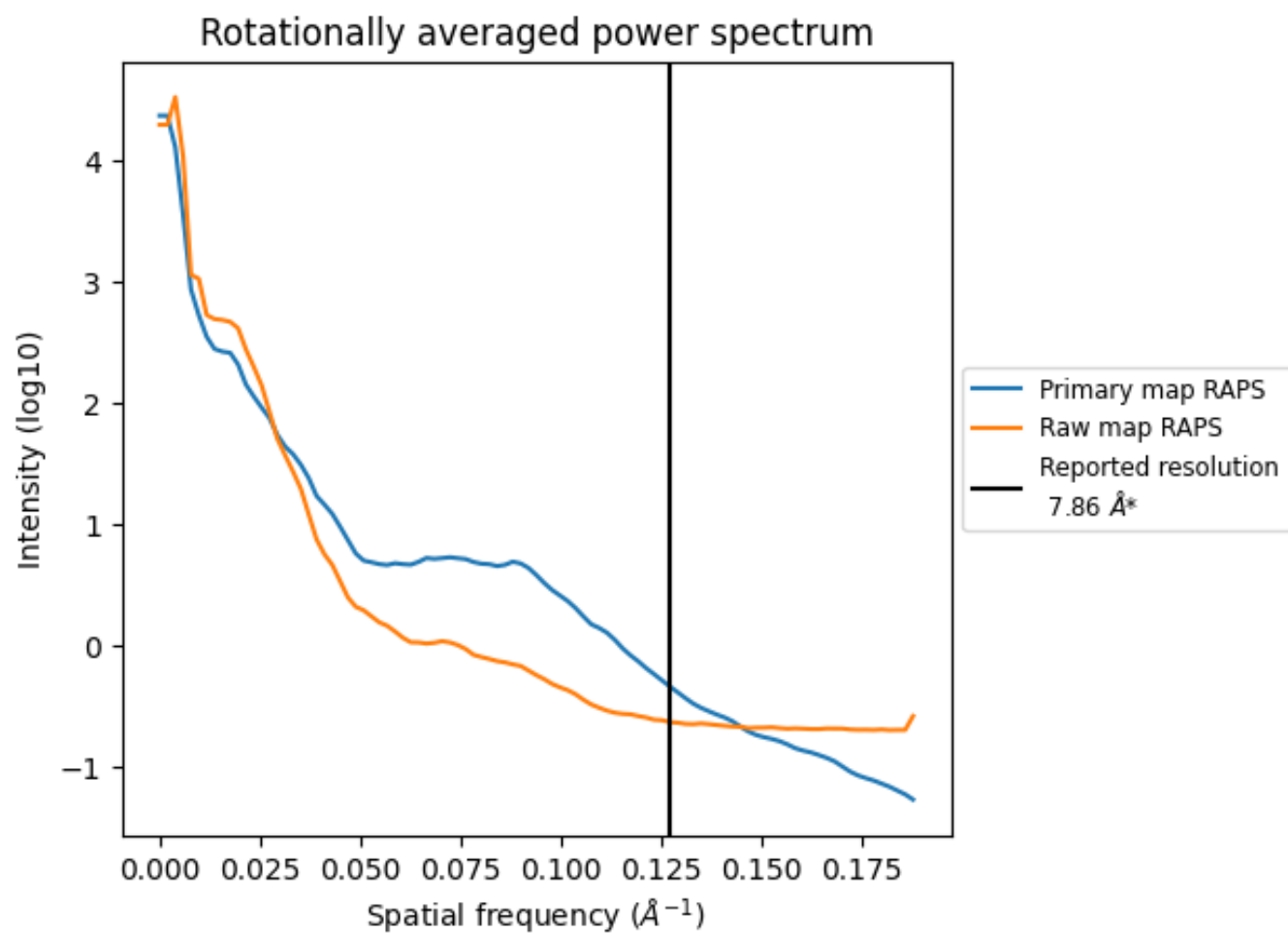
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 117945 nm³; this corresponds to an approximate mass of 106543 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 ⓘ

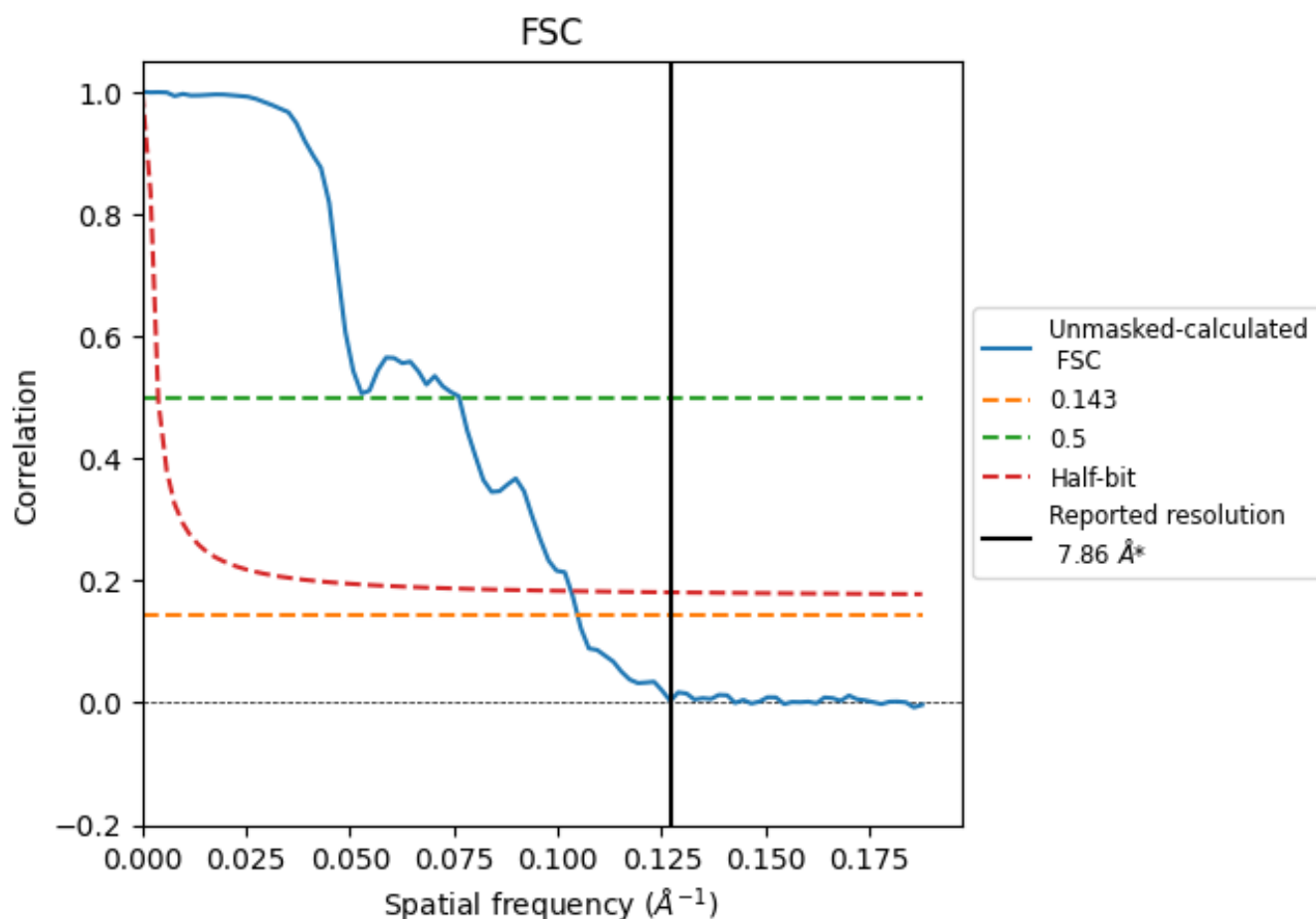


*Reported resolution corresponds to spatial frequency of 0.127 Å⁻¹

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 0.127 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

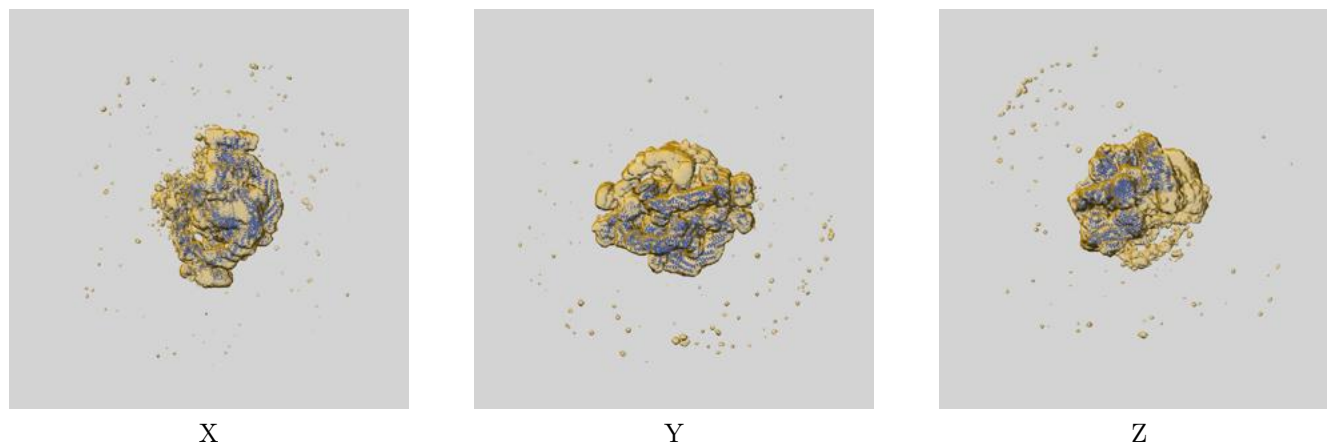
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.86	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.54	13.11	9.69

*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 9.54 differs from the reported value 7.86 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34449 and PDB model 8H33. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0001 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](#)

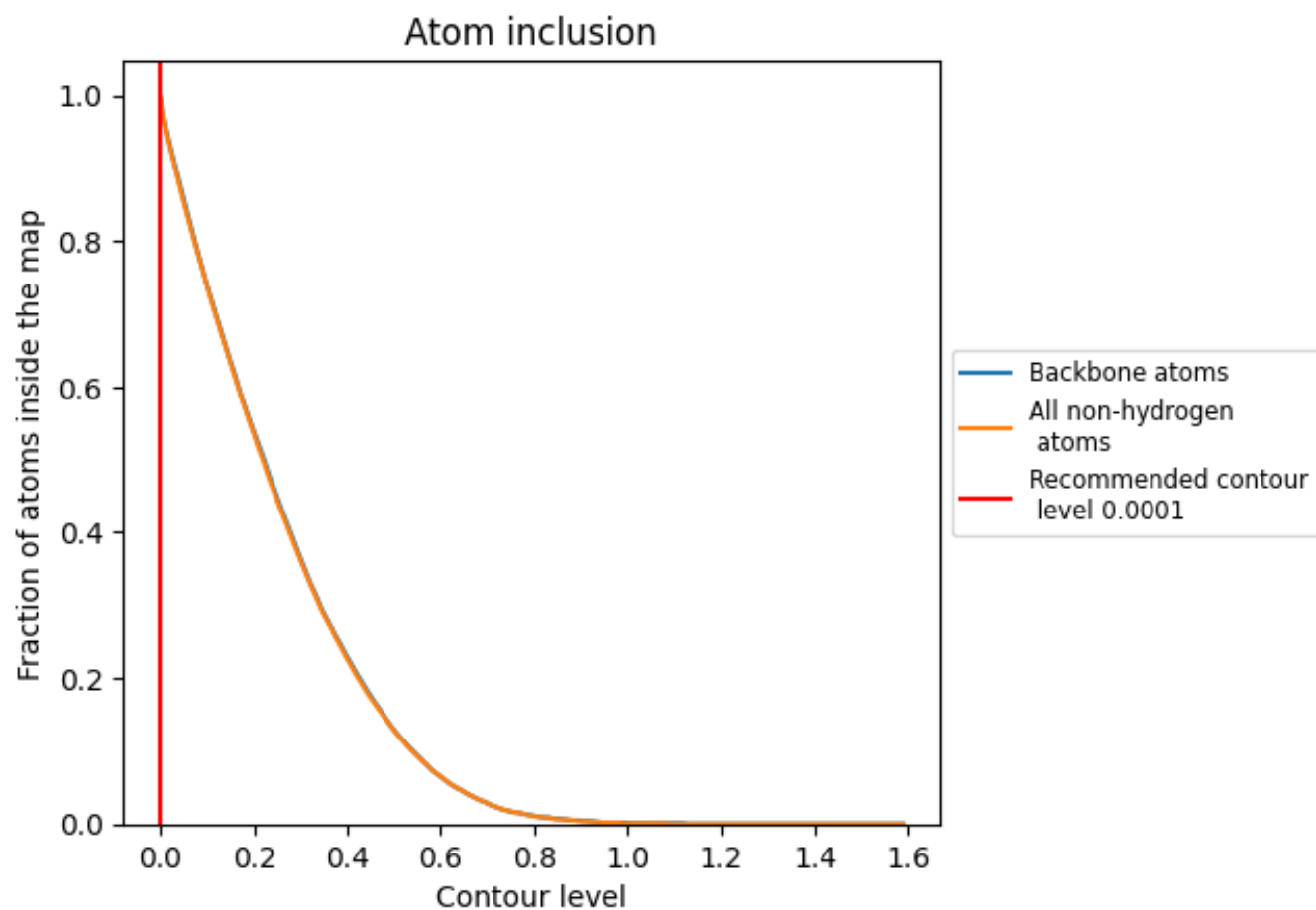


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.0001) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9970	0.0700
A	0.9980	0.0850
B	0.9980	0.0790
C	0.9930	0.0520
D	0.9990	0.0320
E	0.9750	-0.0190
F	0.9980	0.0840
G	0.9990	0.0850
H	0.9990	0.0780
I	0.9990	0.0810
J	0.9970	0.0570
K	0.9670	0.0000
L	0.9990	0.0280

