



Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 01:10 PM JST

PDB ID : 7W68
EMDB ID : EMD-32326
Title : human single hexameric Mcm2-7 complex
Authors : Xu, N.N.; Lin, Q.P.; Liu, C.D.; Tian, H.L.; Xiang, Y.; Zhu, G.
Deposited on : 2021-12-01
Resolution : 4.40 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

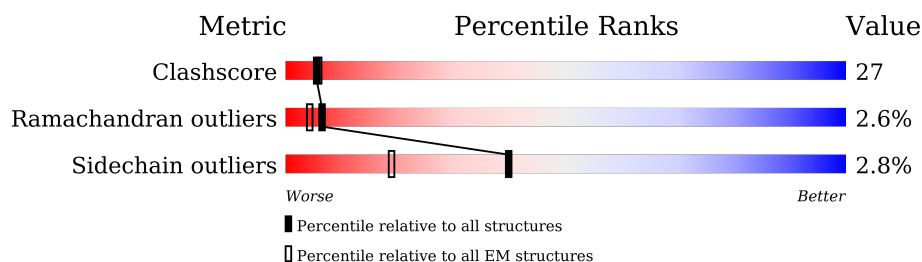
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	904	<div> <div>18%</div> <div>33% 26% . 38%</div> </div>
2	B	808	<div> <div>14%</div> <div>30% 27% . . 38%</div> </div>
3	C	863	<div> <div>14%</div> <div>30% 28% . . 39%</div> </div>
4	D	734	<div> <div>15%</div> <div>29% 27% . 42%</div> </div>
5	E	821	<div> <div>24%</div> <div>40% 35% . . 19%</div> </div>
6	F	719	<div> <div>22%</div> <div>42% 36% . 20%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25833 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	560	Total	C	N	O	S	0	0
			4443	2800	797	823	23		

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	498	Total	C	N	O	S	0	0
			3912	2456	700	733	23		

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	529	Total	C	N	O	S	0	0
			4227	2670	745	788	24		

- Molecule 4 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	426	Total	C	N	O	S	0	0
			3349	2106	591	627	25		

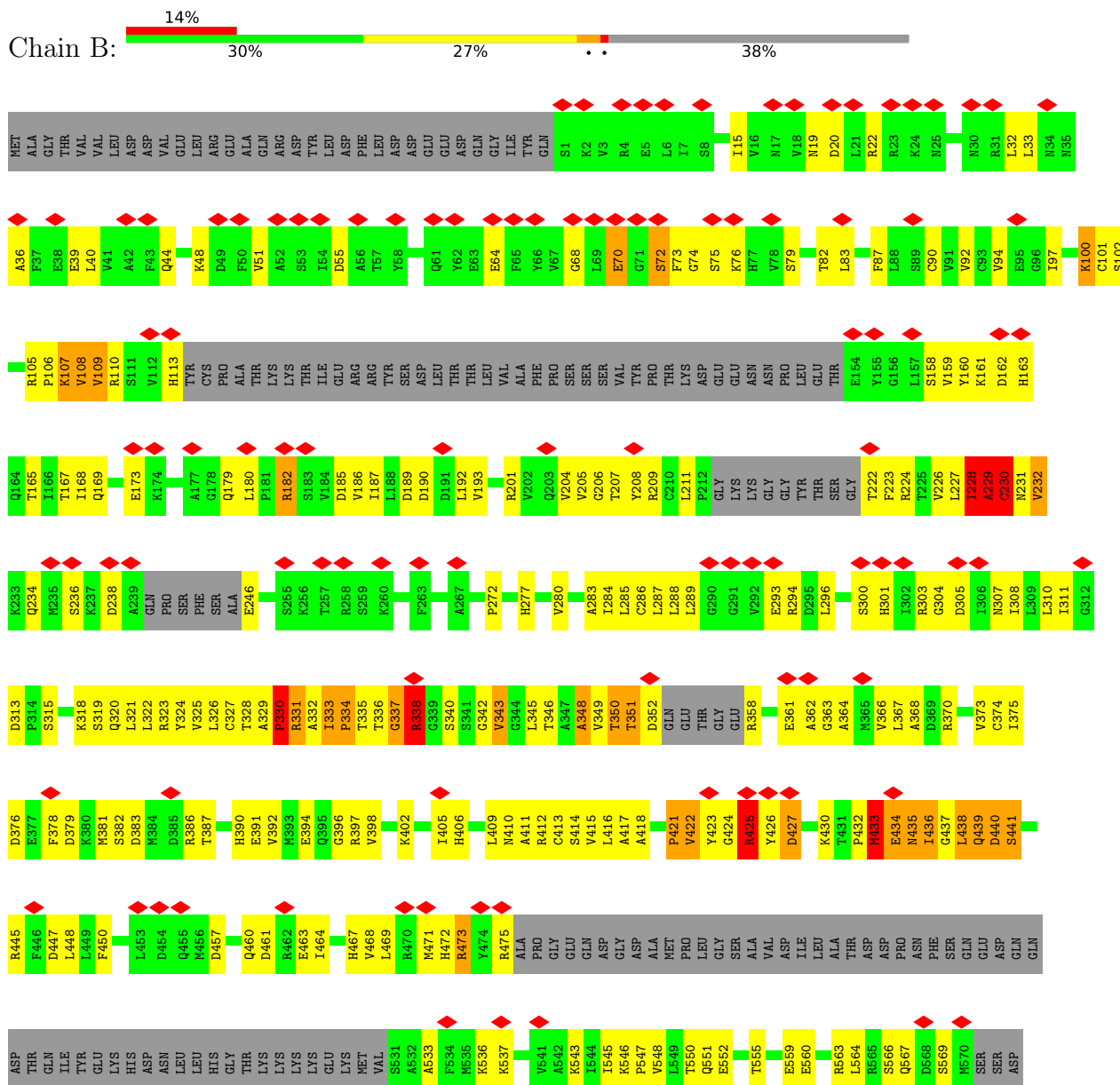
- Molecule 5 is a protein called DNA replication licensing factor MCM6.

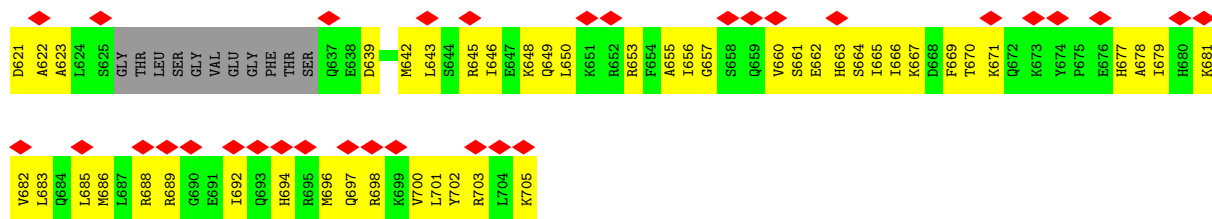
Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	661	Total	C	N	O	S	0	0
			5335	3355	946	1007	27		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

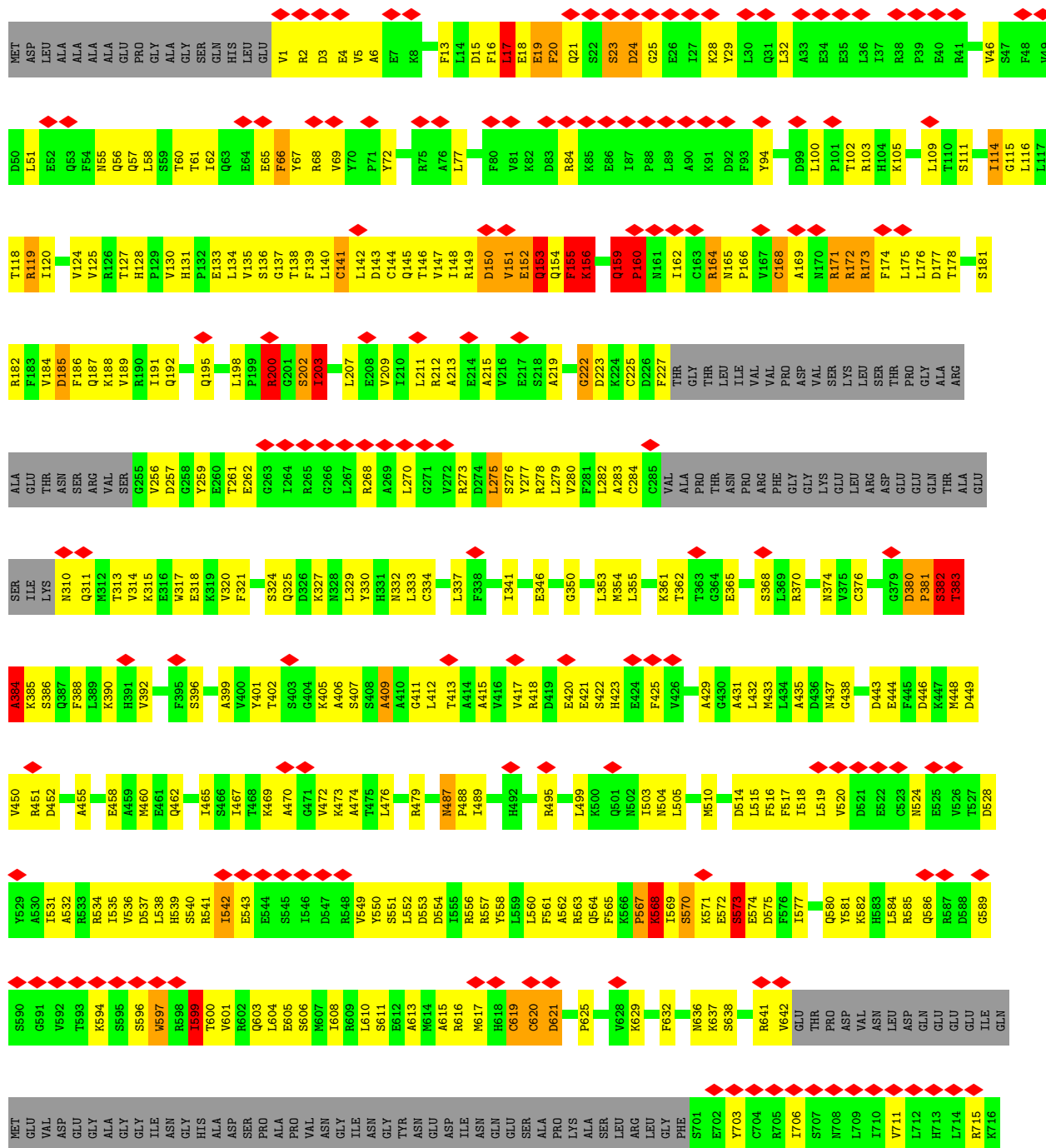
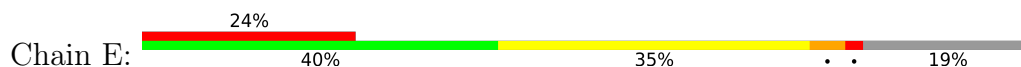
Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	575	Total	C	N	O	S	0	0
			4567	2866	815	861	25		

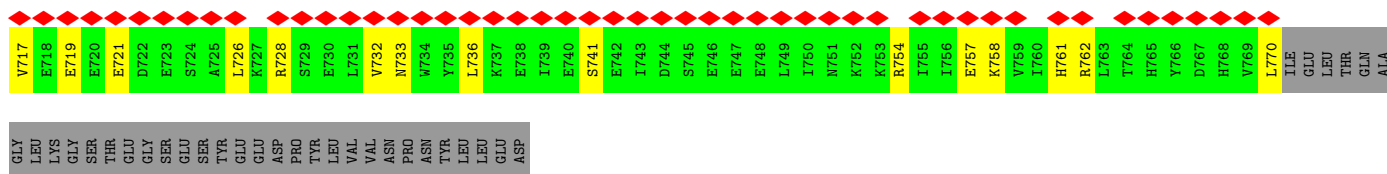
- Molecule 2: DNA replication licensing factor MCM3



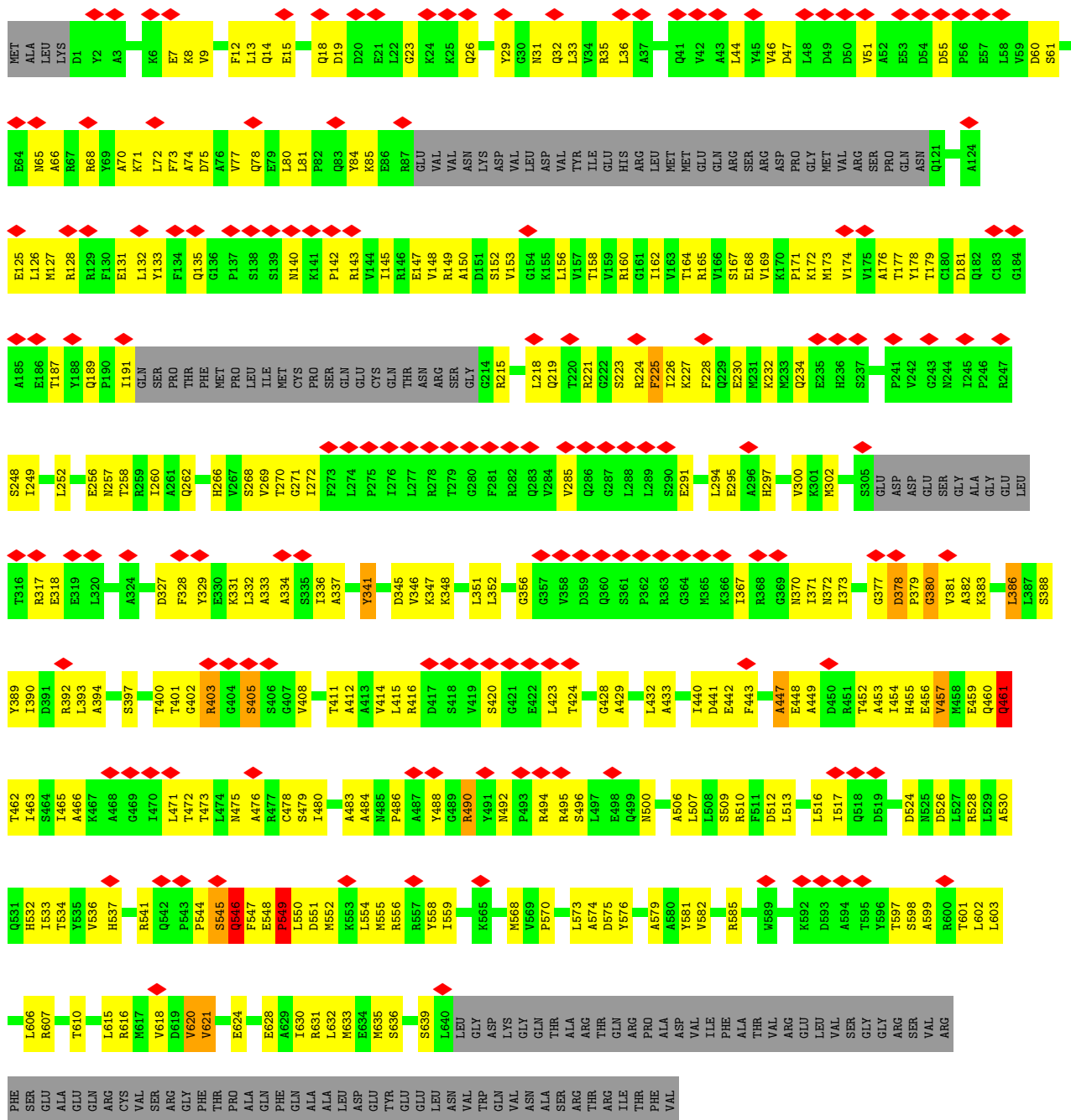


• Molecule 5: DNA replication licensing factor MCM6





• Molecule 6: DNA replication licensing factor MCM7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	186918	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.293	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.14	Depositor
Map size (\AA)	254.4, 254.4, 254.4	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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	0.53	0/4518	0.80	16/6093 (0.3%)
2	B	0.70	8/3965 (0.2%)	0.96	29/5341 (0.5%)
3	C	0.60	1/4299 (0.0%)	0.95	35/5809 (0.6%)
4	D	0.52	0/3390	0.74	4/4541 (0.1%)
5	E	0.67	7/5420 (0.1%)	0.97	24/7302 (0.3%)
6	F	0.56	1/4637 (0.0%)	0.77	8/6257 (0.1%)
All	All	0.60	17/26229 (0.1%)	0.88	116/35343 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	14
2	B	0	8
3	C	0	17
4	D	0	9
5	E	0	13
6	F	0	7
All	All	0	68

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	153	GLN	N-CA	9.22	1.64	1.46
5	E	203	ILE	C-N	8.46	1.50	1.34
5	E	153	GLN	CB-CG	8.16	1.74	1.52
2	B	433	MET	N-CA	-8.14	1.30	1.46
2	B	433	MET	CA-CB	7.39	1.70	1.53
2	B	436	ILE	C-N	7.20	1.46	1.33
5	E	153	GLN	CA-C	-7.12	1.34	1.52
2	B	421	PRO	C-N	7.10	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	378	ASP	N-CA	6.64	1.59	1.46
2	B	433	MET	CA-C	6.29	1.69	1.52
3	C	153	ALA	CA-CB	6.27	1.65	1.52
2	B	436	ILE	CA-CB	6.20	1.69	1.54
5	E	153	GLN	CA-CB	5.73	1.66	1.53
5	E	384	ALA	C-O	5.37	1.33	1.23
2	B	435	ASN	N-CA	-5.33	1.35	1.46
2	B	441	SER	CA-CB	-5.28	1.45	1.52
5	E	385	LYS	N-CA	-5.19	1.35	1.46

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	380	ASP	C-N-CD	-16.07	85.25	120.60
5	E	153	GLN	CA-CB-CG	13.68	143.50	113.40
5	E	384	ALA	N-CA-C	-11.85	79.00	111.00
3	C	151	GLN	N-CA-CB	11.20	130.76	110.60
2	B	436	ILE	CB-CA-C	11.08	133.76	111.60
2	B	433	MET	CB-CA-C	11.00	132.41	110.40
2	B	433	MET	CA-CB-CG	10.84	131.72	113.30
1	A	193	GLY	C-N-CA	10.74	148.55	121.70
5	E	384	ALA	N-CA-CB	9.76	123.77	110.10
4	D	336	LEU	C-N-CD	-9.68	99.31	120.60
5	E	383	THR	N-CA-C	-9.54	85.24	111.00
2	B	421	PRO	O-C-N	-9.29	107.84	122.70
3	C	153	ALA	CB-CA-C	9.23	123.95	110.10
6	F	378	ASP	N-CA-C	9.11	135.59	111.00
5	E	275	LEU	CB-CG-CD2	9.09	126.46	111.00
6	F	380	GLY	N-CA-C	-8.93	90.78	113.10
5	E	153	GLN	N-CA-CB	8.84	126.51	110.60
2	B	106	PRO	O-C-N	-8.48	109.13	122.70
5	E	384	ALA	CB-CA-C	-8.39	97.52	110.10
6	F	378	ASP	C-N-CD	-8.29	102.37	120.60
2	B	427	ASP	C-N-CA	8.26	142.35	121.70
2	B	438	LEU	N-CA-C	-8.15	89.01	111.00
1	A	360	GLY	N-CA-C	-8.14	92.75	113.10
2	B	434	GLU	N-CA-CB	8.13	125.24	110.60
3	C	78	ILE	CG1-CB-CG2	7.90	128.78	111.40
3	C	154	PHE	CB-CA-C	-7.87	94.67	110.40
2	B	439	GLN	C-N-CA	7.79	141.17	121.70
5	E	382	SER	C-N-CA	7.72	141.00	121.70
2	B	473	ARG	NE-CZ-NH2	-7.60	116.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	380	ASP	C-N-CA	7.49	153.44	122.00
3	C	73	LEU	CB-CG-CD2	7.47	123.70	111.00
3	C	77	LEU	C-N-CA	7.29	139.94	121.70
3	C	152	GLU	C-N-CA	7.29	139.93	121.70
3	C	269	VAL	CA-CB-CG2	7.11	121.57	110.90
3	C	77	LEU	CB-CG-CD2	7.09	123.05	111.00
3	C	267	ILE	CG1-CB-CG2	7.05	126.92	111.40
1	A	422	SER	O-C-N	-7.01	111.49	122.70
5	E	114	ILE	CG1-CB-CG2	6.90	126.58	111.40
5	E	20	PHE	N-CA-C	6.84	129.48	111.00
3	C	221	VAL	CG1-CB-CG2	6.81	121.80	110.90
1	A	333	GLY	C-N-CA	6.77	138.62	121.70
5	E	570	SER	CB-CA-C	-6.71	97.36	110.10
3	C	146	LEU	CB-CG-CD2	6.70	122.38	111.00
2	B	228	ILE	N-CA-C	-6.69	92.93	111.00
3	C	152	GLU	N-CA-C	6.66	128.97	111.00
2	B	424	GLY	C-N-CA	6.63	138.28	121.70
3	C	133	LEU	CB-CG-CD2	6.60	122.22	111.00
5	E	153	GLN	CB-CA-C	-6.55	97.29	110.40
1	A	424	ALA	N-CA-CB	6.55	119.27	110.10
3	C	244	ILE	CG1-CB-CG2	6.53	125.76	111.40
1	A	93	VAL	CG1-CB-CG2	6.51	121.31	110.90
3	C	159	VAL	N-CA-C	-6.47	93.52	111.00
6	F	546	GLN	N-CA-C	6.36	128.16	111.00
2	B	101	CYS	CA-CB-SG	-6.35	102.57	114.00
3	C	203	ILE	CG1-CB-CG2	6.34	125.35	111.40
5	E	620	CYS	CA-CB-SG	-6.30	102.66	114.00
5	E	275	LEU	CA-CB-CG	-6.27	100.88	115.30
2	B	330	PRO	O-C-N	6.23	132.66	122.70
3	C	63	CYS	N-CA-C	-6.19	94.30	111.00
3	C	150	MET	C-N-CA	6.18	137.16	121.70
2	B	436	ILE	CB-CG1-CD1	6.08	130.93	113.90
3	C	111	VAL	CG1-CB-CG2	6.05	120.58	110.90
3	C	147	ILE	CG1-CB-CG2	6.03	124.66	111.40
5	E	155	PHE	O-C-N	6.03	132.34	122.70
3	C	241	VAL	C-N-CA	6.03	136.76	121.70
1	A	98	LEU	C-N-CD	-6.02	107.36	120.60
5	E	17	LEU	CA-CB-CG	5.97	129.03	115.30
3	C	150	MET	O-C-N	-5.90	113.25	122.70
2	B	337	GLY	O-C-N	-5.84	113.35	122.70
3	C	269	VAL	CG1-CB-CG2	5.84	120.25	110.90
2	B	590	ARG	NE-CZ-NH1	5.84	123.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	154	PHE	N-CA-CB	5.83	121.10	110.60
1	A	337	THR	CA-CB-CG2	5.83	120.56	112.40
3	C	590	ARG	NE-CZ-NH1	5.82	123.21	120.30
2	B	427	ASP	CB-CA-C	5.82	122.03	110.40
3	C	154	PHE	N-CA-C	-5.79	95.37	111.00
1	A	337	THR	O-C-N	-5.79	113.44	122.70
2	B	101	CYS	N-CA-C	5.76	126.56	111.00
3	C	117	LEU	CB-CG-CD1	5.76	120.80	111.00
3	C	160	CYS	CB-CA-C	5.75	121.90	110.40
5	E	568	LYS	N-CA-C	5.71	126.42	111.00
5	E	567	PRO	N-CA-C	5.69	126.89	112.10
2	B	230	CYS	CB-CA-C	5.68	121.76	110.40
1	A	98	LEU	C-N-CA	5.65	145.73	122.00
3	C	205	LEU	CA-CB-CG	5.65	128.28	115.30
2	B	349	VAL	N-CA-C	5.52	125.90	111.00
3	C	92	VAL	CG1-CB-CG2	5.49	119.68	110.90
6	F	549	PRO	CA-C-O	-5.47	107.06	120.20
2	B	106	PRO	CA-C-N	5.44	129.16	117.20
3	C	117	LEU	CB-CG-CD2	5.42	120.22	111.00
5	E	171	ARG	NE-CZ-NH2	-5.42	117.59	120.30
5	E	573	SER	N-CA-C	5.37	125.50	111.00
2	B	421	PRO	CA-C-N	5.34	128.95	117.20
2	B	473	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	334	ASP	N-CA-CB	5.31	120.15	110.60
4	D	341	THR	O-C-N	-5.28	114.26	122.70
6	F	545	SER	N-CA-C	-5.26	96.80	111.00
5	E	160	PRO	C-N-CA	5.25	134.82	121.70
6	F	377	GLY	C-N-CA	5.22	134.76	121.70
2	B	441	SER	N-CA-C	5.21	125.06	111.00
1	A	3	LEU	N-CA-C	5.18	124.99	111.00
2	B	436	ILE	CA-C-N	5.18	126.57	116.20
3	C	160	CYS	N-CA-CB	5.18	119.92	110.60
3	C	590	ARG	NE-CZ-NH2	-5.17	117.72	120.30
5	E	23	SER	CB-CA-C	5.15	119.88	110.10
6	F	225	PHE	CB-CG-CD1	5.14	124.40	120.80
1	A	334	ASP	N-CA-C	-5.12	97.17	111.00
1	A	422	SER	CA-C-N	5.09	128.41	117.20
1	A	423	LYS	C-N-CA	5.07	134.36	121.70
2	B	182	ARG	NE-CZ-NH1	5.05	122.83	120.30
2	B	425	ARG	N-CA-C	-5.04	97.40	111.00
3	C	270	ILE	N-CA-C	-5.03	97.43	111.00
1	A	423	LYS	N-CA-C	5.02	124.57	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	584	LEU	CA-CB-CG	5.02	126.85	115.30
2	B	229	ALA	C-N-CA	5.02	134.25	121.70
4	D	335	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (68) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	GLU	Peptide
1	A	190	GLU	Peptide
1	A	243	PRO	Peptide
1	A	289	ALA	Peptide
1	A	32	MET	Peptide
1	A	337	THR	Mainchain
1	A	363	ALA	Peptide
1	A	366	LEU	Peptide
1	A	374	PRO	Peptide
1	A	465	SER	Peptide
1	A	530	LEU	Peptide
1	A	532	LYS	Peptide
1	A	539	GLU	Peptide
1	A	594	ASP	Peptide
2	B	105	ARG	Peptide
2	B	107	LYS	Mainchain
2	B	232	VAL	Peptide
2	B	315	SER	Peptide
2	B	342	GLY	Mainchain
2	B	348	ALA	Mainchain
2	B	73	PHE	Peptide
2	B	75	SER	Peptide
3	C	11	ALA	Peptide
3	C	144	SER	Peptide
3	C	145	GLN	Peptide
3	C	148	PRO	Peptide
3	C	185	THR	Peptide
3	C	186	HIS	Peptide
3	C	196	LEU	Peptide
3	C	198	SER	Peptide
3	C	214	ALA	Peptide
3	C	226	HIS	Peptide
3	C	228	ASP	Peptide
3	C	24	PHE	Peptide

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Mol	Chain	Res	Type	Group
3	C	240	ASN	Peptide
3	C	266	HIS	Peptide
3	C	496	ASP	Peptide
3	C	608	ASP	Peptide
3	C	78	ILE	Peptide
4	D	221	ASP	Peptide
4	D	311	ALA	Peptide
4	D	341	THR	Mainchain
4	D	376	SER	Peptide
4	D	384	GLY	Peptide
4	D	455	VAL	Peptide
4	D	479	PRO	Peptide
4	D	486	ASP	Peptide
4	D	63	PRO	Peptide
5	E	102	THR	Peptide
5	E	119	ARG	Peptide
5	E	146	THR	Peptide
5	E	164	ARG	Peptide
5	E	172	ARG	Mainchain
5	E	222	GLY	Peptide
5	E	257	ASP	Peptide
5	E	382	SER	Mainchain
5	E	402	THR	Peptide
5	E	448	MET	Peptide
5	E	470	ALA	Peptide
5	E	570	SER	Mainchain
5	E	77	LEU	Peptide
6	F	156	LEU	Peptide
6	F	269	VAL	Peptide
6	F	271	GLY	Peptide
6	F	447	ALA	Peptide
6	F	457	VAL	Peptide
6	F	461	GLN	Peptide
6	F	537	HIS	Peptide

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	4443	0	4482	208	0
2	B	3912	0	3993	258	0
3	C	4227	0	4258	245	0
4	D	3349	0	3429	199	0
5	E	5335	0	5359	377	0
6	F	4567	0	4622	209	0
All	All	25833	0	26143	1411	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 27.

All (1411) 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)
3:C:552:ARG:CG	5:E:542:ILE:HG13	1.22	1.62
5:E:153:GLN:CB	5:E:153:GLN:CG	1.74	1.59
5:E:594:LYS:HE3	5:E:597:TRP:CD1	1.37	1.59
2:B:436:ILE:CD1	2:B:436:ILE:CG1	1.82	1.54
2:B:386:ARG:NE	2:B:438:LEU:CD2	1.68	1.53
2:B:386:ARG:CD	2:B:438:LEU:CD2	1.91	1.48
2:B:206:GLY:HA2	2:B:230:CYS:SG	1.52	1.47
2:B:386:ARG:HE	2:B:438:LEU:CD2	1.21	1.45
2:B:206:GLY:CA	2:B:230:CYS:SG	2.04	1.43
5:E:152:GLU:N	5:E:159:GLN:CG	1.89	1.34
5:E:594:LYS:CE	5:E:597:TRP:CD1	2.09	1.34
5:E:152:GLU:H	5:E:159:GLN:CG	1.40	1.33
5:E:154:GLN:CB	5:E:156:LYS:HD2	1.58	1.30
3:C:552:ARG:CG	5:E:542:ILE:CG1	2.10	1.29
5:E:151:VAL:CA	5:E:159:GLN:HG3	1.62	1.29
5:E:151:VAL:HA	5:E:159:GLN:CG	1.65	1.26
4:D:331:GLY:CA	4:D:344:GLY:O	1.82	1.26
4:D:332:SER:O	4:D:344:GLY:HA3	1.12	1.25
5:E:154:GLN:CG	5:E:156:LYS:HD2	1.66	1.25
2:B:348:ALA:CB	2:B:405:ILE:HD13	1.69	1.22
3:C:111:VAL:O	3:C:270:ILE:CD1	1.89	1.20
5:E:19:GLU:HG2	5:E:32:LEU:CD1	1.71	1.19
4:D:336:LEU:CB	4:D:337:PRO:HD3	1.70	1.19
5:E:151:VAL:HG23	5:E:160:PRO:CD	1.72	1.19
3:C:112:ARG:HB3	3:C:271:HIS:O	1.42	1.19
5:E:154:GLN:HB2	5:E:156:LYS:CD	1.72	1.18
4:D:332:SER:H	4:D:344:GLY:CA	1.55	1.17
5:E:154:GLN:O	5:E:156:LYS:CG	1.92	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:157:CYS:O	5:E:256:VAL:CG2	1.93	1.17
5:E:19:GLU:OE2	5:E:32:LEU:HD12	1.44	1.17
2:B:386:ARG:NE	2:B:438:LEU:HD21	0.84	1.17
2:B:348:ALA:CB	2:B:405:ILE:CD1	2.22	1.16
5:E:159:GLN:HB2	5:E:160:PRO:HD3	1.26	1.16
5:E:19:GLU:OE2	5:E:32:LEU:CD1	1.94	1.16
3:C:552:ARG:HG3	5:E:542:ILE:HG13	1.27	1.15
5:E:151:VAL:CG2	5:E:160:PRO:HD2	1.76	1.15
3:C:552:ARG:HG3	5:E:542:ILE:CG1	1.76	1.14
5:E:594:LYS:CE	5:E:597:TRP:HD1	1.50	1.14
5:E:19:GLU:HB3	5:E:28:LYS:HG2	1.29	1.14
3:C:157:CYS:O	5:E:256:VAL:HG22	1.46	1.14
5:E:380:ASP:CB	5:E:381:PRO:HD3	1.64	1.13
5:E:594:LYS:CD	5:E:597:TRP:CD1	2.31	1.13
2:B:348:ALA:HB2	2:B:405:ILE:CD1	1.80	1.12
2:B:386:ARG:CD	2:B:438:LEU:HD22	1.78	1.11
5:E:151:VAL:C	5:E:159:GLN:HG3	1.70	1.11
5:E:19:GLU:HG2	5:E:32:LEU:HD11	1.15	1.11
2:B:435:ASN:O	4:D:689:ARG:NH2	1.84	1.10
3:C:552:ARG:CD	5:E:542:ILE:HG13	1.80	1.09
4:D:332:SER:O	4:D:344:GLY:CA	1.98	1.09
1:A:44:TYR:CE2	1:A:99:PRO:HG3	1.85	1.09
2:B:328:THR:O	2:B:330:PRO:HD3	1.50	1.09
5:E:152:GLU:N	5:E:159:GLN:HG2	1.56	1.09
1:A:490:VAL:HG11	5:E:574:GLU:CG	1.83	1.08
2:B:206:GLY:HA3	2:B:230:CYS:SG	1.84	1.08
2:B:386:ARG:HD3	2:B:438:LEU:CD2	1.63	1.08
5:E:151:VAL:HG22	5:E:159:GLN:H	0.90	1.07
4:D:336:LEU:HB3	4:D:337:PRO:HD3	1.08	1.07
5:E:154:GLN:HB2	5:E:156:LYS:HD2	1.11	1.06
4:D:334:LYS:HZ3	4:D:344:GLY:CA	1.67	1.06
5:E:380:ASP:HB3	5:E:381:PRO:CD	1.84	1.06
2:B:329:ALA:HB1	2:B:332:ALA:HB3	1.36	1.06
4:D:336:LEU:HB3	4:D:337:PRO:CD	1.85	1.06
2:B:471:MET:SD	4:D:337:PRO:HG2	1.96	1.05
5:E:154:GLN:C	5:E:156:LYS:HG2	1.75	1.05
5:E:151:VAL:CA	5:E:159:GLN:CG	2.26	1.05
5:E:151:VAL:HG22	5:E:159:GLN:N	1.72	1.05
2:B:386:ARG:HD3	2:B:438:LEU:HD23	1.33	1.05
4:D:331:GLY:N	4:D:344:GLY:O	1.90	1.04
1:A:490:VAL:CG1	5:E:574:GLU:HG3	1.87	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:414:VAL:CG1	6:F:423:LEU:HB3	1.88	1.04
3:C:552:ARG:HG2	5:E:542:ILE:HG13	1.07	1.04
4:D:332:SER:H	4:D:344:GLY:HA2	1.18	1.03
5:E:154:GLN:O	5:E:156:LYS:HG2	1.56	1.03
5:E:154:GLN:O	5:E:156:LYS:HG3	1.57	1.02
5:E:152:GLU:H	5:E:159:GLN:HG2	0.88	1.02
5:E:594:LYS:HD3	5:E:597:TRP:HE1	1.17	1.02
5:E:152:GLU:N	5:E:159:GLN:CD	2.14	1.00
1:A:364:VAL:HG11	1:A:383:ALA:O	1.58	1.00
5:E:151:VAL:HA	5:E:159:GLN:HG3	1.21	1.00
5:E:154:GLN:HB2	5:E:156:LYS:CG	1.91	1.00
1:A:490:VAL:HG11	5:E:574:GLU:HG3	1.00	0.98
2:B:348:ALA:HB2	2:B:405:ILE:HD13	0.99	0.98
2:B:331:ARG:HA	2:B:331:ARG:NH2	1.79	0.98
2:B:423:TYR:CD2	4:D:639:ASP:OD2	2.17	0.98
2:B:348:ALA:HB1	2:B:405:ILE:CD1	1.93	0.98
5:E:19:GLU:CG	5:E:32:LEU:CD1	2.41	0.97
5:E:151:VAL:HA	5:E:159:GLN:CB	1.95	0.97
5:E:154:GLN:CB	5:E:156:LYS:CD	2.33	0.96
5:E:154:GLN:CG	5:E:156:LYS:CD	2.41	0.96
5:E:151:VAL:CG2	5:E:159:GLN:H	1.78	0.96
5:E:151:VAL:C	5:E:159:GLN:CG	2.28	0.96
6:F:541:ARG:HG2	6:F:544:PRO:HB3	1.44	0.95
3:C:552:ARG:HG2	5:E:542:ILE:CG1	1.85	0.95
5:E:19:GLU:CD	5:E:32:LEU:HD12	1.87	0.95
2:B:348:ALA:HB1	2:B:405:ILE:HD11	1.47	0.94
5:E:594:LYS:CD	5:E:597:TRP:NE1	2.29	0.94
4:D:334:LYS:NZ	4:D:344:GLY:HA2	1.82	0.93
5:E:19:GLU:CB	5:E:28:LYS:HG2	1.97	0.93
5:E:154:GLN:HB2	5:E:156:LYS:HG2	1.49	0.93
5:E:159:GLN:HB2	5:E:160:PRO:CD	1.98	0.93
4:D:331:GLY:HA3	4:D:344:GLY:O	1.67	0.93
1:A:1:PRO:HD3	1:A:60:GLU:OE2	1.68	0.93
1:A:44:TYR:CZ	1:A:99:PRO:HG3	2.04	0.92
4:D:334:LYS:HZ3	4:D:344:GLY:HA2	1.34	0.92
2:B:386:ARG:CD	2:B:438:LEU:HD21	1.77	0.92
1:A:334:ASP:OD1	1:A:446:ARG:HG2	1.68	0.92
2:B:348:ALA:CB	2:B:405:ILE:HD11	1.99	0.91
4:D:332:SER:N	4:D:344:GLY:CA	2.33	0.91
5:E:594:LYS:HD2	5:E:597:TRP:CD1	2.06	0.91
3:C:182:CYS:HG	3:C:185:THR:HG1	1.12	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:434:GLU:O	4:D:689:ARG:CZ	2.20	0.90
5:E:594:LYS:HD3	5:E:597:TRP:NE1	1.85	0.90
6:F:334:ALA:HB1	6:F:547:PHE:CD1	2.06	0.90
5:E:380:ASP:HB3	5:E:381:PRO:HD3	0.92	0.89
6:F:380:GLY:O	6:F:383:LYS:N	2.04	0.89
2:B:386:ARG:CG	2:B:438:LEU:HD22	2.03	0.88
5:E:16:PHE:CA	5:E:20:PHE:CZ	2.54	0.87
2:B:386:ARG:CD	2:B:438:LEU:HD23	1.96	0.87
3:C:111:VAL:O	3:C:270:ILE:HD13	1.74	0.87
5:E:173:ARG:HB3	5:E:173:ARG:NH1	1.89	0.87
4:D:332:SER:C	4:D:344:GLY:HA3	1.95	0.86
4:D:334:LYS:NZ	4:D:344:GLY:CA	2.37	0.86
3:C:111:VAL:O	3:C:270:ILE:HD11	1.73	0.86
5:E:173:ARG:HB3	5:E:173:ARG:CZ	2.04	0.86
1:A:578:GLU:O	1:A:582:ARG:NH1	2.07	0.86
4:D:332:SER:O	4:D:343:ARG:O	1.93	0.86
4:D:331:GLY:C	4:D:344:GLY:O	2.13	0.86
5:E:19:GLU:HB3	5:E:28:LYS:CG	2.04	0.86
3:C:552:ARG:HG3	5:E:542:ILE:HG12	1.58	0.85
5:E:355:LEU:O	5:E:563:ARG:NH2	2.10	0.85
5:E:19:GLU:OE2	5:E:32:LEU:HD13	1.75	0.85
2:B:423:TYR:CG	4:D:639:ASP:OD2	2.31	0.84
5:E:154:GLN:HG2	5:E:156:LYS:CD	2.06	0.84
3:C:226:HIS:CD2	3:C:227:ASN:HA	2.13	0.83
2:B:110:ARG:HH11	2:B:113:HIS:CB	1.92	0.83
2:B:329:ALA:HB1	2:B:332:ALA:CB	2.09	0.83
5:E:164:ARG:NE	5:E:165:ASN:O	2.12	0.83
2:B:386:ARG:CZ	2:B:438:LEU:HD21	2.03	0.83
2:B:564:LEU:HD11	2:B:613:VAL:HG13	1.62	0.82
4:D:217:GLN:NE2	4:D:218:LEU:O	2.13	0.82
5:E:16:PHE:HA	5:E:20:PHE:CZ	2.14	0.82
1:A:551:ASP:O	1:A:555:LYS:N	2.13	0.81
5:E:151:VAL:HA	5:E:159:GLN:HB2	1.59	0.81
1:A:44:TYR:CE2	1:A:99:PRO:CG	2.64	0.80
4:D:660:VAL:HG12	4:D:665:ILE:HD12	1.62	0.80
6:F:140:ASN:O	6:F:158:THR:OG1	1.99	0.80
5:E:124:VAL:O	5:E:222:GLY:N	2.14	0.80
5:E:599:ILE:HD13	5:E:599:ILE:H	1.46	0.80
2:B:617:GLN:O	2:B:621:PHE:N	2.14	0.80
3:C:606:ALA:O	3:C:610:GLU:N	2.14	0.80
1:A:364:VAL:CG1	1:A:383:ALA:O	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:304:GLY:O	2:B:590:ARG:NH1	2.16	0.79
5:E:19:GLU:CG	5:E:32:LEU:HD11	2.04	0.79
1:A:214:ASP:O	1:A:217:LYS:NZ	2.14	0.79
5:E:15:ASP:O	5:E:20:PHE:CZ	2.36	0.79
5:E:152:GLU:H	5:E:159:GLN:CD	1.78	0.79
2:B:205:VAL:O	2:B:230:CYS:HB2	1.82	0.79
6:F:370:ASN:O	6:F:607:ARG:NH1	2.16	0.79
2:B:182:ARG:NH2	4:D:221:ASP:OD1	2.16	0.78
3:C:89:ASP:O	3:C:93:ASN:ND2	2.17	0.78
2:B:329:ALA:CB	2:B:332:ALA:HB3	2.11	0.78
3:C:552:ARG:HD2	5:E:542:ILE:CD1	2.13	0.78
5:E:19:GLU:N	5:E:19:GLU:OE1	2.14	0.78
5:E:203:ILE:HD13	5:E:203:ILE:N	1.98	0.78
6:F:581:TYR:OH	6:F:598:SER:O	2.01	0.78
5:E:19:GLU:CG	5:E:32:LEU:HD12	2.11	0.78
4:D:431:GLU:O	4:D:435:GLN:N	2.17	0.77
2:B:205:VAL:O	2:B:229:ALA:O	2.02	0.77
1:A:44:TYR:CD2	1:A:99:PRO:CG	2.67	0.77
1:A:378:GLU:O	1:A:380:THR:OG1	2.02	0.77
4:D:331:GLY:HA3	4:D:344:GLY:C	2.05	0.77
6:F:179:THR:OG1	6:F:181:ASP:OD2	2.02	0.77
5:E:608:ILE:O	5:E:611:SER:OG	2.02	0.77
2:B:370:ARG:N	2:B:412:ARG:O	2.18	0.76
1:A:286:LYS:O	1:A:290:SER:OG	2.04	0.76
2:B:473:ARG:NH2	2:B:475:ARG:O	2.19	0.76
3:C:368:SER:O	3:C:372:GLN:N	2.17	0.76
5:E:154:GLN:HG2	5:E:156:LYS:HD3	1.66	0.76
6:F:390:ILE:O	6:F:394:ALA:N	2.19	0.76
3:C:599:ARG:NH1	3:C:608:ASP:OD2	2.18	0.76
5:E:20:PHE:O	5:E:24:ASP:HA	1.84	0.76
4:D:698:ARG:O	4:D:698:ARG:NH1	2.18	0.76
2:B:591:LEU:HD22	2:B:615:LEU:HD23	1.68	0.76
3:C:197:PHE:O	5:E:111:SER:OG	2.03	0.76
3:C:223:LEU:HD11	3:C:269:VAL:HG22	1.68	0.76
6:F:448:GLU:O	6:F:452:THR:OG1	2.04	0.75
2:B:301:HIS:O	2:B:303:ARG:NH1	2.20	0.75
5:E:61:THR:O	5:E:65:GLU:N	2.19	0.75
5:E:115:GLY:N	5:E:280:VAL:O	2.20	0.75
6:F:429:ALA:O	6:F:433:ALA:N	2.19	0.75
4:D:682:VAL:O	4:D:686:MET:N	2.18	0.75
6:F:495:ARG:O	6:F:500:ASN:ND2	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:THR:C	2:B:330:PRO:HD3	2.05	0.75
3:C:158:GLN:O	3:C:158:GLN:NE2	2.20	0.75
4:D:77:VAL:O	4:D:81:VAL:N	2.19	0.75
1:A:229:HIS:O	1:A:248:VAL:N	2.20	0.75
1:A:346:ILE:O	1:A:350:SER:N	2.20	0.74
6:F:333:ALA:O	6:F:347:LYS:NZ	2.19	0.74
5:E:487:ASN:N	5:E:487:ASN:OD1	2.17	0.74
6:F:341:TYR:O	6:F:528:ARG:NH2	2.20	0.74
1:A:431:GLN:OE1	1:A:433:ARG:NH2	2.20	0.74
6:F:44:LEU:O	6:F:133:TYR:N	2.20	0.74
2:B:102:SER:OG	2:B:165:THR:O	2.02	0.74
3:C:227:ASN:O	3:C:230:VAL:N	2.21	0.74
5:E:16:PHE:CA	5:E:20:PHE:HZ	1.91	0.74
5:E:51:LEU:O	5:E:55:ASN:N	2.19	0.74
5:E:552:LEU:O	5:E:556:ARG:NH1	2.19	0.74
2:B:110:ARG:NH1	2:B:113:HIS:CB	2.51	0.74
2:B:337:GLY:N	2:B:376:ASP:O	2.21	0.74
6:F:414:VAL:HG12	6:F:423:LEU:HB3	1.70	0.74
2:B:473:ARG:O	4:D:544:ARG:NE	2.20	0.74
6:F:172:LYS:N	6:F:226:ILE:O	2.20	0.74
1:A:400:ASP:O	1:A:407:ARG:NH2	2.21	0.74
2:B:107:LYS:HG3	2:B:163:HIS:HB3	1.70	0.73
2:B:364:ALA:O	2:B:368:ALA:N	2.21	0.73
5:E:150:ASP:O	5:E:160:PRO:CG	2.36	0.73
2:B:272:PRO:HG3	4:D:338:ASP:OD2	1.87	0.73
4:D:347:ASN:O	4:D:486:ASP:N	2.21	0.73
6:F:162:ILE:O	6:F:234:GLN:N	2.20	0.73
2:B:234:GLN:OE1	2:B:236:SER:OG	2.06	0.73
5:E:19:GLU:CD	5:E:32:LEU:CD1	2.49	0.73
5:E:625:PRO:O	5:E:629:LYS:N	2.21	0.73
4:D:679:ILE:O	4:D:683:LEU:N	2.22	0.72
6:F:8:LYS:O	6:F:12:PHE:N	2.20	0.72
6:F:270:THR:N	6:F:297:HIS:O	2.22	0.72
6:F:336:ILE:O	6:F:347:LYS:NZ	2.22	0.72
3:C:118:LYS:NZ	3:C:119:THR:O	2.22	0.72
5:E:560:LEU:O	5:E:564:GLN:NE2	2.21	0.72
6:F:632:LEU:O	6:F:636:SER:N	2.21	0.72
3:C:225:ALA:HB2	3:C:268:ASP:HA	1.72	0.72
4:D:338:ASP:OD1	4:D:338:ASP:N	2.17	0.72
5:E:374:ASN:N	5:E:514:ASP:OD2	2.23	0.72
1:A:44:TYR:CD2	1:A:99:PRO:HG2	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:O	1:A:204:LYS:N	2.23	0.72
1:A:118:THR:O	1:A:224:LEU:N	2.23	0.72
6:F:18:GLN:NE2	6:F:84:TYR:OH	2.23	0.72
1:A:33:CYS:SG	1:A:34:LYS:N	2.62	0.71
2:B:44:GLN:NE2	2:B:64:GLU:O	2.22	0.71
2:B:293:GLU:O	2:B:294:ARG:NH1	2.22	0.71
3:C:112:ARG:HA	3:C:270:ILE:HD12	1.72	0.71
4:D:405:MET:SD	4:D:451:SER:OG	2.48	0.71
6:F:148:VAL:O	6:F:149:ARG:NH1	2.23	0.71
1:A:677:ASP:OD2	1:A:681:GLN:NE2	2.23	0.71
3:C:189:ALA:O	3:C:193:ASN:N	2.22	0.71
3:C:450:ALA:HA	3:C:455:ILE:HG23	1.70	0.71
2:B:322:LEU:O	2:B:326:LEU:N	2.23	0.71
5:E:154:GLN:HG3	5:E:156:LYS:HD2	1.72	0.71
3:C:334:GLN:NE2	3:C:464:VAL:O	2.23	0.71
4:D:229:VAL:O	4:D:232:ASN:ND2	2.23	0.71
4:D:290:GLU:O	4:D:294:ARG:N	2.23	0.71
1:A:359:GLN:HA	1:A:359:GLN:OE1	1.91	0.71
2:B:333:ILE:HG13	2:B:334:PRO:HD2	1.71	0.71
5:E:275:LEU:HD12	5:E:278:ARG:HB2	1.71	0.71
5:E:429:ALA:O	5:E:433:MET:N	2.23	0.71
1:A:128:VAL:HG21	1:A:426:ILE:HA	1.73	0.71
1:A:691:TYR:O	1:A:695:LEU:N	2.23	0.71
4:D:92:LEU:O	4:D:96:GLN:N	2.24	0.71
2:B:471:MET:SD	4:D:337:PRO:CG	2.77	0.70
5:E:388:PHE:O	5:E:392:VAL:N	2.23	0.70
6:F:394:ALA:O	6:F:397:SER:OG	2.07	0.70
4:D:656:ILE:HG23	4:D:700:VAL:HG11	1.72	0.70
5:E:374:ASN:O	5:E:514:ASP:N	2.24	0.70
5:E:467:ILE:N	5:E:474:ALA:O	2.24	0.70
6:F:46:VAL:O	6:F:135:GLN:N	2.25	0.70
3:C:225:ALA:HB3	3:C:269:VAL:HG23	1.74	0.70
5:E:613:ALA:O	5:E:617:MET:N	2.24	0.70
6:F:423:LEU:N	6:F:423:LEU:HD12	2.06	0.70
1:A:113:ASN:N	1:A:228:TYR:O	2.23	0.70
5:E:154:GLN:CB	5:E:156:LYS:HG2	2.21	0.70
5:E:136:SER:OG	5:E:149:ARG:O	2.09	0.70
3:C:112:ARG:HA	3:C:270:ILE:CD1	2.22	0.70
3:C:313:LEU:O	3:C:317:LEU:N	2.25	0.70
3:C:230:VAL:O	3:C:232:LYS:NZ	2.23	0.69
4:D:221:ASP:OD1	4:D:222:ARG:NH1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:154:GLN:C	5:E:156:LYS:CG	2.47	0.69
6:F:371:ILE:N	6:F:479:SER:OG	2.25	0.69
1:A:370:VAL:O	1:A:371:GLN:NE2	2.25	0.69
5:E:15:ASP:O	5:E:20:PHE:HZ	1.73	0.69
1:A:35:GLU:O	1:A:37:ARG:NH1	2.25	0.69
1:A:285:GLU:O	1:A:289:ALA:N	2.25	0.69
2:B:110:ARG:HH11	2:B:113:HIS:HB2	1.55	0.69
2:B:110:ARG:NH1	2:B:113:HIS:HB3	2.06	0.69
4:D:662:GLU:OE2	4:D:705:LYS:NZ	2.20	0.69
6:F:461:GLN:N	6:F:476:ALA:O	2.24	0.69
1:A:299:GLU:OE1	1:A:299:GLU:N	2.26	0.69
3:C:510:ASP:O	3:C:514:ALA:N	2.25	0.69
5:E:599:ILE:HD13	5:E:599:ILE:N	2.07	0.69
6:F:541:ARG:CG	6:F:544:PRO:HB3	2.20	0.69
2:B:301:HIS:NE2	2:B:582:ALA:O	2.25	0.69
4:D:413:VAL:HG12	4:D:454:SER:O	1.92	0.69
6:F:423:LEU:HD12	6:F:423:LEU:H	1.58	0.69
1:A:369:TYR:O	1:A:382:GLU:N	2.26	0.69
2:B:435:ASN:C	4:D:689:ARG:NH2	2.46	0.69
2:B:457:ASP:OD2	2:B:460:GLN:NE2	2.26	0.69
3:C:270:ILE:HG13	3:C:270:ILE:O	1.93	0.69
3:C:251:ARG:NH2	3:C:254:PRO:O	2.26	0.69
6:F:456:GLU:O	6:F:459:GLU:N	2.27	0.68
1:A:477:VAL:O	1:A:479:PRO:HD3	1.94	0.68
4:D:535:ALA:O	4:D:539:VAL:N	2.26	0.68
5:E:152:GLU:O	5:E:156:LYS:HG3	1.94	0.68
5:E:151:VAL:CA	5:E:159:GLN:HG2	2.24	0.68
6:F:367:ILE:HG21	6:F:603:LEU:HD23	1.73	0.68
2:B:378:PHE:HD2	2:B:438:LEU:CD1	2.06	0.68
2:B:563:ARG:O	2:B:567:GLN:N	2.25	0.68
3:C:437:VAL:O	3:C:441:VAL:HG23	1.93	0.68
4:D:557:TYR:O	4:D:561:ARG:N	2.26	0.68
5:E:310:ASN:ND2	5:E:313:THR:OG1	2.26	0.68
4:D:646:ILE:O	4:D:650:LEU:N	2.26	0.68
1:A:413:ALA:O	1:A:417:GLN:N	2.26	0.68
2:B:107:LYS:HE2	2:B:110:ARG:HE	1.59	0.68
4:D:405:MET:O	4:D:409:ASP:N	2.27	0.68
5:E:317:TRP:O	5:E:321:PHE:N	2.25	0.68
5:E:594:LYS:CE	5:E:597:TRP:NE1	2.56	0.68
6:F:386:LEU:O	6:F:390:ILE:N	2.26	0.68
2:B:386:ARG:HG3	2:B:438:LEU:HD22	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:332:SER:N	4:D:344:GLY:O	2.27	0.68
3:C:369:GLN:O	3:C:373:TYR:N	2.26	0.68
3:C:163:THR:OG1	5:E:2:ARG:NH2	2.26	0.67
2:B:382:SER:O	2:B:386:ARG:N	2.27	0.67
3:C:139:MET:O	3:C:206:GLN:N	2.27	0.67
3:C:202:MET:HA	3:C:223:LEU:O	1.94	0.67
1:A:375:VAL:HG22	5:E:420:GLU:HB3	1.77	0.67
2:B:545:ILE:O	2:B:597:LYS:NZ	2.28	0.67
4:D:221:ASP:O	4:D:224:LEU:N	2.27	0.67
2:B:410:ASN:OD1	2:B:411:ALA:N	2.27	0.67
3:C:413:ALA:O	3:C:417:SER:OG	2.07	0.67
4:D:417:GLU:N	4:D:458:ALA:O	2.28	0.67
6:F:268:SER:N	6:F:300:VAL:O	2.28	0.67
3:C:75:ARG:O	3:C:79:SER:OG	2.13	0.67
6:F:334:ALA:HB1	6:F:547:PHE:CE1	2.28	0.67
3:C:47:ARG:NE	3:C:50:GLU:OE2	2.28	0.67
3:C:244:ILE:O	3:C:268:ASP:N	2.28	0.67
5:E:637:LYS:O	5:E:641:ARG:N	2.28	0.67
5:E:155:PHE:HZ	5:E:188:LYS:HZ3	1.34	0.67
2:B:379:ASP:O	2:B:386:ARG:NH2	2.28	0.66
2:B:563:ARG:NH1	2:B:567:GLN:OE1	2.28	0.66
3:C:167:GLU:OE2	3:C:174:ALA:HA	1.96	0.66
3:C:554:SER:OG	3:C:556:GLU:OE1	2.09	0.66
3:C:564:ALA:O	3:C:567:ASP:N	2.28	0.66
1:A:385:ALA:O	1:A:389:ALA:N	2.29	0.66
5:E:412:LEU:HD13	5:E:429:ALA:HB1	1.77	0.66
6:F:23:GLY:N	6:F:26:GLN:O	2.28	0.66
3:C:228:ASP:O	3:C:232:LYS:NZ	2.22	0.66
4:D:541:CYS:SG	4:D:596:LYS:HG3	2.35	0.66
5:E:388:PHE:O	5:E:392:VAL:HG23	1.95	0.66
2:B:324:TYR:O	2:B:328:THR:OG1	2.09	0.66
3:C:321:ILE:O	3:C:328:LYS:NZ	2.29	0.66
5:E:20:PHE:O	5:E:24:ASP:OD1	2.14	0.66
3:C:3:ILE:O	3:C:7:ASP:N	2.28	0.66
1:A:33:CYS:O	1:A:84:TYR:OH	2.06	0.66
3:C:124:ASN:O	6:F:227:LYS:NZ	2.29	0.66
5:E:191:ILE:O	5:E:207:LEU:N	2.28	0.66
6:F:624:GLU:O	6:F:628:GLU:N	2.29	0.66
1:A:101:VAL:HA	1:A:117:ARG:O	1.96	0.66
1:A:598:GLU:O	1:A:602:ASN:N	2.29	0.66
3:C:300:LEU:O	3:C:304:SER:N	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:418:ASP:OD1	3:C:461:ARG:N	2.29	0.66
1:A:412:GLU:O	1:A:416:GLN:N	2.28	0.65
4:D:374:TYR:OH	4:D:416:ASP:OD2	2.11	0.65
6:F:378:ASP:CB	6:F:379:PRO:HD3	2.25	0.65
6:F:636:SER:O	6:F:639:SER:OG	2.11	0.65
5:E:152:GLU:CA	5:E:159:GLN:CD	2.65	0.65
5:E:554:ASP:O	5:E:558:TYR:N	2.28	0.65
5:E:558:TYR:O	5:E:562:ALA:N	2.28	0.65
3:C:182:CYS:SG	3:C:185:THR:OG1	2.41	0.65
5:E:330:TYR:O	5:E:334:CYS:N	2.27	0.65
5:E:594:LYS:HE3	5:E:597:TRP:HD1	1.05	0.65
2:B:396:GLY:O	2:B:411:ALA:N	2.28	0.65
5:E:458:GLU:O	5:E:462:GLN:N	2.29	0.65
2:B:51:VAL:O	2:B:55:ASP:N	2.29	0.65
5:E:153:GLN:CG	5:E:153:GLN:HB2	2.15	0.65
6:F:414:VAL:HG11	6:F:423:LEU:HB3	1.76	0.65
1:A:178:THR:O	1:A:182:ASN:N	2.29	0.65
3:C:183:HIS:O	3:C:187:SER:N	2.28	0.65
4:D:615:PHE:O	4:D:619:THR:N	2.29	0.65
3:C:44:TYR:O	3:C:47:ARG:N	2.28	0.65
3:C:311:GLU:OE1	3:C:311:GLU:N	2.29	0.65
4:D:221:ASP:O	4:D:225:CYS:N	2.29	0.65
5:E:275:LEU:HD11	5:E:280:VAL:HG22	1.78	0.65
3:C:605:GLU:OE1	3:C:605:GLU:N	2.30	0.65
5:E:350:GLY:O	5:E:354:MET:N	2.30	0.65
5:E:582:LYS:O	5:E:586:GLN:N	2.28	0.65
6:F:32:GLN:O	6:F:36:LEU:N	2.30	0.65
2:B:410:ASN:OD1	2:B:412:ARG:N	2.29	0.64
4:D:332:SER:N	4:D:344:GLY:HA3	2.06	0.64
4:D:595:SER:O	4:D:599:LEU:N	2.30	0.64
2:B:173:GLU:HG3	2:B:331:ARG:NH2	2.13	0.64
1:A:411:HIS:NE2	1:A:462:PRO:O	2.28	0.64
4:D:304:GLU:O	4:D:308:LYS:N	2.30	0.64
1:A:103:GLU:O	1:A:204:LYS:NZ	2.31	0.64
5:E:154:GLN:CB	5:E:156:LYS:CG	2.66	0.64
3:C:59:LEU:O	3:C:112:ARG:N	2.31	0.64
5:E:155:PHE:CZ	5:E:188:LYS:NZ	2.62	0.64
6:F:442:GLU:N	6:F:483:ALA:O	2.30	0.64
5:E:275:LEU:HD21	5:E:280:VAL:CG2	2.28	0.64
5:E:569:ILE:CG2	5:E:573:SER:HB3	2.28	0.64
5:E:585:ARG:O	5:E:589:GLY:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:71:LYS:NZ	6:F:75:ASP:OD2	2.25	0.64
2:B:303:ARG:NH2	2:B:394:GLU:O	2.30	0.64
1:A:188:ILE:N	1:A:204:LYS:O	2.30	0.64
2:B:555:THR:O	2:B:559:GLU:N	2.31	0.64
4:D:334:LYS:HZ3	4:D:344:GLY:HA3	1.61	0.64
6:F:411:THR:O	6:F:428:GLY:N	2.31	0.64
2:B:461:ASP:HA	2:B:464:ILE:HD12	1.79	0.63
3:C:157:CYS:O	5:E:256:VAL:HG23	1.95	0.63
6:F:402:GLY:N	6:F:441:ASP:O	2.30	0.63
6:F:541:ARG:HG2	6:F:544:PRO:CB	2.25	0.63
1:A:386:LEU:HD23	1:A:434:CYS:SG	2.37	0.63
6:F:528:ARG:O	6:F:532:HIS:N	2.30	0.63
2:B:434:GLU:O	4:D:689:ARG:NH2	2.31	0.63
4:D:64:ALA:O	4:D:68:GLN:NE2	2.31	0.63
2:B:201:ARG:O	2:B:236:SER:N	2.32	0.63
4:D:409:ASP:OD1	4:D:452:ARG:N	2.31	0.63
4:D:419:ASP:O	4:D:426:ARG:NH2	2.32	0.63
3:C:149:GLU:O	3:C:198:SER:N	2.32	0.63
3:C:217:THR:HG23	6:F:472:THR:HG22	1.80	0.63
4:D:336:LEU:CB	4:D:337:PRO:CD	2.53	0.63
5:E:384:ALA:HB1	5:E:519:LEU:HD22	1.81	0.63
5:E:504:ASN:O	5:E:505:LEU:HD23	1.99	0.63
2:B:445:ARG:O	2:B:445:ARG:NH1	2.31	0.62
6:F:31:ASN:OD1	6:F:35:ARG:NH1	2.32	0.62
5:E:632:PHE:O	5:E:636:ASN:N	2.32	0.62
6:F:176:ALA:N	6:F:189:GLN:O	2.32	0.62
1:A:573:THR:OG1	1:A:576:HIS:ND1	2.26	0.62
1:A:574:VAL:O	1:A:578:GLU:N	2.32	0.62
2:B:386:ARG:HD3	2:B:438:LEU:HD22	1.52	0.62
4:D:77:VAL:O	4:D:81:VAL:HG23	1.99	0.62
4:D:665:ILE:O	4:D:669:PHE:N	2.30	0.62
1:A:24:VAL:O	1:A:28:ARG:N	2.32	0.62
3:C:552:ARG:HD2	5:E:542:ILE:CG1	2.30	0.62
3:C:111:VAL:C	3:C:270:ILE:HD11	2.20	0.62
1:A:497:HIS:O	5:E:361:LYS:NZ	2.32	0.62
3:C:544:TYR:O	3:C:548:THR:OG1	2.10	0.62
3:C:552:ARG:HD2	5:E:542:ILE:HG13	1.75	0.62
2:B:308:ILE:O	2:B:417:ALA:N	2.33	0.62
6:F:428:GLY:O	6:F:432:LEU:N	2.31	0.62
1:A:372:ARG:NE	1:A:377:ARG:O	2.32	0.62
5:E:100:LEU:HD23	5:E:119:ARG:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:530:ALA:O	6:F:534:THR:OG1	2.07	0.62
1:A:115:LEU:O	1:A:116:ILE:HD13	2.00	0.62
3:C:330:GLY:O	3:C:334:GLN:N	2.29	0.62
3:C:555:GLU:O	3:C:559:GLN:NE2	2.32	0.61
6:F:174:VAL:N	6:F:224:ARG:O	2.30	0.61
6:F:347:LYS:O	6:F:351:LEU:N	2.31	0.61
2:B:611:GLU:O	2:B:615:LEU:N	2.33	0.61
5:E:703:TYR:CD1	5:E:706:ILE:HD11	2.35	0.61
2:B:107:LYS:O	2:B:160:TYR:HA	2.00	0.61
3:C:420:GLY:O	3:C:463:SER:N	2.32	0.61
5:E:569:ILE:HG23	5:E:573:SER:HB3	1.81	0.61
6:F:126:LEU:O	6:F:224:ARG:NH1	2.33	0.61
6:F:334:ALA:HB1	6:F:547:PHE:CG	2.36	0.61
3:C:186:HIS:O	3:C:189:ALA:N	2.33	0.61
3:C:293:SER:O	3:C:297:VAL:HG23	2.00	0.61
3:C:592:ALA:HB1	3:C:609:VAL:HG22	1.80	0.61
4:D:365:VAL:O	4:D:369:SER:N	2.33	0.61
5:E:518:ILE:CG2	5:E:520:VAL:HG23	2.30	0.61
2:B:330:PRO:HG3	2:B:536:LYS:HE2	1.83	0.61
2:B:425:ARG:HE	2:B:425:ARG:HA	1.65	0.61
1:A:44:TYR:CD2	1:A:99:PRO:HG3	2.29	0.61
1:A:490:VAL:CG1	5:E:574:GLU:CG	2.64	0.61
1:A:532:LYS:HG2	1:A:535:ILE:HD12	1.82	0.61
2:B:383:ASP:O	2:B:387:THR:N	2.34	0.61
4:D:223:TYR:O	4:D:227:LYS:NZ	2.20	0.61
4:D:349:LEU:HD23	4:D:482:LEU:HD13	1.81	0.61
3:C:18:GLN:NE2	3:C:94:GLU:OE1	2.33	0.61
6:F:172:LYS:O	6:F:226:ILE:N	2.34	0.61
6:F:512:ASP:OD1	6:F:513:LEU:N	2.32	0.61
2:B:228:ILE:HG23	2:B:228:ILE:O	2.00	0.61
2:B:345:LEU:O	2:B:363:GLY:N	2.34	0.61
4:D:619:THR:O	4:D:623:ALA:N	2.34	0.61
3:C:156:GLN:OE1	5:E:2:ARG:NH2	2.32	0.61
3:C:186:HIS:O	3:C:190:LEU:N	2.31	0.61
2:B:421:PRO:HB3	2:B:427:ASP:HB3	1.81	0.60
2:B:423:TYR:OH	4:D:643:LEU:CD1	2.49	0.60
4:D:701:LEU:O	4:D:705:LYS:NZ	2.18	0.60
5:E:327:LYS:O	5:E:332:ASN:ND2	2.32	0.60
3:C:113:PRO:HD2	3:C:270:ILE:HG13	1.82	0.60
5:E:320:VAL:O	5:E:324:SER:N	2.33	0.60
1:A:269:GLU:OE2	1:A:272:LYS:NZ	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:325:GLU:N	3:C:325:GLU:OE1	2.32	0.60
4:D:545:LEU:HD11	4:D:588:VAL:HG13	1.83	0.60
5:E:153:GLN:CG	5:E:153:GLN:HB3	2.15	0.60
2:B:162:ASP:N	2:B:190:ASP:OD1	2.34	0.60
6:F:262:GLN:OE1	6:F:475:ASN:ND2	2.34	0.60
1:A:331:LEU:N	1:A:438:ALA:O	2.34	0.60
1:A:587:HIS:O	1:A:591:HIS:N	2.34	0.60
2:B:204:VAL:HG13	2:B:231:ASN:O	2.01	0.60
2:B:322:LEU:HD22	2:B:374:CYS:HB3	1.82	0.60
3:C:74:TYR:O	3:C:77:LEU:N	2.35	0.60
5:E:329:LEU:O	5:E:333:LEU:N	2.34	0.60
4:D:321:LYS:O	4:D:324:ILE:N	2.33	0.60
5:E:21:GLN:HG2	5:E:28:LYS:HE3	1.84	0.60
5:E:585:ARG:HG2	5:E:599:ILE:CG2	2.32	0.60
6:F:318:GLU:N	6:F:318:GLU:OE1	2.34	0.60
1:A:534:ILE:O	1:A:538:LYS:N	2.34	0.60
2:B:405:ILE:HD12	2:B:405:ILE:H	1.66	0.60
2:B:550:THR:HG22	2:B:552:GLU:H	1.66	0.60
5:E:311:GLN:O	5:E:315:LYS:N	2.33	0.60
1:A:465:SER:O	1:A:575:ARG:NH1	2.34	0.60
2:B:319:SER:O	2:B:323:ARG:N	2.32	0.60
5:E:594:LYS:CD	5:E:597:TRP:HE1	1.90	0.60
2:B:205:VAL:C	2:B:229:ALA:O	2.40	0.60
5:E:376:CYS:O	5:E:517:PHE:N	2.34	0.60
3:C:198:SER:O	5:E:111:SER:OG	2.11	0.59
1:A:270:ASP:O	1:A:274:ILE:N	2.33	0.59
5:E:191:ILE:N	5:E:207:LEU:O	2.35	0.59
1:A:274:ILE:O	1:A:278:SER:N	2.35	0.59
2:B:107:LYS:O	2:B:160:TYR:CA	2.51	0.59
5:E:1:VAL:O	5:E:5:VAL:HG22	2.02	0.59
6:F:143:ARG:NH2	6:F:147:GLU:OE1	2.34	0.59
6:F:270:THR:O	6:F:272:ILE:HG22	2.02	0.59
6:F:337:ALA:HB3	6:F:347:LYS:HZ3	1.67	0.59
2:B:234:GLN:O	2:B:238:ASP:N	2.34	0.59
4:D:472:GLU:HA	4:D:482:LEU:HD23	1.84	0.59
4:D:662:GLU:OE1	4:D:662:GLU:N	2.34	0.59
5:E:141:CYS:HB3	5:E:166:PRO:HB2	1.83	0.59
2:B:22:ARG:HA	2:B:32:LEU:HD21	1.85	0.59
3:C:372:GLN:O	3:C:376:ASN:N	2.31	0.59
6:F:603:LEU:O	6:F:607:ARG:N	2.34	0.59
3:C:313:LEU:HD22	3:C:538:LEU:HD21	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:128:HIS:ND1	5:E:188:LYS:O	2.36	0.59
5:E:574:GLU:HA	5:E:577:ILE:HD12	1.83	0.59
5:E:603:GLN:OE1	5:E:603:GLN:N	2.35	0.59
2:B:310:LEU:O	2:B:311:ILE:HD13	2.03	0.59
2:B:211:LEU:HD12	2:B:224:ARG:HD2	1.84	0.59
2:B:587:THR:O	2:B:591:LEU:N	2.35	0.59
3:C:203:ILE:HB	3:C:223:LEU:HD23	1.85	0.59
5:E:524:ASN:O	5:E:528:ASP:N	2.32	0.59
4:D:66:HIS:HA	4:D:69:LEU:HD12	1.85	0.59
5:E:185:ASP:HB3	5:E:213:ALA:HB2	1.85	0.59
6:F:272:ILE:N	6:F:295:GLU:O	2.35	0.59
6:F:352:LEU:O	6:F:356:GLY:N	2.34	0.59
1:A:58:LEU:HD22	1:A:115:LEU:CD2	2.33	0.58
3:C:367:LYS:N	3:C:369:GLN:OE1	2.36	0.58
6:F:176:ALA:HB3	6:F:189:GLN:CG	2.33	0.58
6:F:388:SER:O	6:F:392:ARG:N	2.32	0.58
3:C:331:ILE:O	3:C:335:LEU:N	2.34	0.58
6:F:66:ALA:O	6:F:70:ALA:N	2.34	0.58
6:F:173:MET:HA	6:F:225:PHE:HA	1.85	0.58
4:D:432:ALA:O	4:D:436:GLN:N	2.36	0.58
5:E:120:ILE:HG22	5:E:225:CYS:HB3	1.83	0.58
1:A:473:VAL:O	1:A:473:VAL:HG13	2.03	0.58
2:B:614:GLU:O	2:B:618:TYR:N	2.36	0.58
3:C:535:MET:O	3:C:539:LYS:N	2.32	0.58
2:B:189:ASP:O	2:B:193:VAL:HG23	2.03	0.58
5:E:418:ARG:NE	5:E:421:GLU:O	2.37	0.58
1:A:227:ILE:O	1:A:250:LEU:N	2.36	0.58
1:A:468:ASP:OD1	1:A:469:ILE:N	2.37	0.58
3:C:117:LEU:HG	3:C:118:LYS:N	2.17	0.58
5:E:495:ARG:NE	5:E:495:ARG:O	2.37	0.58
2:B:566:SER:O	2:B:569:SER:OG	2.10	0.58
5:E:94:TYR:CE1	5:E:213:ALA:HB3	2.39	0.58
5:E:154:GLN:O	5:E:156:LYS:N	2.37	0.58
6:F:178:TYR:N	6:F:187:THR:O	2.37	0.58
2:B:430:LYS:HE2	2:B:434:GLU:HB3	1.85	0.57
4:D:604:THR:N	4:D:607:ASP:OD2	2.37	0.57
5:E:754:ARG:O	5:E:758:LYS:N	2.37	0.57
2:B:460:GLN:O	2:B:464:ILE:N	2.37	0.57
3:C:48:LEU:HD13	3:C:99:ARG:NH2	2.19	0.57
4:D:550:ALA:HA	4:D:553:LEU:HD12	1.86	0.57
6:F:630:ILE:O	6:F:633:MET:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:LEU:HD21	2:B:415:VAL:O	2.04	0.57
5:E:435:ALA:O	5:E:438:GLY:N	2.38	0.57
6:F:291:GLU:N	6:F:291:GLU:OE1	2.36	0.57
3:C:111:VAL:O	3:C:270:ILE:HD12	1.96	0.57
4:D:375:THR:CG2	4:D:415:ILE:HA	2.34	0.57
5:E:467:ILE:HD11	5:E:476:LEU:HD11	1.85	0.57
6:F:44:LEU:N	6:F:131:GLU:O	2.37	0.57
1:A:460:THR:O	1:A:464:ILE:N	2.34	0.57
2:B:331:ARG:HA	2:B:331:ARG:CZ	2.35	0.57
2:B:208:TYR:HA	2:B:227:LEU:HD12	1.86	0.57
4:D:667:LYS:O	4:D:671:LYS:N	2.38	0.57
5:E:15:ASP:O	5:E:20:PHE:CE2	2.57	0.57
5:E:535:ILE:O	5:E:539:HIS:N	2.35	0.57
2:B:107:LYS:O	2:B:160:TYR:CB	2.52	0.57
2:B:305:ASP:O	2:B:414:SER:OG	2.18	0.57
2:B:375:ILE:HD12	2:B:415:VAL:HG11	1.87	0.57
3:C:139:MET:N	3:C:206:GLN:O	2.37	0.57
4:D:70:LEU:O	4:D:74:ALA:N	2.36	0.57
5:E:534:ARG:O	5:E:537:ASP:N	2.38	0.57
1:A:122:VAL:HA	1:A:188:ILE:HD13	1.87	0.57
4:D:552:LYS:O	4:D:556:ARG:N	2.33	0.57
4:D:605:GLU:OE2	4:D:605:GLU:N	2.37	0.57
1:A:362:SER:O	1:A:362:SER:OG	2.21	0.57
3:C:391:ALA:HB2	3:C:434:THR:OG1	2.05	0.57
1:A:65:LEU:HA	1:A:68:ILE:HD12	1.87	0.57
5:E:139:PHE:HB2	5:E:173:ARG:HG3	1.85	0.57
2:B:415:VAL:HG12	2:B:416:LEU:O	2.05	0.56
2:B:469:LEU:HD23	2:B:472:HIS:HB2	1.86	0.56
3:C:18:GLN:O	3:C:22:GLN:NE2	2.37	0.56
3:C:226:HIS:CG	3:C:227:ASN:HA	2.39	0.56
5:E:534:ARG:O	5:E:538:LEU:N	2.37	0.56
6:F:257:ASN:HA	6:F:260:ILE:HG21	1.87	0.56
2:B:391:GLU:O	2:B:394:GLU:N	2.38	0.56
5:E:62:ILE:O	5:E:66:PHE:N	2.38	0.56
1:A:121:VAL:N	1:A:189:GLN:O	2.37	0.56
1:A:283:ILE:O	1:A:287:ILE:HG22	2.06	0.56
3:C:401:ASP:O	3:C:405:ARG:N	2.38	0.56
4:D:656:ILE:HD13	4:D:696:MET:CE	2.35	0.56
5:E:383:THR:O	5:E:383:THR:HG22	2.05	0.56
6:F:380:GLY:O	6:F:382:ALA:N	2.38	0.56
6:F:400:THR:O	6:F:441:ASP:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:ARG:HH11	2:B:338:ARG:HB2	1.68	0.56
4:D:655:ALA:O	4:D:697:GLN:NE2	2.38	0.56
6:F:150:ALA:O	6:F:153:VAL:HG12	2.05	0.56
1:A:586:ALA:O	1:A:590:ILE:N	2.38	0.56
5:E:262:GLU:N	5:E:262:GLU:OE1	2.37	0.56
3:C:17:PHE:HA	3:C:73:LEU:HD11	1.87	0.56
5:E:120:ILE:HG21	5:E:227:PHE:HB2	1.88	0.56
6:F:128:ARG:NH2	6:F:223:SER:O	2.37	0.56
6:F:516:LEU:HD23	6:F:517:ILE:N	2.21	0.56
3:C:417:SER:O	3:C:462:THR:OG1	2.12	0.56
3:C:543:ALA:O	3:C:547:SER:N	2.37	0.56
5:E:565:PHE:O	5:E:616:ARG:NH1	2.38	0.56
1:A:457:VAL:HG11	1:A:464:ILE:CD1	2.34	0.56
2:B:33:LEU:N	2:B:39:GLU:OE2	2.38	0.56
3:C:544:TYR:O	3:C:548:THR:N	2.37	0.56
4:D:702:TYR:O	4:D:703:ARG:NE	2.39	0.56
1:A:603:MET:O	1:A:606:ARG:N	2.39	0.55
1:A:398:GLU:N	1:A:439:ALA:O	2.40	0.55
3:C:116:ALA:HB3	3:C:135:THR:OG1	2.06	0.55
3:C:201:GLN:NE2	3:C:231:ASP:OD1	2.38	0.55
4:D:336:LEU:CG	4:D:337:PRO:HD3	2.35	0.55
4:D:352:GLY:O	4:D:460:ASN:ND2	2.38	0.55
4:D:334:LYS:NZ	4:D:344:GLY:N	2.54	0.55
1:A:490:VAL:CG1	5:E:574:GLU:OE1	2.54	0.55
1:A:492:SER:O	1:A:496:HIS:ND1	2.38	0.55
1:A:557:TYR:O	1:A:561:ARG:N	2.36	0.55
3:C:159:VAL:HG13	3:C:159:VAL:O	2.06	0.55
5:E:711:VAL:O	5:E:715:ARG:N	2.40	0.55
6:F:453:ALA:O	6:F:457:VAL:N	2.34	0.55
3:C:589:ILE:O	3:C:593:GLU:N	2.38	0.55
6:F:606:LEU:O	6:F:610:THR:OG1	2.18	0.55
1:A:490:VAL:HG12	5:E:574:GLU:OE1	2.07	0.55
4:D:669:PHE:CE1	4:D:683:LEU:HD22	2.42	0.55
5:E:65:GLU:O	5:E:69:VAL:HG22	2.07	0.55
5:E:449:ASP:OD2	5:E:450:VAL:N	2.38	0.55
1:A:457:VAL:HG12	1:A:459:LEU:N	2.22	0.55
2:B:364:ALA:O	2:B:367:LEU:N	2.40	0.55
2:B:391:GLU:OE2	6:F:401:THR:HG21	2.07	0.55
1:A:410:ILE:HA	1:A:413:ALA:HB3	1.87	0.55
3:C:497:LEU:HD23	3:C:498:ILE:H	1.71	0.55
3:C:550:MET:O	3:C:552:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ASP:OD1	1:A:446:ARG:CG	2.48	0.55
2:B:425:ARG:HA	2:B:425:ARG:NE	2.22	0.55
5:E:275:LEU:HD21	5:E:280:VAL:HG21	1.89	0.55
1:A:396:ILE:N	1:A:437:ILE:O	2.38	0.55
1:A:574:VAL:HG21	1:A:680:ARG:HG3	1.88	0.55
3:C:552:ARG:HD2	5:E:542:ILE:HD11	1.89	0.55
4:D:360:GLN:O	4:D:364:PHE:N	2.37	0.55
6:F:551:ASP:O	6:F:554:LEU:N	2.39	0.55
6:F:555:MET:O	6:F:559:ILE:N	2.40	0.55
1:A:292:ALA:O	1:A:302:LYS:NZ	2.40	0.54
3:C:130:ILE:O	3:C:132:GLN:N	2.40	0.54
4:D:305:VAL:O	4:D:309:SER:OG	2.13	0.54
5:E:56:GLN:O	5:E:60:THR:N	2.39	0.54
5:E:601:VAL:HG23	5:E:604:LEU:HD23	1.90	0.54
1:A:385:ALA:HA	1:A:388:LEU:HD12	1.89	0.54
2:B:76:LYS:HB3	2:B:92:VAL:HA	1.89	0.54
5:E:151:VAL:HG23	5:E:160:PRO:HD2	0.80	0.54
6:F:256:GLU:OE1	6:F:256:GLU:N	2.38	0.54
1:A:570:ILE:N	1:A:571:PRO:HD3	2.21	0.54
2:B:180:LEU:HD23	4:D:445:ILE:HG23	1.90	0.54
3:C:552:ARG:HG2	5:E:542:ILE:CB	2.37	0.54
4:D:323:ALA:O	4:D:327:LEU:N	2.39	0.54
2:B:187:ILE:HD11	2:B:226:VAL:HG21	1.90	0.54
5:E:191:ILE:HD12	5:E:209:VAL:CG1	2.38	0.54
5:E:594:LYS:CD	5:E:597:TRP:HD1	1.91	0.54
4:D:608:VAL:O	4:D:612:LEU:N	2.38	0.54
5:E:465:ILE:HB	5:E:476:LEU:HD12	1.89	0.54
5:E:606:SER:O	5:E:610:LEU:N	2.41	0.54
6:F:127:MET:CE	6:F:132:LEU:HD11	2.38	0.54
6:F:631:ARG:O	6:F:635:MET:N	2.41	0.54
3:C:397:TYR:N	3:C:410:GLN:O	2.40	0.54
3:C:560:ALA:O	3:C:564:ALA:N	2.40	0.54
3:C:594:ALA:O	3:C:598:VAL:N	2.39	0.54
5:E:155:PHE:HZ	5:E:188:LYS:NZ	1.99	0.54
5:E:703:TYR:HD1	5:E:706:ILE:HD11	1.73	0.54
6:F:616:ARG:O	6:F:618:VAL:N	2.40	0.54
2:B:321:LEU:O	2:B:325:VAL:HG23	2.08	0.54
3:C:196:LEU:HD11	5:E:116:LEU:HD21	1.88	0.54
1:A:244:VAL:HG22	5:E:130:VAL:HB	1.90	0.54
5:E:717:VAL:O	5:E:721:GLU:N	2.40	0.54
2:B:109:VAL:HG11	2:B:158:SER:OG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:65:HIS:O	3:C:67:LYS:N	2.41	0.53
4:D:217:GLN:C	4:D:218:LEU:HD12	2.29	0.53
5:E:118:THR:HG23	5:E:120:ILE:HD11	1.91	0.53
2:B:48:LYS:HA	2:B:51:VAL:HG22	1.90	0.53
2:B:386:ARG:CG	2:B:438:LEU:CD2	2.70	0.53
3:C:126:ASN:ND2	3:C:129:ASP:OD1	2.41	0.53
4:D:417:GLU:O	4:D:420:LYS:N	2.40	0.53
5:E:135:VAL:HA	5:E:153:GLN:HA	1.90	0.53
5:E:499:LEU:O	5:E:503:ILE:HG22	2.08	0.53
5:E:154:GLN:CA	5:E:156:LYS:CG	2.87	0.53
3:C:11:ALA:O	3:C:13:CYS:N	2.37	0.53
3:C:544:TYR:CE1	3:C:548:THR:HG21	2.44	0.53
5:E:120:ILE:HD12	5:E:227:PHE:C	2.29	0.53
5:E:124:VAL:HG21	5:E:219:ALA:HB1	1.90	0.53
2:B:423:TYR:OH	4:D:643:LEU:HD13	2.08	0.53
2:B:605:ASP:OD1	2:B:606:LEU:N	2.41	0.53
1:A:331:LEU:HD12	1:A:438:ALA:O	2.09	0.53
4:D:617:VAL:O	4:D:621:ASP:N	2.39	0.53
1:A:418:SER:OG	1:A:431:GLN:NE2	2.42	0.53
3:C:391:ALA:O	3:C:395:THR:N	2.36	0.53
4:D:556:ARG:O	4:D:560:MET:N	2.39	0.53
5:E:581:TYR:CE2	5:E:604:LEU:HD22	2.44	0.53
6:F:266:HIS:ND1	6:F:302:MET:SD	2.82	0.53
3:C:25:ILE:HG22	3:C:45:MET:HB2	1.91	0.53
3:C:121:ASN:O	3:C:124:ASN:ND2	2.39	0.53
5:E:350:GLY:O	5:E:353:LEU:N	2.42	0.53
1:A:8:ARG:O	1:A:12:PHE:N	2.40	0.53
3:C:556:GLU:O	3:C:559:GLN:NE2	2.42	0.53
6:F:176:ALA:HB3	6:F:189:GLN:HG2	1.91	0.53
6:F:466:ALA:HA	6:F:471:LEU:HD23	1.90	0.53
6:F:570:PRO:HD3	6:F:620:VAL:HG12	1.90	0.53
1:A:78:LEU:HD23	1:A:84:TYR:HB2	1.91	0.53
2:B:206:GLY:CA	2:B:227:LEU:HD21	2.39	0.53
3:C:294:GLU:OE2	3:C:294:GLU:N	2.40	0.53
6:F:145:ILE:HD13	6:F:248:SER:HA	1.91	0.53
6:F:415:LEU:O	6:F:423:LEU:HA	2.09	0.53
3:C:297:VAL:O	3:C:301:LYS:N	2.37	0.52
5:E:437:ASN:N	5:E:479:ARG:O	2.40	0.52
6:F:164:THR:O	6:F:232:LYS:N	2.41	0.52
6:F:423:LEU:N	6:F:423:LEU:CD1	2.72	0.52
4:D:304:GLU:OE1	4:D:304:GLU:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:433:MET:CE	4:D:481:ILE:HD11	2.39	0.52
2:B:333:ILE:HG13	2:B:334:PRO:CD	2.37	0.52
3:C:268:ASP:O	3:C:270:ILE:HG22	2.10	0.52
1:A:605:ILE:O	1:A:609:LEU:N	2.34	0.52
4:D:645:ARG:O	4:D:649:GLN:NE2	2.41	0.52
5:E:275:LEU:HD21	5:E:280:VAL:HG22	1.91	0.52
5:E:446:ASP:HB3	5:E:505:LEU:HD21	1.90	0.52
5:E:580:GLN:O	5:E:584:LEU:N	2.36	0.52
1:A:328:ASN:O	1:A:468:ASP:N	2.39	0.52
1:A:384:GLY:O	1:A:387:VAL:N	2.43	0.52
2:B:551:GLN:O	2:B:555:THR:N	2.40	0.52
5:E:154:GLN:CA	5:E:156:LYS:HG2	2.37	0.52
6:F:348:LYS:O	6:F:352:LEU:N	2.39	0.52
5:E:541:ARG:HA	5:E:541:ARG:CZ	2.40	0.52
1:A:288:PHE:HB3	1:A:306:ALA:HB2	1.92	0.52
1:A:490:VAL:CG1	5:E:574:GLU:CD	2.78	0.52
1:A:528:GLU:N	1:A:528:GLU:OE1	2.43	0.52
3:C:71:LYS:HA	3:C:74:TYR:HB3	1.92	0.52
3:C:76:GLN:HA	3:C:79:SER:HB2	1.91	0.52
3:C:293:SER:O	3:C:297:VAL:N	2.36	0.52
3:C:491:LEU:O	3:C:494:ARG:NE	2.39	0.52
4:D:413:VAL:O	4:D:456:LEU:N	2.39	0.52
5:E:20:PHE:CD1	5:E:20:PHE:N	2.77	0.52
5:E:51:LEU:HD11	5:E:58:LEU:HB2	1.91	0.52
1:A:355:PHE:CE1	1:A:395:LEU:HD23	2.45	0.52
1:A:621:MET:O	1:A:625:ARG:NE	2.39	0.52
2:B:464:ILE:O	2:B:468:VAL:N	2.43	0.52
4:D:408:ALA:O	4:D:411:GLY:N	2.39	0.52
2:B:209:ARG:N	2:B:226:VAL:O	2.43	0.52
3:C:456:CYS:HB3	5:E:203:ILE:HG23	1.91	0.52
4:D:611:ALA:HA	4:D:614:LEU:HD12	1.92	0.52
2:B:398:VAL:N	2:B:409:LEU:O	2.39	0.52
3:C:240:ASN:H	3:C:241:VAL:HG23	1.75	0.52
5:E:515:LEU:HD11	5:E:610:LEU:HD11	1.91	0.52
2:B:206:GLY:HA3	2:B:229:ALA:O	2.10	0.51
2:B:378:PHE:CD2	2:B:438:LEU:CD1	2.90	0.51
4:D:336:LEU:CD2	4:D:337:PRO:HD3	2.39	0.51
2:B:206:GLY:O	2:B:227:LEU:HD11	2.09	0.51
3:C:392:VAL:HG12	3:C:397:TYR:HA	1.91	0.51
5:E:19:GLU:HB2	5:E:29:TYR:N	2.25	0.51
6:F:372:ASN:O	6:F:512:ASP:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:HD22	1:A:115:LEU:HD23	1.90	0.51
1:A:462:PRO:O	1:A:466:ARG:NE	2.44	0.51
3:C:223:LEU:CD1	3:C:269:VAL:HG22	2.38	0.51
5:E:346:GLU:OE1	5:E:346:GLU:N	2.38	0.51
1:A:363:ALA:CB	5:E:473:LYS:NZ	2.73	0.51
1:A:457:VAL:HG11	1:A:464:ILE:HD11	1.92	0.51
2:B:284:ILE:CD1	2:B:321:LEU:HD22	2.40	0.51
3:C:364:GLY:O	3:C:369:GLN:NE2	2.40	0.51
5:E:407:SER:O	5:E:407:SER:OG	2.26	0.51
6:F:327:ASP:O	6:F:331:LYS:N	2.34	0.51
1:A:579:SER:O	1:A:582:ARG:N	2.44	0.51
3:C:155:PHE:O	3:C:164:THR:N	2.44	0.51
4:D:661:SER:CB	4:D:701:LEU:HD13	2.41	0.51
5:E:443:ASP:OD1	5:E:444:GLU:N	2.43	0.51
5:E:620:CYS:SG	5:E:621:ASP:N	2.83	0.51
6:F:258:THR:O	6:F:260:ILE:HG23	2.11	0.51
1:A:329:VAL:HG13	1:A:469:ILE:HB	1.93	0.51
3:C:145:GLN:N	3:C:145:GLN:OE1	2.43	0.51
5:E:150:ASP:O	5:E:160:PRO:HG2	2.08	0.51
5:E:150:ASP:O	5:E:160:PRO:CD	2.58	0.51
1:A:303:ARG:O	1:A:307:LEU:N	2.41	0.51
2:B:378:PHE:HD2	2:B:438:LEU:HD12	1.73	0.51
3:C:583:ARG:O	3:C:586:GLU:N	2.44	0.51
5:E:3:ASP:OD2	5:E:4:GLU:N	2.44	0.51
5:E:585:ARG:HG2	5:E:599:ILE:HG22	1.93	0.51
5:E:638:SER:O	5:E:642:VAL:HG13	2.11	0.51
1:A:114:GLN:HB2	1:A:116:ILE:HD11	1.93	0.51
1:A:384:GLY:O	1:A:388:LEU:N	2.33	0.51
1:A:486:ALA:HA	5:E:604:LEU:HD21	1.93	0.51
2:B:68:GLY:HA3	2:B:231:ASN:HB2	1.92	0.51
4:D:92:LEU:HD22	4:D:223:TYR:OH	2.10	0.51
5:E:154:GLN:HA	5:E:154:GLN:HE21	1.75	0.51
1:A:487:ARG:O	1:A:491:GLY:N	2.39	0.51
6:F:74:ALA:O	6:F:78:GLN:N	2.41	0.51
6:F:506:ALA:O	6:F:509:SER:OG	2.28	0.51
2:B:107:LYS:CG	2:B:163:HIS:HB3	2.38	0.51
3:C:89:ASP:O	3:C:108:GLN:NE2	2.44	0.51
3:C:378:VAL:HG12	3:C:380:ARG:N	2.26	0.51
4:D:656:ILE:CG2	4:D:700:VAL:HG11	2.40	0.51
5:E:118:THR:HG21	5:E:282:LEU:O	2.10	0.51
5:E:195:GLN:HA	5:E:198:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:401:THR:HG22	6:F:441:ASP:HB2	1.93	0.51
6:F:624:GLU:N	6:F:624:GLU:OE1	2.41	0.51
1:A:676:VAL:O	1:A:679:ALA:HB3	2.11	0.50
5:E:154:GLN:HA	5:E:154:GLN:NE2	2.26	0.50
5:E:615:ALA:O	5:E:619:CYS:N	2.44	0.50
2:B:179:GLN:N	4:D:446:THR:OG1	2.44	0.50
4:D:332:SER:O	4:D:343:ARG:C	2.48	0.50
4:D:332:SER:N	4:D:344:GLY:HA2	2.04	0.50
4:D:386:THR:O	4:D:388:SER:N	2.43	0.50
5:E:191:ILE:HD12	5:E:209:VAL:HG12	1.93	0.50
5:E:370:ARG:NH2	5:E:460:MET:O	2.43	0.50
1:A:428:THR:OG1	1:A:429:SER:N	2.44	0.50
2:B:423:TYR:OH	4:D:643:LEU:HD11	2.10	0.50
3:C:133:LEU:HG	3:C:244:ILE:HG12	1.93	0.50
4:D:352:GLY:N	4:D:461:SER:OG	2.44	0.50
6:F:554:LEU:O	6:F:558:TYR:N	2.40	0.50
1:A:363:ALA:HB3	5:E:473:LYS:NZ	2.26	0.50
2:B:160:TYR:O	6:F:150:ALA:HB1	2.11	0.50
5:E:551:SER:OG	5:E:553:ASP:N	2.39	0.50
5:E:719:GLU:HG2	5:E:726:LEU:HD11	1.94	0.50
6:F:552:MET:O	6:F:556:ARG:N	2.41	0.50
1:A:101:VAL:O	1:A:101:VAL:HG12	2.12	0.50
3:C:127:PRO:HB2	6:F:225:PHE:HB2	1.92	0.50
3:C:509:TYR:O	3:C:513:LEU:N	2.42	0.50
2:B:246:GLU:N	2:B:246:GLU:OE1	2.44	0.50
5:E:741:SER:O	5:E:741:SER:OG	2.30	0.50
2:B:320:GLN:O	2:B:324:TYR:N	2.36	0.50
2:B:405:ILE:HD12	2:B:405:ILE:N	2.27	0.50
4:D:92:LEU:HD23	4:D:93:GLN:N	2.27	0.50
4:D:661:SER:O	4:D:665:ILE:HG22	2.11	0.50
5:E:541:ARG:HA	5:E:541:ARG:NE	2.26	0.50
2:B:333:ILE:O	2:B:373:VAL:HA	2.12	0.50
5:E:105:LYS:O	5:E:109:LEU:N	2.43	0.50
6:F:463:ILE:HG12	6:F:476:ALA:HB2	1.93	0.50
6:F:378:ASP:HB3	6:F:379:PRO:HD3	1.93	0.50
1:A:233:ASP:N	1:A:239:ALA:HB3	2.27	0.49
1:A:300:ASP:OD1	1:A:300:ASP:N	2.44	0.49
2:B:207:THR:N	2:B:230:CYS:SG	2.85	0.49
2:B:335:THR:OG1	2:B:336:THR:N	2.45	0.49
3:C:225:ALA:HB3	3:C:269:VAL:H	1.78	0.49
3:C:460:ALA:O	3:C:462:THR:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:677:HIS:O	4:D:681:LYS:N	2.43	0.49
5:E:162:ILE:HD13	5:E:256:VAL:HA	1.93	0.49
6:F:373:ILE:N	6:F:480:ILE:O	2.45	0.49
4:D:475:ILE:HG21	4:D:478:MET:HB2	1.93	0.49
6:F:74:ALA:O	6:F:77:VAL:N	2.46	0.49
2:B:381:MET:O	2:B:386:ARG:NH2	2.44	0.49
3:C:202:MET:HA	3:C:224:PHE:HA	1.93	0.49
3:C:327:ILE:HG23	3:C:499:PHE:HD1	1.77	0.49
3:C:543:ALA:O	3:C:546:HIS:N	2.45	0.49
3:C:552:ARG:CD	5:E:542:ILE:CG1	2.64	0.49
4:D:421:MET:O	4:D:426:ARG:NH2	2.45	0.49
5:E:139:PHE:CE1	5:E:176:LEU:HB2	2.46	0.49
5:E:140:LEU:HD22	5:E:148:ILE:HG22	1.93	0.49
5:E:173:ARG:CZ	5:E:173:ARG:CB	2.81	0.49
6:F:345:ASP:N	6:F:345:ASP:OD1	2.45	0.49
1:A:233:ASP:O	1:A:238:THR:OG1	2.12	0.49
3:C:191:ILE:HG21	5:E:67:TYR:CD1	2.48	0.49
3:C:594:ALA:O	3:C:597:LYS:N	2.46	0.49
4:D:559:ILE:O	4:D:562:SER:OG	2.31	0.49
4:D:657:GLY:O	4:D:701:LEU:HD11	2.12	0.49
5:E:575:ASP:OD1	5:E:575:ASP:N	2.44	0.49
5:E:601:VAL:O	5:E:605:GLU:N	2.43	0.49
2:B:323:ARG:O	2:B:327:CYS:N	2.33	0.49
4:D:332:SER:O	4:D:344:GLY:N	2.46	0.49
4:D:618:SER:O	4:D:622:ALA:N	2.45	0.49
5:E:553:ASP:O	5:E:556:ARG:N	2.45	0.49
6:F:329:TYR:CE1	6:F:615:LEU:HD12	2.48	0.49
6:F:628:GLU:O	6:F:632:LEU:N	2.39	0.49
1:A:356:THR:HG21	1:A:366:LEU:HG	1.94	0.49
1:A:386:LEU:HD22	1:A:432:ALA:HB1	1.95	0.49
3:C:21:LEU:O	3:C:48:LEU:HD11	2.13	0.49
1:A:98:LEU:N	1:A:99:PRO:CD	2.69	0.49
1:A:329:VAL:HG22	1:A:468:ASP:OD1	2.13	0.49
1:A:490:VAL:O	1:A:494:VAL:HG23	2.13	0.49
2:B:109:VAL:CG1	2:B:158:SER:OG	2.60	0.49
3:C:518:VAL:HG11	6:F:574:ALA:HB1	1.95	0.49
4:D:336:LEU:HD22	4:D:337:PRO:HD3	1.95	0.49
4:D:648:LYS:O	4:D:653:ARG:N	2.45	0.49
1:A:231:ASN:C	1:A:248:VAL:HG21	2.33	0.48
1:A:234:GLY:H	1:A:239:ALA:HB3	1.78	0.48
3:C:189:ALA:HB1	3:C:193:ASN:ND2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:533:LEU:HD23	3:C:534:ASP:N	2.27	0.48
4:D:92:LEU:HD22	4:D:223:TYR:CZ	2.48	0.48
4:D:375:THR:HG22	4:D:415:ILE:HA	1.94	0.48
6:F:9:VAL:HG22	6:F:13:LEU:HD12	1.95	0.48
6:F:492:ASN:OD1	6:F:494:ARG:N	2.43	0.48
1:A:102:GLU:OE2	1:A:116:ILE:HG21	2.13	0.48
1:A:123:THR:N	1:A:187:ARG:O	2.40	0.48
2:B:346:THR:O	2:B:361:GLU:N	2.43	0.48
2:B:398:VAL:HG23	2:B:409:LEU:O	2.13	0.48
3:C:113:PRO:HB2	3:C:242:THR:HG21	1.96	0.48
3:C:334:GLN:OE1	3:C:465:LEU:HD22	2.13	0.48
5:E:270:LEU:HD23	5:E:273:ARG:HD2	1.96	0.48
1:A:585:GLU:O	1:A:589:ARG:N	2.40	0.48
5:E:159:GLN:CB	5:E:160:PRO:HD3	2.18	0.48
6:F:386:LEU:O	6:F:389:TYR:N	2.46	0.48
1:A:229:HIS:N	1:A:248:VAL:O	2.43	0.48
2:B:373:VAL:HB	2:B:415:VAL:HG13	1.94	0.48
3:C:231:ASP:O	3:C:234:GLN:NE2	2.44	0.48
4:D:661:SER:C	4:D:665:ILE:HG22	2.33	0.48
5:E:133:GLU:O	5:E:184:VAL:HG22	2.13	0.48
6:F:507:LEU:O	6:F:510:ARG:N	2.44	0.48
1:A:182:ASN:O	1:A:210:ALA:HB2	2.12	0.48
1:A:581:ILE:HG23	1:A:582:ARG:N	2.28	0.48
2:B:328:THR:O	2:B:330:PRO:CD	2.41	0.48
3:C:90:MET:O	3:C:94:GLU:N	2.39	0.48
5:E:125:VAL:HG21	5:E:192:GLN:HB3	1.96	0.48
6:F:125:GLU:O	6:F:127:MET:N	2.47	0.48
6:F:599:ALA:O	6:F:602:LEU:N	2.46	0.48
1:A:286:LYS:HA	1:A:289:ALA:HB3	1.95	0.48
2:B:533:ALA:O	2:B:537:LYS:N	2.44	0.48
3:C:87:THR:O	3:C:91:ALA:N	2.41	0.48
3:C:113:PRO:HD3	3:C:270:ILE:HD11	1.96	0.48
5:E:134:LEU:HD13	5:E:181:SER:HB2	1.95	0.48
6:F:9:VAL:HG22	6:F:13:LEU:CD1	2.44	0.48
6:F:345:ASP:OD1	6:F:346:VAL:N	2.46	0.48
1:A:363:ALA:CB	5:E:473:LYS:HZ2	2.26	0.48
5:E:154:GLN:CA	5:E:154:GLN:NE2	2.75	0.48
6:F:486:PRO:HD2	6:F:486:PRO:O	2.13	0.48
1:A:280:ASP:O	1:A:283:ILE:HG22	2.14	0.48
1:A:532:LYS:CG	1:A:535:ILE:HD12	2.43	0.48
2:B:423:TYR:CZ	4:D:643:LEU:HD13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:154:PHE:HA	3:C:165:ARG:HA	1.96	0.48
4:D:306:ILE:O	4:D:310:ILE:HD12	2.13	0.48
5:E:19:GLU:O	5:E:28:LYS:HB3	2.14	0.48
5:E:528:ASP:OD1	5:E:531:ILE:HD12	2.14	0.48
6:F:252:LEU:HB2	6:F:295:GLU:HA	1.95	0.48
6:F:478:CYS:SG	6:F:479:SER:N	2.87	0.48
2:B:386:ARG:HE	2:B:438:LEU:CG	2.11	0.48
5:E:57:GLN:O	5:E:61:THR:OG1	2.26	0.48
5:E:412:LEU:HB2	5:E:431:ALA:HB3	1.95	0.48
5:E:528:ASP:HA	5:E:531:ILE:HD12	1.95	0.48
6:F:176:ALA:HB3	6:F:189:GLN:HG3	1.96	0.48
6:F:443:PHE:HB3	6:F:484:ALA:HB2	1.96	0.48
6:F:461:GLN:O	6:F:473:THR:HG21	2.14	0.48
3:C:335:LEU:HD11	3:C:377:LEU:HD23	1.96	0.48
3:C:428:ASP:OD1	3:C:428:ASP:N	2.47	0.48
3:C:584:GLN:O	3:C:588:LEU:N	2.39	0.48
4:D:664:SER:O	4:D:667:LYS:N	2.44	0.48
1:A:275:THR:O	1:A:278:SER:OG	2.29	0.47
1:A:370:VAL:HG11	1:A:426:ILE:HD12	1.95	0.47
2:B:329:ALA:CA	2:B:332:ALA:HB3	2.43	0.47
5:E:568:LYS:HG3	5:E:568:LYS:O	2.14	0.47
6:F:465:ILE:N	6:F:472:THR:O	2.43	0.47
1:A:605:ILE:O	1:A:608:MET:N	2.47	0.47
2:B:107:LYS:N	2:B:161:LYS:O	2.42	0.47
2:B:379:ASP:OD1	2:B:379:ASP:N	2.47	0.47
5:E:134:LEU:HD11	5:E:136:SER:O	2.14	0.47
6:F:454:ILE:O	6:F:457:VAL:N	2.47	0.47
1:A:609:LEU:O	1:A:613:ILE:N	2.34	0.47
3:C:45:MET:HA	3:C:48:LEU:HD12	1.96	0.47
6:F:447:ALA:O	6:F:449:ALA:N	2.47	0.47
6:F:452:THR:O	6:F:455:HIS:N	2.47	0.47
1:A:422:SER:HA	1:A:427:VAL:HG23	1.96	0.47
2:B:100:LYS:HG2	4:D:443:ALA:HB1	1.95	0.47
2:B:551:GLN:O	2:B:555:THR:OG1	2.26	0.47
2:B:586:GLU:HA	2:B:589:ILE:HD12	1.96	0.47
5:E:321:PHE:O	5:E:325:GLN:N	2.42	0.47
6:F:14:GLN:HG3	6:F:80:LEU:HD21	1.95	0.47
1:A:300:ASP:OD1	1:A:301:ILE:N	2.46	0.47
2:B:108:VAL:HG13	2:B:160:TYR:CZ	2.49	0.47
2:B:173:GLU:OE1	2:B:331:ARG:HA	2.15	0.47
2:B:331:ARG:CZ	2:B:331:ARG:CB	2.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:121:ASN:O	3:C:123:ARG:N	2.47	0.47
4:D:642:MET:C	4:D:646:ILE:HD12	2.34	0.47
6:F:149:ARG:O	6:F:152:SER:OG	2.26	0.47
6:F:403:ARG:NH1	6:F:405:SER:O	2.47	0.47
6:F:616:ARG:O	6:F:618:VAL:HG23	2.14	0.47
1:A:285:GLU:O	1:A:288:PHE:N	2.45	0.47
3:C:517:LEU:O	3:C:521:TYR:N	2.48	0.47
4:D:610:GLU:O	4:D:614:LEU:N	2.44	0.47
5:E:120:ILE:HD13	5:E:283:ALA:CB	2.44	0.47
5:E:399:ALA:HB1	5:E:401:TYR:CE1	2.49	0.47
1:A:423:LYS:N	1:A:426:ILE:O	2.47	0.47
2:B:580:VAL:O	2:B:584:THR:OG1	2.26	0.47
3:C:498:ILE:HD12	3:C:498:ILE:N	2.30	0.47
5:E:198:LEU:HD13	5:E:202:SER:CB	2.45	0.47
6:F:15:GLU:O	6:F:19:ASP:N	2.48	0.47
6:F:29:TYR:OH	6:F:47:ASP:N	2.48	0.47
6:F:490:ARG:HA	6:F:490:ARG:HD3	1.66	0.47
2:B:546:LYS:O	2:B:548:VAL:N	2.48	0.47
3:C:76:GLN:HA	3:C:79:SER:CB	2.45	0.47
3:C:84:VAL:O	3:C:88:PHE:N	2.40	0.47
3:C:140:VAL:HG21	3:C:237:ASP:HB2	1.96	0.47
5:E:127:THR:HA	5:E:189:VAL:HG13	1.97	0.47
1:A:459:LEU:HD11	1:A:463:ILE:HG21	1.96	0.47
4:D:678:ALA:O	4:D:682:VAL:N	2.47	0.47
5:E:569:ILE:CG2	5:E:573:SER:CB	2.92	0.47
6:F:496:SER:O	6:F:500:ASN:N	2.36	0.47
2:B:44:GLN:O	2:B:48:LYS:N	2.45	0.47
3:C:225:ALA:CB	3:C:268:ASP:HA	2.41	0.47
5:E:413:THR:OG1	5:E:451:ARG:NH1	2.46	0.47
6:F:585:ARG:NH2	6:F:597:THR:O	2.48	0.47
3:C:254:PRO:O	5:E:268:ARG:NE	2.42	0.46
5:E:415:ALA:HB3	5:E:425:PHE:CB	2.45	0.46
6:F:252:LEU:N	6:F:294:LEU:O	2.39	0.46
6:F:573:LEU:O	6:F:576:TYR:N	2.47	0.46
1:A:561:ARG:HA	1:A:572:ILE:HG21	1.97	0.46
3:C:565:TYR:CE1	5:E:532:ALA:HB3	2.51	0.46
4:D:299:LEU:HD23	4:D:302:VAL:HG23	1.98	0.46
4:D:419:ASP:OD1	4:D:420:LYS:N	2.48	0.46
4:D:694:HIS:O	4:D:698:ARG:N	2.44	0.46
5:E:144:CYS:SG	5:E:171:ARG:NH2	2.86	0.46
2:B:206:GLY:C	2:B:227:LEU:HD21	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:60:ASP:OD1	6:F:61:SER:N	2.48	0.46
2:B:173:GLU:CG	2:B:331:ARG:NH2	2.79	0.46
5:E:168:CYS:SG	5:E:169:ALA:N	2.88	0.46
6:F:127:MET:HE1	6:F:132:LEU:HD11	1.96	0.46
3:C:248:VAL:O	3:C:264:LYS:N	2.37	0.46
3:C:372:GLN:O	3:C:376:ASN:ND2	2.48	0.46
4:D:79:ASP:OD1	4:D:85:ARG:NH2	2.49	0.46
4:D:536:TYR:O	4:D:540:LYS:N	2.49	0.46
4:D:663:HIS:O	4:D:666:ILE:HD11	2.15	0.46
5:E:19:GLU:HG2	5:E:32:LEU:HD12	1.68	0.46
5:E:138:THR:HG21	5:E:147:VAL:HG22	1.97	0.46
5:E:446:ASP:OD1	5:E:446:ASP:N	2.48	0.46
6:F:541:ARG:CD	6:F:544:PRO:HB3	2.45	0.46
1:A:13:LEU:HD12	1:A:72:ALA:HB1	1.98	0.46
1:A:549:ASP:OD1	1:A:552:LYS:NZ	2.32	0.46
5:E:184:VAL:HG23	5:E:185:ASP:H	1.81	0.46
2:B:463:GLU:O	2:B:467:HIS:N	2.41	0.46
4:D:362:LEU:O	4:D:366:GLU:N	2.43	0.46
1:A:485:LEU:O	1:A:489:VAL:HG23	2.16	0.46
2:B:19:ASN:OD1	2:B:20:ASP:N	2.48	0.46
2:B:167:THR:HA	2:B:185:ASP:HA	1.97	0.46
3:C:154:PHE:HB3	3:C:185:THR:HG22	1.97	0.46
5:E:314:VAL:O	5:E:318:GLU:N	2.44	0.46
6:F:29:TYR:O	6:F:33:LEU:HD23	2.16	0.46
6:F:68:ARG:O	6:F:72:LEU:N	2.40	0.46
1:A:212:LEU:HD11	1:A:252:ASN:HA	1.98	0.46
2:B:460:GLN:O	2:B:463:GLU:N	2.48	0.46
3:C:399:MET:O	3:C:408:VAL:N	2.47	0.46
4:D:297:ALA:CB	4:D:599:LEU:HD12	2.45	0.46
5:E:259:TYR:O	5:E:261:THR:HG23	2.16	0.46
1:A:588:ALA:O	1:A:592:LEU:N	2.45	0.46
2:B:100:LYS:HE3	4:D:443:ALA:HB1	1.98	0.46
2:B:277:HIS:O	2:B:280:VAL:N	2.49	0.46
5:E:13:PHE:HB3	5:E:17:LEU:HD22	1.97	0.46
1:A:98:LEU:HA	1:A:99:PRO:HD2	1.14	0.45
2:B:375:ILE:HG21	2:B:378:PHE:CD1	2.50	0.45
2:B:591:LEU:HD22	2:B:615:LEU:CD2	2.44	0.45
3:C:61:VAL:O	3:C:114:PHE:N	2.48	0.45
3:C:435:ARG:H	3:C:437:VAL:HG12	1.80	0.45
3:C:583:ARG:O	3:C:587:SER:N	2.44	0.45
4:D:415:ILE:O	4:D:458:ALA:N	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:82:GLN:O	3:C:82:GLN:NE2	2.49	0.45
3:C:217:THR:HG21	6:F:471:LEU:H	1.81	0.45
3:C:225:ALA:HB3	3:C:269:VAL:N	2.30	0.45
3:C:422:CYS:N	3:C:463:SER:O	2.46	0.45
1:A:478:ASP:N	1:A:482:ASP:OD2	2.49	0.45
1:A:490:VAL:HG11	5:E:574:GLU:CD	2.33	0.45
2:B:94:VAL:N	2:B:204:VAL:O	2.49	0.45
4:D:660:VAL:CG1	4:D:665:ILE:HD12	2.41	0.45
1:A:103:GLU:N	1:A:106:SER:OG	2.40	0.45
1:A:532:LYS:CB	1:A:535:ILE:HD12	2.46	0.45
5:E:139:PHE:CD1	5:E:176:LEU:HB2	2.51	0.45
5:E:211:LEU:HD23	5:E:215:ALA:O	2.17	0.45
5:E:333:LEU:HD23	5:E:550:TYR:OH	2.16	0.45
6:F:230:GLU:HB2	6:F:420:SER:O	2.17	0.45
1:A:485:LEU:O	1:A:489:VAL:N	2.47	0.45
1:A:498:PRO:HD2	5:E:568:LYS:HB3	1.99	0.45
1:A:626:LYS:O	1:A:630:ARG:N	2.48	0.45
2:B:192:LEU:HD21	2:B:231:ASN:HA	1.99	0.45
3:C:65:HIS:C	3:C:67:LYS:H	2.20	0.45
4:D:332:SER:CA	4:D:344:GLY:HA3	2.46	0.45
4:D:399:ILE:O	4:D:401:GLU:N	2.49	0.45
5:E:758:LYS:O	5:E:762:ARG:N	2.47	0.45
6:F:61:SER:O	6:F:65:ASN:N	2.45	0.45
6:F:164:THR:N	6:F:232:LYS:O	2.46	0.45
6:F:177:THR:N	6:F:223:SER:OG	2.46	0.45
4:D:685:LEU:HD13	4:D:688:ARG:CZ	2.47	0.45
5:E:433:MET:SD	5:E:476:LEU:HD13	2.56	0.45
6:F:167:SER:HG	6:F:230:GLU:H	1.64	0.45
6:F:383:LYS:HA	6:F:386:LEU:HD23	1.97	0.45
6:F:414:VAL:HG13	6:F:423:LEU:O	2.16	0.45
6:F:453:ALA:O	6:F:457:VAL:HG23	2.17	0.45
6:F:546:GLN:HG2	6:F:546:GLN:O	2.17	0.45
1:A:100:LEU:CD1	1:A:100:LEU:C	2.85	0.45
1:A:465:SER:O	1:A:466:ARG:NH1	2.49	0.45
1:A:530:LEU:HD23	1:A:531:LYS:HA	1.98	0.45
3:C:77:LEU:HG	3:C:78:ILE:H	1.82	0.45
4:D:365:VAL:HG11	4:D:456:LEU:HD11	1.99	0.45
4:D:472:GLU:OE1	4:D:472:GLU:N	2.50	0.45
4:D:666:ILE:O	4:D:670:THR:N	2.43	0.45
5:E:212:ARG:NH2	5:E:284:CYS:SG	2.85	0.45
1:A:102:GLU:O	1:A:118:THR:OG1	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:44:TYR:O	3:C:48:LEU:N	2.47	0.45
3:C:244:ILE:N	3:C:268:ASP:O	2.48	0.45
3:C:553:LEU:HD11	3:C:609:VAL:HG21	1.99	0.45
5:E:405:LYS:O	5:E:407:SER:N	2.50	0.45
5:E:543:GLU:OE1	5:E:543:GLU:HA	2.17	0.45
6:F:533:ILE:O	6:F:536:VAL:N	2.48	0.45
1:A:234:GLY:N	1:A:239:ALA:HB3	2.32	0.45
3:C:435:ARG:N	3:C:437:VAL:HG12	2.32	0.45
4:D:332:SER:N	4:D:344:GLY:C	2.70	0.45
6:F:81:LEU:O	6:F:85:LYS:N	2.50	0.45
2:B:79:SER:N	2:B:82:THR:OG1	2.43	0.45
2:B:167:THR:O	2:B:168:ILE:HD13	2.17	0.45
2:B:437:GLY:O	2:B:439:GLN:N	2.50	0.45
2:B:583:ARG:O	2:B:586:GLU:N	2.46	0.45
3:C:308:ASP:O	3:C:312:ARG:N	2.41	0.45
3:C:417:SER:O	3:C:420:GLY:N	2.50	0.45
5:E:341:ILE:O	5:E:534:ARG:NH2	2.50	0.45
5:E:412:LEU:HD13	5:E:429:ALA:CB	2.45	0.45
6:F:9:VAL:HA	6:F:12:PHE:HB3	1.98	0.45
4:D:350:MET:HG2	4:D:488:ILE:HG21	1.99	0.44
5:E:155:PHE:O	5:E:155:PHE:CD1	2.70	0.44
5:E:156:LYS:NZ	5:E:156:LYS:HB3	2.30	0.44
5:E:541:ARG:NE	5:E:541:ARG:CA	2.80	0.44
6:F:548:GLU:HA	6:F:549:PRO:HD2	1.55	0.44
4:D:543:PRO:HG2	4:D:592:GLU:OE1	2.17	0.44
4:D:581:VAL:O	4:D:584:LEU:HB2	2.16	0.44
5:E:452:ASP:HA	5:E:455:ALA:HB3	2.00	0.44
5:E:536:VAL:O	5:E:540:SER:N	2.50	0.44
6:F:401:THR:HG22	6:F:441:ASP:CB	2.47	0.44
1:A:303:ARG:O	1:A:306:ALA:HB3	2.17	0.44
2:B:422:VAL:HG23	2:B:436:ILE:HA	1.99	0.44
3:C:161:ALA:HB2	5:E:256:VAL:N	2.31	0.44
5:E:558:TYR:O	5:E:561:PHE:N	2.50	0.44
1:A:551:ASP:HA	1:A:554:ALA:HB3	2.00	0.44
2:B:100:LYS:HD2	2:B:361:GLU:HA	1.98	0.44
3:C:245:TYR:OH	3:C:265:THR:OG1	2.15	0.44
3:C:318:ALA:O	3:C:328:LYS:NZ	2.44	0.44
4:D:656:ILE:HD13	4:D:696:MET:HE1	2.00	0.44
6:F:73:PHE:O	6:F:77:VAL:HG23	2.17	0.44
6:F:440:ILE:HD13	6:F:443:PHE:CD1	2.53	0.44
1:A:364:VAL:HG21	1:A:388:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:ALA:HB1	1:A:684:ILE:O	2.17	0.44
1:A:679:ALA:O	1:A:683:ASN:N	2.50	0.44
2:B:396:GLY:C	2:B:411:ALA:HB3	2.38	0.44
4:D:299:LEU:HD23	4:D:302:VAL:HB	1.99	0.44
4:D:415:ILE:N	4:D:456:LEU:O	2.46	0.44
6:F:142:PRO:O	6:F:160:ARG:NH1	2.51	0.44
6:F:189:GLN:NE2	6:F:191:ILE:O	2.51	0.44
1:A:118:THR:HG22	1:A:228:TYR:OH	2.18	0.44
2:B:222:THR:HG23	2:B:223:PHE:HD1	1.83	0.44
3:C:201:GLN:N	3:C:224:PHE:O	2.50	0.44
3:C:554:SER:O	3:C:556:GLU:N	2.50	0.44
1:A:573:THR:HG1	1:A:576:HIS:CE1	2.28	0.44
2:B:375:ILE:CD1	2:B:415:VAL:HG11	2.47	0.44
2:B:471:MET:SD	4:D:337:PRO:CB	3.05	0.44
5:E:140:LEU:HD22	5:E:148:ILE:CG2	2.48	0.44
5:E:384:ALA:O	5:E:386:SER:N	2.50	0.44
6:F:575:ASP:O	6:F:579:ALA:N	2.40	0.44
1:A:691:TYR:O	1:A:694:GLU:N	2.50	0.44
2:B:83:LEU:CD1	2:B:92:VAL:HG21	2.48	0.44
2:B:209:ARG:HB2	2:B:226:VAL:HG23	2.00	0.44
2:B:287:LEU:HD22	2:B:308:ILE:HD12	2.00	0.44
2:B:373:VAL:HG12	2:B:374:CYS:N	2.33	0.44
3:C:143:THR:HG22	3:C:203:ILE:CD1	2.48	0.44
3:C:153:ALA:HB2	3:C:186:HIS:CE1	2.53	0.44
4:D:319:ASP:OD2	4:D:320:MET:N	2.51	0.44
4:D:483:SER:OG	4:D:484:ARG:NH1	2.51	0.44
1:A:490:VAL:CB	5:E:574:GLU:HG3	2.45	0.43
2:B:204:VAL:HG22	2:B:232:VAL:HG23	1.99	0.43
2:B:350:THR:HA	2:B:358:ARG:HD3	2.00	0.43
3:C:189:ALA:O	3:C:192:HIS:N	2.51	0.43
3:C:246:ARG:N	3:C:266:HIS:O	2.50	0.43
4:D:305:VAL:O	4:D:309:SER:N	2.45	0.43
4:D:607:ASP:O	4:D:611:ALA:N	2.44	0.43
4:D:669:PHE:CZ	4:D:683:LEU:HD22	2.53	0.43
5:E:125:VAL:HG21	5:E:192:GLN:CB	2.48	0.43
6:F:78:GLN:HB3	6:F:126:LEU:HD11	2.00	0.43
1:A:104:LEU:HD22	1:A:190:GLU:N	2.33	0.43
3:C:77:LEU:HG	3:C:78:ILE:N	2.33	0.43
3:C:158:GLN:O	3:C:158:GLN:CG	2.67	0.43
5:E:18:GLU:O	5:E:18:GLU:HG2	2.18	0.43
5:E:390:LYS:HZ3	5:E:401:TYR:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:332:LEU:HB3	6:F:351:LEU:HD21	1.99	0.43
2:B:36:ALA:O	2:B:40:LEU:N	2.39	0.43
2:B:272:PRO:CG	4:D:338:ASP:OD2	2.61	0.43
4:D:541:CYS:SG	4:D:596:LYS:HA	2.58	0.43
5:E:21:GLN:CG	5:E:28:LYS:HE3	2.47	0.43
5:E:417:VAL:O	5:E:423:HIS:N	2.41	0.43
4:D:403:GLY:N	4:D:406:VAL:HG21	2.34	0.43
6:F:541:ARG:CD	6:F:544:PRO:CB	2.97	0.43
1:A:109:GLN:OE1	1:A:109:GLN:N	2.47	0.43
1:A:454:SER:HA	1:A:457:VAL:HG21	2.00	0.43
2:B:186:VAL:HG22	2:B:227:LEU:CB	2.49	0.43
2:B:448:LEU:HD13	2:B:450:PHE:CE1	2.53	0.43
3:C:128:GLU:O	3:C:130:ILE:N	2.51	0.43
5:E:145:GLN:HB2	5:E:166:PRO:HG3	2.01	0.43
5:E:503:ILE:HG21	5:E:510:MET:SD	2.59	0.43
2:B:173:GLU:CD	2:B:331:ARG:HH22	2.21	0.43
3:C:161:ALA:HB2	5:E:256:VAL:H	1.84	0.43
3:C:457:GLN:C	3:C:458:LEU:HD22	2.39	0.43
5:E:273:ARG:O	5:E:277:TYR:N	2.49	0.43
5:E:728:ARG:O	5:E:732:VAL:HG22	2.19	0.43
6:F:457:VAL:HG22	6:F:462:THR:OG1	2.18	0.43
1:A:348:LYS:NZ	5:E:365:GLU:O	2.52	0.43
1:A:574:VAL:O	1:A:577:ILE:N	2.51	0.43
4:D:425:ASP:O	4:D:429:ILE:N	2.39	0.43
5:E:124:VAL:HG23	5:E:223:ASP:O	2.18	0.43
1:A:227:ILE:N	1:A:250:LEU:O	2.51	0.43
2:B:307:ASN:O	2:B:447:ASP:N	2.39	0.43
2:B:547:PRO:O	2:B:604:VAL:HG23	2.19	0.43
3:C:19:ARG:O	3:C:23:ARG:N	2.51	0.43
3:C:551:PRO:HB3	3:C:596:ALA:HB3	2.00	0.43
6:F:12:PHE:CZ	6:F:51:VAL:HG13	2.53	0.43
1:A:361:ALA:O	1:A:363:ALA:N	2.52	0.43
1:A:389:ALA:HB1	1:A:434:CYS:HB3	2.01	0.43
2:B:109:VAL:HA	2:B:159:VAL:O	2.19	0.43
2:B:206:GLY:C	2:B:230:CYS:SG	2.90	0.43
3:C:565:TYR:OH	5:E:528:ASP:O	2.25	0.43
2:B:109:VAL:HG13	2:B:109:VAL:O	2.18	0.43
3:C:302:GLU:O	3:C:306:LYS:N	2.51	0.43
4:D:611:ALA:O	4:D:615:PHE:N	2.45	0.43
6:F:393:LEU:O	6:F:556:ARG:NH2	2.52	0.43
1:A:14:ARG:NH1	1:A:76:VAL:HG22	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:ILE:HG22	2:B:169:GLN:O	2.19	0.42
4:D:594:LEU:HD22	4:D:607:ASP:HB3	2.01	0.42
5:E:18:GLU:HG2	5:E:25:GLY:O	2.19	0.42
5:E:46:VAL:O	5:E:46:VAL:HG13	2.19	0.42
5:E:429:ALA:O	5:E:432:LEU:N	2.47	0.42
5:E:469:LYS:N	5:E:472:VAL:O	2.44	0.42
5:E:516:PHE:HB2	5:E:642:VAL:HG11	2.01	0.42
5:E:518:ILE:HG23	5:E:520:VAL:HG23	2.00	0.42
6:F:266:HIS:O	6:F:302:MET:N	2.45	0.42
2:B:87:PHE:O	2:B:90:CYS:N	2.52	0.42
3:C:321:ILE:C	3:C:328:LYS:HZ1	2.21	0.42
4:D:433:MET:HE3	4:D:481:ILE:HD11	1.99	0.42
5:E:114:ILE:HG23	5:E:280:VAL:HB	2.01	0.42
5:E:411:GLY:O	5:E:451:ARG:NH2	2.45	0.42
2:B:288:LEU:O	2:B:543:LYS:NZ	2.40	0.42
2:B:432:PRO:O	2:B:433:MET:C	2.56	0.42
3:C:143:THR:HG22	3:C:203:ILE:HG12	2.01	0.42
3:C:550:MET:N	3:C:602:ASN:OD1	2.51	0.42
4:D:437:THR:OG1	4:D:449:LEU:O	2.28	0.42
5:E:273:ARG:O	5:E:276:SER:N	2.53	0.42
5:E:754:ARG:O	5:E:757:GLU:N	2.52	0.42
1:A:586:ALA:HA	1:A:589:ARG:HB2	2.02	0.42
2:B:392:VAL:HG13	2:B:397:ARG:O	2.19	0.42
3:C:227:ASN:O	3:C:229:LEU:N	2.53	0.42
3:C:317:LEU:HD11	3:C:332:LEU:HB2	2.01	0.42
3:C:454:ILE:HG23	5:E:203:ILE:CG2	2.48	0.42
4:D:692:ILE:HD12	4:D:692:ILE:H	1.85	0.42
5:E:151:VAL:CG2	5:E:159:GLN:N	2.56	0.42
6:F:328:PHE:O	6:F:332:LEU:N	2.47	0.42
6:F:620:VAL:O	6:F:621:VAL:HG23	2.19	0.42
2:B:318:LYS:NZ	2:B:376:ASP:OD1	2.46	0.42
3:C:65:HIS:C	3:C:67:LYS:N	2.72	0.42
3:C:301:LYS:O	3:C:305:ARG:N	2.43	0.42
1:A:2:ARG:H	1:A:2:ARG:HG2	1.72	0.42
1:A:351:SER:OG	1:A:352:ARG:N	2.52	0.42
3:C:17:PHE:CA	3:C:73:LEU:HD11	2.48	0.42
3:C:380:ARG:NH1	3:C:418:ASP:O	2.49	0.42
3:C:514:ALA:O	3:C:518:VAL:N	2.37	0.42
4:D:378:LYS:HB3	4:D:420:LYS:O	2.19	0.42
4:D:661:SER:O	4:D:665:ILE:N	2.40	0.42
5:E:120:ILE:HD13	5:E:283:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:51:VAL:HG12	6:F:55:ASP:O	2.20	0.42
6:F:524:ASP:O	6:F:528:ARG:N	2.47	0.42
6:F:526:ASP:O	6:F:530:ALA:N	2.45	0.42
1:A:122:VAL:HG22	1:A:186:ILE:HD11	2.02	0.42
1:A:254:VAL:HG12	1:A:255:ALA:O	2.19	0.42
1:A:570:ILE:O	1:A:570:ILE:HG13	2.18	0.42
2:B:110:ARG:NH1	2:B:113:HIS:CG	2.87	0.42
2:B:158:SER:OG	6:F:285:VAL:HG22	2.20	0.42
3:C:112:ARG:HA	3:C:270:ILE:HD11	1.98	0.42
3:C:592:ALA:CB	3:C:609:VAL:HG22	2.46	0.42
4:D:426:ARG:HA	4:D:429:ILE:HG22	2.01	0.42
5:E:557:ARG:O	5:E:561:PHE:N	2.46	0.42
6:F:176:ALA:HB1	6:F:218:LEU:HG	2.02	0.42
1:A:369:TYR:N	1:A:382:GLU:O	2.51	0.42
2:B:294:ARG:HB3	2:B:296:LEU:HD21	2.02	0.42
3:C:160:CYS:O	3:C:160:CYS:SG	2.77	0.42
5:E:362:THR:OG1	5:E:368:SER:N	2.53	0.42
5:E:503:ILE:HG23	5:E:505:LEU:H	1.84	0.42
5:E:728:ARG:NH1	5:E:770:LEU:O	2.53	0.42
1:A:532:LYS:HA	1:A:535:ILE:HD12	2.02	0.42
5:E:6:ALA:HB1	5:E:72:TYR:CG	2.55	0.42
5:E:215:ALA:HB1	5:E:227:PHE:CE2	2.55	0.42
5:E:572:GLU:O	5:E:574:GLU:N	2.53	0.42
6:F:378:ASP:OD1	6:F:483:ALA:HB1	2.19	0.42
2:B:387:THR:O	2:B:390:HIS:N	2.48	0.42
3:C:364:GLY:O	3:C:366:SER:N	2.50	0.42
3:C:507:GLU:HB2	6:F:582:VAL:HG13	2.02	0.42
5:E:203:ILE:HD13	5:E:203:ILE:H	1.82	0.42
1:A:223:GLU:H	1:A:255:ALA:HB3	1.84	0.41
1:A:490:VAL:CB	5:E:574:GLU:CG	2.97	0.41
1:A:567:THR:O	1:A:567:THR:HG22	2.20	0.41
2:B:375:ILE:O	2:B:418:ALA:N	2.48	0.41
6:F:545:SER:O	6:F:547:PHE:N	2.52	0.41
2:B:411:ALA:O	2:B:413:CYS:N	2.53	0.41
2:B:440:ASP:OD1	2:B:440:ASP:N	2.50	0.41
2:B:580:VAL:O	2:B:584:THR:N	2.40	0.41
3:C:552:ARG:HG2	5:E:542:ILE:HG21	2.03	0.41
4:D:475:ILE:HG22	4:D:476:ASP:N	2.34	0.41
5:E:135:VAL:HB	5:E:182:ARG:HB2	2.03	0.41
5:E:173:ARG:O	5:E:173:ARG:HG2	2.20	0.41
5:E:418:ARG:HD2	5:E:422:SER:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:597:TRP:CD1	5:E:597:TRP:N	2.89	0.41
6:F:145:ILE:HG23	6:F:249:ILE:HB	2.01	0.41
6:F:228:PHE:HA	6:F:258:THR:HG21	2.02	0.41
1:A:460:THR:O	1:A:463:ILE:N	2.54	0.41
3:C:151:GLN:HG2	3:C:198:SER:CA	2.50	0.41
3:C:598:VAL:HG12	3:C:599:ARG:N	2.35	0.41
4:D:584:LEU:O	4:D:588:VAL:HG23	2.21	0.41
5:E:143:ASP:HB2	5:E:172:ARG:NH2	2.35	0.41
5:E:757:GLU:O	5:E:761:HIS:ND1	2.50	0.41
1:A:581:ILE:HG23	1:A:582:ARG:HG3	2.01	0.41
3:C:437:VAL:C	3:C:441:VAL:HG23	2.41	0.41
4:D:619:THR:HA	4:D:622:ALA:HB3	2.02	0.41
5:E:130:VAL:HG22	5:E:187:GLN:HB3	2.03	0.41
5:E:145:GLN:HB2	5:E:166:PRO:CG	2.50	0.41
5:E:415:ALA:HB2	5:E:469:LYS:NZ	2.35	0.41
1:A:304:GLY:O	1:A:308:ALA:N	2.42	0.41
1:A:418:SER:OG	1:A:430:LEU:O	2.30	0.41
2:B:392:VAL:HG13	2:B:397:ARG:C	2.40	0.41
2:B:434:GLU:O	4:D:689:ARG:NH1	2.52	0.41
5:E:19:GLU:HB2	5:E:28:LYS:C	2.41	0.41
6:F:168:GLU:OE2	6:F:169:VAL:N	2.53	0.41
6:F:541:ARG:CG	6:F:544:PRO:CB	2.93	0.41
1:A:44:TYR:CD1	1:A:99:PRO:CD	3.04	0.41
1:A:619:SER:C	1:A:623:SER:HG	2.16	0.41
2:B:285:LEU:O	2:B:289:LEU:N	2.48	0.41
2:B:580:VAL:HB	2:B:583:ARG:HB3	2.01	0.41
3:C:449:ILE:O	3:C:456:CYS:N	2.46	0.41
3:C:559:GLN:OE1	3:C:559:GLN:N	2.45	0.41
6:F:164:THR:HG23	6:F:232:LYS:HB3	2.03	0.41
6:F:408:VAL:HG12	6:F:412:ALA:CA	2.50	0.41
6:F:568:MET:O	6:F:620:VAL:HG13	2.20	0.41
2:B:15:ILE:HB	2:B:70:GLU:CD	2.41	0.41
2:B:287:LEU:HB2	2:B:308:ILE:HD12	2.02	0.41
2:B:430:LYS:CE	2:B:434:GLU:HB3	2.48	0.41
4:D:543:PRO:CG	4:D:592:GLU:OE1	2.68	0.41
5:E:131:HIS:O	5:E:186:PHE:N	2.51	0.41
5:E:337:LEU:HD21	5:E:355:LEU:HD11	2.02	0.41
5:E:396:SER:HA	5:E:556:ARG:HD2	2.03	0.41
6:F:379:PRO:HB2	6:F:490:ARG:HH22	1.86	0.41
1:A:32:MET:HA	1:A:33:CYS:CB	2.51	0.41
1:A:615:THR:O	1:A:615:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:ALA:O	2:B:286:CYS:N	2.53	0.41
2:B:362:ALA:HB1	2:B:366:VAL:HG11	2.03	0.41
3:C:127:PRO:HB3	6:F:171:PRO:HB2	2.03	0.41
3:C:363:PRO:O	3:C:365:THR:N	2.54	0.41
3:C:398:VAL:HG21	3:C:451:LYS:HE3	2.02	0.41
5:E:19:GLU:HB3	5:E:28:LYS:CD	2.50	0.41
1:A:25:PHE:O	1:A:29:ILE:HG22	2.20	0.41
2:B:187:ILE:CD1	2:B:226:VAL:HG21	2.51	0.41
2:B:457:ASP:O	2:B:460:GLN:N	2.50	0.41
3:C:153:ALA:H	3:C:167:GLU:HB2	1.86	0.41
3:C:245:TYR:HH	3:C:265:THR:HG1	1.42	0.41
3:C:324:HIS:HB3	3:C:327:ILE:HD12	2.03	0.41
4:D:201:GLN:HG2	4:D:230:PRO:CB	2.51	0.41
4:D:683:LEU:O	4:D:694:HIS:NE2	2.53	0.41
5:E:152:GLU:O	5:E:154:GLN:N	2.53	0.41
5:E:200:ARG:NH1	5:E:200:ARG:HG3	2.36	0.41
5:E:332:ASN:O	5:E:549:VAL:HG11	2.21	0.41
6:F:7:GLU:OE2	6:F:7:GLU:N	2.49	0.41
6:F:598:SER:N	6:F:601:THR:OG1	2.37	0.41
1:A:574:VAL:HA	1:A:577:ILE:HD12	2.02	0.41
2:B:533:ALA:O	2:B:536:LYS:N	2.54	0.41
2:B:617:GLN:O	2:B:617:GLN:NE2	2.49	0.41
3:C:151:GLN:HG2	3:C:198:SER:HA	2.03	0.41
4:D:303:TYR:O	4:D:307:SER:N	2.50	0.41
4:D:423:GLU:OE1	4:D:423:GLU:N	2.53	0.41
4:D:646:ILE:CD1	4:D:682:VAL:HG11	2.51	0.41
6:F:164:THR:OG1	6:F:165:ARG:N	2.51	0.41
1:A:692:ASP:N	1:A:692:ASP:OD1	2.54	0.40
5:E:719:GLU:HG3	5:E:726:LEU:HD21	2.02	0.40
6:F:178:TYR:O	6:F:187:THR:OG1	2.31	0.40
6:F:334:ALA:CB	6:F:547:PHE:CE1	3.02	0.40
2:B:83:LEU:HD13	2:B:92:VAL:HG21	2.02	0.40
2:B:108:VAL:HA	2:B:160:TYR:CD2	2.56	0.40
2:B:310:LEU:HD11	2:B:416:LEU:HD21	2.04	0.40
2:B:601:SER:OG	2:B:603:THR:O	2.37	0.40
3:C:247:ALA:HB2	3:C:265:THR:HA	2.03	0.40
4:D:438:ILE:O	4:D:449:LEU:N	2.52	0.40
1:A:597:ILE:HG23	1:A:600:ASP:H	1.87	0.40
2:B:173:GLU:OE1	2:B:331:ARG:CA	2.70	0.40
2:B:173:GLU:CD	2:B:331:ARG:NH2	2.74	0.40
2:B:423:TYR:CE1	4:D:643:LEU:HD13	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:560:GLU:OE1	2:B:563:ARG:NE	2.52	0.40
3:C:17:PHE:CZ	3:C:21:LEU:HD21	2.57	0.40
3:C:547:SER:HB3	3:C:548:THR:HG23	2.04	0.40
3:C:565:TYR:CZ	5:E:532:ALA:HB3	2.56	0.40
4:D:201:GLN:OE1	4:D:201:GLN:CA	2.69	0.40
4:D:553:LEU:O	4:D:556:ARG:N	2.54	0.40
5:E:137:GLY:O	5:E:150:ASP:N	2.54	0.40
5:E:569:ILE:HG23	5:E:573:SER:CB	2.48	0.40
6:F:189:GLN:HE22	6:F:218:LEU:HD11	1.87	0.40
6:F:546:GLN:O	6:F:546:GLN:CG	2.69	0.40
1:A:199:ARG:NH1	1:A:200:LEU:O	2.54	0.40
1:A:363:ALA:HB3	5:E:473:LYS:HZ1	1.85	0.40
2:B:402:LYS:O	2:B:406:HIS:NE2	2.55	0.40
3:C:199:ASP:HB3	3:C:226:HIS:CE1	2.56	0.40
4:D:338:ASP:O	4:D:340:LEU:N	2.55	0.40
5:E:176:LEU:O	5:E:178:THR:N	2.55	0.40
5:E:409:ALA:O	5:E:451:ARG:NH2	2.55	0.40
5:E:733:ASN:OD1	5:E:736:LEU:HD22	2.22	0.40
6:F:219:GLN:OE1	6:F:221:ARG:NH2	2.55	0.40
6:F:509:SER:OG	6:F:510:ARG:N	2.54	0.40
2:B:90:CYS:O	2:B:208:TYR:N	2.49	0.40
2:B:107:LYS:O	2:B:160:TYR:HB3	2.20	0.40
2:B:185:ASP:N	2:B:185:ASP:OD1	2.54	0.40
2:B:296:LEU:HD13	2:B:300:SER:HA	2.02	0.40
2:B:343:VAL:O	2:B:364:ALA:N	2.47	0.40
2:B:351:THR:O	2:B:351:THR:HG23	2.20	0.40
3:C:449:ILE:N	3:C:456:CYS:O	2.53	0.40
4:D:394:SER:H	4:D:394:SER:HG	1.61	0.40
5:E:518:ILE:HD11	5:E:642:VAL:HA	2.02	0.40
6:F:12:PHE:HZ	6:F:51:VAL:HG13	1.86	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	546/904 (60%)	454 (83%)	79 (14%)	13 (2%)	5	28
2	B	484/808 (60%)	402 (83%)	67 (14%)	15 (3%)	3	23
3	C	515/863 (60%)	400 (78%)	100 (19%)	15 (3%)	3	24
4	D	410/734 (56%)	355 (87%)	50 (12%)	5 (1%)	11	43
5	E	653/821 (80%)	517 (79%)	109 (17%)	27 (4%)	2	18
6	F	567/719 (79%)	484 (85%)	74 (13%)	9 (2%)	8	37
All	All	3175/4849 (66%)	2612 (82%)	479 (15%)	84 (3%)	6	26

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	PRO
1	A	374	PRO
1	A	424	ALA
2	B	229	ALA
2	B	230	CYS
2	B	340	SER
2	B	343	VAL
2	B	350	THR
2	B	422	VAL
2	B	440	ASP
2	B	441	SER
3	C	66	ILE
3	C	145	GLN
3	C	152	GLU
3	C	154	PHE
4	D	337	PRO
4	D	339	GLY
4	D	343	ARG
5	E	156	LYS
5	E	159	GLN
5	E	160	PRO
5	E	200	ARG
5	E	381	PRO
5	E	383	THR
5	E	384	ALA
5	E	409	ALA
5	E	567	PRO

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Mol	Chain	Res	Type
5	E	568	LYS
5	E	573	SER
5	E	621	ASP
6	F	381	VAL
6	F	488	TYR
6	F	546	GLN
6	F	621	VAL
1	A	100	LEU
1	A	423	LYS
2	B	109	VAL
3	C	122	MET
3	C	161	ALA
3	C	211	ASP
3	C	228	ASP
3	C	322	TYR
5	E	542	ILE
5	E	599	ILE
6	F	550	LEU
1	A	101	VAL
2	B	72	SER
2	B	330	PRO
2	B	338	ARG
3	C	12	ALA
3	C	227	ASN
4	D	541	CYS
5	E	152	GLU
5	E	153	GLN
5	E	155	PHE
5	E	382	SER
5	E	597	TRP
6	F	461	GLN
1	A	33	CYS
2	B	351	THR
3	C	323	GLU
3	C	364	GLY
5	E	19	GLU
5	E	141	CYS
5	E	185	ASP
1	A	243	PRO
1	A	244	VAL
1	A	375	VAL
2	B	334	PRO

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Mol	Chain	Res	Type
3	C	497	LEU
5	E	17	LEU
5	E	23	SER
5	E	177	ASP
5	E	406	ALA
6	F	460	GLN
6	F	549	PRO
1	A	340	SER
1	A	571	PRO
1	A	365	GLY
2	B	74	GLY
3	C	270	ILE
5	E	489	ILE
4	D	300	PRO
6	F	620	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	488/781 (62%)	476 (98%)	12 (2%)	42	62
2	B	429/707 (61%)	416 (97%)	13 (3%)	36	57
3	C	470/753 (62%)	461 (98%)	9 (2%)	52	70
4	D	364/625 (58%)	357 (98%)	7 (2%)	52	70
5	E	595/724 (82%)	566 (95%)	29 (5%)	21	43
6	F	494/619 (80%)	484 (98%)	10 (2%)	50	69
All	All	2840/4209 (68%)	2760 (97%)	80 (3%)	40	59

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	3	LEU
1	A	100	LEU

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Mol	Chain	Res	Type
1	A	125	CYS
1	A	334	ASP
1	A	362	SER
1	A	364	VAL
1	A	472	VAL
1	A	474	ARG
1	A	475	ASP
1	A	476	THR
1	A	570	ILE
2	B	70	GLU
2	B	72	SER
2	B	100	LYS
2	B	108	VAL
2	B	228	ILE
2	B	313	ASP
2	B	331	ARG
2	B	333	ILE
2	B	338	ARG
2	B	352	ASP
2	B	425	ARG
2	B	426	TYR
2	B	433	MET
3	C	23	ARG
3	C	63	CYS
3	C	64	GLU
3	C	152	GLU
3	C	159	VAL
3	C	160	CYS
3	C	182	CYS
3	C	270	ILE
3	C	497	LEU
4	D	201	GLN
4	D	235	THR
4	D	338	ASP
4	D	342	ARG
4	D	345	ASP
4	D	540	LYS
4	D	543	PRO
5	E	17	LEU
5	E	24	ASP
5	E	66	PHE
5	E	68	ARG

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Mol	Chain	Res	Type
5	E	84	ARG
5	E	103	ARG
5	E	142	LEU
5	E	150	ASP
5	E	151	VAL
5	E	153	GLN
5	E	156	LYS
5	E	159	GLN
5	E	160	PRO
5	E	168	CYS
5	E	173	ARG
5	E	174	PHE
5	E	175	LEU
5	E	200	ARG
5	E	202	SER
5	E	203	ILE
5	E	279	LEU
5	E	383	THR
5	E	487	ASN
5	E	488	PRO
5	E	571	LYS
5	E	596	SER
5	E	599	ILE
5	E	600	THR
5	E	619	CYS
6	F	215	ARG
6	F	317	ARG
6	F	341	TYR
6	F	386	LEU
6	F	403	ARG
6	F	405	SER
6	F	416	ARG
6	F	424	THR
6	F	490	ARG
6	F	546	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	431	GLN
1	A	546	ASN

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Mol	Chain	Res	Type
1	A	547	GLN
1	A	681	GLN
1	A	683	ASN
2	B	298	ASN
2	B	395	GLN
2	B	420	ASN
2	B	540	HIS
3	C	18	GLN
3	C	82	GLN
3	C	93	ASN
3	C	186	HIS
3	C	206	GLN
3	C	226	HIS
3	C	376	ASN
3	C	469	ASN
4	D	93	GLN
4	D	217	GLN
4	D	460	ASN
5	E	21	GLN
5	E	154	GLN
5	E	310	ASN
5	E	423	HIS
5	E	504	ASN
5	E	708	ASN
6	F	18	GLN
6	F	189	GLN
6	F	460	GLN
6	F	627	ASN

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

There are no ligands in this entry.

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.

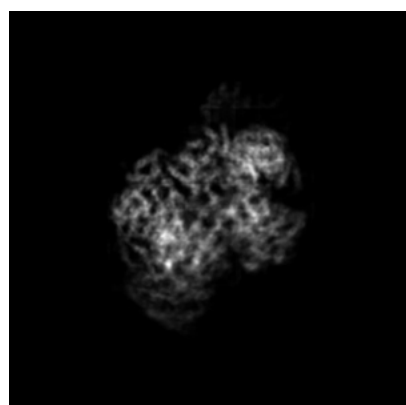
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32326. These allow visual inspection of the internal detail of the map and identification of artifacts.

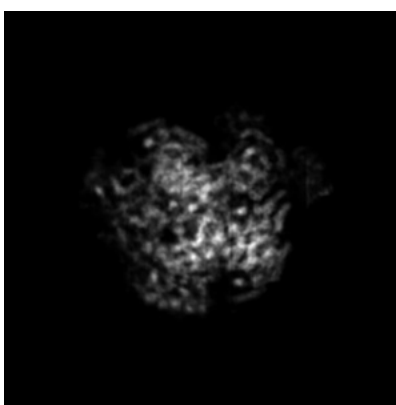
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

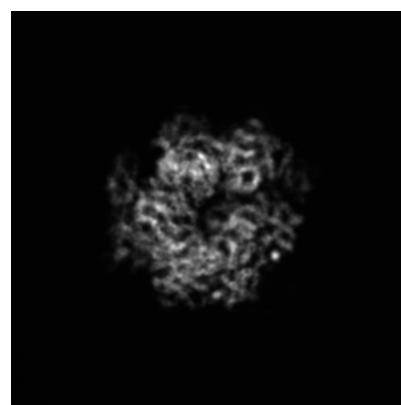
6.1.1 Primary map



X



Y

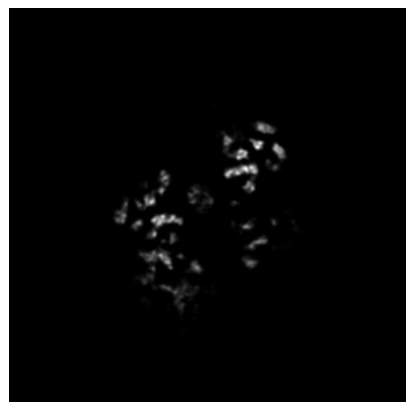


Z

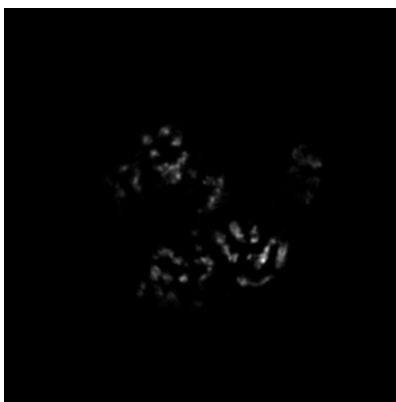
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

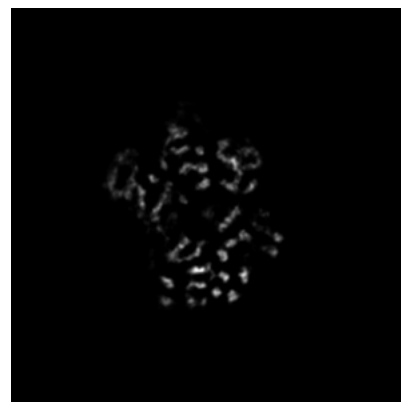
6.2.1 Primary map



X Index: 120



Y Index: 120

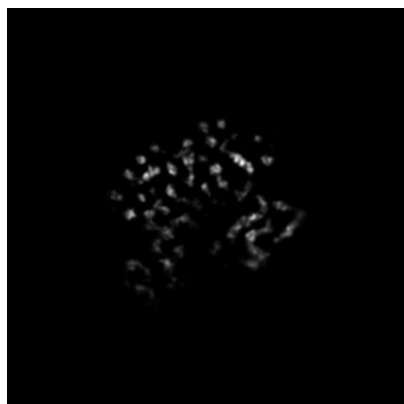


Z Index: 120

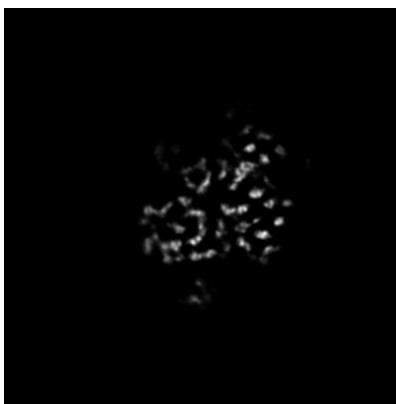
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 98



Y Index: 146

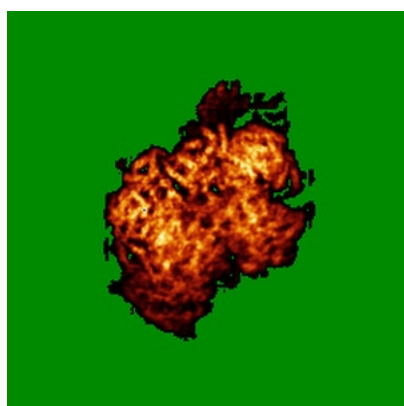


Z Index: 119

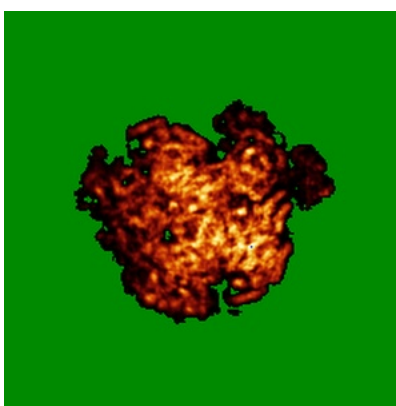
The images above show the largest variance slices of the map in three orthogonal directions.

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

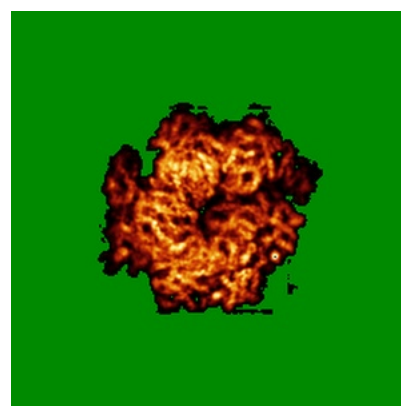
6.4.1 Primary map



X



Y

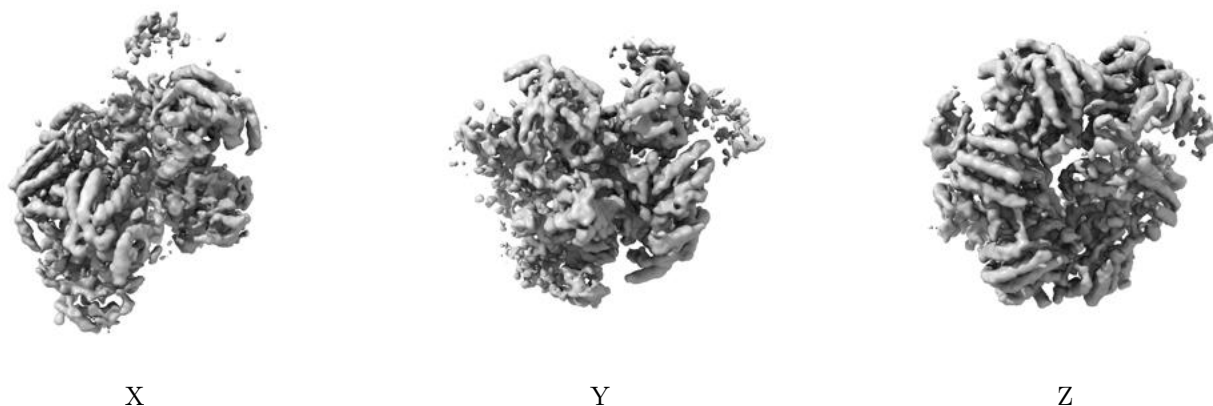


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

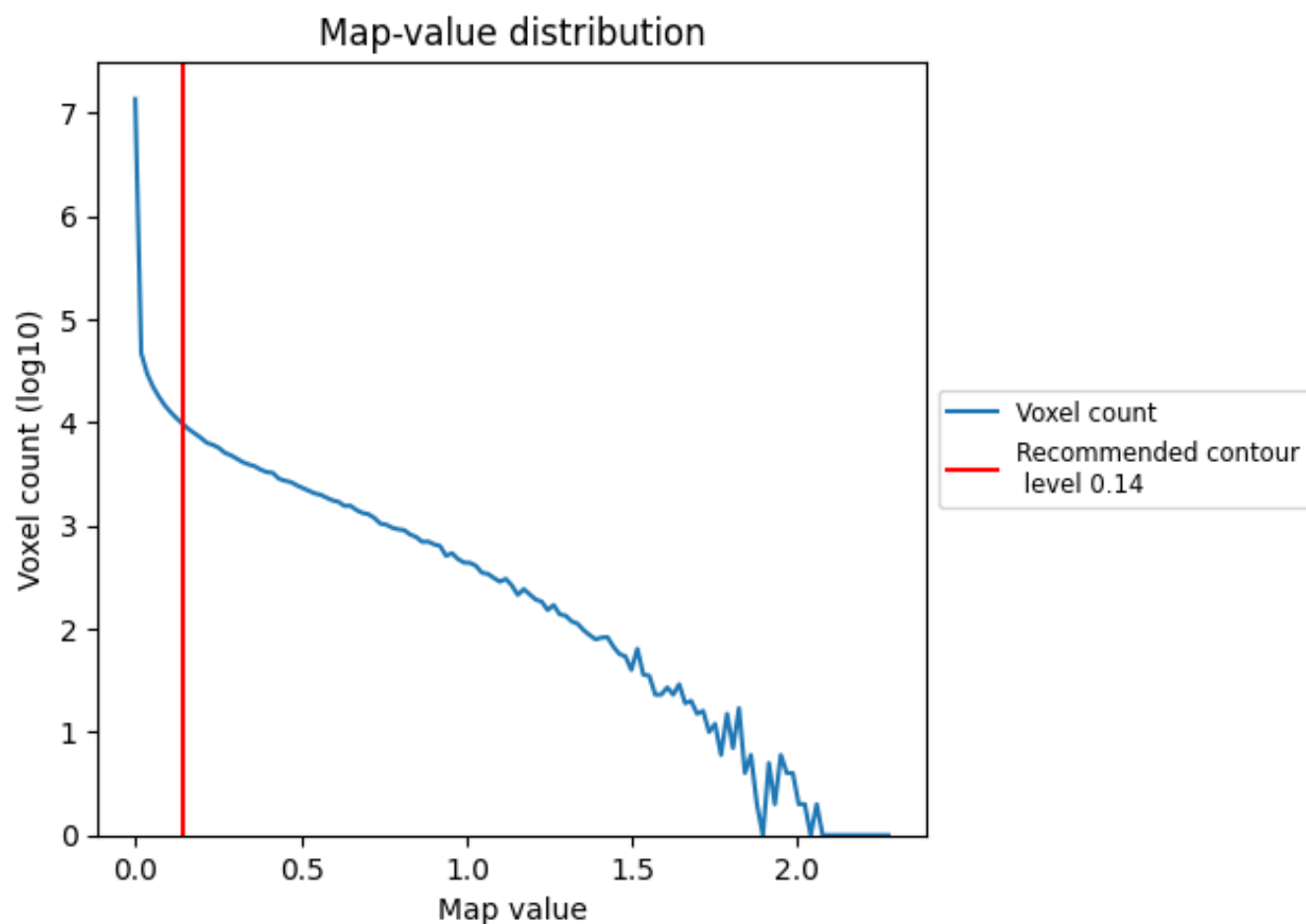
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

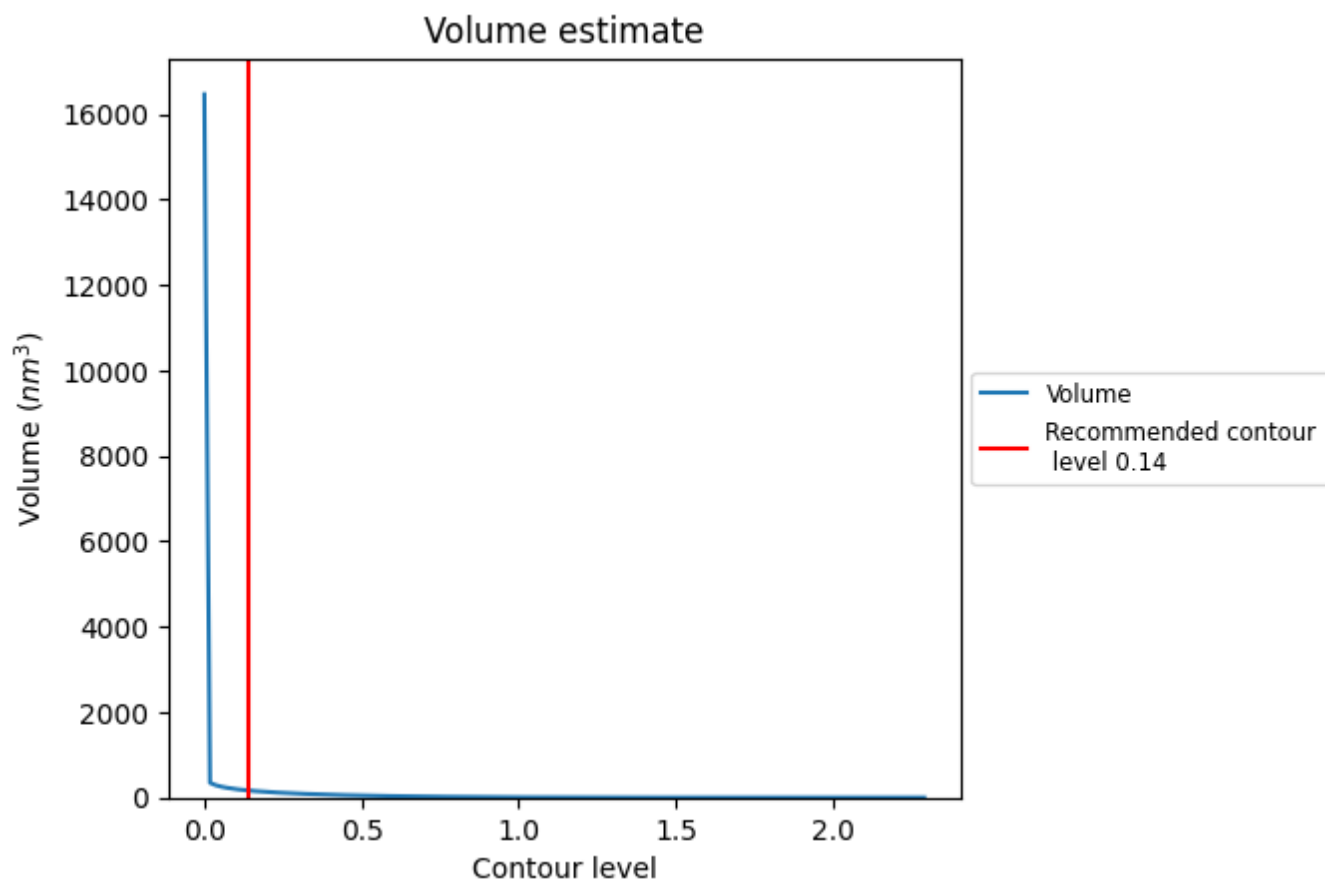
This section contains the results of statistical analysis of the map.

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.

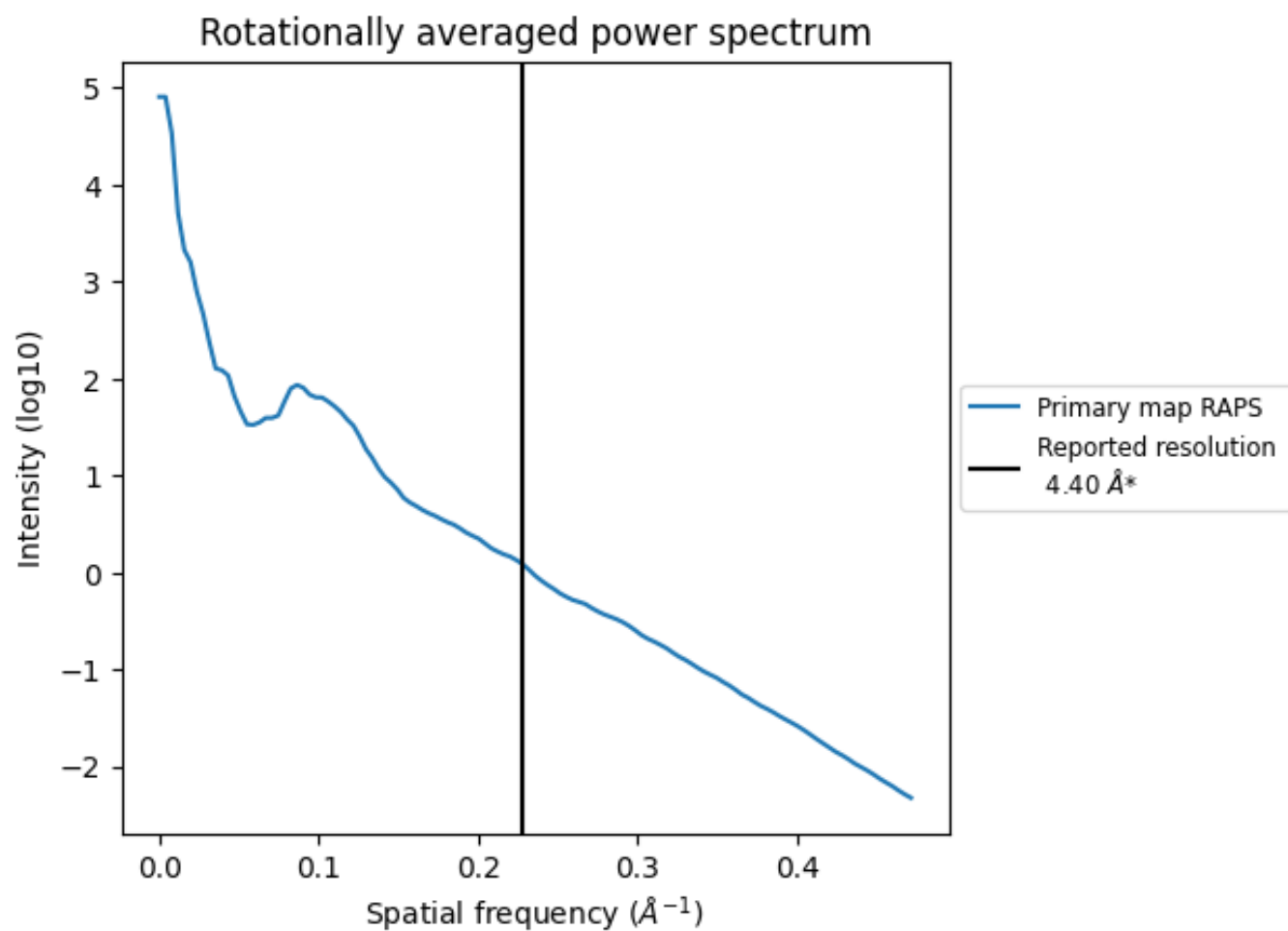
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 165 nm^3 ; this corresponds to an approximate mass of 149 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 ⓘ

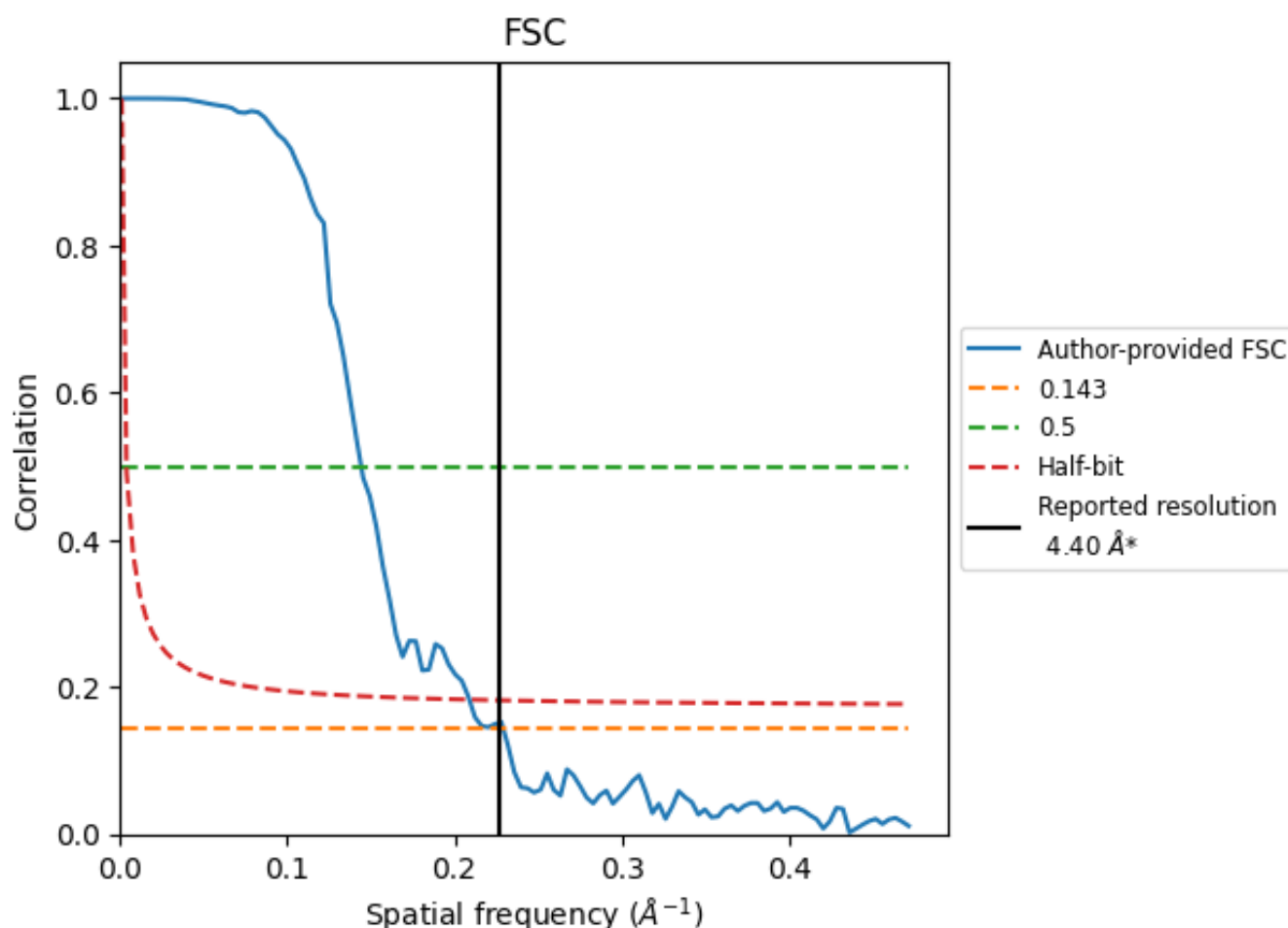


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

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 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

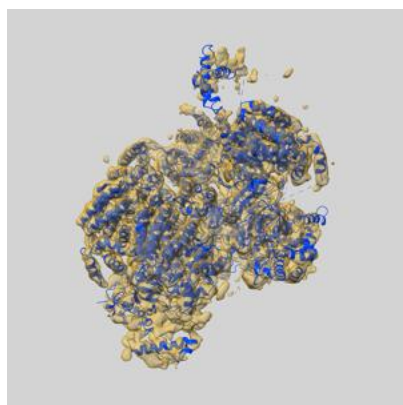
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.36	6.93	4.79
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

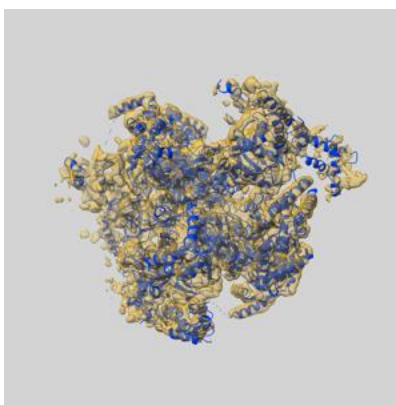
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32326 and PDB model 7W68. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

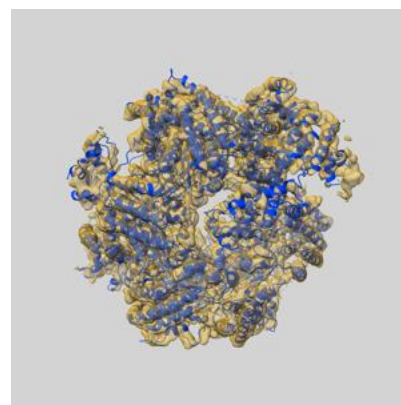
9.1 Map-model overlay [i](#)



X



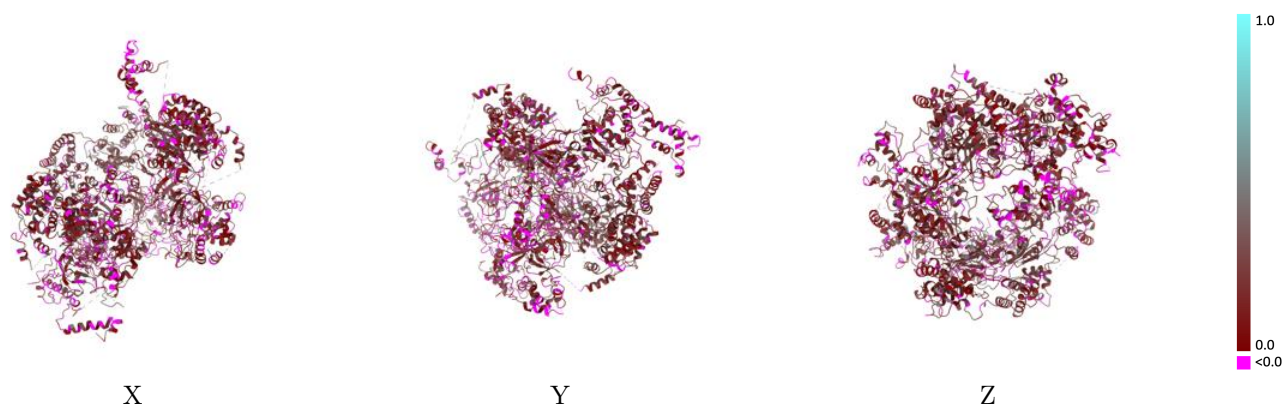
Y



Z

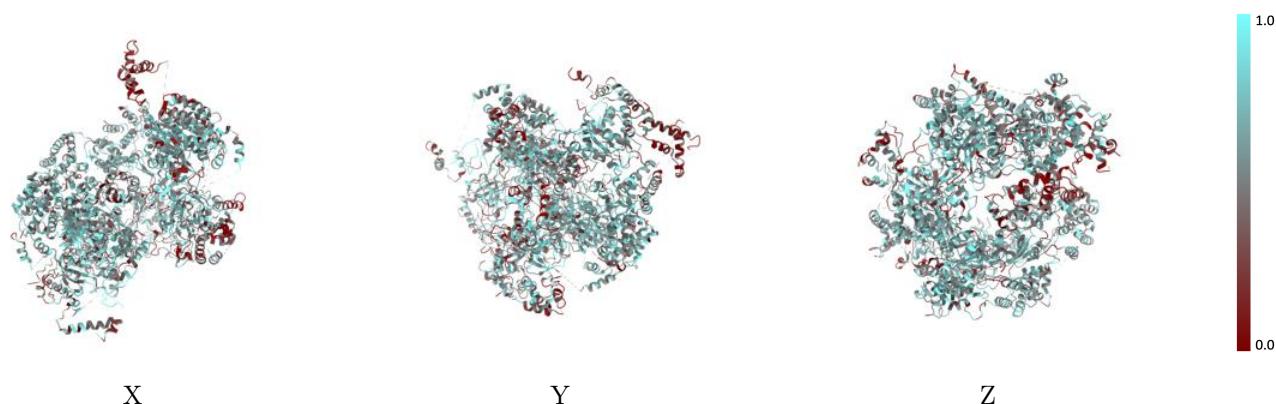
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



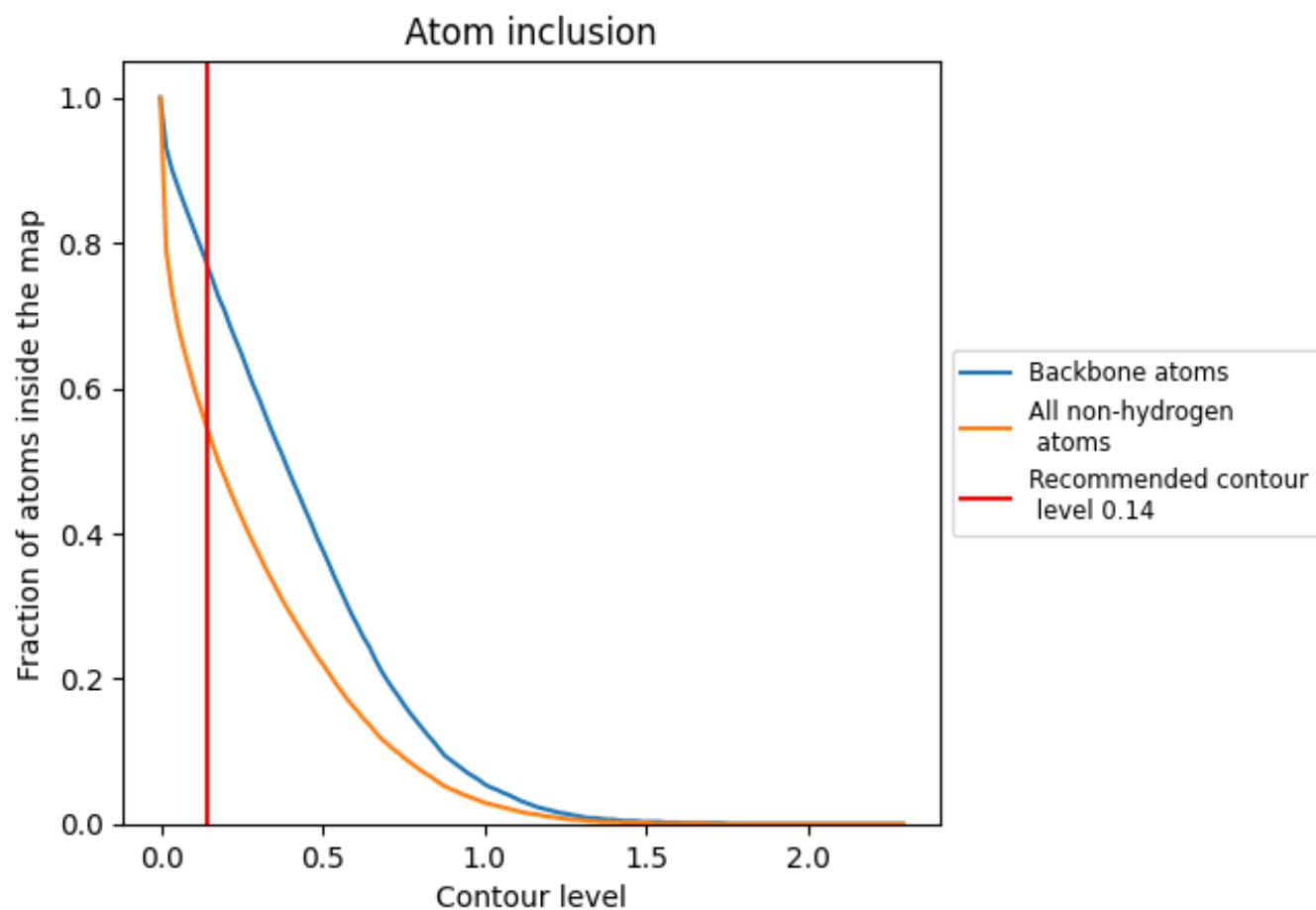
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.14).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 55% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.5480	<div><div></div></div> 0.1490
A	<div><div></div></div> 0.5300	<div><div></div></div> 0.1370
B	<div><div></div></div> 0.5780	<div><div></div></div> 0.1690
C	<div><div></div></div> 0.5760	<div><div></div></div> 0.1560
D	<div><div></div></div> 0.5560	<div><div></div></div> 0.1460
E	<div><div></div></div> 0.5200	<div><div></div></div> 0.1450
F	<div><div></div></div> 0.5370	<div><div></div></div> 0.1440

1.0

0.0

<0.0