



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:04 PM UTC

PDB ID : 7W68 / pdb_00007w68
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:

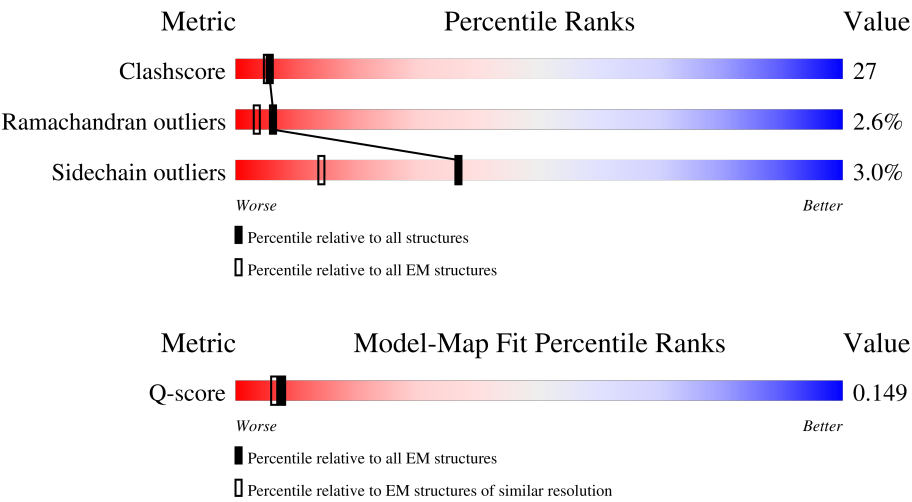
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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

Mol	Chain	Length	Quality of chain
1	A	904	18% 32%26%38%
2	B	808	14% 30%26%38%
3	C	863	14% 30%27%39%
4	D	734	15% 29%27%42%

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Mol	Chain	Length	Quality of chain
5	E	821	
6	F	719	

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		

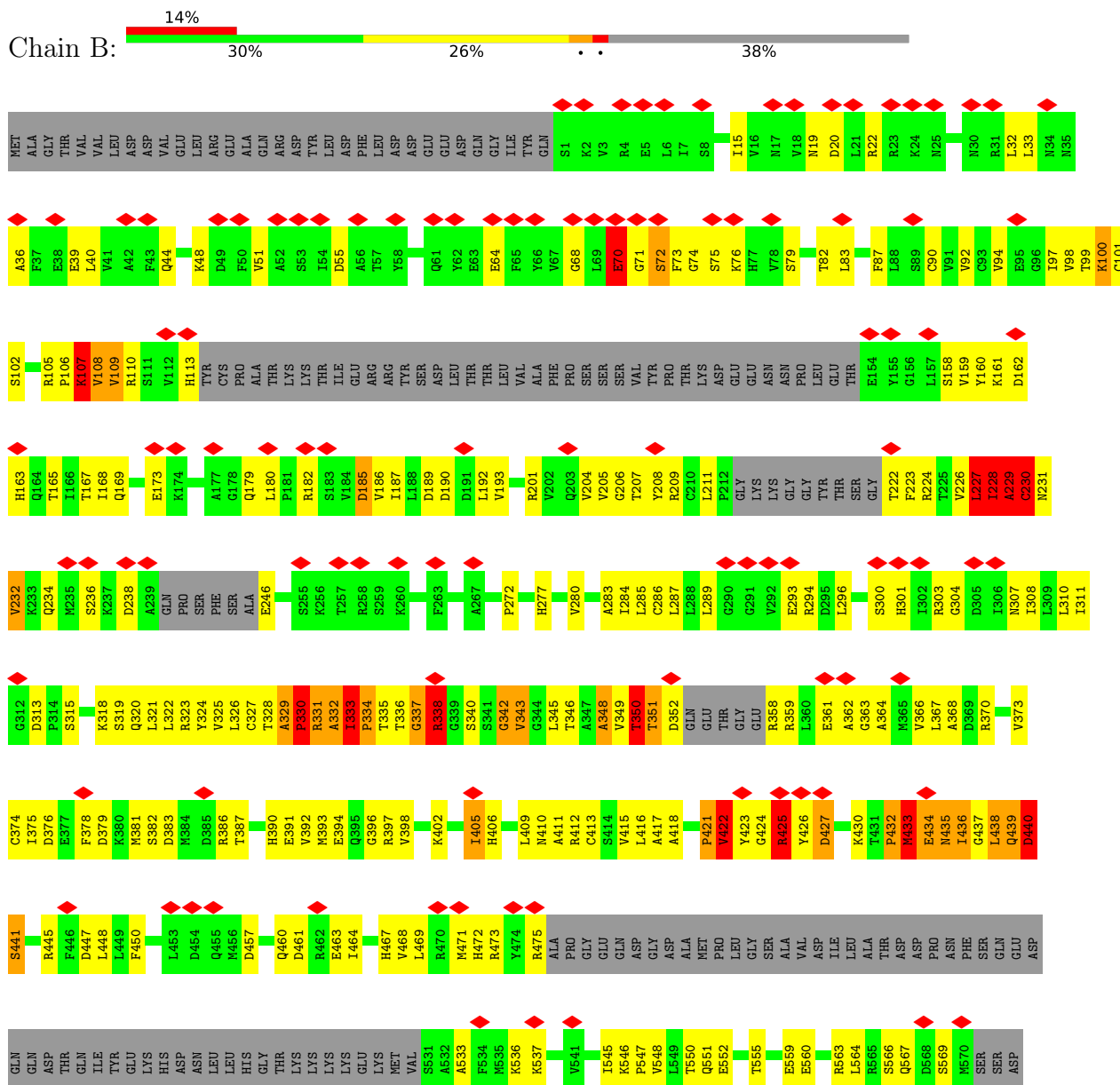
- Molecule 5 is a protein called DNA replication licensing factor MCM6.

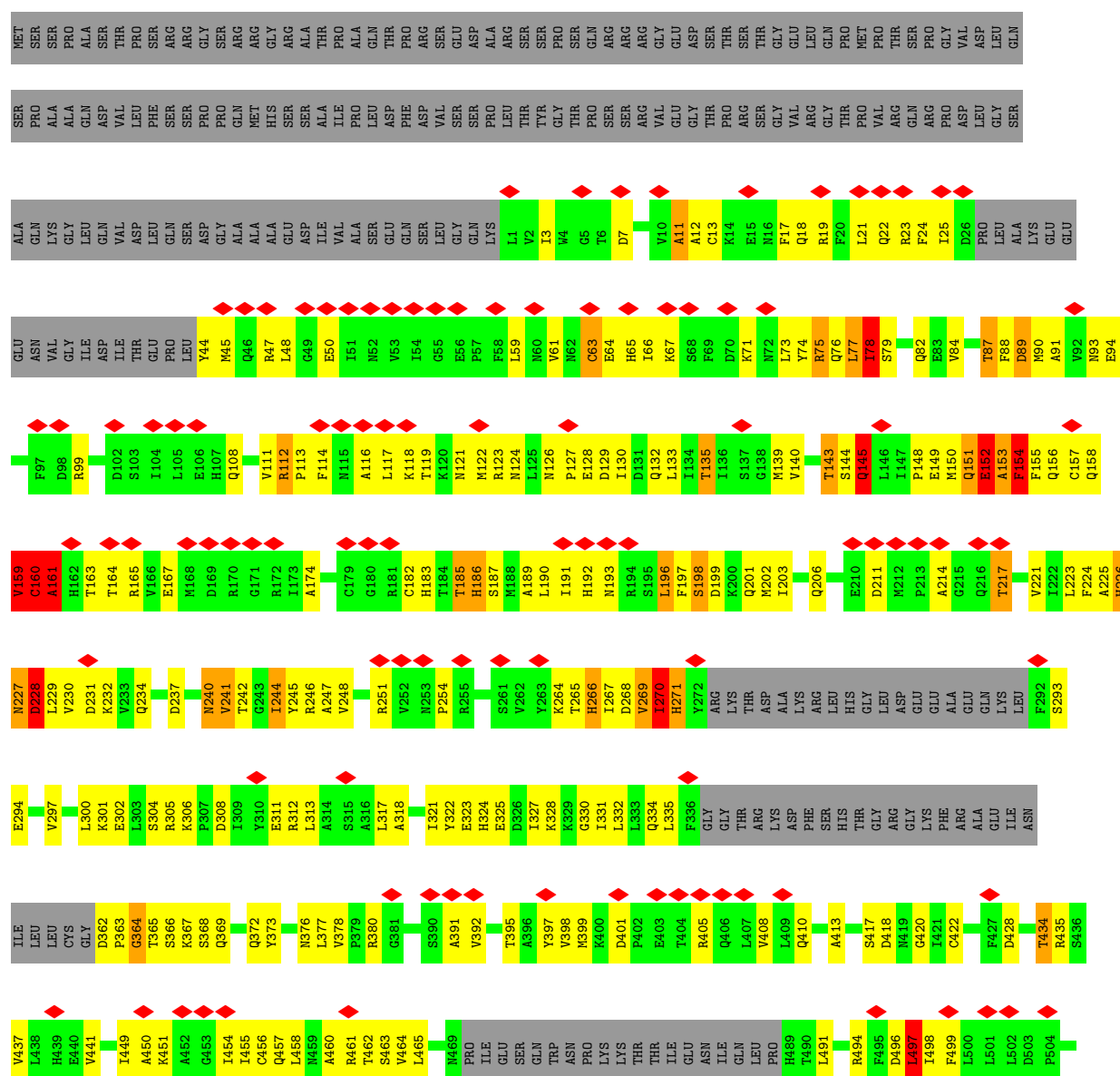
Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	661	Total	C	N	O	S	0	0
			5335	3355	946	1007	27		

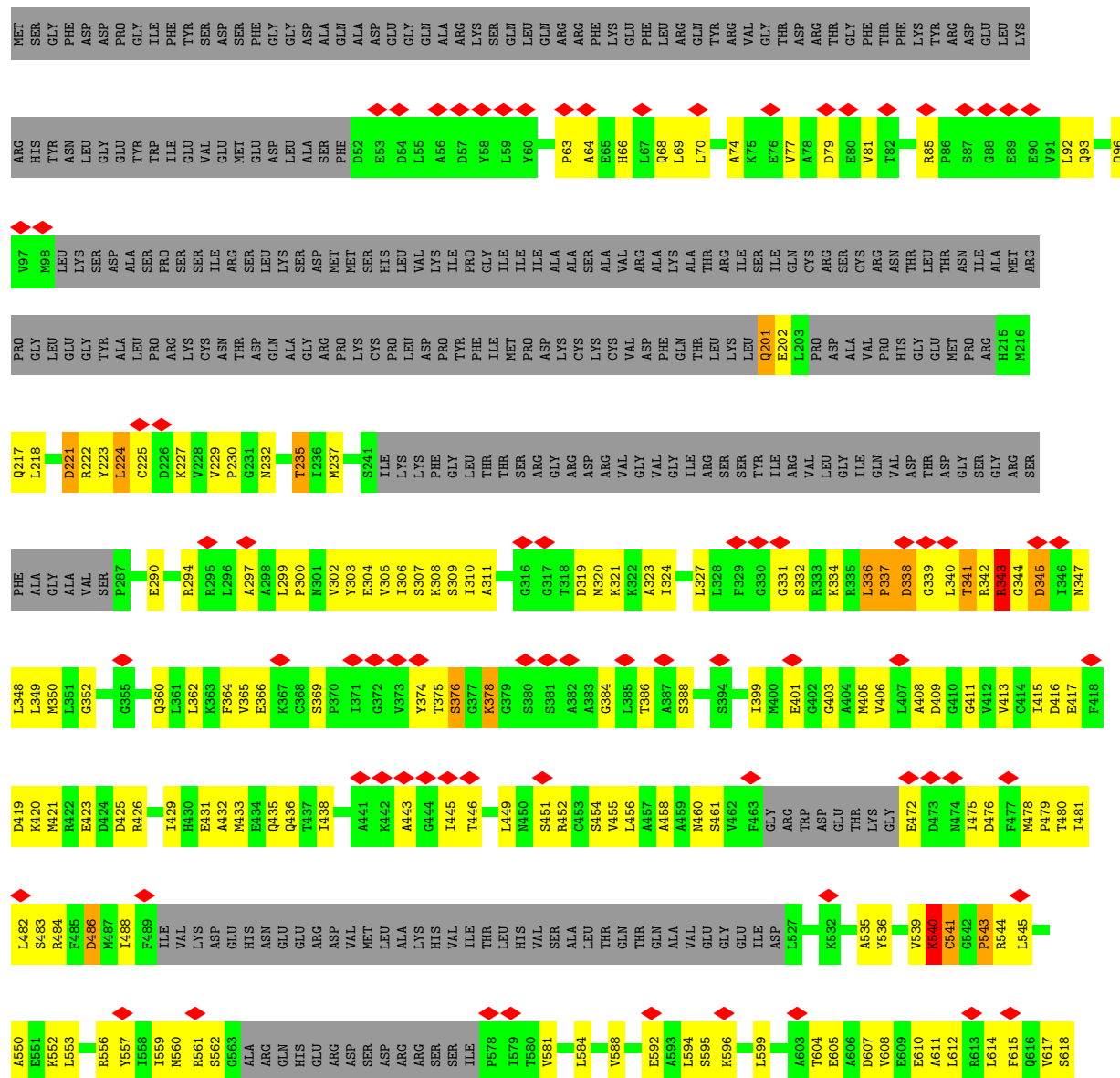
- Molecule 6 is a protein called DNA replication licensing factor MCM7.

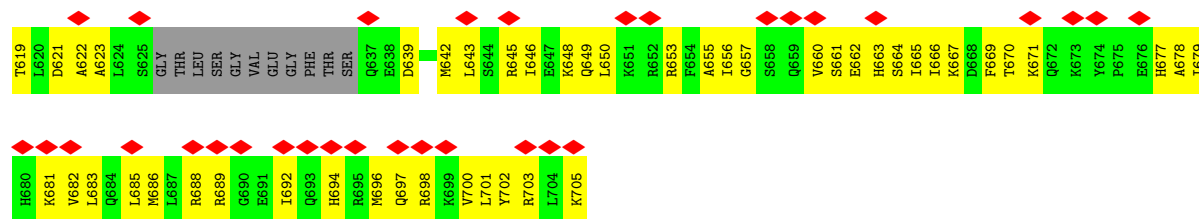
Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	575	Total	C	N	O	S	0	0
			4567	2866	815	861	25		

- Molecule 2: DNA replication licensing factor MCM3

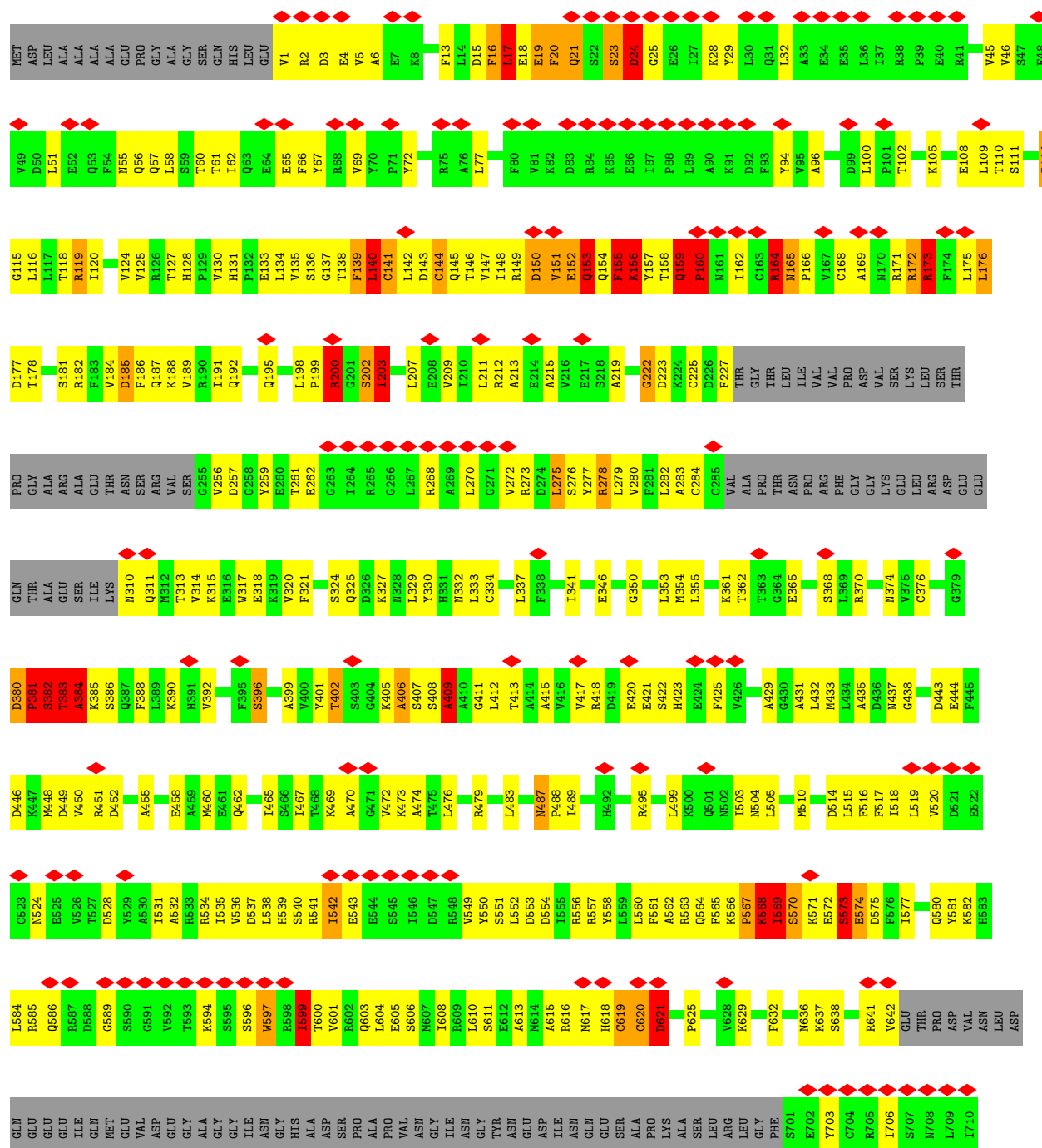


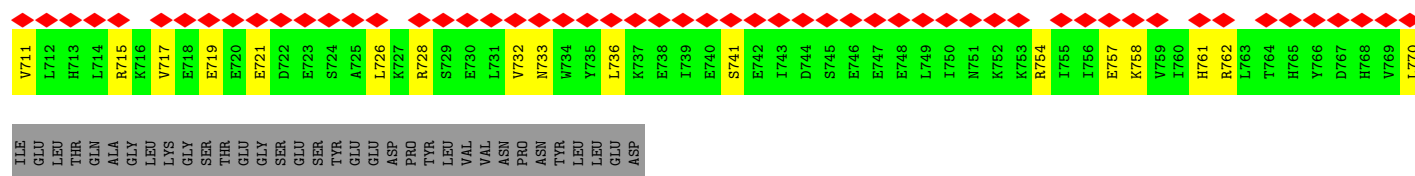




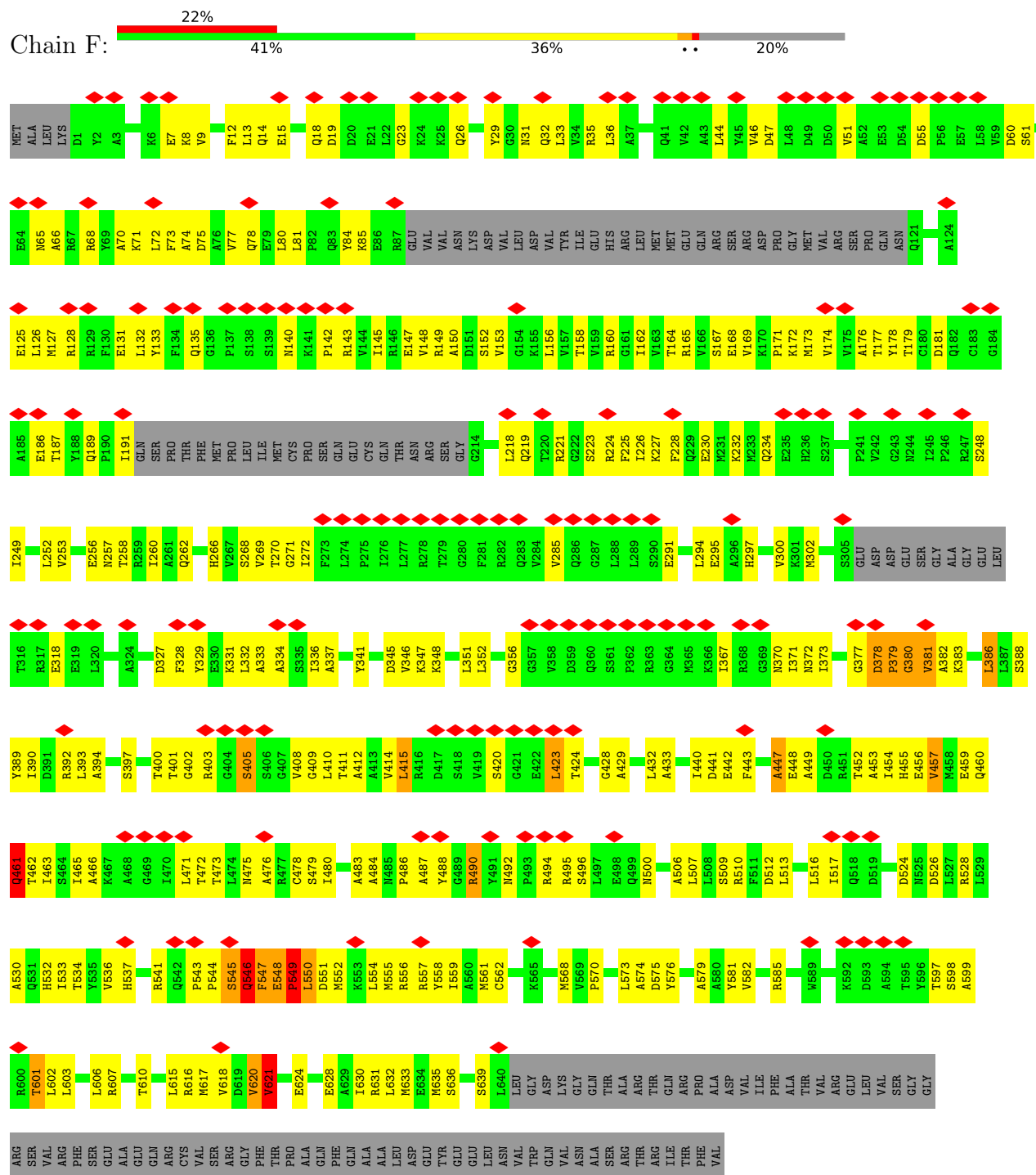


• Molecule 5: DNA replication licensing factor MCM6





• 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 (Å)	254.4, 254.4, 254.4	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.64	3/4518 (0.1%)	1.01	30/6093 (0.5%)
2	B	0.98	22/3965 (0.6%)	1.21	58/5341 (1.1%)
3	C	0.73	6/4299 (0.1%)	1.07	39/5809 (0.7%)
4	D	0.61	3/3390 (0.1%)	0.87	6/4541 (0.1%)
5	E	0.88	16/5420 (0.3%)	1.24	76/7302 (1.0%)
6	F	0.69	4/4637 (0.1%)	0.90	18/6257 (0.3%)
All	All	0.77	54/26229 (0.2%)	1.07	227/35343 (0.6%)

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 (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	153	GLN	N-CA	14.41	1.64	1.46
5	E	203	ILE	C-N	13.83	1.50	1.33
5	E	153	GLN	CA-C	-13.68	1.34	1.52
2	B	436	ILE	CA-CB	12.73	1.69	1.54
2	B	433	MET	N-CA	-12.42	1.30	1.46
2	B	421	PRO	C-N	12.31	1.50	1.33
2	B	433	MET	CA-C	11.80	1.69	1.52
6	F	378	ASP	N-CA	9.57	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	433	MET	CA-CB	9.46	1.70	1.53
2	B	436	ILE	CA-C	9.14	1.65	1.52
5	E	385	LYS	N-CA	-8.70	1.35	1.46
2	B	436	ILE	C-N	8.57	1.46	1.33
2	B	435	ASN	N-CA	-8.42	1.35	1.46
3	C	153	ALA	CA-CB	8.35	1.65	1.53
2	B	427	ASP	CA-C	8.23	1.63	1.52
2	B	436	ILE	CG1-CD1	7.99	1.82	1.51
4	D	345	ASP	CA-C	7.91	1.61	1.52
2	B	439	GLN	C-O	-7.80	1.14	1.24
5	E	153	GLN	CA-CB	7.74	1.66	1.53
5	E	384	ALA	C-O	7.60	1.33	1.24
6	F	378	ASP	CA-C	7.42	1.62	1.52
5	E	153	GLN	CB-CG	7.38	1.74	1.52
2	B	432	PRO	C-N	-7.34	1.24	1.33
5	E	157	TYR	CA-C	7.31	1.57	1.53
6	F	543	PRO	C-N	7.08	1.42	1.34
3	C	161	ALA	C-O	-7.04	1.15	1.24
3	C	153	ALA	CA-C	-7.00	1.44	1.53
3	C	271	HIS	CA-CB	6.81	1.64	1.53
2	B	433	MET	C-O	-6.64	1.15	1.24
4	D	376	SER	CA-C	-6.52	1.44	1.52
5	E	621	ASP	CA-C	-6.42	1.44	1.52
3	C	151	GLN	CA-C	-6.36	1.44	1.52
6	F	380	GLY	C-O	6.26	1.30	1.24
5	E	385	LYS	CA-C	-6.15	1.46	1.53
2	B	436	ILE	N-CA	-6.09	1.38	1.46
1	A	335	PRO	CA-C	-6.06	1.43	1.52
1	A	334	ASP	CA-C	6.03	1.59	1.52
4	D	540	LYS	N-CA	-5.99	1.42	1.46
3	C	154	PHE	N-CA	-5.93	1.38	1.46
2	B	440	ASP	C-O	-5.79	1.16	1.24
2	B	436	ILE	CB-CG1	5.78	1.65	1.53
2	B	333	ILE	CA-C	-5.70	1.47	1.52
5	E	173	ARG	N-CA	5.69	1.53	1.46
5	E	396	SER	N-CA	-5.67	1.38	1.46
5	E	160	PRO	CA-C	5.67	1.60	1.52
2	B	99	THR	CA-C	-5.63	1.45	1.53
2	B	342	GLY	C-O	-5.56	1.16	1.23
1	A	335	PRO	C-O	-5.33	1.17	1.24
5	E	203	ILE	CA-C	5.31	1.58	1.52
2	B	439	GLN	CA-C	-5.26	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	574	GLU	C-O	-5.20	1.17	1.24
2	B	333	ILE	CA-CB	-5.15	1.50	1.55
2	B	98	VAL	CA-C	-5.08	1.46	1.52
5	E	159	GLN	CA-C	5.05	1.59	1.52

All (227) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	380	ASP	CA-C-N	26.88	153.44	119.84
5	E	380	ASP	C-N-CA	26.88	153.44	119.84
1	A	98	LEU	CA-C-N	20.71	145.73	119.84
1	A	98	LEU	C-N-CA	20.71	145.73	119.84
2	B	436	ILE	CB-CA-C	18.20	133.76	111.20
5	E	20	PHE	N-CA-C	16.62	129.48	111.03
4	D	336	LEU	CA-C-N	16.39	140.32	119.84
4	D	336	LEU	C-N-CA	16.39	140.32	119.84
5	E	384	ALA	N-CA-C	-14.93	79.00	110.80
5	E	153	GLN	CA-CB-CG	14.70	143.50	114.10
6	F	380	GLY	N-CA-C	-14.46	90.78	111.03
1	A	193	GLY	CA-C-N	13.12	148.55	121.91
1	A	193	GLY	C-N-CA	13.12	148.55	121.91
6	F	548	GLU	CA-C-N	12.99	136.08	119.84
6	F	548	GLU	C-N-CA	12.99	136.08	119.84
2	B	329	ALA	CA-C-N	12.87	135.92	119.84
2	B	329	ALA	C-N-CA	12.87	135.92	119.84
2	B	101	CYS	N-CA-C	12.58	126.56	110.33
3	C	77	LEU	CA-C-N	12.53	139.94	121.02
3	C	77	LEU	C-N-CA	12.53	139.94	121.02
2	B	438	LEU	N-CA-C	-12.27	89.01	108.63
5	E	383	THR	N-CA-C	-12.00	85.24	110.80
6	F	378	ASP	N-CA-C	11.67	135.59	109.81
2	B	427	ASP	CA-C-N	11.62	142.35	122.36
2	B	427	ASP	C-N-CA	11.62	142.35	122.36
5	E	159	GLN	CA-C-N	11.54	134.26	119.84
5	E	159	GLN	C-N-CA	11.54	134.26	119.84
2	B	106	PRO	O-C-N	-11.07	109.13	122.86
3	C	151	GLN	N-CA-CB	10.97	130.76	111.13
2	B	421	PRO	O-C-N	-10.96	107.84	122.64
3	C	63	CYS	N-CA-C	-10.51	94.30	109.96
2	B	433	MET	CB-CA-C	10.47	132.41	110.32
2	B	439	GLN	CA-C-N	10.28	141.17	121.54
2	B	439	GLN	C-N-CA	10.28	141.17	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	382	SER	CA-C-N	10.19	141.00	121.54
5	E	382	SER	C-N-CA	10.19	141.00	121.54
2	B	70	GLU	N-CA-C	10.13	122.28	111.03
3	C	152	GLU	CA-C-N	10.12	139.93	122.12
3	C	152	GLU	C-N-CA	10.12	139.93	122.12
1	A	92	HIS	CA-C-N	9.82	134.00	120.35
1	A	92	HIS	C-N-CA	9.82	134.00	120.35
5	E	380	ASP	C-N-CD	-9.70	85.25	125.00
5	E	153	GLN	N-CA-CB	9.48	126.51	110.49
3	C	241	VAL	CA-C-N	9.47	136.76	122.65
3	C	241	VAL	C-N-CA	9.47	136.76	122.65
5	E	569	ILE	N-CA-C	9.19	121.44	109.58
2	B	433	MET	CA-CB-CG	8.81	131.72	114.10
1	A	422	SER	O-C-N	-8.77	111.49	121.84
2	B	424	GLY	CA-C-N	8.77	138.28	121.54
2	B	424	GLY	C-N-CA	8.77	138.28	121.54
6	F	545	SER	N-CA-C	-8.70	96.80	109.59
2	B	228	ILE	N-CA-C	-8.67	92.93	106.72
1	A	360	GLY	N-CA-C	-8.62	92.75	113.18
5	E	140	LEU	N-CA-C	8.60	122.97	110.42
3	C	150	MET	CA-C-N	8.60	137.16	122.37
3	C	150	MET	C-N-CA	8.60	137.16	122.37
3	C	152	GLU	N-CA-C	8.53	128.97	110.80
2	B	436	ILE	CB-CG1-CD1	8.16	130.93	113.80
6	F	546	GLN	N-CA-C	8.15	128.16	110.80
3	C	150	MET	O-C-N	-8.14	113.25	122.86
6	F	379	PRO	CA-C-N	8.02	128.93	120.43
6	F	379	PRO	C-N-CA	8.02	128.93	120.43
2	B	349	VAL	N-CA-C	7.96	125.90	109.34
1	A	337	THR	O-C-N	-7.95	113.44	122.75
3	C	154	PHE	CB-CA-C	-7.91	94.67	110.42
5	E	384	ALA	N-CA-CB	7.86	123.77	110.49
2	B	434	GLU	N-CA-CB	7.64	125.24	110.88
5	E	203	ILE	CA-C-N	7.63	128.66	120.11
5	E	203	ILE	C-N-CA	7.63	128.66	120.11
3	C	159	VAL	N-CA-C	-7.61	93.52	109.34
1	A	425	GLY	N-CA-C	-7.52	103.39	112.49
5	E	385	LYS	CA-C-O	-7.51	112.37	122.44
3	C	160	CYS	CB-CA-C	7.50	121.90	111.86
5	E	160	PRO	CA-C-N	7.49	134.82	122.62
5	E	160	PRO	C-N-CA	7.49	134.82	122.62
6	F	549	PRO	CA-C-O	-7.44	107.06	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	330	PRO	O-C-N	7.43	132.66	122.64
1	A	123	THR	N-CA-C	-7.42	104.36	113.41
5	E	165	ASN	N-CA-C	7.40	122.23	112.17
5	E	384	ALA	CA-C-N	-7.39	111.27	122.21
5	E	384	ALA	C-N-CA	-7.39	111.27	122.21
2	B	435	ASN	N-CA-C	-7.35	102.64	111.69
5	E	155	PHE	O-C-N	7.33	132.34	122.59
5	E	568	LYS	N-CA-C	7.33	126.42	110.80
2	B	107	LYS	N-CA-C	-7.30	99.65	110.46
5	E	21	GLN	N-CA-C	7.30	119.74	110.33
3	C	154	PHE	N-CA-C	-7.25	95.37	110.80
2	B	337	GLY	O-C-N	-7.19	113.35	122.70
5	E	272	VAL	CA-C-N	7.05	132.66	120.68
5	E	272	VAL	C-N-CA	7.05	132.66	120.68
1	A	3	LEU	N-CA-C	7.03	124.99	114.09
4	D	336	LEU	N-CA-C	7.01	120.91	110.39
5	E	567	PRO	N-CA-C	7.00	126.89	112.47
5	E	573	SER	N-CA-C	6.90	125.50	110.80
2	B	424	GLY	N-CA-C	-6.73	103.35	112.57
1	A	423	LYS	CA-C-N	6.71	134.36	121.54
1	A	423	LYS	C-N-CA	6.71	134.36	121.54
2	B	441	SER	N-CA-C	6.69	125.06	110.80
2	B	342	GLY	CA-C-N	6.67	133.98	121.97
2	B	342	GLY	C-N-CA	6.67	133.98	121.97
1	A	333	GLY	CA-C-N	6.66	138.62	122.31
1	A	333	GLY	C-N-CA	6.66	138.62	122.31
2	B	229	ALA	CA-C-N	6.65	134.25	121.54
2	B	229	ALA	C-N-CA	6.65	134.25	121.54
2	B	228	ILE	N-CA-CB	6.64	120.18	112.15
5	E	153	GLN	CB-CA-C	-6.60	97.29	110.42
3	C	75	ARG	CA-C-N	6.58	133.23	120.99
3	C	75	ARG	C-N-CA	6.58	133.23	120.99
3	C	269	VAL	CA-CB-CG2	6.57	121.57	110.40
5	E	144	CYS	N-CA-C	6.55	122.16	114.04
5	E	620	CYS	N-CA-C	6.49	118.15	111.14
5	E	384	ALA	CB-CA-C	-6.49	97.52	110.42
1	A	423	LYS	N-CA-C	6.46	124.57	110.80
2	B	330	PRO	N-CA-C	-6.46	99.17	112.47
1	A	336	GLY	N-CA-C	-6.40	104.58	112.77
1	A	337	THR	N-CA-C	-6.39	102.06	110.43
2	B	425	ARG	N-CA-C	-6.29	97.40	110.80
6	F	381	VAL	N-CA-C	6.29	122.42	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ASP	CB-CA-C	6.29	118.56	109.45
3	C	154	PHE	N-CA-CB	6.28	121.10	110.49
4	D	336	LEU	C-N-CD	-6.27	99.31	125.00
2	B	337	GLY	CA-C-N	6.25	133.49	121.54
2	B	337	GLY	C-N-CA	6.25	133.49	121.54
5	E	385	LYS	CA-C-N	-6.22	110.85	120.31
5	E	385	LYS	C-N-CA	-6.22	110.85	120.31
4	D	341	THR	O-C-N	-6.17	114.26	122.59
2	B	422	VAL	N-CA-C	6.15	122.14	109.34
5	E	153	GLN	N-CA-C	6.13	123.85	110.80
5	E	158	THR	N-CA-C	6.08	118.40	110.43
3	C	89	ASP	CA-C-N	6.07	130.72	120.88
3	C	89	ASP	C-N-CA	6.07	130.72	120.88
2	B	230	CYS	N-CA-C	-6.07	97.87	110.80
5	E	155	PHE	CA-C-N	6.05	133.09	121.54
5	E	155	PHE	C-N-CA	6.05	133.09	121.54
5	E	409	ALA	CA-C-N	6.04	132.23	120.99
5	E	409	ALA	C-N-CA	6.04	132.23	120.99
2	B	333	ILE	CA-C-N	-6.03	112.30	119.84
2	B	333	ILE	C-N-CA	-6.03	112.30	119.84
5	E	157	TYR	O-C-N	-6.03	116.95	121.47
3	C	78	ILE	CG1-CB-CG2	6.03	128.78	110.70
3	C	153	ALA	N-CA-C	5.97	119.11	109.86
1	A	98	LEU	O-C-N	5.96	128.17	121.32
5	E	153	GLN	CB-CG-CD	5.92	122.67	112.60
3	C	271	HIS	CA-CB-CG	5.92	119.72	113.80
1	A	337	THR	CA-CB-CG2	5.92	120.56	110.50
5	E	620	CYS	CA-C-N	5.87	132.75	121.54
5	E	620	CYS	C-N-CA	5.87	132.75	121.54
2	B	350	THR	N-CA-C	5.86	123.28	110.80
2	B	427	ASP	CB-CA-C	5.84	122.03	110.42
6	F	380	GLY	CA-C-O	5.84	126.47	120.98
2	B	101	CYS	N-CA-CB	-5.83	102.36	110.29
3	C	153	ALA	CA-C-O	-5.82	114.22	121.50
6	F	487	ALA	CA-C-O	-5.78	115.45	120.88
6	F	547	PHE	N-CA-C	5.76	119.03	109.46
3	C	270	ILE	N-CA-C	-5.72	97.43	109.34
2	B	230	CYS	CB-CA-C	5.70	121.76	110.42
5	E	153	GLN	CA-C-N	-5.69	109.27	121.45
5	E	153	GLN	C-N-CA	-5.69	109.27	121.45
1	A	295	ILE	N-CA-C	-5.66	107.75	113.47
5	E	155	PHE	N-CA-C	5.64	122.82	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	143	THR	OG1-CB-CG2	5.64	120.58	109.30
5	E	164	ARG	CA-C-N	5.64	126.09	119.83
5	E	164	ARG	C-N-CA	5.64	126.09	119.83
3	C	87	THR	OG1-CB-CG2	5.60	120.50	109.30
5	E	383	THR	CA-C-N	5.59	132.22	121.54
5	E	383	THR	C-N-CA	5.59	132.22	121.54
2	B	436	ILE	N-CA-C	-5.59	107.54	112.90
1	A	358	GLY	O-C-N	-5.56	116.76	122.60
3	C	434	THR	N-CA-C	-5.55	101.29	109.18
5	E	278	ARG	N-CA-C	5.54	118.29	109.81
6	F	378	ASP	C-N-CD	-5.52	102.37	125.00
5	E	570	SER	CB-CA-C	-5.51	97.36	110.02
2	B	227	LEU	O-C-N	-5.49	115.34	122.97
2	B	359	ARG	CA-C-N	5.49	131.68	123.23
2	B	359	ARG	C-N-CA	5.49	131.68	123.23
5	E	23	SER	N-CA-C	-5.45	99.19	110.80
5	E	24	ASP	N-CA-C	5.43	116.79	108.42
4	D	343	ARG	N-CA-C	5.43	122.36	110.80
3	C	267	ILE	CG1-CB-CG2	5.41	126.92	110.70
1	A	335	PRO	CA-C-N	5.39	125.93	120.00
1	A	335	PRO	C-N-CA	5.39	125.93	120.00
3	C	271	HIS	N-CA-C	-5.37	102.25	110.14
5	E	566	LYS	CA-C-N	-5.35	113.16	119.84
5	E	566	LYS	C-N-CA	-5.35	113.16	119.84
5	E	618	HIS	O-C-N	-5.33	115.16	122.46
2	B	405	ILE	CA-C-N	-5.32	115.70	122.77
2	B	405	ILE	C-N-CA	-5.32	115.70	122.77
6	F	377	GLY	CA-C-N	5.31	134.76	121.80
6	F	377	GLY	C-N-CA	5.31	134.76	121.80
5	E	114	ILE	CG1-CB-CG2	5.29	126.58	110.70
5	E	165	ASN	N-CA-CB	-5.29	105.36	110.39
3	C	160	CYS	N-CA-CB	5.27	119.92	111.91
1	A	362	SER	N-CA-C	-5.26	99.60	110.80
5	E	16	PHE	CA-C-N	5.25	131.57	121.54
5	E	16	PHE	C-N-CA	5.25	131.57	121.54
5	E	275	LEU	CB-CG-CD2	5.25	126.46	110.70
3	C	151	GLN	O-C-N	5.24	129.68	123.33
5	E	139	PHE	CB-CA-C	-5.23	103.02	111.28
5	E	381	PRO	CA-N-CD	-5.22	104.69	112.00
2	B	71	GLY	N-CA-C	5.22	125.55	113.18
6	F	377	GLY	N-CA-C	5.20	125.51	113.18
1	A	424	ALA	N-CA-CB	5.20	119.27	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	441	SER	CA-C-O	-5.20	113.08	120.51
5	E	381	PRO	N-CA-C	5.19	123.16	112.47
5	E	160	PRO	N-CA-C	5.19	123.16	112.47
5	E	406	ALA	N-CA-C	-5.18	99.78	110.80
5	E	408	SER	O-C-N	5.17	127.39	122.07
5	E	199	PRO	CA-C-O	-5.17	114.45	120.85
2	B	101	CYS	CA-CB-SG	-5.14	102.57	114.40
5	E	569	ILE	CA-C-N	5.14	130.10	120.95
5	E	569	ILE	C-N-CA	5.14	130.10	120.95
2	B	436	ILE	CA-CB-CG1	5.13	119.13	110.40
1	A	364	VAL	N-CA-C	-5.13	98.67	109.34
2	B	350	THR	CB-CA-C	-5.11	100.26	110.42
5	E	620	CYS	CA-CB-SG	-5.11	102.66	114.40
2	B	332	ALA	N-CA-C	5.10	116.34	107.93
5	E	156	LYS	N-CA-C	5.09	121.64	110.80
3	C	151	GLN	CA-C-N	5.07	131.22	121.54
3	C	151	GLN	C-N-CA	5.07	131.22	121.54
3	C	112	ARG	N-CA-C	5.06	116.05	108.76
6	F	423	LEU	N-CA-C	5.05	118.30	111.17
2	B	99	THR	N-CA-CB	5.04	118.00	110.19
3	C	87	THR	CA-CB-CG2	5.03	119.06	110.50
2	B	421	PRO	CA-C-N	5.03	131.02	121.97
2	B	421	PRO	C-N-CA	5.03	131.02	121.97
3	C	244	ILE	CG1-CB-CG2	5.02	125.76	110.70
1	A	101	VAL	N-CA-C	5.02	119.77	109.34

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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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	4483	211	0
2	B	3912	0	3993	259	0
3	C	4227	0	4258	249	0
4	D	3349	0	3429	201	0
5	E	5335	0	5360	381	0
6	F	4567	0	4622	212	0
All	All	25833	0	26145	1427	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 (1427) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:151:VAL:C	5:E:159:GLN:HG3	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:386:ARG:CD	2:B:438:LEU:HD22	1.78	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
5:E:154:GLN:C	5:E:156:LYS:HG2	1.75	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: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
5:E:152:GLU:N	5:E:159:GLN:CD	2.14	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
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:151:VAL:C	5:E:159:GLN:CG	2.28	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
5:E:19:GLU:CD	5:E:32:LEU:HD12	1.87	0.99
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
4:D:332:SER:C	4:D:344:GLY:HA3	1.95	0.91
2:B:348:ALA:CB	2:B:405:ILE:HD11	1.99	0.91
4:D:331:GLY:C	4:D:344:GLY:O	2.13	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:332:SER:O	4:D:343:ARG:O	1.93	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
5:E:152:GLU:H	5:E:159:GLN:CD	1.78	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
4:D:331:GLY:HA3	4:D:344:GLY:C	2.05	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
2:B:328:THR:C	2:B:330:PRO:HD3	2.05	0.79
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:19:GLU:CG	5:E:32:LEU:HD12	2.11	0.78
5:E:19:GLU:CD	5:E:32:LEU:CD1	2.49	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
2:B:102:SER:OG	2:B:165:THR:O	2.02	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
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
3:C:227:ASN:O	3:C:230:VAL:N	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:435:ASN:C	4:D:689:ARG:NH2	2.46	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
5:E:154:GLN:C	5:E:156:LYS:CG	2.47	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
6:F:550:LEU:HB2	6:F:555:MET:HE2	1.71	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:228:ASP:O	3:C:232:LYS:NZ	2.22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:656:ILE:HD13	4:D:696:MET:HE3	1.73	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
4:D:221:ASP:OD1	4:D:222:ARG:NH1	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:C:198:SER:O	5:E:111:SER:OG	2.11	0.68
3:C:544:TYR:O	3:C:548:THR:OG1	2.10	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
3:C:230:VAL:O	3:C:232:LYS:NZ	2.23	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
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
5:E:354:MET:HE1	5:E:483:LEU:HA	1.75	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
6:F:530:ALA:O	6:F:534:THR:OG1	2.07	0.67
2:B:410:ASN:OD1	2:B:411:ALA:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:111:VAL:C	3:C:270:ILE:HD11	2.20	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:E:152:GLU:CA	5:E:159:GLN:CD	2.65	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
3:C:413:ALA:O	3:C:417:SER:OG	2.07	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
2:B:205:VAL:C	2:B:229:ALA:O	2.40	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
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
3:C:417:SER:O	3:C:462:THR:OG1	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:E:16:PHE:CA	5:E:20:PHE:HZ	1.91	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:363:ALA:HB3	5:E:473:LYS:HZ1	1.64	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
1:A:497:HIS:O	5:E:361:LYS:NZ	2.32	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:273:MET:O	1:A:276:SER:OG	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:E:376:CYS:O	5:E:517:PHE:N	2.34	0.60
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:217:GLN:C	4:D:218:LEU:HD12	2.29	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:120:ILE:HD12	5:E:227:PHE:C	2.29	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:490:VAL:CG1	5:E:574:GLU:CD	2.78	0.56
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
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:543:ALA:O	3:C:547:SER:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:332:SER:O	4:D:343:ARG:C	2.48	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
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
3:C:130:ILE:O	3:C:132:GLN:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:E:151:VAL:C	5:E:159:GLN:HG2	2.13	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
6:F:636:SER:O	6:F:639:SER:OG	2.11	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
3:C:65:HIS:O	3:C:67:LYS:N	2.41	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
1:A:231:ASN:C	1:A:248:VAL:HG21	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:154:GLN:CA	5:E:156:LYS:CG	2.87	0.53
6:F:337:ALA:HB3	6:F:347:LYS:HZ3	1.73	0.53
2:B:580:VAL:O	2:B:584:THR:OG1	2.26	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: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
4:D:661:SER:C	4:D:665:ILE:HG22	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
4:D:642:MET:C	4:D:646:ILE:HD12	2.34	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:364:GLY:O	3:C:369:GLN:NE2	2.40	0.51
6:F:327:ASP:O	6:F:331:LYS:N	2.34	0.51
1:A:292:ALA:O	1:A:302:LYS:NZ	2.40	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
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
4:D:235:THR:CG2	4:D:237:MET:HE2	2.40	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:275:THR:O	1:A:278:SER:OG	2.29	0.51
1:A:303:ARG:O	1:A:307:LEU:N	2.41	0.51
2:B:206:GLY:C	2:B:227:LEU:HD21	2.36	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
1:A:490:VAL:HG11	5:E:574:GLU:CD	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
1:A:549:ASP:OD1	1:A:552:LYS:NZ	2.32	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
3:C:65:HIS:C	3:C:67:LYS:H	2.20	0.50
6:F:378:ASP:HB3	6:F:379:PRO:HD3	1.93	0.50
1:A:100:LEU:CD1	1:A:100:LEU:C	2.85	0.49
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
1:A:469:ILE:HD11	1:A:583:MET:HE2	1.94	0.49
4:D:332:SER:N	4:D:344:GLY:C	2.70	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
4:D:677:HIS:O	4:D:681:LYS:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:E:620:CYS:SG	5:E:621:ASP:N	2.83	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:87:THR:HA	3:C:90:MET:HE3	1.94	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
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
2:B:396:GLY:C	2:B:411:ALA:HB3	2.38	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: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
3:C:533:LEU:HD23	3:C:534:ASP:N	2.27	0.48

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:321:ILE:C	3:C:328:LYS:HZ1	2.20	0.48
3:C:335:LEU:HD11	3:C:377:LEU:HD23	1.96	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: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:173:GLU:CD	2:B:331:ARG:HH22	2.21	0.47
2:B:206:GLY:C	2:B:230:CYS:SG	2.90	0.47
2:B:379:ASP:OD1	2:B:379:ASP:N	2.47	0.47
3:C:428:ASP:OD1	3:C:428: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
3:C:457:GLN:C	3:C:458:LEU:HD22	2.39	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
6:F:557:ARG:O	6:F:561:MET:HE2	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:ARG:CZ	2:B:331:ARG:CB	2.91	0.47
3:C:121:ASN:O	3:C:123:ARG:N	2.47	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
2:B:432:PRO:O	2:B:433:MET:C	2.56	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:390:HIS:HA	2:B:393:MET:HE3	1.96	0.47
3:C:65:HIS:C	3:C:67:LYS:N	2.72	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:345:ASP:OD1	6:F:345:ASP:N	2.45	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
6:F:562:CYS:SG	6:F:617:MET:HE3	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:318:LYS:NZ	2:B:376:ASP:OD1	2.46	0.46
5:E:168:CYS:SG	5:E:169:ALA:N	2.88	0.46
2:B:15:ILE:HB	2:B:70:GLU:CD	2.41	0.46
2:B:392:VAL:HG13	2:B:397:ARG:C	2.40	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
3:C:437:VAL:C	3:C:441:VAL:HG23	2.41	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
5:E:19:GLU:HB2	5:E:28:LYS:C	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:362:ASP:O	3:C:367:LYS:NZ	2.39	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
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:363:ALA:CB	5:E:473:LYS:HZ1	2.26	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:173:GLU:CD	2:B:331:ARG:NH2	2.74	0.45
2:B:192:LEU:HD21	2:B:231:ASN:HA	1.99	0.45
4:D:399:ILE:O	4:D:401:GLU:N	2.49	0.45
5:E:407:SER:O	5:E:407:SER:OG	2.26	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:423:TYR:CD2	2:B:423:TYR:C	2.95	0.45
3:C:435:ARG:N	3:C:437:VAL:HG12	2.32	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
3:C:155:PHE:C	3:C:185:THR:HG21	2.42	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:245:TYR:OH	3:C:265:THR:OG1	2.15	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
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
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
5:E:45:VAL:HG23	5:E:96:ALA:C	2.42	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:202:GLU:CD	4:D:202:GLU:C	2.85	0.44
4:D:319:ASP:OD2	4:D:320:MET:N	2.51	0.44
4:D:480:THR:O	4:D:483:SER:OG	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:741:SER:O	5:E:741:SER:OG	2.30	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
2:B:107:LYS:C	2:B:160:TYR:CD2	2.96	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
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:332:SER:CA	4:D:344:GLY:HA3	2.46	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:160:TYR:C	6:F:150:ALA:HB1	2.44	0.43
3:C:161:ALA:HB2	5:E:256:VAL:H	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:565:TYR:OH	5:E:528:ASP:O	2.25	0.43
6:F:167:SER:HG	6:F:230:GLU:H	1.64	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
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
4:D:348:LEU:O	4:D:350:MET:HE2	2.19	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
1:A:578:GLU:C	1:A:581:ILE:HG22	2.45	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
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:548:MET:HE3	1:A:549:ASP:OD2	2.19	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
6:F:409:GLY:C	6:F:410:LEU:HD12	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:418:ARG:HD2	5:E:422:SER:HA	2.02	0.41
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:152:GLU:HB3	3:C:167:GLU:C	2.45	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:434:GLU:O	4:D:689:ARG:NH1	2.52	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
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: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
3:C:318:ALA:O	3:C:328:LYS:NZ	2.44	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
2:B:283:ALA:O	2:B:286:CYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:108:GLU:C	5:E:110:THR:HG23	2.46	0.41
5:E:152:GLU:O	5:E:154:GLN:N	2.53	0.41
5:E:173:ARG:O	5:E:173:ARG:HG2	2.20	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
1:A:615:THR:O	1:A:615:THR:HG22	2.21	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
5:E:390:LYS:NZ	5:E:402:THR:O	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:GLU:OE1	2:B:331:ARG:CA	2.70	0.40
2:B:423:TYR:CE1	4:D:643:LEU:HD13	2.56	0.40
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
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
1:A:233:ASP:O	1:A:238:THR:OG1	2.12	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: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:201:GLN:CD	4:D:201:GLN:N	2.79	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	546/904 (60%)	454 (83%)	79 (14%)	13 (2%)	4	27
2	B	484/808 (60%)	402 (83%)	67 (14%)	15 (3%)	3	22
3	C	515/863 (60%)	400 (78%)	100 (19%)	15 (3%)	3	23
4	D	410/734 (56%)	355 (87%)	50 (12%)	5 (1%)	10	42
5	E	653/821 (80%)	517 (79%)	109 (17%)	27 (4%)	2	18
6	F	567/719 (79%)	484 (85%)	74 (13%)	9 (2%)	7	36
All	All	3175/4849 (66%)	2612 (82%)	479 (15%)	84 (3%)	6	25

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%)	475 (97%)	13 (3%)	39	59
2	B	429/707 (61%)	414 (96%)	15 (4%)	32	53
3	C	470/753 (62%)	460 (98%)	10 (2%)	47	65
4	D	364/625 (58%)	355 (98%)	9 (2%)	42	62
5	E	595/724 (82%)	568 (96%)	27 (4%)	24	46
6	F	494/619 (80%)	484 (98%)	10 (2%)	48	66
All	All	2840/4209 (68%)	2756 (97%)	84 (3%)	37	57

All (84) 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	233	ASP
1	A	334	ASP
1	A	340	SER
1	A	362	SER
1	A	364	VAL
1	A	472	VAL
1	A	473	VAL
1	A	474	ARG
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	185	ASP
2	B	227	LEU
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	63	CYS
3	C	64	GLU
3	C	135	THR
3	C	152	GLU
3	C	159	VAL
3	C	160	CYS
3	C	217	THR
3	C	221	VAL
3	C	270	ILE
3	C	497	LEU
4	D	201	GLN
4	D	224	LEU
4	D	235	THR
4	D	338	ASP
4	D	342	ARG
4	D	345	ASP
4	D	378	LYS

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Mol	Chain	Res	Type
4	D	540	LYS
4	D	543	PRO
5	E	17	LEU
5	E	24	ASP
5	E	140	LEU
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	173	ARG
5	E	175	LEU
5	E	176	LEU
5	E	200	ARG
5	E	202	SER
5	E	203	ILE
5	E	279	LEU
5	E	381	PRO
5	E	383	THR
5	E	487	ASN
5	E	488	PRO
5	E	569	ILE
5	E	571	LYS
5	E	596	SER
5	E	599	ILE
5	E	600	THR
5	E	619	CYS
6	F	186	GLU
6	F	253	VAL
6	F	386	LEU
6	F	405	SER
6	F	415	LEU
6	F	424	THR
6	F	490	ARG
6	F	546	GLN
6	F	601	THR
6	F	621	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	182	ASN
1	A	417	GLN
1	A	546	ASN
1	A	547	GLN
1	A	683	ASN
2	B	10	ASN
2	B	35	ASN
2	B	275	HIS
2	B	540	HIS
3	C	18	GLN
3	C	72	ASN
3	C	76	GLN
3	C	82	GLN
3	C	115	ASN
3	C	151	GLN
3	C	186	HIS
3	C	226	HIS
3	C	227	ASN
3	C	419	ASN
3	C	469	ASN
3	C	546	HIS
4	D	217	GLN
4	D	360	GLN
4	D	460	ASN
5	E	21	GLN
5	E	98	GLN
5	E	154	GLN
5	E	192	GLN
5	E	195	GLN
5	E	310	ASN
5	E	618	HIS
5	E	636	ASN
5	E	708	ASN
6	F	18	GLN
6	F	189	GLN
6	F	262	GLN
6	F	461	GLN
6	F	475	ASN
6	F	518	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

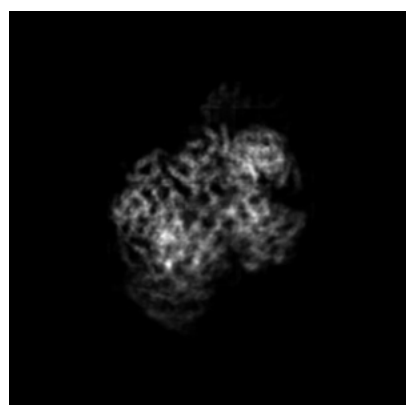
6 Map visualisation [i](#)

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

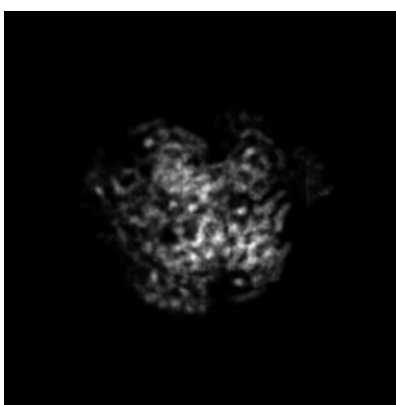
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

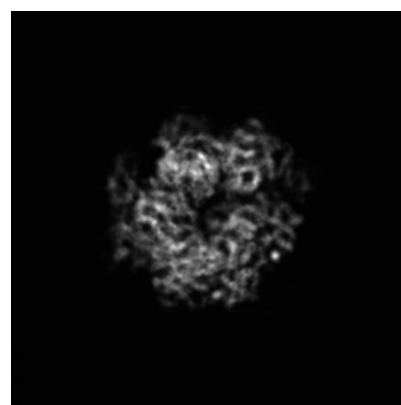
6.1.1 Primary map



X



Y

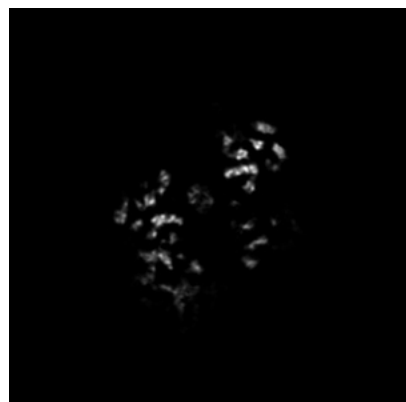


Z

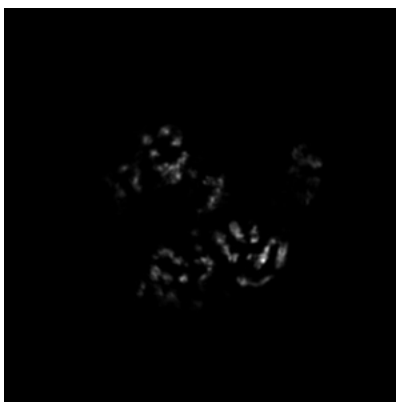
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

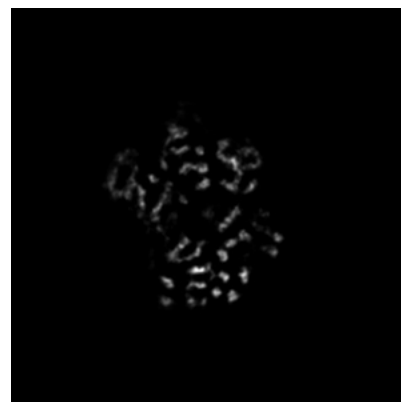
6.2.1 Primary map



X Index: 120



Y Index: 120

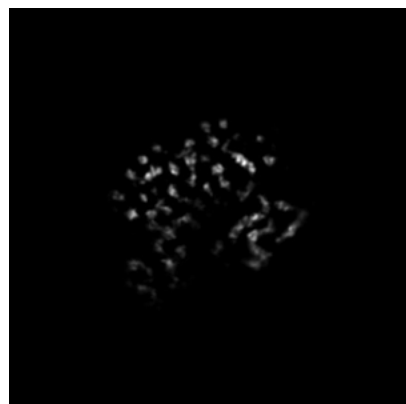


Z Index: 120

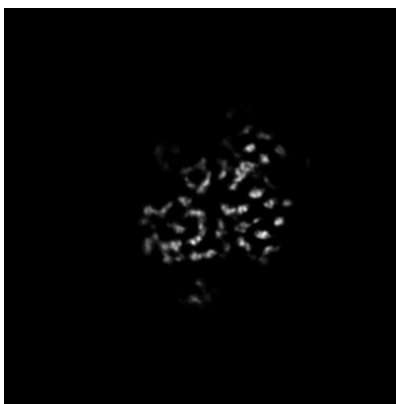
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 98



Y Index: 146

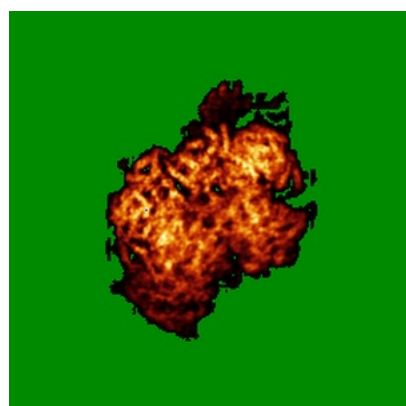


Z Index: 119

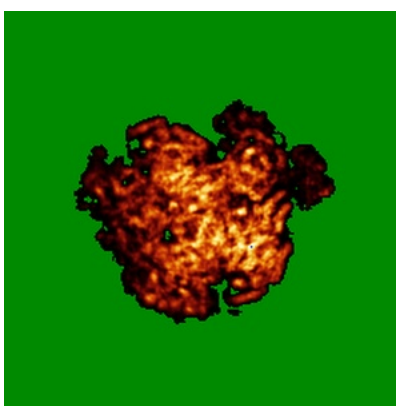
The images above show the largest variance slices of the map in three orthogonal directions.

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

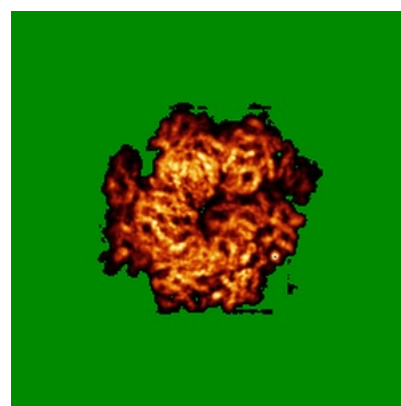
6.4.1 Primary map



X



Y

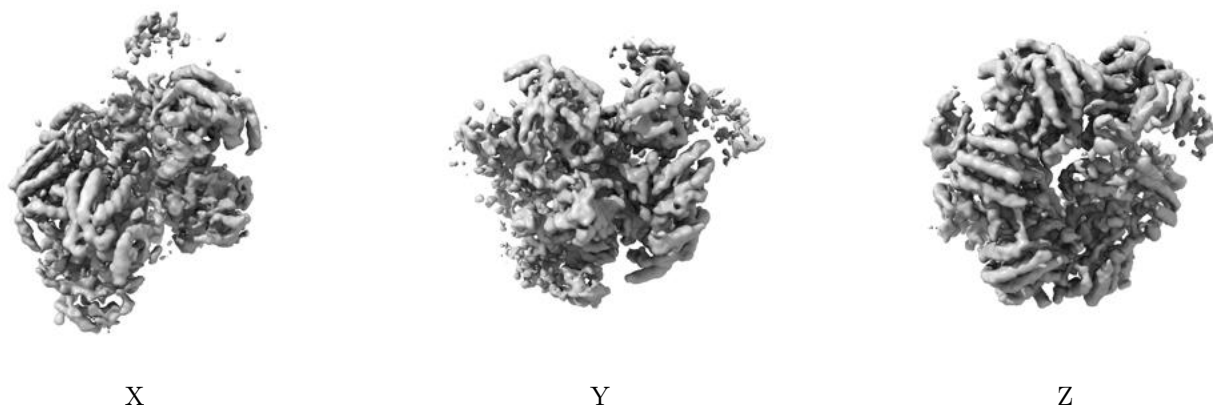


Z

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.

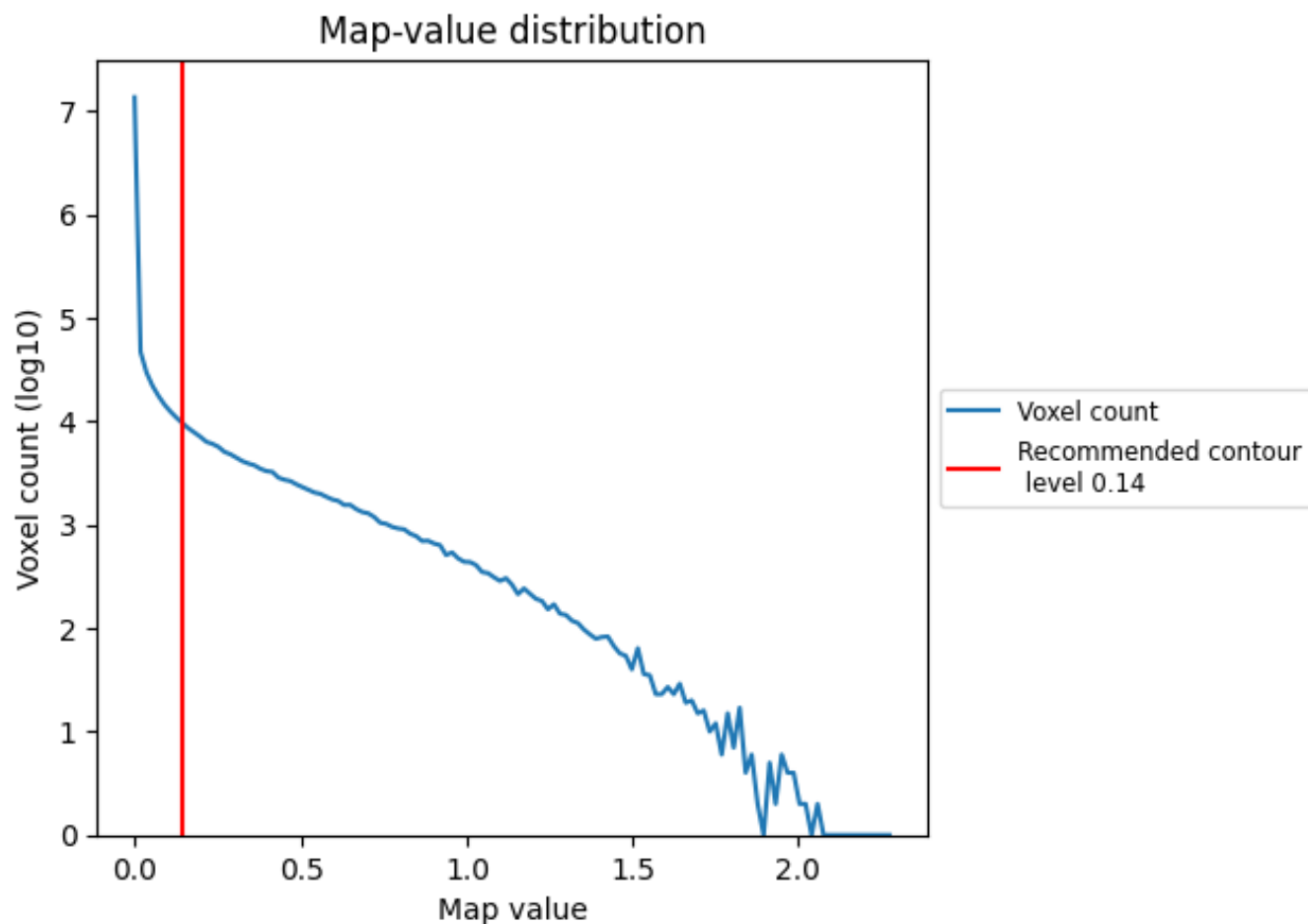
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

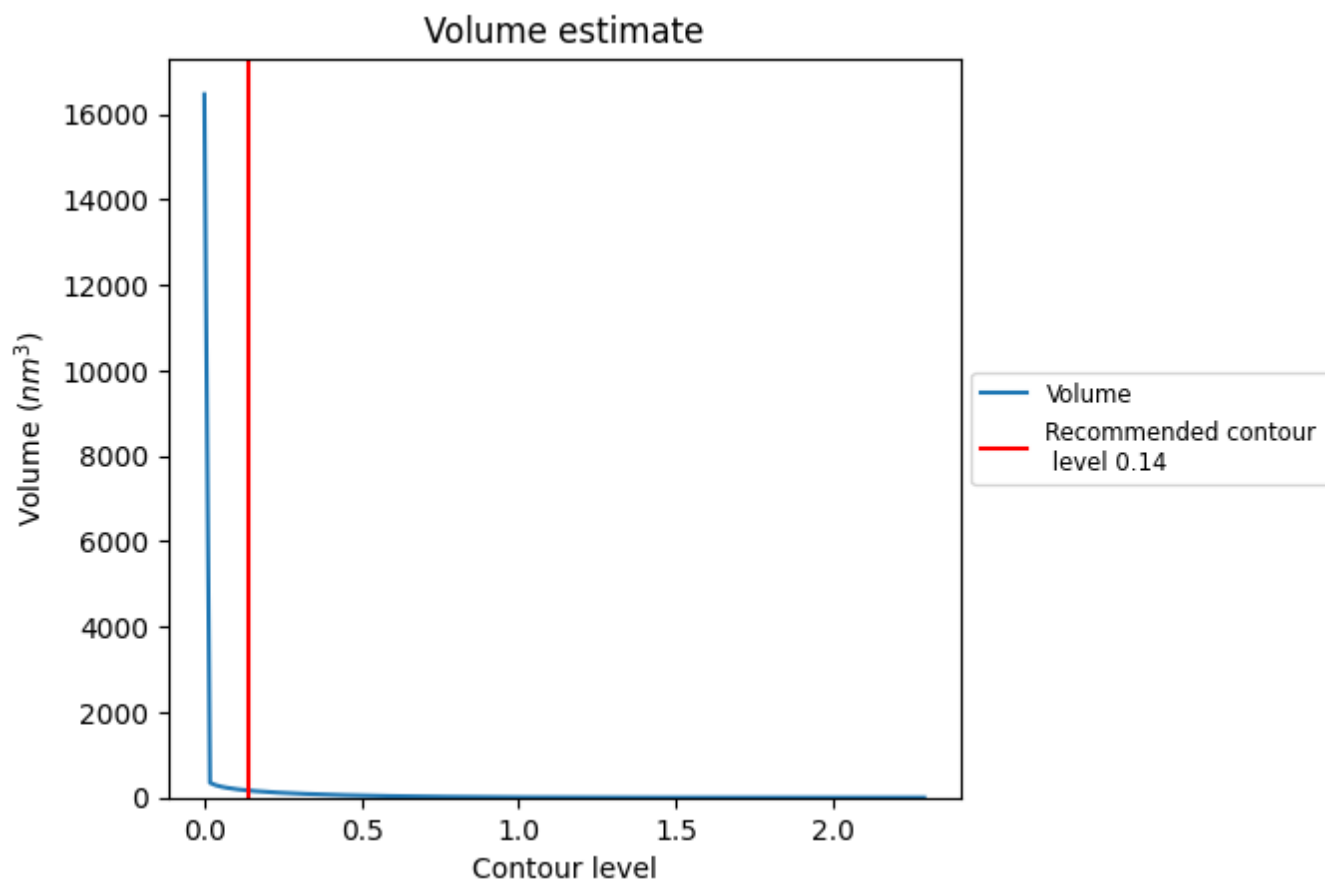
This section contains the results of statistical analysis of the map.

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.

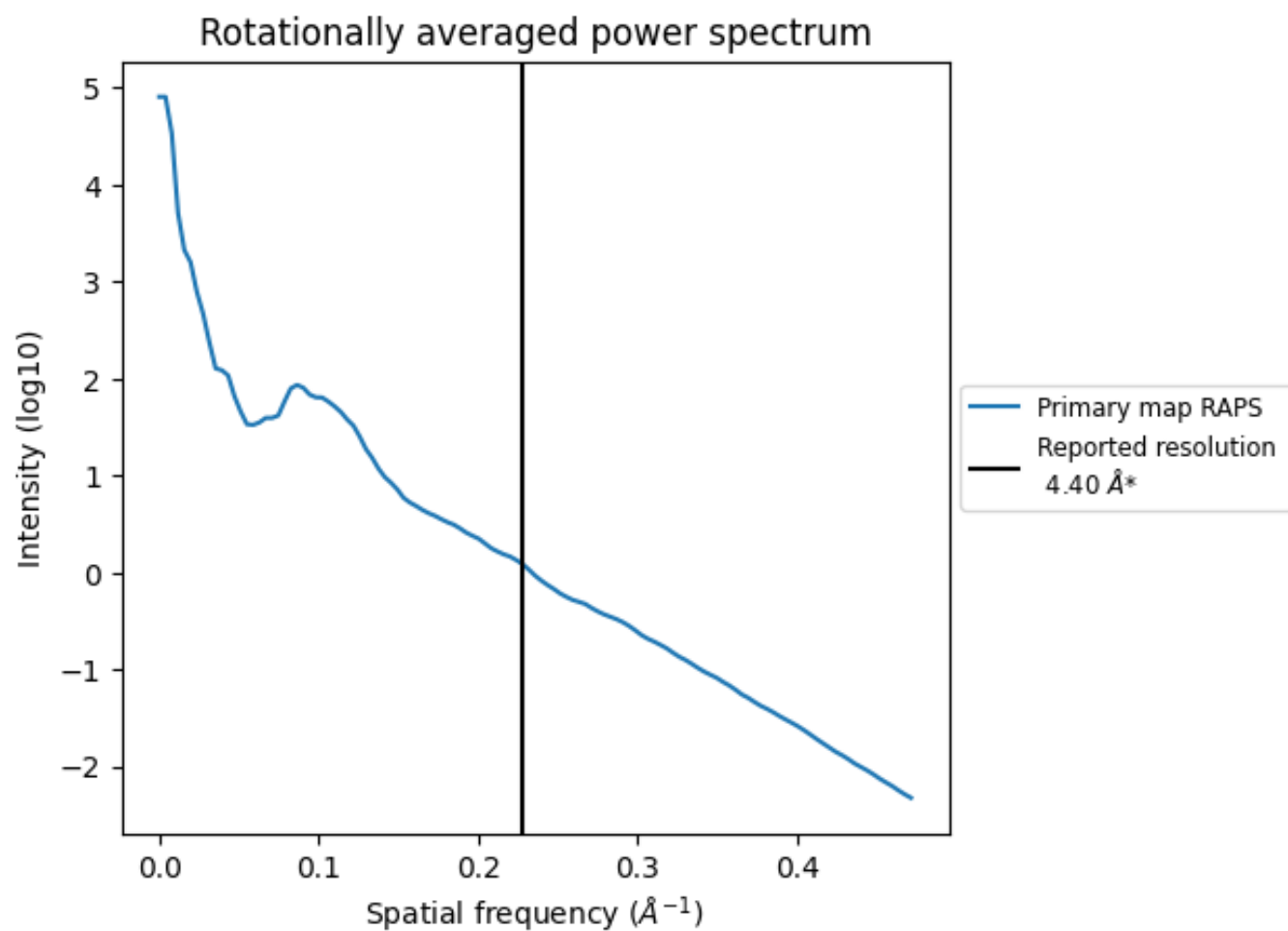
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 165 nm³; 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 ⓘ

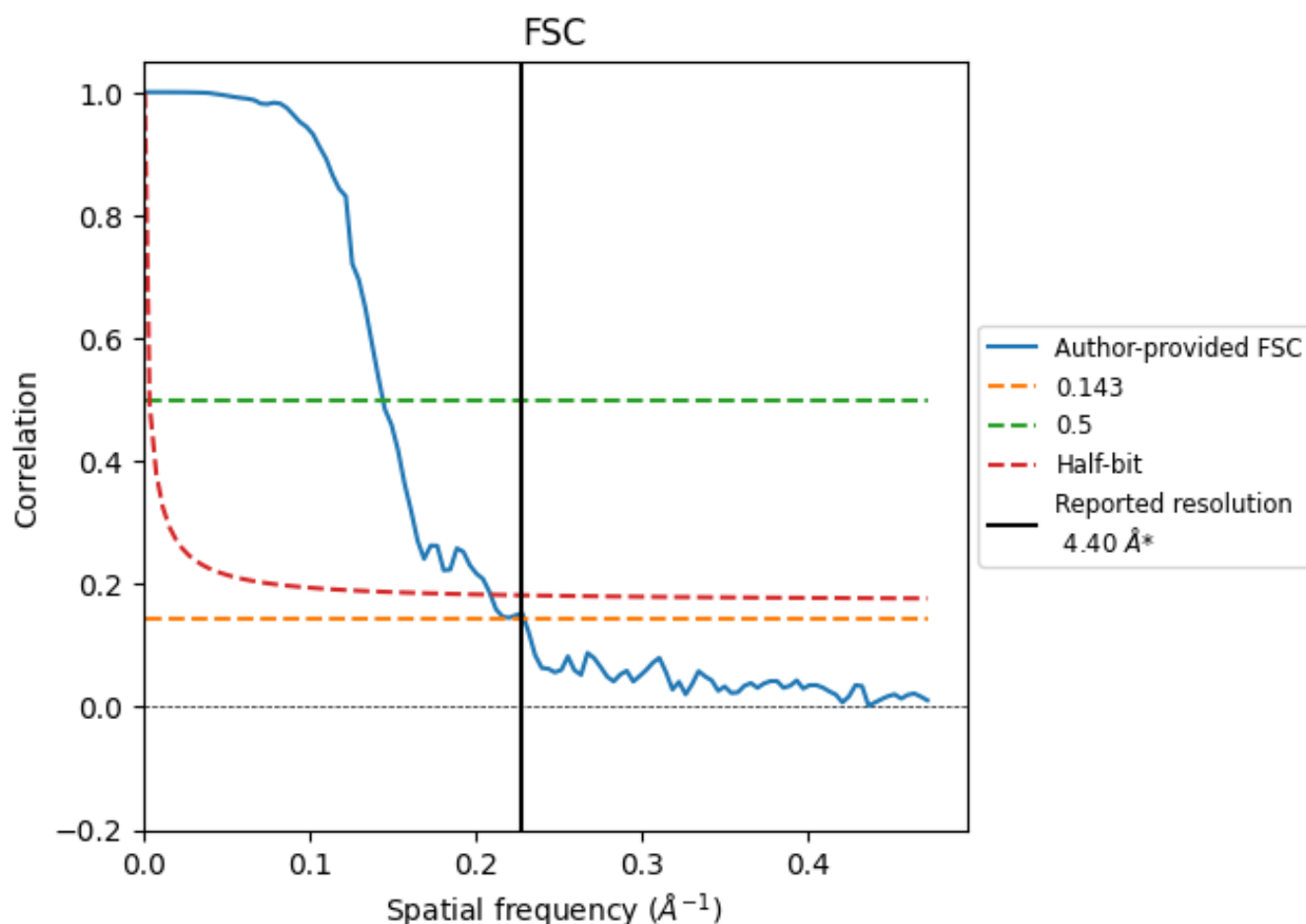


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

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](#)

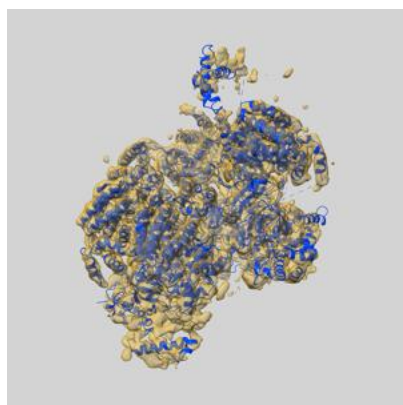
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.36	6.93	4.79
Unmasked-calculated*	-	-	-

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

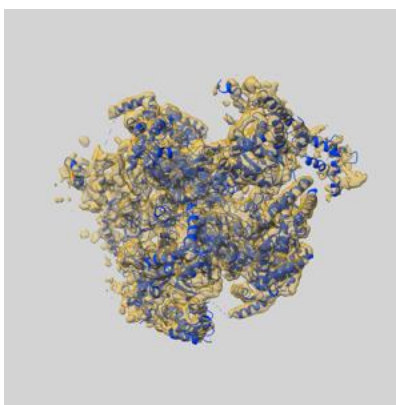
9 Map-model fit [i](#)

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 5.

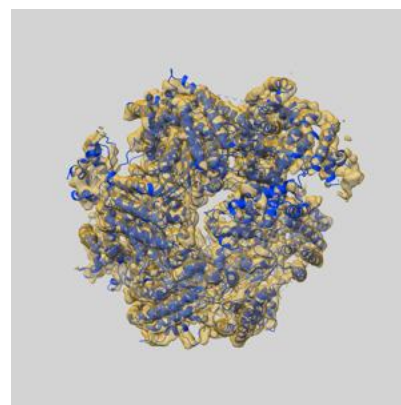
9.1 Map-model overlay [i](#)



X



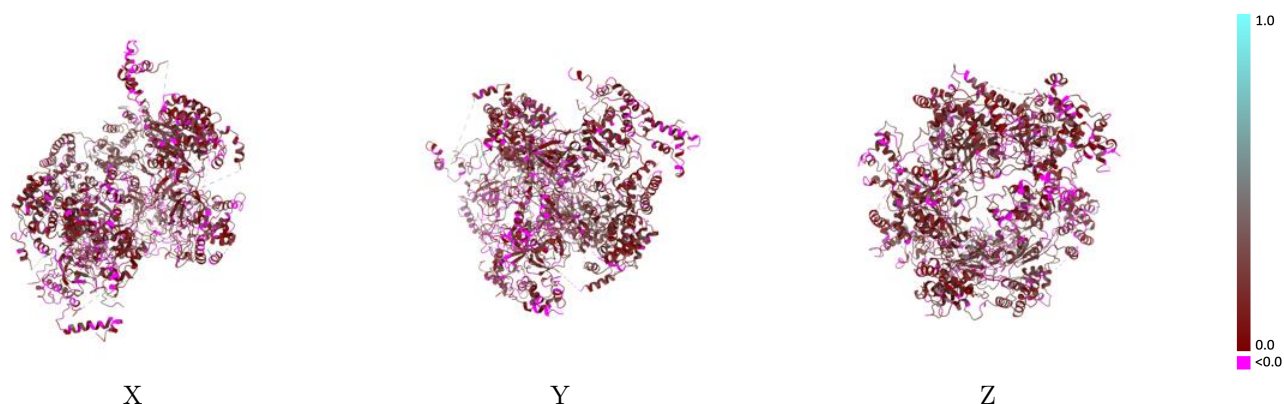
Y



Z

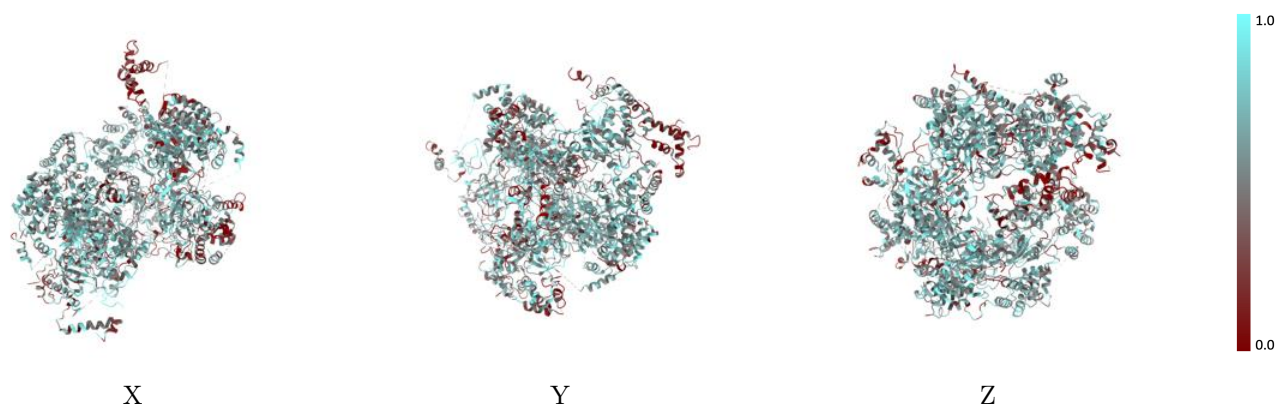
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



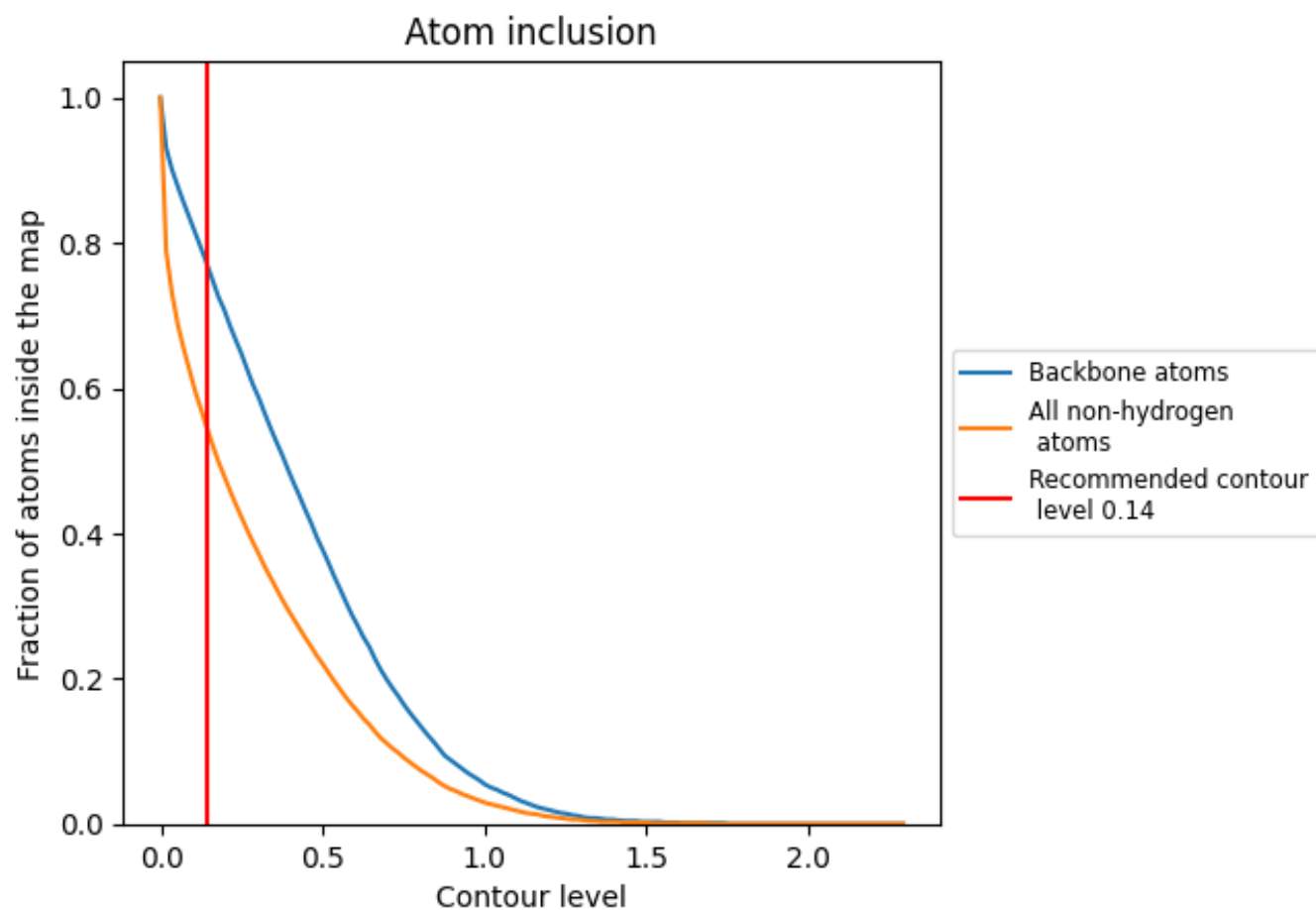
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.5480	0.1490
A	0.5300	0.1370
B	0.5780	0.1690
C	0.5760	0.1560
D	0.5560	0.1460
E	0.5200	0.1450
F	0.5370	0.1440

1.0

0.0

<0.0