



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:50 AM UTC

PDB ID : 8XCG / pdb_00008xcg
EMDB ID : EMD-38242
Title : Tail tip complex of bacteriophage lambda in the open state
Authors : Ge, X.F.; Wang, J.W.
Deposited on : 2023-12-09
Resolution : 3.46 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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

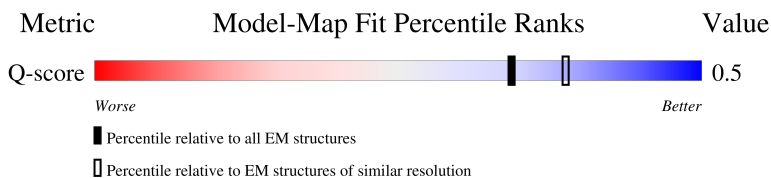
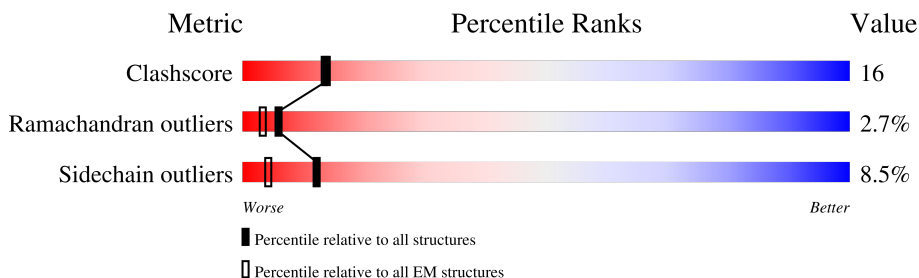
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.46 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	13788 (2.96 - 3.96)

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	E	109	
1	K	109	
1	M	109	
1	Y	109	

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Mol	Chain	Length	Quality of chain
1	e	109	
1	m	109	
2	F	1132	
2	J	1132	
2	Z	1132	
3	I	223	
3	P	223	
3	h	223	
4	L	232	
4	N	232	
4	f	232	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 25941 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 Tail tip protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	109	Total	C	N	O	S	0	0
			884	569	154	157	4		
1	K	109	Total	C	N	O	S	0	0
			884	569	154	157	4		
1	M	109	Total	C	N	O	S	0	0
			884	569	154	157	4		
1	Y	109	Total	C	N	O	S	0	0
			884	569	154	157	4		
1	e	109	Total	C	N	O	S	0	0
			884	569	154	157	4		
1	m	109	Total	C	N	O	S	0	0
			884	569	154	157	4		

- Molecule 2 is a protein called Tip attachment protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	594	Total	C	N	O	S	0	0
			4627	2884	815	909	19		
2	J	598	Total	C	N	O	S	0	0
			4657	2903	819	916	19		
2	Z	597	Total	C	N	O	S	0	0
			4650	2899	818	914	19		

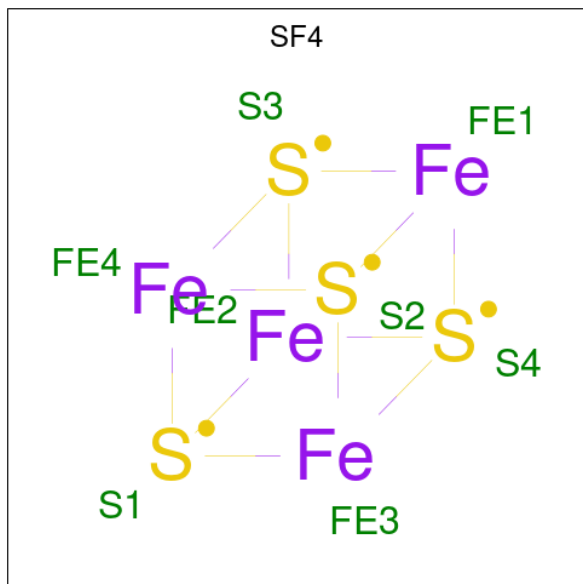
- Molecule 3 is a protein called Tail tip assembly protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	56	Total	C	N	O	S	0	0
			412	251	71	88	2		
3	P	59	Total	C	N	O	S	0	0
			436	266	75	93	2		
3	h	58	Total	C	N	O	S	0	0
			428	260	74	92	2		

- Molecule 4 is a protein called Tail tip protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	232	Total	C	N	O	S	0	0
			1801	1117	309	362	13		
4	N	232	Total	C	N	O	S	0	0
			1801	1117	309	362	13		
4	f	232	Total	C	N	O	S	0	0
			1801	1117	309	362	13		

- Molecule 5 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

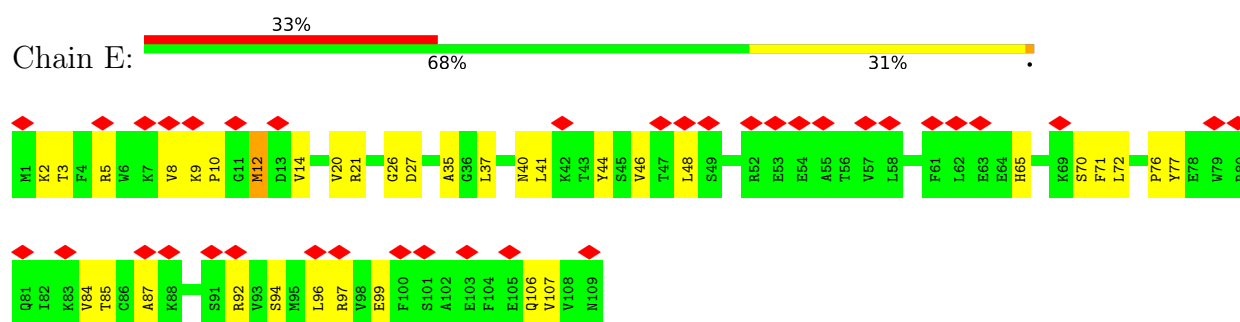


Mol	Chain	Residues	Atoms			AltConf
5	L	1	Total	Fe	S	0
			8	4	4	
5	N	1	Total	Fe	S	0
			8	4	4	
5	f	1	Total	Fe	S	0
			8	4	4	

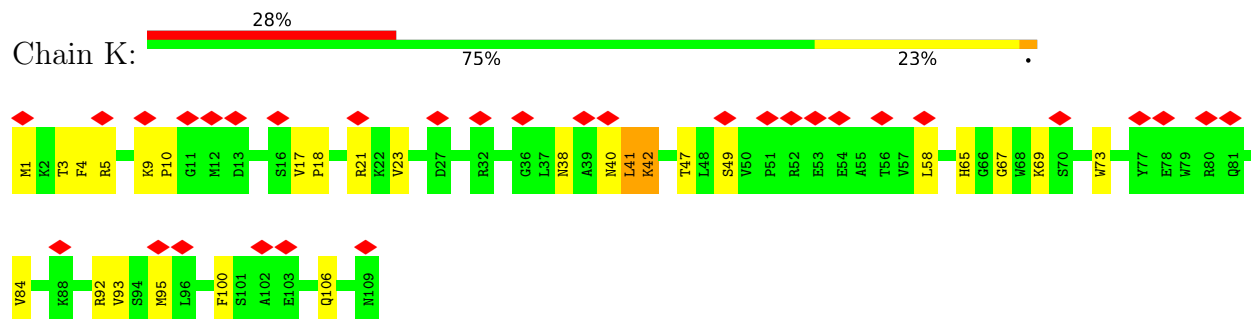
3 Residue-property plots [i](#)

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

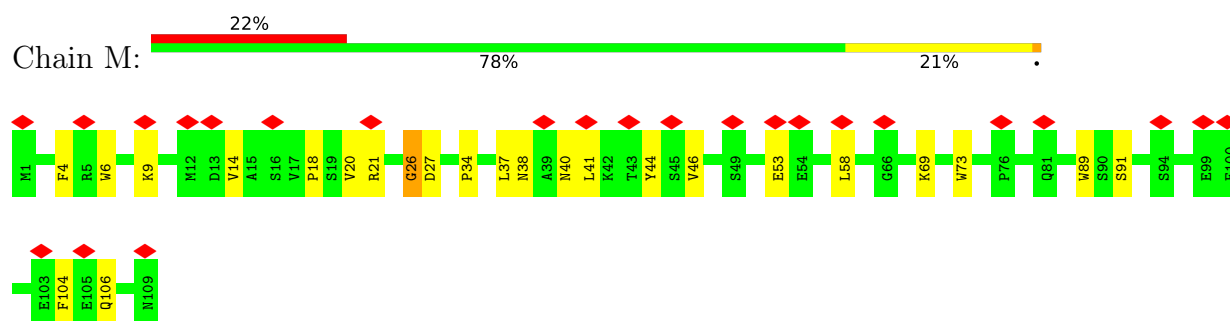
- Molecule 1: Tail tip protein M



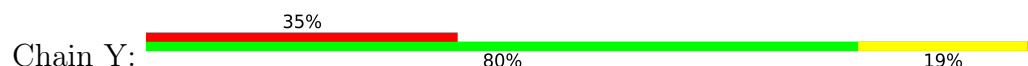
- Molecule 1: Tail tip protein M

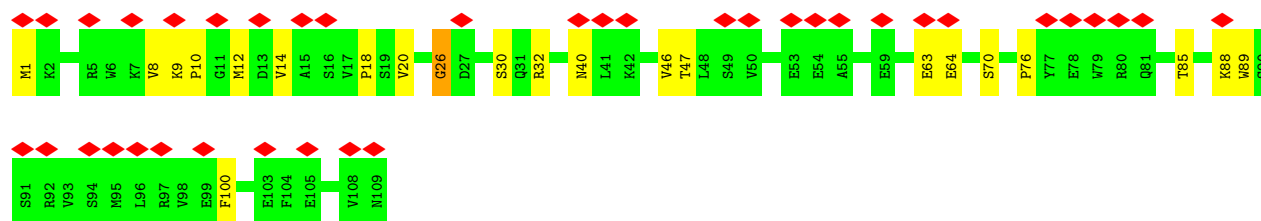


- Molecule 1: Tail tip protein M

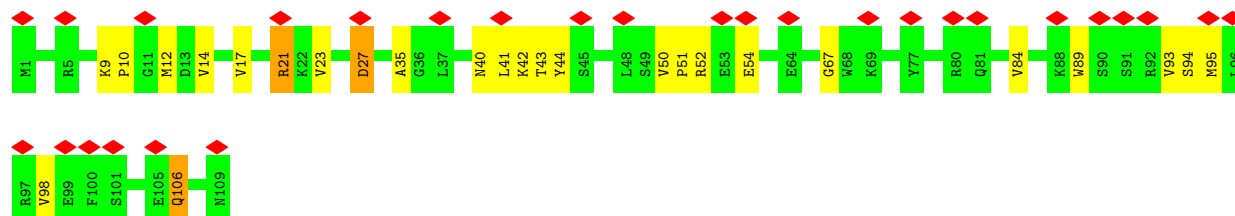
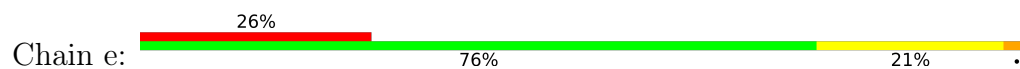


- Molecule 1: Tail tip protein M

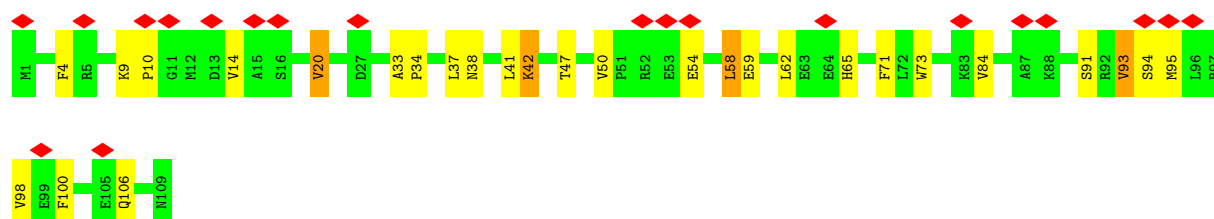
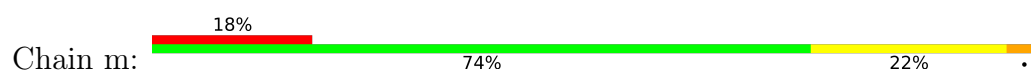




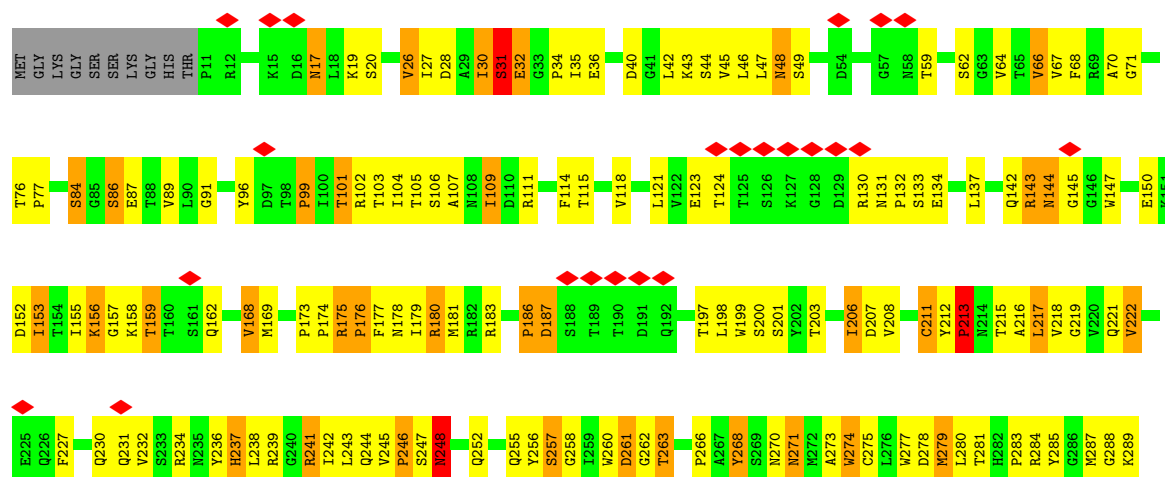
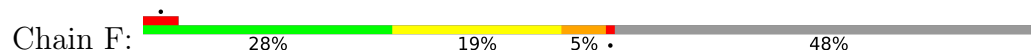
• Molecule 1: Tail tip protein M

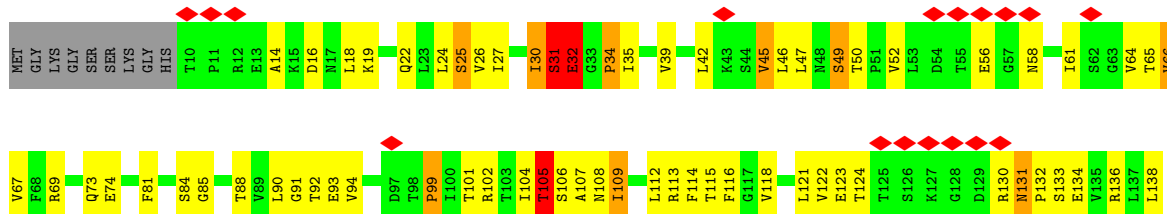
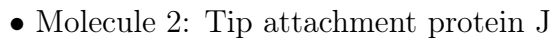


• Molecule 1: Tail tip protein M



• Molecule 2: Tip attachment protein J

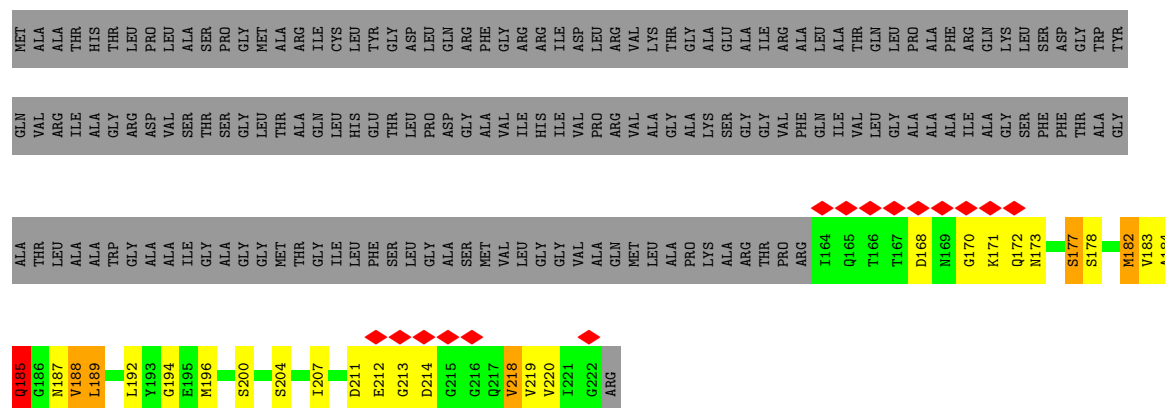




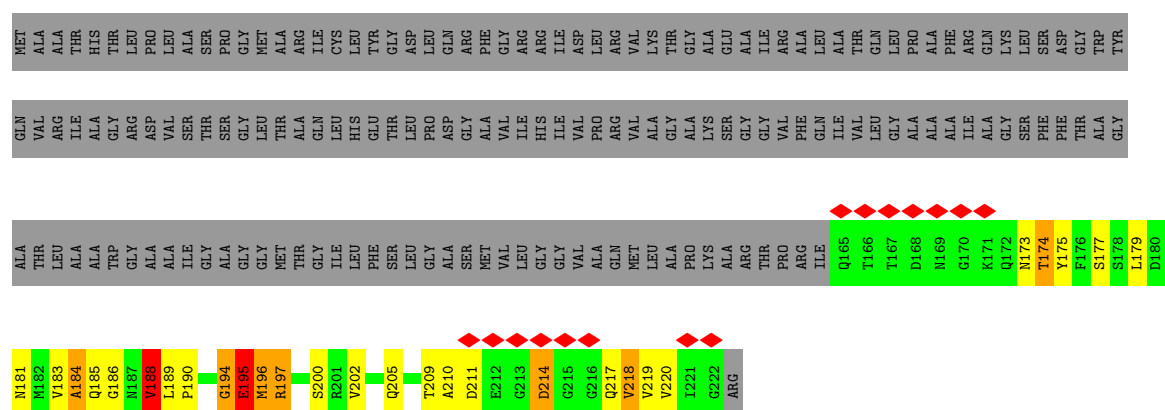




- Molecule 3: Tail tip assembly protein I

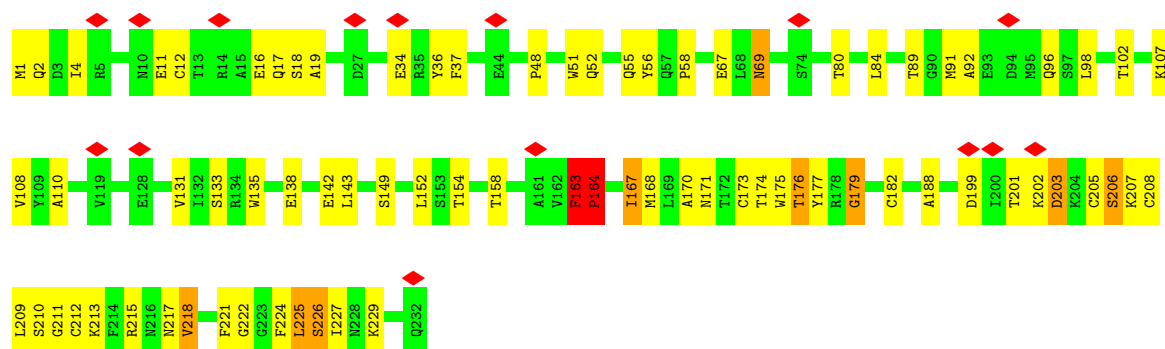


- Molecule 3: Tail tip assembly protein I

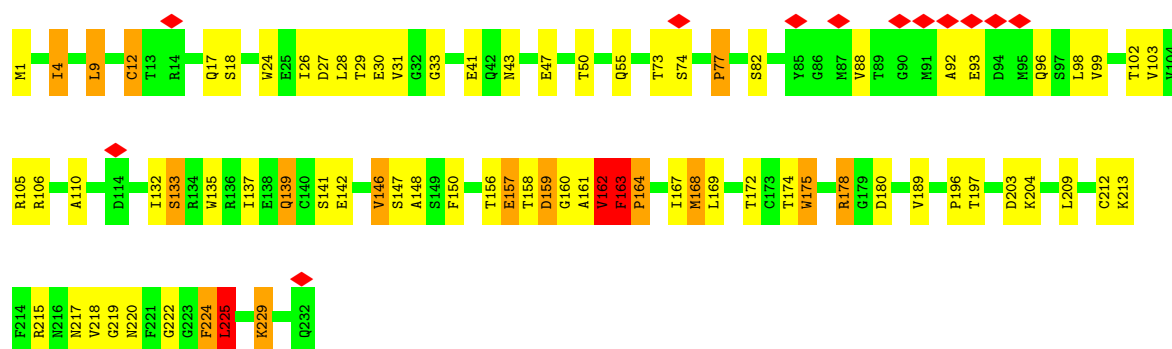


- Molecule 4: Tail tip protein L

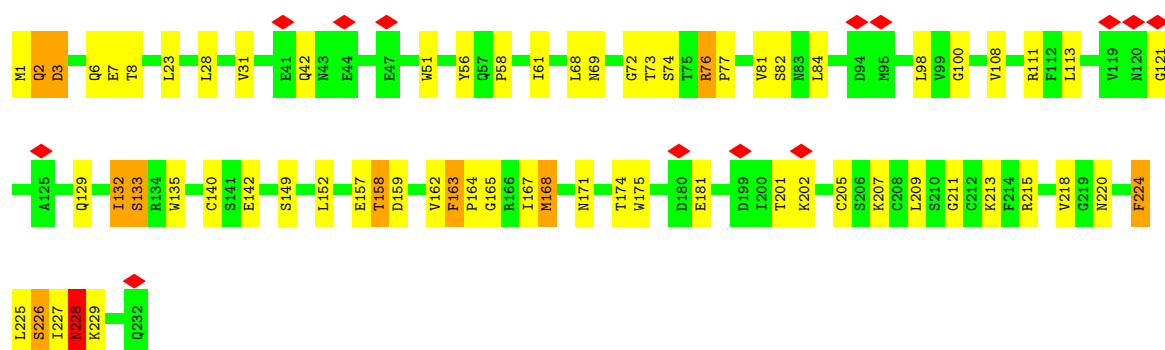




• Molecule 4: Tail tip protein L



• Molecule 4: Tail tip protein L



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	358235	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	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	3.933	Depositor
Minimum map value	-1.412	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.4	Depositor
Map size ($\text{\AA}$)	343.74402, 343.74402, 343.74402	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4

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	E	1.11	0/909	1.34	0/1231
1	K	1.11	0/909	1.35	0/1231
1	M	1.08	0/909	1.35	0/1231
1	Y	1.12	0/909	1.30	0/1231
1	e	1.10	0/909	1.32	0/1231
1	m	1.08	0/909	1.34	2/1231 (0.2%)
2	F	1.15	8/4722 (0.2%)	1.58	39/6430 (0.6%)
2	J	1.13	3/4753 (0.1%)	1.52	25/6473 (0.4%)
2	Z	1.08	0/4746	1.43	12/6462 (0.2%)
3	I	1.20	1/415 (0.2%)	1.64	6/561 (1.1%)
3	P	1.22	0/439	1.51	2/594 (0.3%)
3	h	1.15	0/431	1.37	0/583
4	L	1.10	2/1836 (0.1%)	1.48	4/2487 (0.2%)
4	N	1.10	1/1836 (0.1%)	1.48	10/2487 (0.4%)
4	f	1.06	0/1836	1.39	5/2487 (0.2%)
All	All	1.11	15/26468 (0.1%)	1.46	105/35950 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	5
2	J	0	3
2	Z	0	2
3	I	0	2
3	P	0	1
4	L	0	1
4	f	0	3
All	All	0	17

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	475	PRO	C-O	-6.51	1.15	1.23
2	F	293	ALA	C-O	6.32	1.31	1.23
2	F	357	LEU	C-O	-6.27	1.16	1.24
2	J	205	ILE	C-O	-6.11	1.17	1.24
4	N	77	PRO	C-O	-6.04	1.16	1.24
2	F	445	HIS	CE1-NE2	6.01	1.38	1.32
2	F	31	SER	CA-CB	-6.00	1.43	1.53
2	J	266	PRO	C-O	-5.41	1.17	1.23
2	F	321	PRO	C-O	-5.32	1.17	1.23
2	F	266	PRO	C-O	-5.31	1.17	1.23
4	L	173	CYS	C-O	-5.27	1.17	1.23
3	I	195	GLU	C-O	-5.20	1.17	1.24
2	F	352	TRP	C-O	-5.20	1.17	1.23
2	J	25	SER	C-O	5.11	1.29	1.23
4	L	212	CYS	C-O	5.05	1.29	1.24

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	177	PHE	CB-CA-C	-11.66	87.21	110.42
2	F	268	TYR	CA-C-O	-9.27	110.12	120.69
4	N	175	TRP	CA-C-O	-8.54	112.22	121.44
2	F	241	ARG	CA-C-O	-8.46	112.57	121.87
2	J	235	ASN	CB-CA-C	-8.40	99.11	110.79
4	N	163	PHE	CA-CB-CG	-8.37	105.43	113.80
2	F	348	CYS	CB-CA-C	-7.43	95.63	110.42
2	F	241	ARG	O-C-N	7.41	131.42	122.75
4	L	176	THR	CA-CB-OG1	-7.26	98.71	109.60
4	N	163	PHE	N-CA-CB	7.08	122.97	110.37
3	P	192	LEU	CA-C-O	-6.87	112.89	120.38
2	F	244	GLN	CB-CG-CD	-6.79	101.06	112.60
2	Z	227	PHE	CA-C-N	6.54	127.91	121.57
2	Z	227	PHE	C-N-CA	6.54	127.91	121.57
4	f	175	TRP	CA-C-O	-6.54	114.62	121.55
2	F	213	PRO	N-CA-C	6.38	125.60	112.47
2	J	105	THR	CB-CA-C	-6.33	97.82	110.42
2	J	27	ILE	CA-C-O	-6.32	114.59	120.22
2	Z	574	VAL	N-CA-C	-6.30	106.64	111.62
2	J	274	TRP	CA-CB-CG	-6.29	101.66	113.60
3	I	197	ARG	CA-C-O	-6.26	113.37	120.32
4	f	121	GLY	CA-C-O	-6.19	118.19	122.22
2	Z	32	GLU	CA-C-O	-6.18	114.84	121.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	174	THR	CA-C-O	-6.13	114.39	120.82
2	F	589	VAL	CA-C-O	-6.11	115.86	121.72
4	N	164	PRO	CB-CA-C	6.11	121.64	111.56
3	I	193	TYR	CA-C-O	-6.10	114.06	120.58
2	Z	274	TRP	CA-CB-CG	-6.04	102.13	113.60
2	F	35	ILE	CA-C-O	-6.01	114.89	121.92
2	J	399	VAL	CA-C-O	-6.00	114.92	121.28
2	F	463	ASP	CA-C-O	-5.98	113.90	120.36
4	f	77	PRO	CB-CA-C	-5.96	103.43	111.12
2	F	460	GLN	CB-CG-CD	-5.95	102.49	112.60
2	F	301	LEU	N-CA-C	-5.93	104.72	111.07
2	F	237	HIS	CA-C-O	-5.88	115.29	122.41
4	L	188	ALA	CA-C-O	-5.88	115.08	121.44
2	F	246	PRO	CA-C-O	-5.81	114.41	121.03
4	L	208	CYS	CB-CA-C	-5.80	97.78	109.68
2	F	302	TYR	CA-C-O	-5.78	114.75	120.82
3	I	195	GLU	CA-C-O	-5.77	112.26	120.51
2	J	292	GLY	CA-C-O	-5.74	118.27	122.23
2	F	256	TYR	CA-C-O	-5.72	114.19	120.43
2	F	168	VAL	CA-C-O	-5.72	115.67	121.67
2	F	302	TYR	O-C-N	5.71	127.95	122.07
2	F	295	ASP	N-CA-C	-5.68	105.93	112.92
2	F	84	SER	CA-C-N	5.67	128.30	121.38
2	F	84	SER	C-N-CA	5.67	128.30	121.38
2	J	69	ARG	CA-C-O	-5.67	114.02	120.32
2	F	360	VAL	CA-C-O	-5.67	114.51	120.57
2	J	30	ILE	N-CA-CB	-5.63	105.92	112.34
2	F	270	ASN	CA-CB-CG	-5.62	106.98	112.60
2	Z	68	PHE	CA-CB-CG	-5.61	108.19	113.80
2	J	339	LEU	N-CA-C	-5.60	105.27	111.71
2	J	34	PRO	CA-C-O	-5.54	114.43	120.92
2	F	590	GLN	CA-C-O	-5.50	115.82	121.87
4	L	96	GLN	N-CA-C	-5.49	106.63	113.55
2	J	173	PRO	N-CA-C	5.48	117.39	110.70
2	J	157	GLY	CA-C-O	-5.44	117.88	122.29
2	F	26	VAL	CA-C-O	-5.43	115.85	121.93
2	Z	69	ARG	CA-C-O	-5.40	114.73	120.40
2	F	477	ASP	CA-C-O	-5.38	115.63	121.44
2	F	274	TRP	CA-CB-CG	-5.36	103.41	113.60
2	F	176	PRO	N-CA-C	-5.35	104.56	112.26
2	F	390	SER	CA-C-O	-5.34	114.66	120.81
2	F	271	ASN	CA-CB-CG	-5.34	107.26	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	204	GLU	CA-C-O	-5.33	114.61	120.69
4	N	172	THR	CA-CB-OG1	-5.33	101.60	109.60
2	J	159	THR	CA-C-N	5.30	128.12	120.38
2	J	159	THR	C-N-CA	5.30	128.12	120.38
4	N	224	PHE	CA-C-O	-5.30	115.85	121.78
3	I	189	LEU	CA-C-O	-5.27	115.86	119.29
2	J	214	ASN	CA-CB-CG	-5.27	107.33	112.60
2	Z	439	THR	CA-CB-OG1	-5.26	101.71	109.60
3	I	203	VAL	N-CA-C	-5.26	107.64	111.90
4	f	100	GLY	CA-C-N	5.25	124.96	119.92
4	f	100	GLY	C-N-CA	5.25	124.96	119.92
2	J	287	MET	N-CA-C	-5.20	107.10	112.93
2	J	168	VAL	CA-C-O	-5.20	117.57	121.68
4	N	162	VAL	CA-C-O	-5.20	114.29	120.78
2	F	203	THR	CA-C-O	-5.19	115.24	121.11
2	F	333	ARG	CA-C-O	-5.19	115.56	121.68
2	F	569	ARG	CB-CA-C	-5.18	105.18	111.82
1	m	38	ASN	CA-C-N	5.18	127.48	120.38
1	m	38	ASN	C-N-CA	5.18	127.48	120.38
2	F	588	ALA	CA-C-O	-5.17	115.27	121.11
2	F	275	CYS	CB-CA-C	-5.16	103.02	110.96
2	J	228	GLY	CA-C-N	5.15	128.84	120.60
2	J	228	GLY	C-N-CA	5.15	128.84	120.60
2	F	351	VAL	CA-C-O	-5.14	116.17	121.93
2	Z	359	PHE	CA-CB-CG	-5.14	108.66	113.80
3	I	189	LEU	O-C-N	5.13	125.39	121.23
2	F	48	ASN	CA-CB-CG	-5.12	107.48	112.60
2	J	429	ASN	CB-CA-C	-5.12	100.88	109.48
2	F	571	PHE	CB-CA-C	-5.11	101.25	109.89
2	Z	429	ASN	CB-CA-C	-5.10	101.93	110.19
2	F	345	ALA	CA-C-O	-5.09	115.16	120.55
3	P	189	LEU	N-CA-CB	-5.07	101.35	110.37
2	J	49	SER	N-CA-C	-5.05	106.96	114.64
2	J	220	VAL	O-C-N	5.04	125.86	121.98
2	Z	420	THR	CB-CA-C	5.02	118.76	110.88
2	J	329	LEU	CA-C-O	-5.02	114.76	120.58
4	N	174	THR	CB-CA-C	5.02	118.76	110.88
2	Z	11	PRO	CA-N-CD	-5.02	104.97	112.00
4	N	139	GLN	CA-C-O	-5.01	115.13	120.75
2	F	408	ASN	N-CA-C	-5.01	104.14	111.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	174	PRO	Peptide
2	F	175	ARG	Peptide
2	F	176	PRO	Peptide
2	F	31	SER	Peptide
2	F	348	CYS	Peptide
3	I	176	PHE	Peptide
3	I	182	MET	Peptide
2	J	174	PRO	Peptide
2	J	175	ARG	Peptide
2	J	31	SER	Peptide
4	L	163	PHE	Peptide
3	P	182	MET	Peptide
2	Z	175	ARG	Peptide
2	Z	31	SER	Peptide
4	f	163	PHE	Peptide
4	f	224	PHE	Peptide
4	f	226	SER	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	E	884	0	881	18	0
1	K	884	0	881	18	0
1	M	884	0	881	15	0
1	Y	884	0	881	14	0
1	e	884	0	881	17	0
1	m	884	0	881	21	0
2	F	4627	0	4526	203	0
2	J	4657	0	4548	197	0
2	Z	4650	0	4542	169	0
3	I	412	0	396	30	0
3	P	436	0	422	21	0
3	h	428	0	411	39	0
4	L	1801	0	1716	58	0
4	N	1801	0	1715	61	0
4	f	1801	0	1715	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	8	0	0	0	0
5	N	8	0	0	0	0
5	f	8	0	0	0	0
All	All	25941	0	25277	807	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 16.

All (807) 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)
2:F:31:SER:OG	2:F:32:GLU:N	1.90	0.98
2:J:35:ILE:HB	2:J:240:GLY:O	1.68	0.94
2:J:433:MET:HE3	2:J:451:LEU:HD22	1.49	0.93
2:J:105:THR:O	2:J:105:THR:OG1	1.78	0.92
2:J:34:PRO:HD2	2:J:241:ARG:HH12	1.42	0.84
2:Z:396:HIS:CE1	2:Z:431:THR:HG21	2.13	0.83
3:I:173:ASN:OD1	3:I:174:THR:N	2.12	0.82
2:F:245:VAL:HG22	2:F:246:PRO:HD2	1.61	0.82
2:J:469:GLU:HA	4:L:12:CYS:SG	2.19	0.82
4:N:163:PHE:HB3	4:N:164:PRO:HD3	1.59	0.82
2:Z:224:SER:OG	3:h:174:THR:O	1.99	0.80
2:Z:304:ILE:CG2	2:Z:346:MET:HE2	2.13	0.79
2:Z:269:SER:O	2:Z:270:ASN:HB3	1.81	0.78
2:Z:279:MET:HE2	2:Z:338:VAL:HG12	1.64	0.78
2:F:173:PRO:HD2	2:F:177:PHE:CE1	2.18	0.78
2:F:42:LEU:HD11	2:F:66:VAL:CG1	2.14	0.77
2:J:272:MET:HE3	2:J:325:CYS:HA	1.66	0.77
2:Z:153:ILE:HG22	3:h:220:VAL:HG12	1.67	0.76
2:F:142:GLN:HB2	2:F:178:ASN:HB3	1.68	0.75
4:f:168:MET:HE3	3:h:183:VAL:HG21	1.68	0.75
2:F:19:LYS:NZ	3:P:171:LYS:O	2.15	0.74
4:N:24:TRP:CH2	4:N:105:ARG:HD3	2.23	0.74
1:E:9:LYS:O	1:m:95:MET:HE3	1.88	0.73
2:F:398:ALA:O	2:F:430:VAL:HA	1.87	0.73
2:F:247:SER:O	2:F:248:ASN:HB3	1.87	0.72
2:F:173:PRO:HD2	2:F:177:PHE:CZ	2.24	0.72
3:I:218:VAL:HG22	2:J:155:ILE:HD12	1.71	0.72
2:Z:173:PRO:HD2	2:Z:177:PHE:CZ	2.24	0.72
3:I:180:ASP:OD2	3:I:180:ASP:C	2.32	0.72
4:L:206:SER:OG	4:L:211:GLY:HA3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:31:SER:HA	3:h:190:PRO:O	1.90	0.72
2:F:239:ARG:HD3	2:F:268:TYR:OH	1.89	0.71
4:L:203:ASP:O	4:L:203:ASP:OD2	2.08	0.71
2:J:134:GLU:HA	2:J:155:ILE:O	1.91	0.71
2:F:30:ILE:HG12	2:F:216:ALA:O	1.91	0.70
2:J:159:THR:HG21	2:J:163:TYR:HB2	1.73	0.70
2:J:433:MET:HE3	2:J:451:LEU:CD2	2.22	0.70
2:Z:18:LEU:HB2	2:Z:159:THR:HG22	1.73	0.69
2:F:230:GLN:O	2:F:232:VAL:N	2.24	0.69
4:N:217:ASN:O	4:N:217:ASN:ND2	2.25	0.69
2:F:104:ILE:CG1	2:F:177:PHE:HD2	2.06	0.69
4:N:163:PHE:O	4:N:164:PRO:C	2.33	0.69
3:I:217:GLN:O	2:J:155:ILE:HA	1.93	0.69
2:Z:32:GLU:O	2:Z:33:GLY:O	2.10	0.69
2:F:137:LEU:HB2	2:F:153:ILE:HD11	1.75	0.68
2:J:99:PRO:HB3	2:J:180:ARG:HD3	1.75	0.68
2:J:172:LEU:HB3	2:J:177:PHE:HZ	1.57	0.68
2:Z:31:SER:O	3:h:189:LEU:HD11	1.93	0.68
2:F:36:GLU:OE1	2:F:239:ARG:NH1	2.25	0.68
2:F:479:ILE:HD12	2:F:481:ILE:HD11	1.76	0.68
3:I:177:SER:OG	3:I:178:SER:N	2.23	0.68
2:F:247:SER:O	2:F:248:ASN:CB	2.41	0.67
2:F:354:GLY:O	4:N:133:SER:HA	1.94	0.67
1:m:41:LEU:O	1:m:106:GLN:HG2	1.94	0.67
2:Z:421:GLN:N	2:Z:421:GLN:OE1	2.27	0.67
2:J:30:ILE:O	2:J:31:SER:C	2.37	0.67
4:N:178:ARG:NH1	4:N:203:ASP:OD2	2.27	0.67
2:F:464:PHE:O	2:F:464:PHE:CD2	2.48	0.67
2:J:30:ILE:HG22	2:J:31:SER:N	2.10	0.67
2:Z:396:HIS:ND1	2:Z:431:THR:HG21	2.10	0.67
4:f:167:ILE:HG23	3:h:186:GLY:HA2	1.75	0.67
2:J:260:TRP:O	2:J:261:ASP:HB3	1.93	0.66
2:F:109:ILE:HG22	2:F:175:ARG:HH11	1.60	0.66
2:F:111:ARG:NH1	2:F:207:ASP:OD1	2.28	0.66
2:Z:218:VAL:HG11	2:Z:236:TYR:CE1	2.30	0.65
2:F:104:ILE:HG13	2:F:177:PHE:HD2	1.58	0.65
2:J:247:SER:O	2:J:248:ASN:ND2	2.29	0.65
2:J:218:VAL:HG12	2:J:219:GLY:N	2.12	0.65
2:F:17:ASN:N	2:F:17:ASN:OD1	2.29	0.65
2:F:260:TRP:O	2:F:261:ASP:OD1	2.13	0.65
3:I:186:GLY:HA2	4:L:167:ILE:HG22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:28:ASP:OD2	3:h:200:SER:CB	2.45	0.65
2:Z:308:CYS:HB2	2:Z:323:ILE:HB	1.77	0.65
4:L:203:ASP:OD2	4:L:203:ASP:C	2.39	0.64
2:J:35:ILE:HA	2:J:241:ARG:HA	1.78	0.64
4:L:224:PHE:O	4:L:225:LEU:C	2.41	0.64
4:f:132:ILE:N	4:f:132:ILE:HD12	2.13	0.64
2:J:30:ILE:HD13	2:J:238:LEU:HD11	1.78	0.64
2:F:147:TRP:CZ3	2:F:180:ARG:HB2	2.31	0.64
2:Z:304:ILE:HG22	2:Z:346:MET:HE2	1.78	0.64
2:J:409:GLY:O	2:J:411:GLU:N	2.31	0.63
3:I:180:ASP:OD2	3:I:180:ASP:O	2.17	0.63
1:Y:12:MET:HE1	1:Y:76:PRO:HD2	1.81	0.63
2:Z:332:GLN:NE2	4:f:162:VAL:HG21	2.12	0.63
1:e:23:VAL:HG11	4:f:82:SER:HB2	1.80	0.63
4:L:224:PHE:O	4:L:225:LEU:O	2.15	0.63
2:Z:184:MET:HE3	2:Z:184:MET:HA	1.79	0.63
2:F:212:TYR:HD2	2:F:217:LEU:HD22	1.63	0.63
3:I:175:TYR:O	3:I:177:SER:N	2.32	0.63
2:Z:66:VAL:HG12	2:Z:220:VAL:HG22	1.81	0.63
2:Z:269:SER:O	2:Z:270:ASN:CB	2.47	0.63
2:J:162:GLN:HE21	2:J:164:LEU:HD21	1.63	0.62
2:J:433:MET:HE1	2:J:451:LEU:HB2	1.79	0.62
2:J:399:VAL:HG23	2:J:452:ILE:HD11	1.81	0.62
2:Z:304:ILE:HG21	2:Z:346:MET:HE2	1.81	0.62
2:F:121:LEU:HG	2:F:133:SER:HB2	1.79	0.62
2:F:592:VAL:HG22	2:F:592:VAL:O	2.00	0.62
3:I:180:ASP:OD2	3:I:202:VAL:HG21	1.99	0.62
4:f:227:ILE:O	4:f:228:ASN:HB2	1.98	0.62
2:F:20:SER:HA	3:P:211:ASP:HA	1.81	0.62
2:Z:464:PHE:O	2:Z:464:PHE:CD2	2.53	0.62
2:F:103:THR:HA	2:F:178:ASN:HA	1.82	0.61
2:J:121:LEU:HD23	2:J:157:GLY:O	1.99	0.61
2:F:261:ASP:CG	2:F:261:ASP:O	2.41	0.61
2:F:539:THR:HB	2:F:543:LYS:HB2	1.81	0.61
2:Z:521:ILE:HD11	2:Z:559:TRP:HE3	1.66	0.61
4:f:205:CYS:HA	4:f:215:ARG:NH2	2.14	0.61
1:e:89:TRP:O	1:e:89:TRP:CD1	2.54	0.61
4:N:27:ASP:HB3	4:N:102:THR:HG22	1.83	0.61
2:F:347:ARG:HG2	2:F:450:TRP:CE2	2.35	0.60
2:F:143:ARG:HG3	2:F:143:ARG:HH11	1.65	0.60
2:F:352:TRP:NE1	2:F:354:GLY:HA2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:183:ARG:HH21	2:J:187:ASP:HA	1.65	0.60
1:e:9:LYS:HE2	1:e:10:PRO:HD2	1.84	0.60
2:J:116:PHE:HB3	2:J:181:MET:HE2	1.83	0.60
1:E:77:TYR:OH	1:m:59:GLU:HG3	2.02	0.60
2:F:42:LEU:HD11	2:F:66:VAL:HG13	1.84	0.59
1:e:14:VAL:HG22	1:e:44:TYR:HD1	1.66	0.59
2:F:101:THR:HG22	2:F:180:ARG:HG3	1.83	0.59
2:J:74:GLU:N	2:J:74:GLU:OE1	2.34	0.59
2:Z:297:ASP:HB2	2:Z:358:THR:HG22	1.84	0.59
2:F:64:VAL:HG22	2:F:222:VAL:HG12	1.85	0.59
2:F:419:ASP:C	2:F:419:ASP:OD1	2.45	0.59
2:J:104:ILE:CD1	2:J:109:ILE:HD13	2.32	0.59
2:Z:597:ALA:O	2:Z:601:ASN:HB2	2.02	0.59
2:F:144:ASN:OD1	2:F:145:GLY:N	2.36	0.59
2:F:222:VAL:HG21	2:F:232:VAL:HG21	1.83	0.59
2:F:260:TRP:CZ2	2:F:262:GLY:HA2	2.38	0.59
2:J:272:MET:HG2	2:J:346:MET:HE2	1.85	0.59
2:F:124:THR:HG22	2:F:130:ARG:HG2	1.83	0.59
2:F:347:ARG:HG2	2:F:450:TRP:CZ2	2.38	0.58
3:I:172:GLN:HA	3:I:172:GLN:HE21	1.68	0.58
2:Z:11:PRO:HG2	2:Z:129:ASP:CG	2.27	0.58
2:Z:173:PRO:HD2	2:Z:177:PHE:CE2	2.38	0.58
2:Z:253:THR:HG23	2:Z:255:GLN:HB2	1.85	0.58
3:I:175:TYR:CE2	2:J:164:LEU:HD23	2.38	0.58
2:J:104:ILE:HD12	2:J:109:ILE:HG21	1.85	0.58
2:F:257:SER:OG	2:F:258:GLY:N	2.34	0.58
2:J:314:ASP:OD1	2:J:320:GLU:HB2	2.03	0.58
2:Z:67:VAL:HG21	2:Z:78:PRO:HB3	1.86	0.58
1:E:92:ARG:HB3	1:E:99:GLU:HB2	1.84	0.58
3:h:195:GLU:O	3:h:196:MET:CB	2.50	0.58
2:F:32:GLU:OE1	3:P:189:LEU:HD23	2.03	0.58
4:N:106:ARG:HG2	4:N:132:ILE:HD13	1.85	0.58
2:Z:470:GLY:HA3	2:Z:584:TYR:CD1	2.39	0.58
2:F:212:TYR:CD2	2:F:217:LEU:HD22	2.38	0.58
3:I:174:THR:O	2:J:224:SER:OG	2.22	0.58
2:F:575:SER:OG	2:F:587:THR:HG22	2.04	0.57
2:J:433:MET:HG2	2:J:434:ASP:N	2.18	0.57
2:Z:28:ASP:OD2	3:h:200:SER:HB2	2.04	0.57
2:Z:133:SER:O	2:Z:134:GLU:HB3	2.04	0.57
2:J:124:THR:HG22	2:J:130:ARG:HG3	1.86	0.57
3:I:183:VAL:HG12	4:L:227:ILE:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:14:ALA:HB2	2:J:130:ARG:HB2	1.86	0.57
2:J:108:ASN:OD1	4:L:209:LEU:HD23	2.05	0.57
2:F:230:GLN:C	2:F:232:VAL:H	2.12	0.57
2:F:295:ASP:N	2:F:295:ASP:OD1	2.37	0.57
2:J:223:ASP:OD1	2:J:224:SER:N	2.38	0.57
2:Z:155:ILE:CG2	3:h:218:VAL:HG12	2.34	0.57
2:J:30:ILE:HG21	2:J:238:LEU:CD1	2.35	0.57
2:Z:108:ASN:HB3	2:Z:206:ILE:HD13	1.85	0.57
2:F:472:ARG:HB2	4:N:4:ILE:HD11	1.86	0.57
2:F:239:ARG:HD3	2:F:268:TYR:HH	1.70	0.57
1:E:65:HIS:CE1	1:E:71:PHE:HB3	2.40	0.56
2:F:42:LEU:CD1	2:F:66:VAL:CG1	2.82	0.56
2:F:245:VAL:CG2	2:F:246:PRO:HD2	2.33	0.56
2:J:277:TRP:HB2	2:J:301:LEU:HD13	1.87	0.56
2:F:378:MET:SD	2:F:384:PRO:HG3	2.46	0.56
2:J:231:GLN:CD	2:J:231:GLN:H	2.12	0.56
2:Z:229:SER:O	2:Z:230:GLN:O	2.22	0.56
2:J:114:PHE:CE2	2:J:179:ILE:HD12	2.40	0.56
2:F:248:ASN:OD1	2:F:248:ASN:C	2.47	0.56
2:J:290:ARG:H	2:J:290:ARG:HD2	1.71	0.56
2:Z:279:MET:HE2	2:Z:338:VAL:CG1	2.35	0.56
4:f:209:LEU:HD13	4:f:225:LEU:HD21	1.87	0.56
2:F:239:ARG:HD3	2:F:268:TYR:CZ	2.41	0.56
4:L:18:SER:HB2	4:L:110:ALA:HB3	1.88	0.56
4:L:163:PHE:CD2	4:L:164:PRO:HD3	2.40	0.56
2:Z:172:LEU:HB3	2:Z:177:PHE:CZ	2.40	0.56
2:F:123:GLU:O	2:F:131:ASN:N	2.37	0.56
2:F:372:ASN:OD1	2:F:373:ARG:N	2.39	0.56
3:I:204:SER:O	2:J:26:VAL:HA	2.06	0.56
2:J:118:VAL:HG22	2:J:163:TYR:HB3	1.88	0.56
2:Z:325:CYS:O	2:Z:437:GLY:O	2.23	0.56
2:F:67:VAL:HG22	2:F:68:PHE:H	1.71	0.55
2:F:325:CYS:O	2:F:326:ASN:HB2	2.06	0.55
2:F:351:VAL:HG22	2:F:358:THR:HG23	1.89	0.55
1:m:9:LYS:HB3	1:m:10:PRO:HD2	1.89	0.55
2:F:472:ARG:CB	4:N:4:ILE:HD11	2.36	0.55
2:J:286:GLY:C	2:J:287:MET:HE2	2.31	0.55
4:L:11:GLU:O	4:L:17:GLN:HG2	2.07	0.55
2:F:44:SER:HB2	2:F:237:HIS:HB3	1.87	0.55
1:K:9:LYS:HB3	1:K:10:PRO:HD2	1.89	0.55
2:J:540:ASP:OD1	2:J:541:GLY:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:45:VAL:HG13	2:F:236:TYR:HD1	1.73	0.54
4:f:211:GLY:O	4:f:215:ARG:NH1	2.40	0.54
2:F:247:SER:OG	2:F:263:THR:O	2.22	0.54
4:L:135:TRP:HB3	4:L:152:LEU:HB3	1.89	0.54
2:F:325:CYS:O	2:F:326:ASN:CB	2.55	0.54
2:J:136:ARG:NH1	2:J:184:MET:HE2	2.22	0.54
2:J:243:LEU:H	2:J:243:LEU:HD23	1.73	0.54
2:J:113:ARG:HB2	2:J:168:VAL:HG12	1.89	0.54
2:F:378:MET:HE3	2:F:382:GLY:HA2	1.90	0.54
2:Z:210:GLN:HG2	2:Z:212:TYR:CZ	2.42	0.54
2:J:123:GLU:O	2:J:130:ARG:HA	2.08	0.54
2:J:132:PRO:HB3	2:J:157:GLY:H	1.72	0.54
2:Z:123:GLU:HG3	2:Z:193:LEU:HD12	1.88	0.54
3:h:188:VAL:HG12	3:h:188:VAL:O	2.06	0.54
2:F:464:PHE:O	2:F:464:PHE:CG	2.61	0.54
2:J:433:MET:CE	2:J:451:LEU:HB2	2.38	0.53
3:h:183:VAL:HG13	3:h:202:VAL:O	2.08	0.53
2:F:181:MET:HE2	2:F:199:TRP:CD2	2.43	0.53
2:J:46:LEU:H	2:J:46:LEU:HD12	1.72	0.53
2:J:416:LEU:HD13	2:J:416:LEU:C	2.33	0.53
1:Y:9:LYS:HB2	1:Y:10:PRO:HD3	1.90	0.53
4:f:61:ILE:HG13	4:f:81:VAL:HG22	1.89	0.53
4:L:36:TYR:HE2	4:L:91:MET:SD	2.31	0.53
2:Z:268:TYR:HE1	3:h:194:GLY:HA2	1.73	0.53
4:f:227:ILE:O	4:f:228:ASN:CB	2.55	0.53
1:Y:26:GLY:HA2	2:Z:378:MET:HE2	1.90	0.53
4:L:80:THR:HG22	4:L:149:SER:HB3	1.90	0.53
4:L:143:LEU:C	4:L:143:LEU:HD23	2.34	0.53
4:N:133:SER:HB2	4:N:135:TRP:HE1	1.73	0.53
2:F:87:GLU:OE2	3:P:207:ILE:HD12	2.09	0.53
2:F:332:GLN:HA	4:N:164:PRO:HD2	1.91	0.53
1:K:41:LEU:O	1:K:42:LYS:O	2.27	0.53
2:F:283:PRO:HA	2:F:288:GLY:HA3	1.90	0.53
3:h:195:GLU:O	3:h:196:MET:HB3	2.08	0.53
2:F:104:ILE:HD12	2:F:105:THR:N	2.24	0.52
2:F:153:ILE:HA	3:P:219:VAL:O	2.09	0.52
2:J:242:ILE:HG23	2:J:267:ALA:C	2.34	0.52
2:F:248:ASN:ND2	2:F:260:TRP:HA	2.24	0.52
2:F:486:TYR:CE1	4:L:89:THR:HG23	2.43	0.52
2:J:206:ILE:HD13	4:L:225:LEU:HB3	1.91	0.52
2:Z:575:SER:OG	2:Z:577:ARG:NH1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:181:MET:CE	2:F:199:TRP:CG	2.93	0.52
4:L:19:ALA:HB2	1:M:34:PRO:HG2	1.91	0.52
1:M:20:VAL:HG11	1:e:67:GLY:HA3	1.91	0.52
4:N:28:LEU:HB2	4:N:33:GLY:HA3	1.91	0.52
1:m:93:VAL:HA	1:m:98:VAL:HG12	1.90	0.52
2:F:103:THR:HG22	2:F:178:ASN:CG	2.34	0.52
2:F:28:ASP:OD1	3:P:200:SER:HB2	2.10	0.52
3:I:191:VAL:O	2:J:329:LEU:HD12	2.10	0.52
2:J:310:GLN:OE1	2:J:322:ARG:NH2	2.42	0.52
4:N:30:GLU:OE1	4:N:31:VAL:HG13	2.09	0.52
4:N:168:MET:HE2	3:P:189:LEU:HA	1.91	0.52
4:N:209:LEU:HG	4:N:213:LYS:HD2	1.91	0.52
4:f:42:GLN:HG2	4:f:58:PRO:HB3	1.92	0.52
1:m:41:LEU:O	1:m:42:LYS:O	2.27	0.52
2:J:52:VAL:HG22	2:J:61:ILE:HD11	1.92	0.52
2:Z:208:VAL:HB	4:f:218:VAL:HG11	1.91	0.52
2:F:492:GLY:HA2	2:F:559:TRP:CH2	2.45	0.52
3:I:218:VAL:HG22	2:J:155:ILE:CD1	2.39	0.52
2:J:471:LEU:HD13	4:L:131:VAL:HG21	1.90	0.52
2:Z:22:GLN:OE1	3:h:209:THR:OG1	2.27	0.52
2:Z:250:ASN:OD1	2:Z:253:THR:HG22	2.10	0.52
2:Z:138:LEU:HD13	2:Z:184:MET:HG2	1.90	0.52
2:Z:396:HIS:CG	2:Z:431:THR:HG23	2.44	0.52
2:J:503:ARG:HB2	2:J:549:VAL:HG23	1.91	0.52
4:L:67:GLU:OE2	4:L:69:ASN:ND2	2.43	0.52
2:F:96:TYR:HB2	2:F:186:PRO:O	2.10	0.51
2:F:454:THR:HG22	2:F:595:LYS:NZ	2.25	0.51
2:F:104:ILE:HG13	2:F:177:PHE:CD2	2.42	0.51
2:F:152:ASP:N	2:F:152:ASP:OD1	2.43	0.51
2:J:268:TYR:C	2:J:268:TYR:CD2	2.88	0.51
4:N:217:ASN:C	4:N:217:ASN:HD22	2.18	0.51
2:Z:396:HIS:CG	2:Z:431:THR:CG2	2.92	0.51
1:M:53:GLU:OE1	1:M:53:GLU:N	2.42	0.51
2:Z:327:ALA:C	3:h:196:MET:CE	2.83	0.51
4:f:2:GLN:OE1	4:f:3:ASP:N	2.44	0.51
1:E:8:VAL:HG11	1:E:46:VAL:HG13	1.93	0.51
2:F:277:TRP:O	2:F:281:THR:OG1	2.27	0.51
2:J:247:SER:HA	2:J:265:LYS:HD3	1.92	0.51
1:Y:88:LYS:HG2	1:e:17:VAL:CG1	2.41	0.51
2:Z:14:ALA:O	2:Z:158:LYS:HD2	2.11	0.51
2:Z:105:THR:HA	2:Z:175:ARG:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:423:ILE:HD13	2:Z:428:ARG:HG3	1.92	0.51
2:Z:469:GLU:O	2:Z:472:ARG:HB3	2.10	0.51
2:J:172:LEU:HB3	2:J:177:PHE:CZ	2.43	0.51
1:K:23:VAL:HG11	4:N:82:SER:OG	2.11	0.51
4:N:224:PHE:O	4:N:225:LEU:C	2.53	0.51
2:Z:24:LEU:HB3	2:Z:222:VAL:HG22	1.93	0.51
2:Z:114:PHE:CE2	2:Z:199:TRP:CZ2	2.99	0.51
1:K:9:LYS:HE3	1:K:49:SER:HB2	1.93	0.51
2:Z:279:MET:HG2	4:f:163:PHE:CE1	2.45	0.51
2:Z:280:LEU:O	2:Z:287:MET:HB2	2.10	0.51
2:F:241:ARG:HD3	2:F:285:TYR:OH	2.11	0.51
2:J:465:SER:HA	2:J:585:ALA:HA	1.92	0.51
1:K:84:VAL:HA	1:K:106:GLN:HA	1.92	0.51
2:F:358:THR:OG1	2:F:359:PHE:N	2.44	0.51
2:F:581:ASP:HB2	2:F:583:THR:HG22	1.93	0.51
2:J:104:ILE:HD12	2:J:109:ILE:HD13	1.92	0.51
4:N:163:PHE:HB3	4:N:164:PRO:CD	2.38	0.51
2:Z:42:LEU:HD12	2:Z:52:VAL:HG21	1.92	0.51
2:J:260:TRP:O	2:J:261:ASP:CB	2.59	0.51
2:Z:503:ARG:HD2	2:Z:548:ARG:HA	1.92	0.51
2:J:399:VAL:O	2:J:416:LEU:HD22	2.11	0.50
2:Z:396:HIS:CE1	2:Z:431:THR:CG2	2.91	0.50
2:Z:507:LEU:HD12	2:Z:559:TRP:CD1	2.46	0.50
2:F:335:ALA:HB2	4:N:161:ALA:O	2.10	0.50
4:L:182:CYS:O	4:L:217:ASN:ND2	2.44	0.50
2:J:35:ILE:HG22	2:J:241:ARG:HG3	1.94	0.50
2:J:354:GLY:O	4:L:133:SER:HA	2.11	0.50
2:Z:155:ILE:HG22	3:h:218:VAL:HG13	1.93	0.50
2:J:320:GLU:HG3	2:J:321:PRO:HD2	1.93	0.50
1:e:52:ARG:NH1	1:e:95:MET:O	2.44	0.50
2:F:32:GLU:OE2	2:F:284:ARG:NH1	2.44	0.50
2:J:30:ILE:HG21	2:J:238:LEU:HD12	1.92	0.50
1:K:92:ARG:NH1	1:K:93:VAL:O	2.45	0.50
1:e:84:VAL:HA	1:e:106:GLN:HA	1.93	0.50
3:h:194:GLY:O	3:h:195:GLU:O	2.29	0.50
2:F:493:GLY:HA3	2:F:509:ARG:HH12	1.77	0.50
2:J:116:PHE:HE1	2:J:167:VAL:HG12	1.77	0.50
4:N:4:ILE:HD12	4:N:9:LEU:HG	1.93	0.50
1:E:2:LYS:O	1:E:72:LEU:N	2.43	0.50
1:E:70:SER:HB3	1:E:85:THR:HG23	1.94	0.50
2:F:332:GLN:CG	4:N:162:VAL:HB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:67:GLY:HA3	1:Y:20:VAL:HG11	1.93	0.50
2:J:138:LEU:HB2	2:J:182:ARG:HB3	1.94	0.50
2:Z:179:ILE:HD12	2:Z:179:ILE:O	2.12	0.50
2:Z:410:TRP:CZ3	3:h:196:MET:HA	2.46	0.50
2:Z:536:GLN:HE22	2:Z:547:SER:HA	1.77	0.50
4:f:168:MET:CE	3:h:183:VAL:HG21	2.41	0.50
4:f:229:LYS:O	3:h:185:GLN:NE2	2.45	0.50
4:N:163:PHE:CB	4:N:164:PRO:HD3	2.38	0.50
2:F:106:SER:OG	2:F:107:ALA:N	2.45	0.49
2:F:227:PHE:CE1	2:F:232:VAL:HG22	2.46	0.49
2:J:45:VAL:O	2:J:45:VAL:HG12	2.12	0.49
4:N:158:THR:C	4:N:160:GLY:H	2.20	0.49
2:Z:19:LYS:O	3:h:211:ASP:OD2	2.30	0.49
2:F:27:ILE:HA	2:F:219:GLY:HA2	1.94	0.49
2:F:396:HIS:HA	2:F:429:ASN:HB3	1.94	0.49
2:J:249:TYR:HE1	2:J:309:ASP:OD2	1.95	0.49
2:Z:293:ALA:O	2:Z:294:ALA:HB3	2.12	0.49
2:Z:474:VAL:O	2:Z:475:PRO:C	2.55	0.49
4:f:69:ASN:HB3	4:f:72:GLY:O	2.12	0.49
2:J:109:ILE:HG23	2:J:175:ARG:HD3	1.94	0.49
1:M:89:TRP:O	1:M:89:TRP:CD1	2.66	0.49
3:h:189:LEU:HD12	3:h:190:PRO:HD2	1.93	0.49
2:J:30:ILE:CG2	2:J:31:SER:N	2.75	0.49
2:J:279:MET:HG3	4:L:163:PHE:CE2	2.47	0.49
1:Y:63:GLU:HB2	1:e:40:ASN:ND2	2.28	0.49
2:Z:212:TYR:N	2:Z:212:TYR:CD1	2.80	0.49
2:Z:239:ARG:HD2	3:h:195:GLU:OE1	2.11	0.49
2:F:279:MET:HG2	4:N:163:PHE:CE1	2.47	0.49
2:F:353:ASN:O	2:F:355:GLN:N	2.46	0.49
2:J:147:TRP:CZ3	2:J:180:ARG:HB2	2.47	0.49
2:F:396:HIS:HA	2:F:429:ASN:CB	2.42	0.49
2:J:106:SER:OG	2:J:107:ALA:N	2.43	0.49
4:L:210:SER:OG	4:L:211:GLY:N	2.44	0.49
4:N:88:VAL:HG11	4:N:148:ALA:CB	2.42	0.49
2:F:479:ILE:CD1	2:F:481:ILE:HD11	2.40	0.49
1:M:91:SER:HB3	1:m:14:VAL:HB	1.95	0.49
3:P:187:ASN:O	3:P:188:VAL:HG12	2.13	0.49
2:Z:101:THR:HA	2:Z:179:ILE:O	2.12	0.49
2:Z:367:LYS:NZ	4:f:1:MET:HE2	2.27	0.49
1:m:41:LEU:O	1:m:106:GLN:CG	2.60	0.49
2:F:87:GLU:O	2:F:87:GLU:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:92:ALA:O	4:N:93:GLU:HG2	2.13	0.49
2:Z:172:LEU:HB3	2:Z:177:PHE:CE2	2.47	0.49
2:Z:274:TRP:HA	2:Z:274:TRP:CE3	2.47	0.49
1:m:58:LEU:HD21	1:m:100:PHE:CE1	2.48	0.49
2:F:99:PRO:HB3	2:F:180:ARG:HD3	1.95	0.49
3:I:190:PRO:O	2:J:31:SER:HA	2.13	0.49
2:J:509:ARG:NH2	1:M:27:ASP:OD1	2.45	0.49
4:N:217:ASN:ND2	4:N:220:ASN:HB2	2.27	0.49
2:Z:11:PRO:HG2	2:Z:129:ASP:CB	2.42	0.49
2:Z:17:ASN:OD1	3:h:217:GLN:NE2	2.45	0.49
2:Z:134:GLU:HA	2:Z:155:ILE:O	2.13	0.49
2:Z:155:ILE:HG22	3:h:218:VAL:CG1	2.43	0.49
2:Z:209:LYS:O	2:Z:210:GLN:HB2	2.13	0.49
2:Z:210:GLN:NE2	4:f:225:LEU:HD12	2.27	0.49
2:Z:268:TYR:CE1	3:h:194:GLY:HA2	2.47	0.49
2:Z:339:LEU:HD12	2:Z:339:LEU:O	2.12	0.49
4:f:133:SER:HB2	4:f:135:TRP:HE1	1.76	0.49
2:F:294:ALA:HB3	2:F:295:ASP:OD1	2.12	0.49
4:f:158:THR:OG1	4:f:159:ASP:N	2.45	0.49
4:L:4:ILE:CG2	4:L:131:VAL:HG22	2.43	0.48
4:N:189:VAL:HG21	4:N:215:ARG:HG3	1.94	0.48
2:Z:31:SER:OG	2:Z:32:GLU:N	2.46	0.48
2:J:32:GLU:O	2:J:241:ARG:HD2	2.13	0.48
2:J:45:VAL:O	2:J:52:VAL:HG23	2.13	0.48
2:J:312:VAL:HG12	2:J:313:PRO:HD2	1.95	0.48
2:Z:139:VAL:HG22	2:Z:151:LYS:HB2	1.95	0.48
2:F:17:ASN:HA	3:P:214:ASP:OD1	2.13	0.48
2:J:109:ILE:HD11	2:J:112:LEU:HB2	1.94	0.48
1:m:84:VAL:HA	1:m:106:GLN:HA	1.95	0.48
2:F:399:VAL:HG23	2:F:452:ILE:HG13	1.94	0.48
2:J:461:THR:HG22	2:J:589:VAL:HG23	1.94	0.48
1:K:95:MET:HE2	1:K:95:MET:N	2.28	0.48
2:Z:172:LEU:HD23	2:Z:177:PHE:CZ	2.49	0.48
4:f:218:VAL:HG12	4:f:218:VAL:O	2.14	0.48
4:L:205:CYS:SG	4:L:207:LYS:HD3	2.54	0.48
2:Z:20:SER:HB2	3:h:210:ALA:O	2.14	0.48
2:Z:606:ASP:OD1	2:Z:606:ASP:N	2.47	0.48
2:F:181:MET:HE3	2:F:199:TRP:HB2	1.95	0.48
2:F:469:GLU:HA	4:N:12:CYS:SG	2.54	0.48
2:J:333:ARG:HE	2:J:338:VAL:HG12	1.79	0.48
4:L:225:LEU:O	4:L:226:SER:OG	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:183:VAL:O	3:P:184:ALA:HB3	2.14	0.48
2:Z:42:LEU:HB2	2:Z:53:LEU:HD11	1.96	0.48
2:F:181:MET:CE	2:F:199:TRP:HB2	2.44	0.48
2:F:603:ALA:O	2:F:604:HIS:O	2.32	0.48
2:J:482:CYS:HB2	2:J:560:GLU:OE1	2.14	0.48
4:N:96:GLN:HG3	2:Z:392:LEU:HD23	1.96	0.48
4:N:167:ILE:HA	3:P:188:VAL:HA	1.95	0.48
2:F:70:ALA:O	2:F:216:ALA:HA	2.14	0.48
3:I:188:VAL:HG21	2:J:332:GLN:HB2	1.96	0.48
1:M:4:PHE:HB3	1:M:73:TRP:CD1	2.48	0.48
2:Z:155:ILE:HA	3:h:217:GLN:O	2.14	0.47
2:F:465:SER:HA	2:F:585:ALA:HA	1.97	0.47
2:J:274:TRP:HA	2:J:274:TRP:CE3	2.49	0.47
1:K:3:THR:O	1:K:5:ARG:NH2	2.47	0.47
4:L:48:PRO:HB2	4:L:55:GLN:HG3	1.96	0.47
2:Z:30:ILE:O	2:Z:216:ALA:HB3	2.14	0.47
4:f:209:LEU:HD13	4:f:225:LEU:CD2	2.44	0.47
2:F:369:TRP:H	2:F:369:TRP:CD1	2.32	0.47
2:F:260:TRP:O	2:F:260:TRP:CD1	2.67	0.47
2:F:42:LEU:CD1	2:F:66:VAL:HG11	2.43	0.47
2:F:155:ILE:HG22	3:P:218:VAL:HG22	1.96	0.47
2:J:246:PRO:HD3	2:J:274:TRP:CE2	2.49	0.47
1:E:9:LYS:HG3	1:E:10:PRO:HD3	1.96	0.47
2:F:134:GLU:HG3	2:F:156:LYS:HG2	1.96	0.47
3:I:193:TYR:HB3	2:J:275:CYS:SG	2.54	0.47
2:J:93:GLU:HA	2:J:198:LEU:HA	1.96	0.47
2:J:115:THR:HG22	2:J:164:LEU:HD12	1.97	0.47
2:J:173:PRO:HD2	2:J:177:PHE:CZ	2.48	0.47
2:F:118:VAL:HG12	2:F:197:THR:HG22	1.96	0.47
2:J:31:SER:OG	2:J:32:GLU:N	2.48	0.47
2:J:56:GLU:HB2	2:J:58:ASN:OD1	2.14	0.47
2:J:85:GLY:HA2	2:J:205:ILE:HA	1.95	0.47
2:J:276:LEU:HD23	2:J:301:LEU:HD21	1.96	0.47
1:K:9:LYS:CE	1:K:49:SER:HB2	2.45	0.47
1:Y:18:PRO:HB3	1:Y:40:ASN:HB3	1.97	0.47
2:F:143:ARG:HG3	2:F:143:ARG:NH1	2.30	0.47
2:F:343:CYS:O	2:F:348:CYS:HB2	2.15	0.47
4:N:99:VAL:HG22	4:N:139:GLN:HA	1.97	0.47
2:Z:438:CYS:SG	2:Z:443:GLN:HB3	2.53	0.47
3:h:183:VAL:O	3:h:184:ALA:HB3	2.15	0.47
2:F:376:VAL:HG11	2:F:385:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:16:ASP:OD1	2:J:159:THR:HA	2.15	0.47
1:M:6:TRP:CD2	1:M:58:LEU:HD13	2.49	0.47
2:Z:25:SER:HB3	2:Z:81:PHE:CE2	2.50	0.47
4:f:171:ASN:CG	4:f:171:ASN:O	2.58	0.47
1:m:65:HIS:HD2	1:m:71:PHE:HD2	1.60	0.47
2:F:510:GLU:HA	2:F:541:GLY:O	2.15	0.47
2:J:222:VAL:HG11	2:J:232:VAL:HG11	1.97	0.47
2:J:241:ARG:HG2	2:J:241:ARG:HH11	1.80	0.47
2:J:280:LEU:O	2:J:287:MET:HB2	2.14	0.47
2:Z:155:ILE:CG2	3:h:218:VAL:CG1	2.93	0.47
4:f:157:GLU:O	4:f:158:THR:C	2.58	0.47
1:E:3:THR:O	1:E:5:ARG:NH2	2.48	0.46
2:F:211:CYS:HG	4:N:219:GLY:C	2.22	0.46
2:F:489:ILE:HD12	2:F:489:ILE:O	2.16	0.46
2:J:18:LEU:HB2	2:J:159:THR:OG1	2.15	0.46
2:Z:328:TYR:N	3:h:196:MET:HE3	2.29	0.46
2:F:34:PRO:HD2	2:F:241:ARG:NH2	2.30	0.46
4:N:169:LEU:HA	3:P:185:GLN:HG2	1.98	0.46
1:m:47:THR:HA	1:m:100:PHE:O	2.15	0.46
2:F:495:VAL:HG22	2:F:557:SER:H	1.79	0.46
2:J:163:TYR:C	2:J:164:LEU:HD22	2.41	0.46
2:J:462:VAL:HG11	2:J:481:ILE:CD1	2.46	0.46
4:L:209:LEU:HD11	4:L:218:VAL:HG13	1.97	0.46
2:Z:135:VAL:CG1	2:Z:195:ASN:HB3	2.45	0.46
2:Z:396:HIS:ND1	2:Z:455:GLU:OE1	2.49	0.46
2:Z:402:ASN:HB2	2:Z:434:ASP:OD1	2.16	0.46
1:e:14:VAL:HG22	1:e:44:TYR:CD1	2.49	0.46
2:F:268:TYR:CD2	2:F:268:TYR:C	2.91	0.46
2:F:271:ASN:ND2	2:F:274:TRP:HD1	2.14	0.46
3:I:186:GLY:HA2	4:L:167:ILE:CG2	2.44	0.46
3:I:189:LEU:HD11	2:J:215:THR:HG22	1.96	0.46
2:Z:279:MET:HG2	4:f:163:PHE:CZ	2.50	0.46
2:F:147:TRP:H	2:F:147:TRP:CD1	2.33	0.46
3:I:194:GLY:HA3	2:J:270:ASN:OD1	2.15	0.46
2:J:464:PHE:O	2:J:465:SER:C	2.58	0.46
2:Z:89:VAL:HG11	3:h:177:SER:O	2.15	0.46
2:F:389:PHE:N	2:F:389:PHE:CD1	2.84	0.46
2:J:140:GLN:HB3	2:J:147:TRP:HB3	1.97	0.46
2:J:151:LYS:HG3	2:J:167:VAL:HG21	1.97	0.46
3:P:172:GLN:N	3:P:172:GLN:CD	2.74	0.46
1:M:41:LEU:O	1:M:106:GLN:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:89:TRP:O	1:Y:89:TRP:CD1	2.68	0.46
2:Z:527:SER:HA	4:f:6:GLN:HG3	1.98	0.46
1:e:21:ARG:HD2	1:e:35:ALA:HA	1.97	0.46
2:J:18:LEU:HD11	2:J:156:LYS:O	2.15	0.46
1:K:58:LEU:HD23	1:K:100:PHE:CE2	2.50	0.46
2:Z:139:VAL:HG12	2:Z:181:MET:HE3	1.98	0.46
2:Z:521:ILE:HD11	2:Z:559:TRP:CE3	2.49	0.46
4:f:76:ARG:HB3	4:f:152:LEU:O	2.16	0.46
1:E:37:LEU:HD13	4:N:43:ASN:HA	1.98	0.46
2:F:278:ASP:OD2	2:F:285:TYR:OH	2.27	0.46
2:J:90:LEU:O	2:J:92:THR:N	2.48	0.46
2:J:470:GLY:HA3	2:J:584:TYR:CG	2.50	0.46
1:m:65:HIS:NE2	1:m:71:PHE:HB3	2.31	0.46
2:J:124:THR:CG2	2:J:130:ARG:HG3	2.45	0.46
2:J:239:ARG:HG2	2:J:268:TYR:CE1	2.51	0.46
2:F:147:TRP:CD1	2:F:180:ARG:NH2	2.84	0.45
2:F:273:ALA:HB1	2:F:301:LEU:HD22	1.97	0.45
2:Z:13:GLU:HA	2:Z:130:ARG:HG2	1.98	0.45
2:Z:400:GLU:HB3	2:Z:414:THR:CG2	2.46	0.45
4:f:205:CYS:SG	4:f:207:LYS:N	2.82	0.45
3:I:185:GLN:NE2	4:L:229:LYS:HA	2.31	0.45
4:L:211:GLY:O	4:L:215:ARG:NH1	2.50	0.45
4:L:224:PHE:C	4:L:225:LEU:O	2.59	0.45
2:F:260:TRP:NE1	2:F:262:GLY:O	2.49	0.45
2:F:513:LEU:HD13	2:F:514:PRO:HD2	1.99	0.45
2:J:66:VAL:HA	2:J:220:VAL:HA	1.98	0.45
2:J:131:ASN:OD1	2:J:131:ASN:N	2.50	0.45
2:J:279:MET:HG3	4:L:163:PHE:CZ	2.51	0.45
1:K:17:VAL:HG22	1:K:17:VAL:O	2.16	0.45
4:N:41:GLU:N	4:N:41:GLU:OE1	2.49	0.45
2:Z:137:LEU:HB2	2:Z:153:ILE:HD11	1.98	0.45
2:Z:320:GLU:OE2	2:Z:446:ARG:NH2	2.48	0.45
2:Z:577:ARG:O	2:Z:584:TYR:HA	2.16	0.45
1:E:27:ASP:OD1	2:F:373:ARG:NH1	2.49	0.45
2:F:260:TRP:CE2	2:F:262:GLY:HA2	2.50	0.45
2:F:594:GLU:HB3	2:F:598:ILE:HD11	1.98	0.45
4:N:50:THR:OG1	4:N:55:GLN:OE1	2.32	0.45
4:N:175:TRP:NE1	4:N:222:GLY:HA2	2.31	0.45
4:N:212:CYS:SG	4:N:218:VAL:HA	2.56	0.45
2:Z:409:GLY:O	2:Z:411:GLU:N	2.48	0.45
2:Z:464:PHE:O	2:Z:465:SER:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:586:ILE:HG22	2:F:587:THR:N	2.32	0.45
1:M:18:PRO:HB3	1:M:40:ASN:HB3	1.98	0.45
4:N:217:ASN:HD21	4:N:220:ASN:HB2	1.81	0.45
2:Z:119:GLN:OE1	2:Z:119:GLN:HA	2.16	0.45
1:e:94:SER:OG	1:e:95:MET:N	2.50	0.45
2:J:272:MET:HE3	2:J:325:CYS:SG	2.56	0.45
4:N:158:THR:O	4:N:160:GLY:N	2.42	0.45
2:J:351:VAL:CG2	2:J:358:THR:HG23	2.46	0.45
2:J:353:ASN:OD1	4:L:2:GLN:NE2	2.50	0.45
1:m:50:VAL:HG13	1:m:54:GLU:HB3	1.99	0.45
2:F:230:GLN:C	2:F:232:VAL:N	2.75	0.45
3:I:183:VAL:HG21	4:L:168:MET:HE1	1.98	0.45
3:I:218:VAL:HA	2:J:155:ILE:HD13	1.99	0.45
4:L:163:PHE:HD1	4:L:163:PHE:HA	1.69	0.45
4:N:189:VAL:O	4:N:197:THR:N	2.50	0.45
2:Z:28:ASP:OD2	3:h:200:SER:HB3	2.14	0.45
2:Z:114:PHE:HE2	2:Z:199:TRP:CZ2	2.33	0.45
2:Z:406:PRO:HB3	2:Z:410:TRP:CH2	2.51	0.45
2:F:218:VAL:HG11	2:F:236:TYR:CE1	2.51	0.45
2:J:540:ASP:CG	2:J:541:GLY:H	2.25	0.45
2:Z:103:THR:HA	2:Z:178:ASN:HA	1.98	0.45
2:Z:578:GLU:HG2	2:Z:584:TYR:CE2	2.51	0.45
1:e:93:VAL:HA	1:e:98:VAL:HG12	1.99	0.45
2:F:566:LEU:HA	2:F:566:LEU:HD23	1.80	0.45
2:J:138:LEU:HD12	2:J:182:ARG:HD2	1.99	0.45
2:J:325:CYS:O	2:J:326:ASN:CB	2.65	0.45
4:L:84:LEU:HD23	4:L:84:LEU:HA	1.76	0.45
2:Z:135:VAL:HG11	2:Z:195:ASN:HB3	1.99	0.45
2:Z:260:TRP:NE1	2:Z:262:GLY:O	2.50	0.45
4:f:23:LEU:HD22	4:f:56:TYR:CD1	2.51	0.45
2:J:279:MET:CG	4:L:163:PHE:CZ	2.99	0.44
4:N:73:THR:HB	4:N:157:GLU:OE2	2.17	0.44
2:Z:474:VAL:HG12	4:f:68:LEU:CD1	2.48	0.44
2:F:132:PRO:HA	2:F:157:GLY:O	2.17	0.44
2:F:421:GLN:OE1	2:F:421:GLN:HA	2.15	0.44
2:J:499:ASN:O	2:J:503:ARG:HA	2.17	0.44
3:P:212:GLU:OE1	3:P:212:GLU:N	2.51	0.44
2:Z:271:ASN:HD22	2:Z:274:TRP:CD1	2.36	0.44
4:f:73:THR:HG23	4:f:73:THR:O	2.16	0.44
2:F:372:ASN:OD1	2:F:372:ASN:C	2.60	0.44
2:J:132:PRO:HB3	2:J:157:GLY:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:169:MET:HE2	2:J:169:MET:HB3	1.90	0.44
2:J:312:VAL:HG21	2:J:322:ARG:HD3	1.98	0.44
4:N:137:ILE:HG23	4:N:150:PHE:HB3	2.00	0.44
4:N:18:SER:HB3	4:N:110:ALA:HB3	1.98	0.44
2:Z:82:GLU:O	2:Z:83:SER:OG	2.34	0.44
2:Z:465:SER:HA	2:Z:585:ALA:HA	1.99	0.44
2:F:252:GLN:OE1	2:F:252:GLN:HA	2.17	0.44
2:F:338:VAL:HG21	4:N:163:PHE:HB2	1.99	0.44
2:F:404:ILE:N	2:F:404:ILE:HD12	2.32	0.44
2:J:104:ILE:O	2:J:106:SER:N	2.51	0.44
2:Z:142:GLN:HB3	2:Z:178:ASN:HB3	2.00	0.44
2:F:285:TYR:CD2	2:F:285:TYR:C	2.95	0.44
2:J:66:VAL:HG23	2:J:218:VAL:HG13	2.00	0.44
4:L:80:THR:HG22	4:L:149:SER:CB	2.48	0.44
4:f:7:GLU:HB2	4:f:129:GLN:OE1	2.18	0.44
2:F:89:VAL:HA	2:F:201:SER:CB	2.47	0.44
2:F:109:ILE:HG22	2:F:175:ARG:NH1	2.31	0.44
2:F:236:TYR:CB	2:F:238:LEU:HD13	2.48	0.44
2:F:293:ALA:O	2:F:294:ALA:HB2	2.18	0.44
2:J:183:ARG:NH2	2:J:187:ASP:HA	2.32	0.44
4:N:12:CYS:O	4:N:17:GLN:NE2	2.49	0.44
4:N:229:LYS:HB2	4:N:229:LYS:NZ	2.31	0.44
3:P:168:ASP:C	3:P:170:GLY:H	2.25	0.44
1:E:41:LEU:O	1:E:106:GLN:HB3	2.18	0.44
2:F:104:ILE:O	2:F:105:THR:HG22	2.18	0.44
2:F:173:PRO:O	2:F:175:ARG:HD3	2.18	0.44
2:F:217:LEU:H	2:F:217:LEU:HG	1.56	0.44
3:P:214:ASP:OD1	3:P:214:ASP:N	2.50	0.44
2:Z:179:ILE:HD12	2:Z:179:ILE:C	2.43	0.44
4:f:133:SER:HB2	4:f:135:TRP:NE1	2.33	0.44
1:m:65:HIS:CD2	1:m:71:PHE:HB3	2.53	0.44
2:F:291:LEU:HD23	2:F:291:LEU:HA	1.86	0.44
2:J:212:TYR:CD2	2:J:217:LEU:HD22	2.52	0.44
2:J:377:VAL:HG22	2:J:465:SER:O	2.18	0.44
2:Z:42:LEU:O	2:Z:52:VAL:HG22	2.18	0.44
2:Z:73:GLN:NE2	4:f:181:GLU:HA	2.32	0.44
1:e:50:VAL:HB	1:e:54:GLU:OE2	2.18	0.44
2:F:102:ARG:NH1	2:F:102:ARG:HA	2.33	0.43
2:F:271:ASN:HD22	2:F:274:TRP:HD1	1.65	0.43
2:J:250:ASN:OD1	2:J:253:THR:HG22	2.17	0.43
2:F:86:SER:HB2	3:P:182:MET:HE1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:89:VAL:HG23	2:F:201:SER:HB3	2.01	0.43
2:J:272:MET:CE	2:J:325:CYS:SG	3.06	0.43
2:Z:39:VAL:HG12	2:Z:44:SER:HB2	2.00	0.43
2:F:40:ASP:HB3	2:F:43:LYS:HB2	1.98	0.43
2:F:124:THR:CG2	2:F:130:ARG:HG2	2.48	0.43
2:J:34:PRO:CD	2:J:241:ARG:HH12	2.23	0.43
2:J:94:VAL:HB	2:J:197:THR:HG23	2.00	0.43
4:L:225:LEU:O	4:L:226:SER:CB	2.66	0.43
1:E:87:ALA:O	1:K:18:PRO:HD2	2.18	0.43
3:I:194:GLY:HA2	2:J:268:TYR:HE1	1.83	0.43
2:Z:164:LEU:HD23	3:h:175:TYR:CD2	2.53	0.43
2:Z:361:GLN:HG2	2:Z:363:ARG:HG3	1.99	0.43
4:f:168:MET:HG2	4:f:224:PHE:CD1	2.53	0.43
2:F:332:GLN:HG3	4:N:162:VAL:HB	1.99	0.43
2:F:503:ARG:NH1	2:F:546:VAL:O	2.47	0.43
2:J:101:THR:HA	2:J:179:ILE:O	2.18	0.43
2:Z:285:TYR:O	4:f:165:GLY:N	2.52	0.43
3:I:172:GLN:HA	3:I:172:GLN:NE2	2.32	0.43
2:J:141:ILE:HG12	2:J:179:ILE:HG22	2.00	0.43
2:J:183:ARG:HD3	2:J:197:THR:HG22	2.00	0.43
2:J:241:ARG:HG2	2:J:241:ARG:NH1	2.33	0.43
4:N:43:ASN:HD21	4:N:47:GLU:HB2	1.83	0.43
2:F:345:ALA:HB2	2:F:436:PHE:HB3	2.01	0.43
2:J:30:ILE:O	2:J:31:SER:O	2.35	0.43
2:J:378:MET:HE2	1:M:26:GLY:HA2	2.00	0.43
2:J:384:PRO:HB2	2:J:385:PHE:CD1	2.53	0.43
2:J:508:ASP:OD1	2:J:508:ASP:N	2.42	0.43
1:M:14:VAL:HG22	1:M:44:TYR:CD1	2.54	0.43
2:Z:95:LYS:O	2:Z:183:ARG:HB3	2.19	0.43
2:J:42:LEU:CD1	2:J:66:VAL:HG13	2.49	0.43
2:J:470:GLY:HA3	2:J:584:TYR:CD1	2.54	0.43
1:K:1:MET:SD	1:K:65:HIS:CE1	3.12	0.43
1:m:20:VAL:HG23	1:m:33:ALA:O	2.19	0.43
2:F:137:LEU:HB2	2:F:153:ILE:CD1	2.45	0.43
2:J:114:PHE:HE2	2:J:179:ILE:HD12	1.84	0.43
2:J:396:HIS:HA	2:J:429:ASN:CB	2.49	0.43
4:N:224:PHE:O	4:N:225:LEU:O	2.37	0.43
2:Z:208:VAL:O	2:Z:209:LYS:CB	2.67	0.43
2:Z:323:ILE:HD13	2:Z:346:MET:HA	2.00	0.43
1:e:27:ASP:OD1	1:e:27:ASP:N	2.51	0.43
3:I:185:GLN:HE21	4:L:229:LYS:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:24:LEU:O	2:J:221:GLN:HA	2.19	0.43
2:J:94:VAL:HG12	2:J:183:ARG:HB3	2.00	0.43
2:J:239:ARG:HG2	2:J:268:TYR:CZ	2.54	0.43
2:J:566:LEU:C	2:J:566:LEU:HD12	2.44	0.43
2:F:101:THR:HA	2:F:179:ILE:O	2.18	0.42
4:N:26:ILE:HG12	4:N:103:VAL:HG22	2.01	0.42
2:F:158:LYS:C	2:F:159:THR:O	2.62	0.42
2:F:353:ASN:O	2:F:354:GLY:C	2.62	0.42
2:J:185:THR:O	2:J:186:PRO:C	2.61	0.42
2:J:287:MET:HE2	2:J:287:MET:N	2.33	0.42
2:J:351:VAL:O	2:J:351:VAL:HG23	2.19	0.42
2:J:351:VAL:HG23	2:J:358:THR:HG23	2.01	0.42
1:Y:30:SER:OG	1:Y:32:ARG:NH1	2.52	0.42
2:Z:246:PRO:HD3	2:Z:274:TRP:CE2	2.54	0.42
2:F:183:ARG:HD2	2:F:197:THR:OG1	2.19	0.42
2:F:410:TRP:H	2:F:410:TRP:CD1	2.37	0.42
2:J:416:LEU:HD11	2:J:418:GLU:CG	2.50	0.42
1:K:47:THR:HA	1:K:100:PHE:O	2.18	0.42
3:P:184:ALA:O	3:P:187:ASN:HB2	2.19	0.42
1:Y:1:MET:N	1:Y:64:GLU:OE2	2.49	0.42
1:E:14:VAL:HG22	1:E:44:TYR:HD1	1.83	0.42
2:F:28:ASP:OD2	2:F:236:TYR:OH	2.35	0.42
2:F:158:LYS:HD2	2:F:159:THR:N	2.35	0.42
2:F:410:TRP:CD1	2:F:410:TRP:N	2.87	0.42
4:L:2:GLN:HB3	4:L:4:ILE:HG12	2.00	0.42
3:P:172:GLN:N	3:P:172:GLN:OE1	2.50	0.42
2:Z:23:LEU:HD12	2:Z:222:VAL:O	2.19	0.42
2:Z:236:TYR:O	3:h:197:ARG:HA	2.20	0.42
2:J:25:SER:HB3	2:J:81:PHE:HE1	1.84	0.42
2:J:245:VAL:HB	2:J:246:PRO:HD2	2.02	0.42
2:J:352:TRP:NE1	4:L:154:THR:HG23	2.34	0.42
4:L:199:ASP:OD1	4:L:202:LYS:N	2.51	0.42
4:N:175:TRP:CD1	4:N:222:GLY:HA3	2.54	0.42
1:Y:89:TRP:O	1:Y:89:TRP:CG	2.73	0.42
2:Z:367:LYS:HZ1	4:f:1:MET:HE2	1.84	0.42
2:F:28:ASP:OD2	2:F:234:ARG:NE	2.52	0.42
2:F:280:LEU:O	2:F:287:MET:HB3	2.19	0.42
2:J:207:ASP:OD1	2:J:207:ASP:N	2.29	0.42
2:J:438:CYS:SG	2:J:443:GLN:HB3	2.59	0.42
4:L:51:TRP:CE2	4:L:52:GLN:HG3	2.55	0.42
1:M:6:TRP:CE2	1:M:58:LEU:HD13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:155:ILE:HG23	3:h:218:VAL:HG12	2.01	0.42
2:Z:451:LEU:O	2:Z:454:THR:HG22	2.19	0.42
1:E:26:GLY:HA3	2:F:373:ARG:O	2.20	0.42
2:F:456:LEU:HD23	2:F:456:LEU:HA	1.90	0.42
2:J:438:CYS:SG	2:J:439:THR:N	2.93	0.42
4:L:206:SER:OG	4:L:211:GLY:CA	2.63	0.42
2:Z:139:VAL:CG1	2:Z:181:MET:HE3	2.50	0.42
2:Z:277:TRP:O	2:Z:281:THR:HG22	2.19	0.42
1:m:94:SER:OG	1:m:95:MET:N	2.53	0.42
1:E:8:VAL:HG12	1:E:48:LEU:HD23	2.02	0.42
2:J:142:GLN:OE1	2:J:142:GLN:HA	2.20	0.42
4:N:204:LYS:O	4:N:215:ARG:NH2	2.53	0.42
1:Y:8:VAL:HG22	1:Y:46:VAL:HG13	2.02	0.42
2:F:153:ILE:O	2:F:153:ILE:HD12	2.19	0.42
2:F:402:ASN:OD1	2:F:414:THR:OG1	2.33	0.42
2:J:364:PRO:HG3	2:J:593:PRO:O	2.19	0.42
4:L:170:ALA:O	4:L:171:ASN:C	2.61	0.42
1:m:33:ALA:HB1	1:m:34:PRO:HD2	2.02	0.42
2:F:353:ASN:HB3	2:F:474:VAL:HG11	2.01	0.42
2:J:522:SER:HB3	2:J:562:LYS:HE2	2.02	0.42
2:Z:152:ASP:OD1	2:Z:152:ASP:N	2.53	0.42
2:Z:244:GLN:HB3	2:Z:264:PHE:HB3	2.02	0.42
2:J:93:GLU:OE1	2:J:93:GLU:N	2.53	0.41
2:J:138:LEU:HD22	2:J:149:THR:CG2	2.50	0.41
2:Z:30:ILE:HG21	2:Z:238:LEU:HD12	2.01	0.41
2:Z:137:LEU:HD21	2:Z:197:THR:HG21	2.02	0.41
3:I:213:GLY:N	2:J:19:LYS:O	2.54	0.41
2:J:253:THR:HG23	2:J:255:GLN:HB2	2.02	0.41
4:L:221:PHE:CE2	4:L:225:LEU:HD21	2.55	0.41
2:Z:159:THR:O	2:Z:159:THR:OG1	2.38	0.41
2:Z:505:LEU:HD11	2:Z:523:LEU:HD21	2.02	0.41
4:f:201:THR:HG23	4:f:202:LYS:HG3	2.02	0.41
1:E:12:MET:HE1	1:E:76:PRO:HD2	2.01	0.41
2:F:242:ILE:HA	2:F:268:TYR:HA	2.01	0.41
2:J:279:MET:HG2	4:L:163:PHE:CE1	2.55	0.41
2:J:399:VAL:HG23	2:J:452:ILE:CD1	2.47	0.41
4:L:92:ALA:HB2	4:L:98:LEU:HG	2.01	0.41
2:Z:104:ILE:O	2:Z:105:THR:C	2.64	0.41
2:Z:250:ASN:HB3	2:Z:253:THR:CG2	2.49	0.41
2:Z:270:ASN:ND2	2:Z:326:ASN:OD1	2.53	0.41
2:Z:314:ASP:OD2	2:Z:314:ASP:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:37:PHE:HB3	4:L:56:TYR:CD1	2.55	0.41
2:Z:105:THR:O	2:Z:105:THR:HG23	2.21	0.41
1:m:37:LEU:HD12	1:m:37:LEU:HA	1.97	0.41
2:F:114:PHE:CE2	2:F:179:ILE:HD12	2.55	0.41
2:F:571:PHE:HB3	2:F:588:ALA:HB1	2.02	0.41
4:f:51:TRP:CE3	4:f:113:LEU:HD23	2.56	0.41
2:F:76:THR:O	2:F:77:PRO:C	2.64	0.41
2:F:158:LYS:O	2:F:159:THR:O	2.38	0.41
2:F:255:GLN:OE1	2:F:255:GLN:HA	2.19	0.41
2:F:586:ILE:CG2	2:F:587:THR:N	2.83	0.41
1:K:38:ASN:HB3	1:K:41:LEU:HD21	2.02	0.41
1:M:37:LEU:HD23	1:M:37:LEU:HA	1.96	0.41
4:N:98:LEU:HD12	4:N:150:PHE:CE1	2.55	0.41
2:Z:396:HIS:CD2	2:Z:431:THR:CG2	3.03	0.41
2:Z:466:VAL:HG22	2:Z:467:GLY:H	1.85	0.41
1:e:51:PRO:HD2	1:e:54:GLU:OE2	2.21	0.41
3:h:214:ASP:OD1	3:h:214:ASP:N	2.54	0.41
2:F:47:LEU:O	2:F:49:SER:N	2.53	0.41
2:F:173:PRO:CD	2:F:177:PHE:CE1	2.98	0.41
1:Y:47:THR:HA	1:Y:100:PHE:O	2.21	0.41
2:Z:102:ARG:HB2	2:Z:179:ILE:HD11	2.03	0.41
2:F:236:TYR:HB2	2:F:238:LEU:HD13	2.03	0.41
2:F:301:LEU:HD23	2:F:301:LEU:HA	1.79	0.41
2:F:575:SER:OG	2:F:587:THR:CG2	2.69	0.41
2:J:122:VAL:HA	2:J:158:LYS:HZ3	1.85	0.41
2:J:416:LEU:HD11	2:J:418:GLU:OE2	2.21	0.41
4:L:175:TRP:NE1	4:L:222:GLY:CA	2.84	0.41
3:P:168:ASP:OD1	3:P:168:ASP:N	2.53	0.41
2:Z:172:LEU:H	2:Z:172:LEU:HD12	1.85	0.41
2:Z:398:ALA:O	2:Z:430:VAL:HA	2.20	0.41
1:e:41:LEU:O	1:e:106:GLN:HG2	2.21	0.41
2:F:84:SER:O	2:F:206:ILE:HB	2.20	0.41
2:F:339:LEU:C	2:F:339:LEU:HD23	2.45	0.41
2:F:406:PRO:HB3	2:F:410:TRP:CH2	2.56	0.41
2:F:571:PHE:CD1	2:F:590:GLN:HA	2.56	0.41
2:J:138:LEU:HD22	2:J:149:THR:HG21	2.02	0.41
2:J:290:ARG:H	2:J:290:ARG:CD	2.34	0.41
2:J:403:TRP:CD1	2:J:403:TRP:N	2.88	0.41
2:J:423:ILE:HG23	2:J:428:ARG:HB2	2.03	0.41
2:J:453:LYS:HD3	2:J:453:LYS:HA	1.90	0.41
2:J:464:PHE:O	2:J:464:PHE:CG	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:21:ARG:CG	2:Z:382:GLY:HA3	2.51	0.41
1:M:46:VAL:HG21	1:M:104:PHE:CE2	2.56	0.41
4:N:159:ASP:C	4:N:159:ASP:OD1	2.64	0.41
2:Z:372:ASN:HD22	2:Z:560:GLU:HG2	1.85	0.41
2:Z:571:PHE:HB3	2:Z:588:ALA:HB1	2.03	0.41
3:h:179:LEU:HD23	3:h:179:LEU:HA	1.80	0.41
1:m:4:PHE:HB3	1:m:73:TRP:CD1	2.56	0.41
1:m:62:LEU:HD23	1:m:62:LEU:HA	1.97	0.41
2:F:563:LEU:H	2:F:563:LEU:HD22	1.86	0.41
3:I:185:GLN:NE2	4:L:229:LYS:O	2.54	0.41
2:J:364:PRO:HB3	2:J:593:PRO:HB3	2.01	0.41
4:L:48:PRO:HB3	4:L:58:PRO:HD3	2.03	0.41
4:L:177:TYR:C	4:L:179:GLY:H	2.28	0.41
2:Z:43:LYS:O	2:Z:51:PRO:HB3	2.21	0.41
2:Z:135:VAL:O	2:Z:154:THR:HA	2.21	0.41
2:J:73:GLN:O	2:J:73:GLN:NE2	2.54	0.40
2:J:217:LEU:H	2:J:217:LEU:HG	1.51	0.40
2:J:329:LEU:HD12	2:J:329:LEU:H	1.86	0.40
4:N:146:VAL:HG12	4:N:147:SER:N	2.35	0.40
2:F:45:VAL:HG13	2:F:236:TYR:CD1	2.54	0.40
2:J:351:VAL:HG12	2:J:475:PRO:HB2	2.03	0.40
4:N:218:VAL:O	4:N:218:VAL:HG12	2.20	0.40
2:Z:28:ASP:N	2:Z:28:ASP:OD1	2.55	0.40
2:Z:211:CYS:O	2:Z:212:TYR:C	2.63	0.40
4:f:28:LEU:HD13	4:f:98:LEU:CD2	2.50	0.40
4:N:229:LYS:NZ	4:N:229:LYS:CB	2.84	0.40
1:Y:70:SER:HB3	1:Y:85:THR:HG23	2.02	0.40
1:E:94:SER:HB3	1:E:97:ARG:O	2.21	0.40
2:F:115:THR:HG22	2:F:200:SER:OG	2.21	0.40
2:F:150:GLU:HG2	2:F:169:MET:SD	2.62	0.40
2:J:90:LEU:HD23	2:J:201:SER:HA	2.03	0.40
1:K:4:PHE:HB3	1:K:73:TRP:CD1	2.57	0.40
2:Z:36:GLU:HB3	2:Z:239:ARG:HB3	2.03	0.40
4:f:84:LEU:HD12	4:f:84:LEU:HA	1.93	0.40
2:F:268:TYR:CD2	2:F:268:TYR:O	2.74	0.40
2:J:90:LEU:HD13	2:J:102:ARG:HD3	2.04	0.40
4:L:34:GLU:OE1	4:L:34:GLU:N	2.55	0.40
2:Z:209:LYS:O	2:Z:210:GLN:CB	2.69	0.40
2:Z:567:ARG:HD2	2:Z:567:ARG:HA	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	107/109 (98%)	87 (81%)	19 (18%)	1 (1%)	14	46
1	K	107/109 (98%)	90 (84%)	16 (15%)	1 (1%)	14	46
1	M	107/109 (98%)	88 (82%)	17 (16%)	2 (2%)	6	33
1	Y	107/109 (98%)	91 (85%)	15 (14%)	1 (1%)	14	46
1	e	107/109 (98%)	94 (88%)	12 (11%)	1 (1%)	14	46
1	m	107/109 (98%)	94 (88%)	12 (11%)	1 (1%)	14	46
2	F	592/1132 (52%)	489 (83%)	81 (14%)	22 (4%)	2	21
2	J	596/1132 (53%)	495 (83%)	87 (15%)	14 (2%)	5	30
2	Z	595/1132 (53%)	501 (84%)	80 (13%)	14 (2%)	4	29
3	I	54/223 (24%)	39 (72%)	12 (22%)	3 (6%)	1	13
3	P	57/223 (26%)	37 (65%)	12 (21%)	8 (14%)	0	3
3	h	56/223 (25%)	43 (77%)	8 (14%)	5 (9%)	0	7
4	L	230/232 (99%)	202 (88%)	23 (10%)	5 (2%)	5	30
4	N	230/232 (99%)	198 (86%)	26 (11%)	6 (3%)	4	27
4	f	230/232 (99%)	200 (87%)	25 (11%)	5 (2%)	5	30
All	All	3282/5415 (61%)	2748 (84%)	445 (14%)	89 (3%)	6	27

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	159	THR
2	F	213	PRO
2	F	231	GLN
2	F	294	ALA
2	F	326	ASN
2	F	348	CYS
3	I	176	PHE
2	J	31	SER

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Mol	Chain	Res	Type
2	J	91	GLY
2	J	242	ILE
2	J	326	ASN
2	J	410	TRP
4	L	225	LEU
4	N	163	PHE
4	N	225	LEU
3	P	185	GLN
2	Z	209	LYS
2	Z	210	GLN
2	Z	230	GLN
4	f	158	THR
4	f	228	ASN
3	h	195	GLU
1	m	42	LYS
2	F	32	GLU
2	F	48	ASN
2	F	354	GLY
2	F	355	GLN
2	F	409	GLY
2	F	433	MET
3	I	188	VAL
3	I	194	GLY
2	J	32	GLU
2	J	105	THR
1	K	42	LYS
4	L	164	PRO
4	L	179	GLY
4	N	159	ASP
3	P	188	VAL
3	P	204	SER
2	Z	33	GLY
4	f	140	CYS
4	f	164	PRO
2	F	71	GLY
2	F	99	PRO
2	F	143	ARG
2	F	187	ASP
2	F	263	THR
2	F	503	ARG
2	J	173	PRO
1	M	69	LYS

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Mol	Chain	Res	Type
4	N	74	SER
4	N	77	PRO
3	P	194	GLY
2	Z	14	ALA
2	Z	91	GLY
2	Z	103	THR
2	Z	325	CYS
1	E	35	ALA
2	F	144	ASN
2	J	144	ASN
3	P	177	SER
1	Y	26	GLY
2	Z	127	LYS
1	e	42	LYS
3	h	184	ALA
3	h	188	VAL
3	h	194	GLY
3	h	196	MET
2	F	248	ASN
2	F	257	SER
2	J	99	PRO
4	L	163	PHE
4	L	226	SER
3	P	196	MET
3	P	213	GLY
2	Z	49	SER
2	Z	212	TYR
4	f	3	ASP
2	J	176	PRO
4	N	196	PRO
2	Z	83	SER
2	Z	99	PRO
2	Z	101	THR
2	J	218	VAL
1	M	26	GLY
2	J	186	PRO
2	F	91	GLY
2	J	45	VAL
3	P	218	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	E	96/96 (100%)	89 (93%)	7 (7%)	13	39
1	K	96/96 (100%)	93 (97%)	3 (3%)	35	61
1	M	96/96 (100%)	93 (97%)	3 (3%)	35	61
1	Y	96/96 (100%)	95 (99%)	1 (1%)	68	76
1	e	96/96 (100%)	91 (95%)	5 (5%)	21	49
1	m	96/96 (100%)	92 (96%)	4 (4%)	26	53
2	F	514/958 (54%)	452 (88%)	62 (12%)	5	23
2	J	517/958 (54%)	467 (90%)	50 (10%)	8	31
2	Z	516/958 (54%)	482 (93%)	34 (7%)	15	43
3	I	46/162 (28%)	38 (83%)	8 (17%)	2	12
3	P	49/162 (30%)	44 (90%)	5 (10%)	7	28
3	h	48/162 (30%)	38 (79%)	10 (21%)	1	6
4	L	198/198 (100%)	180 (91%)	18 (9%)	9	32
4	N	198/198 (100%)	181 (91%)	17 (9%)	10	34
4	f	198/198 (100%)	181 (91%)	17 (9%)	10	34
All	All	2860/4530 (63%)	2616 (92%)	244 (8%)	12	35

All (244) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	12	MET
1	E	20	VAL
1	E	21	ARG
1	E	40	ASN
1	E	84	VAL
1	E	96	LEU
1	E	107	VAL
2	F	17	ASN
2	F	26	VAL
2	F	30	ILE

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Mol	Chain	Res	Type
2	F	46	LEU
2	F	59	THR
2	F	62	SER
2	F	66	VAL
2	F	86	SER
2	F	101	THR
2	F	109	ILE
2	F	153	ILE
2	F	156	LYS
2	F	162	GLN
2	F	168	VAL
2	F	180	ARG
2	F	186	PRO
2	F	187	ASP
2	F	198	LEU
2	F	206	ILE
2	F	208	VAL
2	F	211	CYS
2	F	213	PRO
2	F	215	THR
2	F	217	LEU
2	F	221	GLN
2	F	222	VAL
2	F	243	LEU
2	F	248	ASN
2	F	261	ASP
2	F	279	MET
2	F	289	LYS
2	F	295	ASP
2	F	304	ILE
2	F	306	GLN
2	F	312	VAL
2	F	334	LYS
2	F	346	MET
2	F	347	ARG
2	F	348	CYS
2	F	351	VAL
2	F	358	THR
2	F	364	PRO
2	F	368	THR
2	F	376	VAL
2	F	388	SER

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Mol	Chain	Res	Type
2	F	393	LYS
2	F	412	THR
2	F	416	LEU
2	F	420	THR
2	F	461	THR
2	F	466	VAL
2	F	471	LEU
2	F	489	ILE
2	F	544	VAL
2	F	551	ASP
2	F	563	LEU
2	F	567	ARG
2	F	576	ILE
2	F	586	ILE
2	F	592	VAL
2	F	599	VAL
2	F	604	HIS
3	I	171	LYS
3	I	177	SER
3	I	178	SER
3	I	187	ASN
3	I	188	VAL
3	I	197	ARG
3	I	203	VAL
3	I	212	GLU
2	J	22	GLN
2	J	32	GLU
2	J	39	VAL
2	J	47	LEU
2	J	49	SER
2	J	50	THR
2	J	64	VAL
2	J	65	THR
2	J	66	VAL
2	J	67	VAL
2	J	84	SER
2	J	88	THR
2	J	109	ILE
2	J	131	ASN
2	J	133	SER
2	J	156	LYS
2	J	167	VAL

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Mol	Chain	Res	Type
2	J	169	MET
2	J	175	ARG
2	J	187	ASP
2	J	190	THR
2	J	198	LEU
2	J	203	THR
2	J	206	ILE
2	J	207	ASP
2	J	208	VAL
2	J	215	THR
2	J	217	LEU
2	J	222	VAL
2	J	245	VAL
2	J	248	ASN
2	J	268	TYR
2	J	279	MET
2	J	280	LEU
2	J	325	CYS
2	J	329	LEU
2	J	330	THR
2	J	339	LEU
2	J	378	MET
2	J	404	ILE
2	J	407	ASN
2	J	430	VAL
2	J	439	THR
2	J	456	LEU
2	J	461	THR
2	J	463	ASP
2	J	511	ILE
2	J	523	LEU
2	J	596	GLU
2	J	601	ASN
1	K	40	ASN
1	K	41	LEU
1	K	69	LYS
4	L	1	MET
4	L	16	GLU
4	L	69	ASN
4	L	102	THR
4	L	107	LYS
4	L	108	VAL

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Mol	Chain	Res	Type
4	L	138	GLU
4	L	142	GLU
4	L	158	THR
4	L	164	PRO
4	L	167	ILE
4	L	174	THR
4	L	176	THR
4	L	201	THR
4	L	203	ASP
4	L	206	SER
4	L	213	LYS
4	L	218	VAL
1	M	9	LYS
1	M	21	ARG
1	M	38	ASN
4	N	1	MET
4	N	4	ILE
4	N	9	LEU
4	N	12	CYS
4	N	29	THR
4	N	133	SER
4	N	141	SER
4	N	142	GLU
4	N	146	VAL
4	N	156	THR
4	N	157	GLU
4	N	162	VAL
4	N	168	MET
4	N	178	ARG
4	N	180	ASP
4	N	225	LEU
4	N	229	LYS
3	P	173	ASN
3	P	177	SER
3	P	178	SER
3	P	185	GLN
3	P	220	VAL
1	Y	14	VAL
2	Z	27	ILE
2	Z	28	ASP
2	Z	47	LEU
2	Z	48	ASN

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Mol	Chain	Res	Type
2	Z	50	THR
2	Z	65	THR
2	Z	67	VAL
2	Z	97	ASP
2	Z	103	THR
2	Z	110	ASP
2	Z	150	GLU
2	Z	164	LEU
2	Z	181	MET
2	Z	197	THR
2	Z	212	TYR
2	Z	215	THR
2	Z	222	VAL
2	Z	236	TYR
2	Z	248	ASN
2	Z	314	ASP
2	Z	316	PHE
2	Z	339	LEU
2	Z	377	VAL
2	Z	418	GLU
2	Z	429	ASN
2	Z	432	LYS
2	Z	451	LEU
2	Z	452	ILE
2	Z	461	THR
2	Z	465	SER
2	Z	562	LYS
2	Z	572	ARG
2	Z	594	GLU
2	Z	606	ASP
1	e	12	MET
1	e	21	ARG
1	e	27	ASP
1	e	43	THR
1	e	106	GLN
4	f	2	GLN
4	f	8	THR
4	f	31	VAL
4	f	74	SER
4	f	76	ARG
4	f	108	VAL
4	f	111	ARG

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Mol	Chain	Res	Type
4	f	132	ILE
4	f	133	SER
4	f	142	GLU
4	f	149	SER
4	f	168	MET
4	f	174	THR
4	f	213	LYS
4	f	220	ASN
4	f	226	SER
4	f	228	ASN
3	h	173	ASN
3	h	174	THR
3	h	181	ASN
3	h	188	VAL
3	h	195	GLU
3	h	197	ARG
3	h	205	GLN
3	h	214	ASP
3	h	218	VAL
3	h	219	VAL
1	m	20	VAL
1	m	58	LEU
1	m	91	SER
1	m	93	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	48	ASN
2	F	75	GLN
2	F	171	ASN
2	F	443	GLN
2	F	445	HIS
3	I	172	GLN
3	I	185	GLN
2	J	108	ASN
2	J	162	GLN
2	J	306	GLN
4	L	2	GLN
4	L	6	GLN
4	L	10	ASN
4	L	57	GLN

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Mol	Chain	Res	Type
4	L	69	ASN
1	M	31	GLN
1	M	81	GLN
1	M	109	ASN
4	N	6	GLN
4	N	96	GLN
4	N	217	ASN
3	P	185	GLN
1	Y	106	GLN
2	Z	17	ASN
2	Z	221	GLN
2	Z	270	ASN
2	Z	326	ASN
2	Z	332	GLN
2	Z	361	GLN
2	Z	372	ASN
2	Z	443	GLN
2	Z	529	ASN
2	Z	536	GLN
1	e	38	ASN
4	f	2	GLN
4	f	6	GLN
4	f	55	GLN
4	f	232	GLN
3	h	205	GLN
3	h	217	GLN
1	m	65	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SF4	f	301	4	0,12,12	-	-	-		
5	SF4	L	301	4	0,12,12	-	-	-		
5	SF4	N	301	4	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SF4	f	301	4	-	-	0/6/5/5
5	SF4	L	301	4	-	-	0/6/5/5
5	SF4	N	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

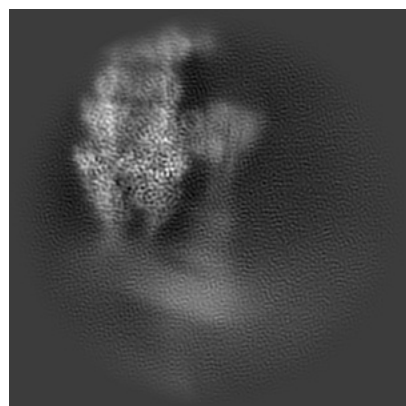
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38242. These allow visual inspection of the internal detail of the map and identification of artifacts.

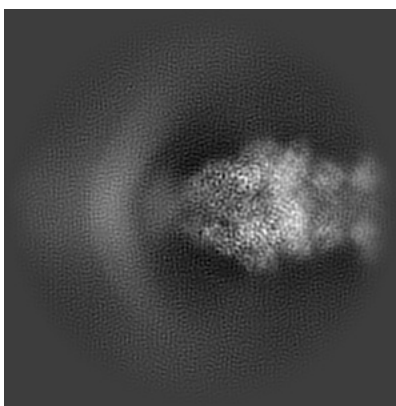
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

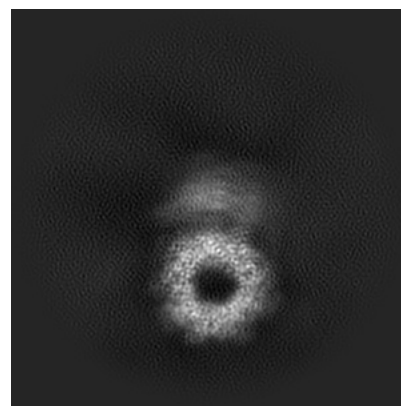
6.1.1 Primary map



X

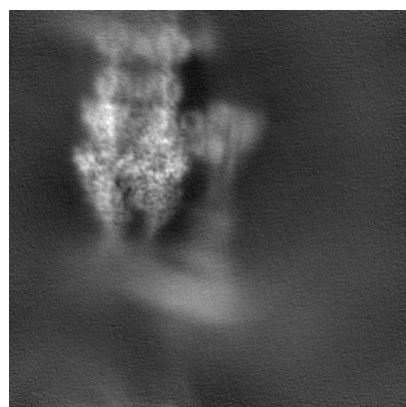


Y

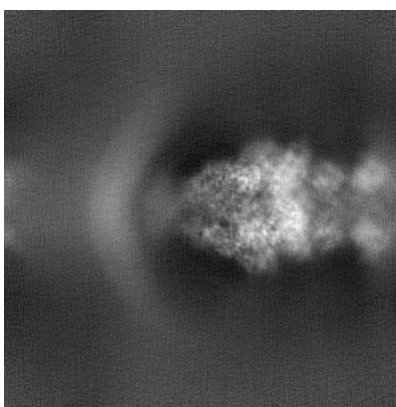


Z

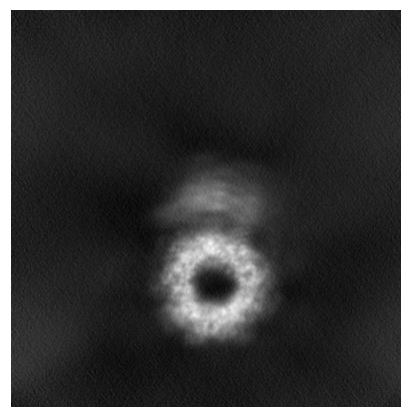
6.1.2 Raw map



X



Y

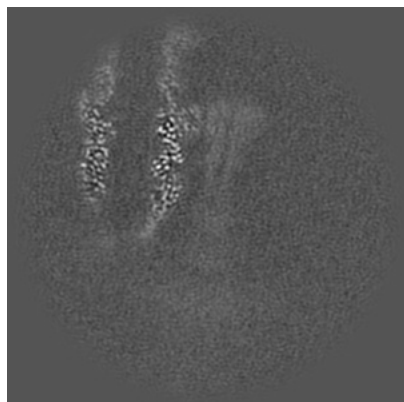


Z

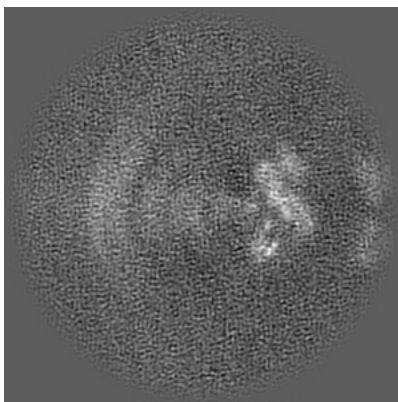
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

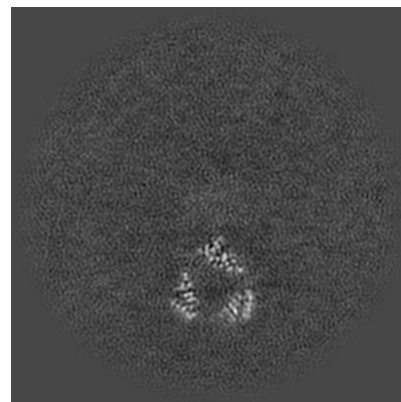
6.2.1 Primary map



X Index: 160

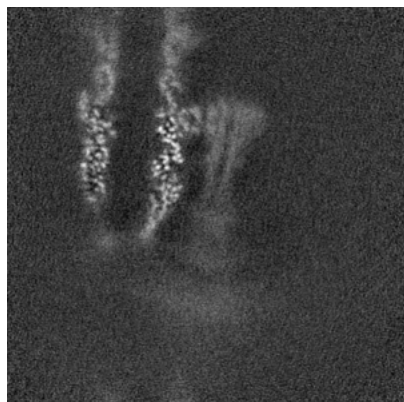


Y Index: 160

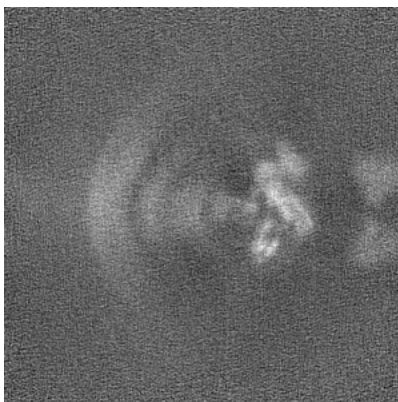


Z Index: 160

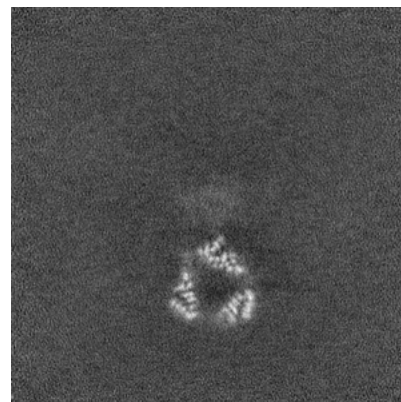
6.2.2 Raw map



X Index: 160



Y Index: 160

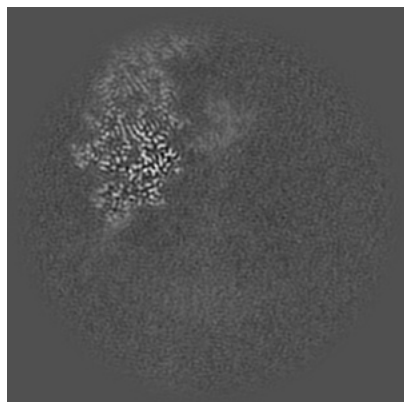


Z Index: 160

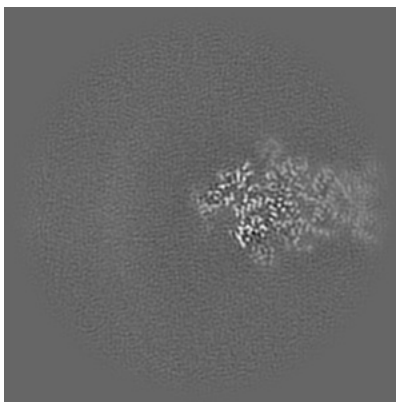
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

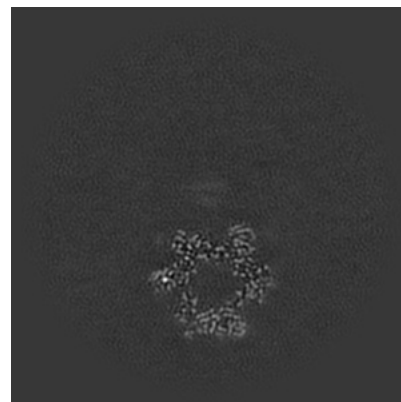
6.3.1 Primary map



X Index: 141

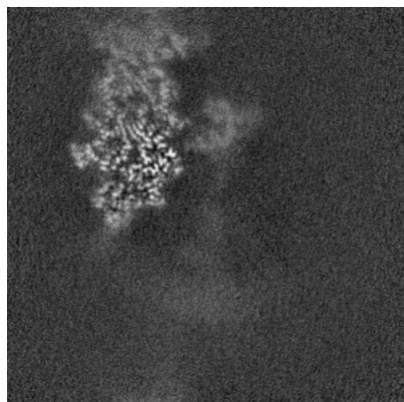


Y Index: 126

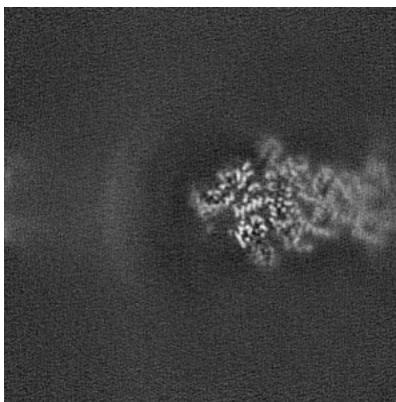


Z Index: 193

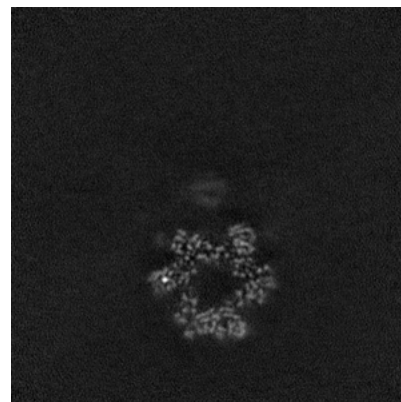
6.3.2 Raw map



X Index: 141



Y Index: 126

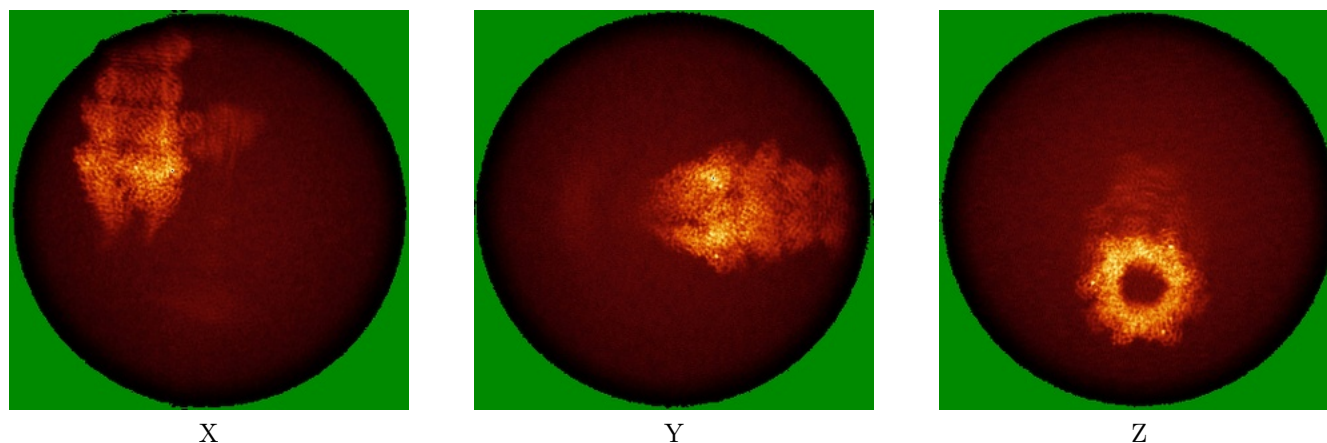


Z Index: 193

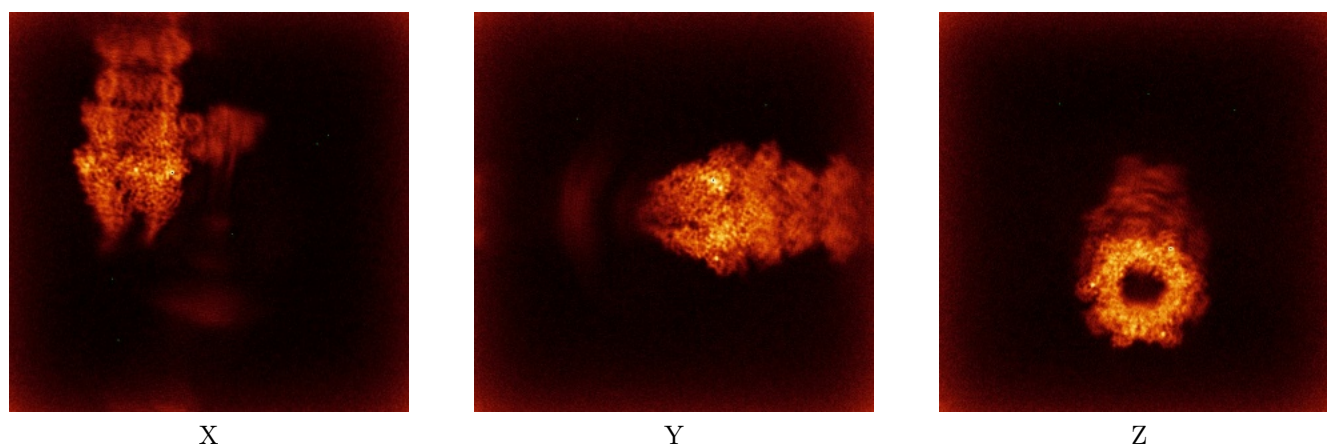
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

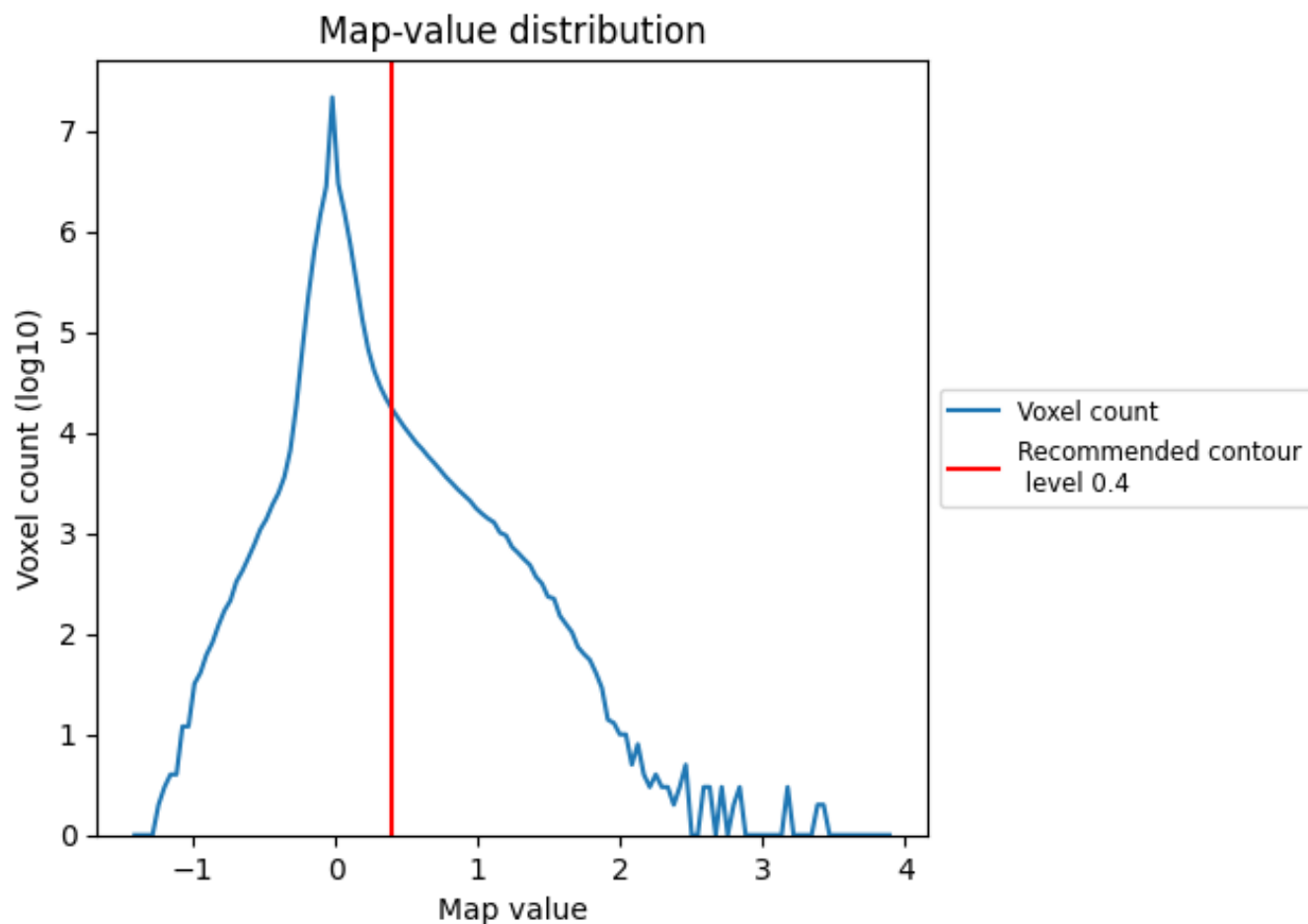
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

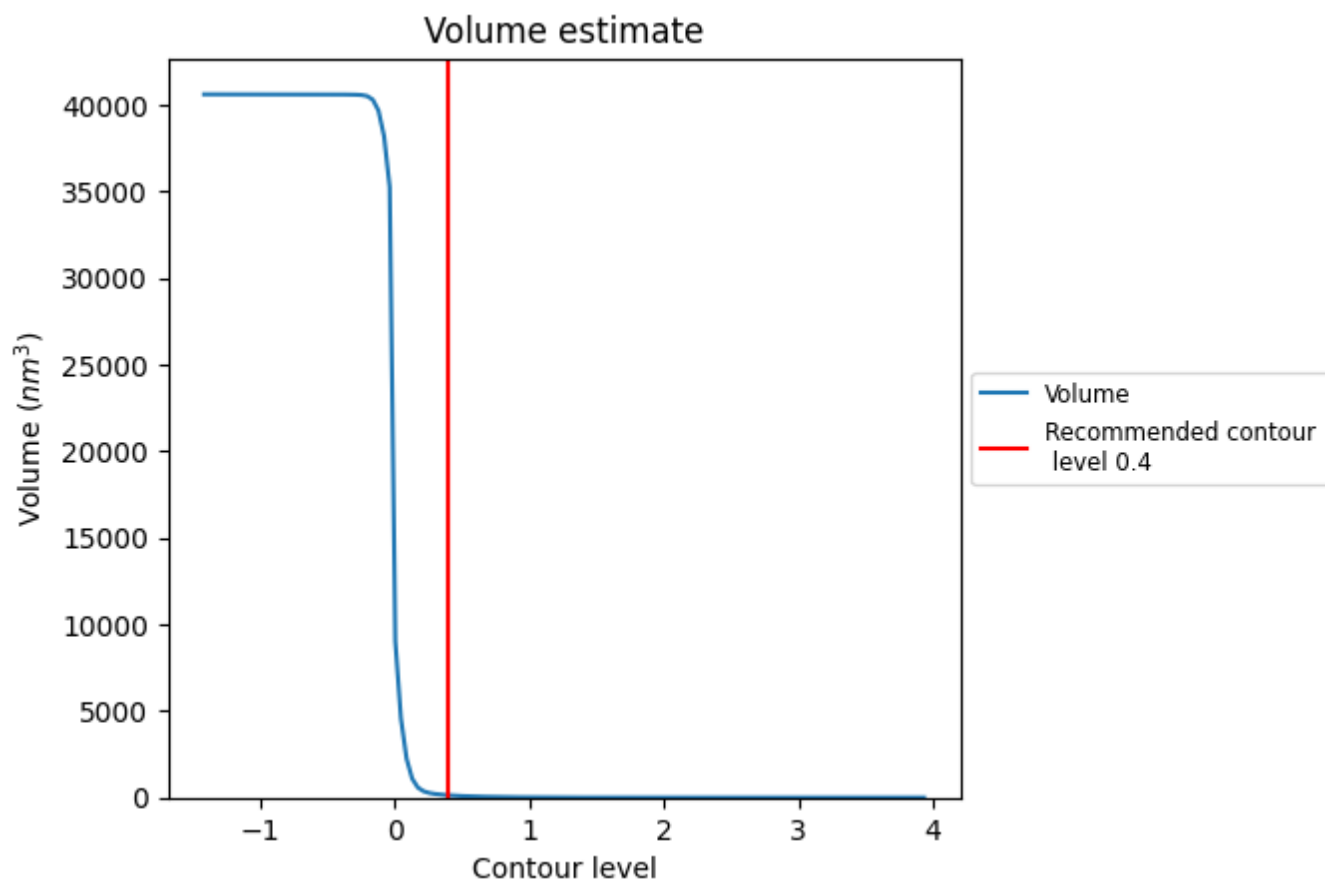
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

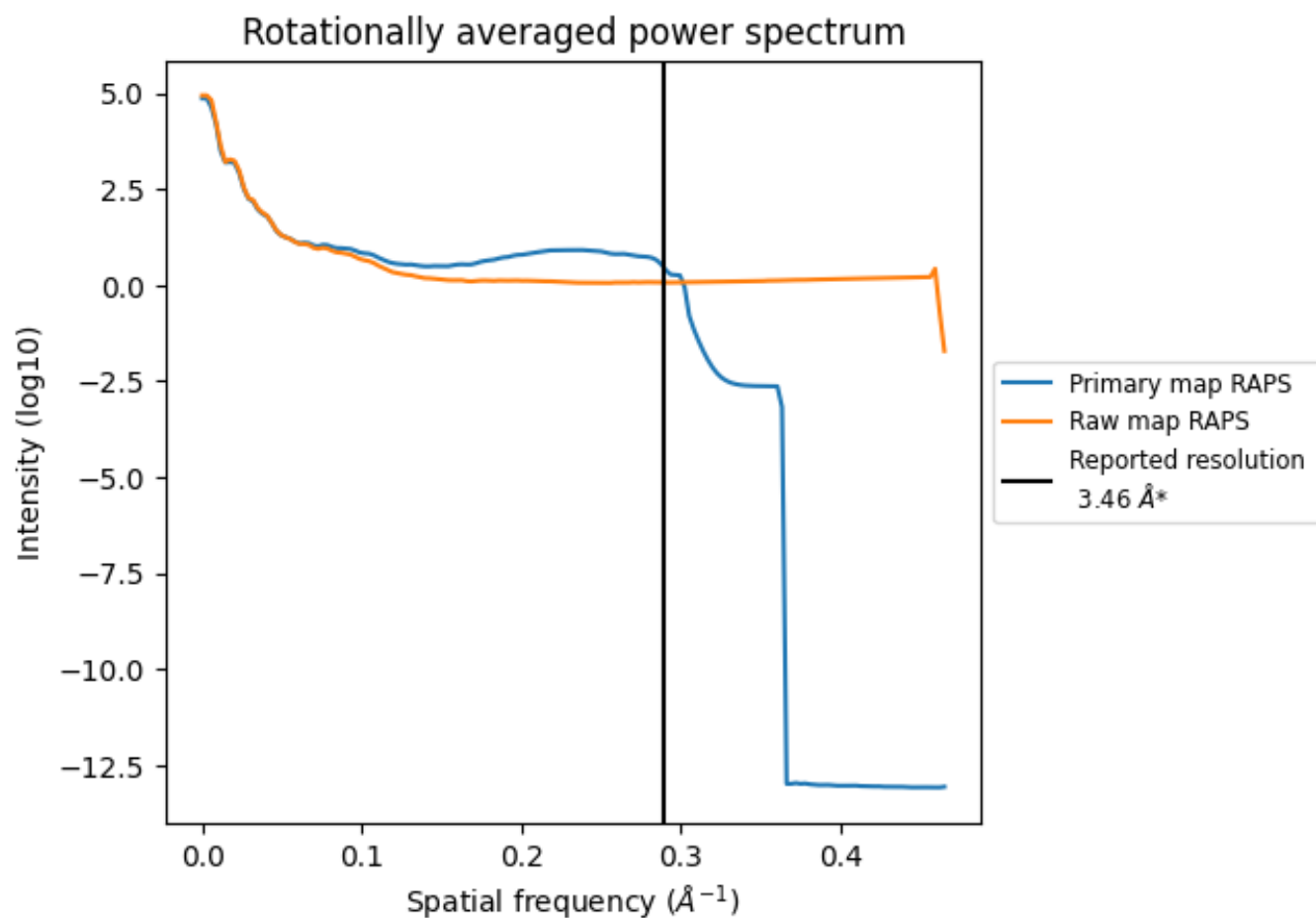
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 133 nm^3 ; this corresponds to an approximate mass of 120 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 ⓘ

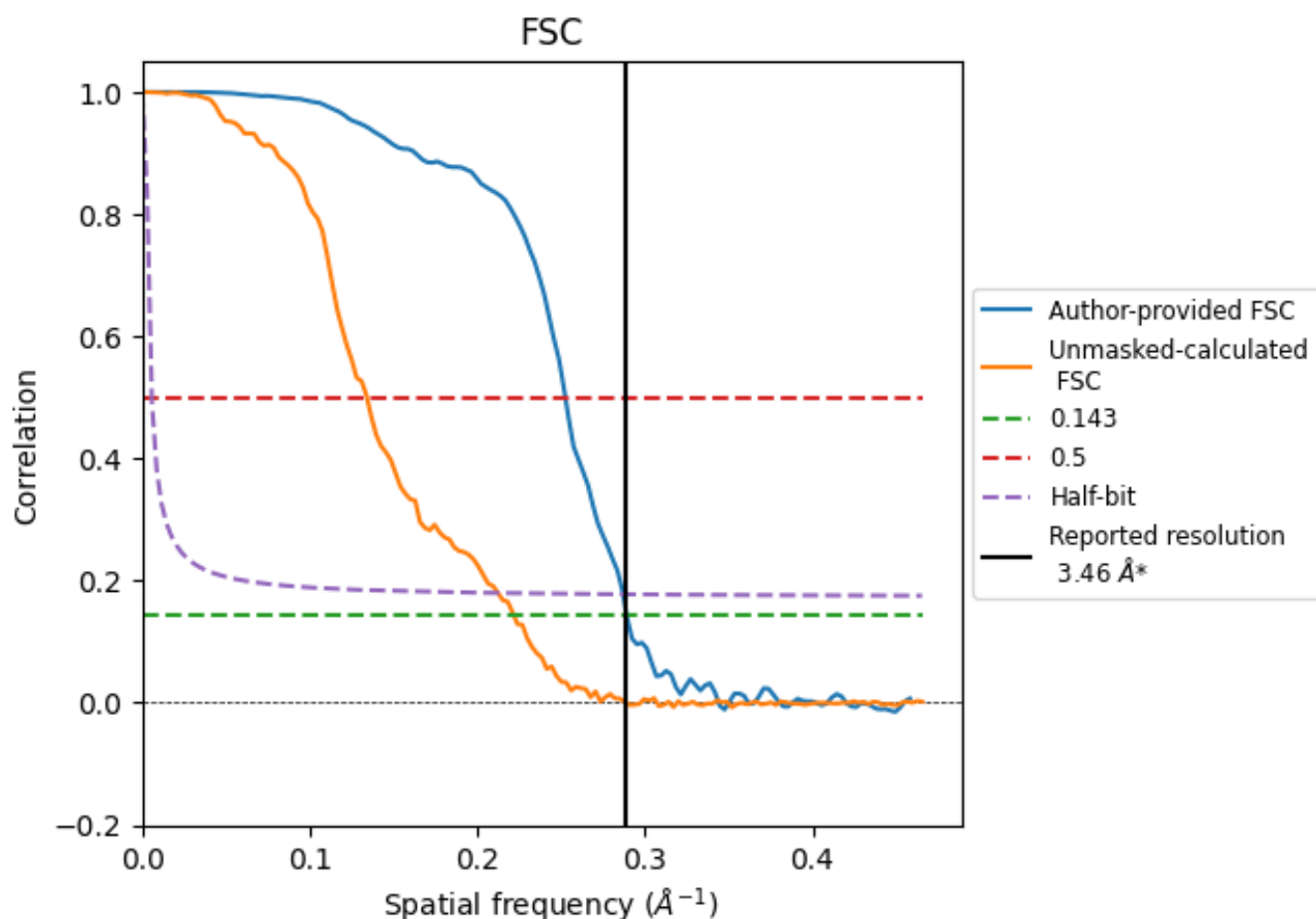


*Reported resolution corresponds to spatial frequency of 0.289 Å⁻¹

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 0.289 Å⁻¹

8.2 Resolution estimates [i](#)

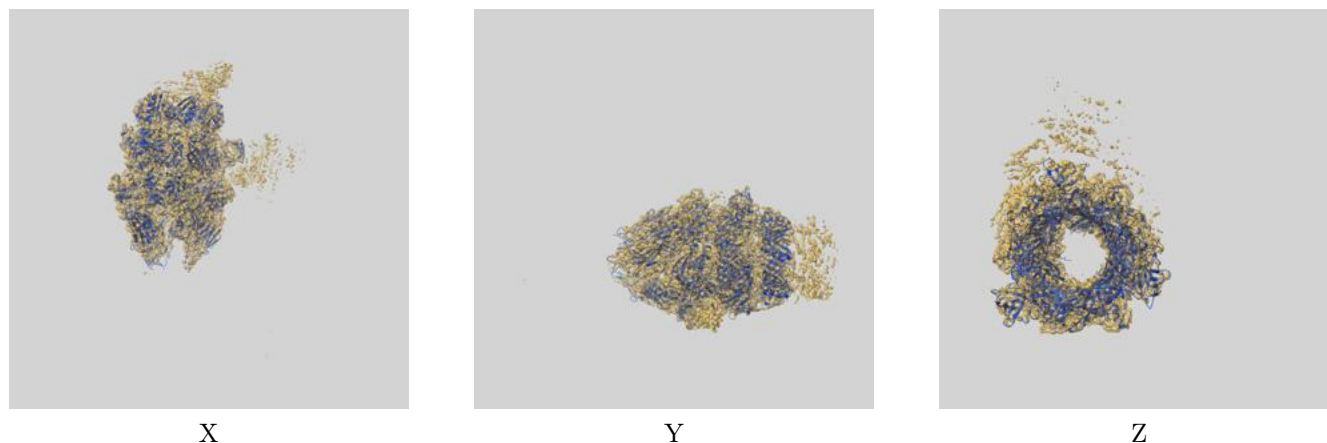
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	3.46	3.96	3.48
Unmasked-calculated*	4.51	7.46	4.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.51 differs from the reported value 3.46 by more than 10 %

9 Map-model fit [i](#)

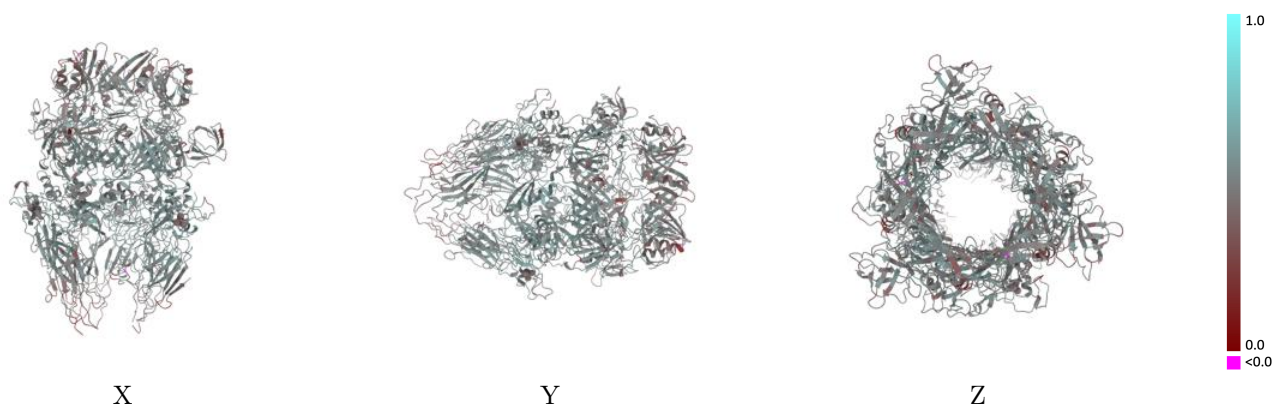
This section contains information regarding the fit between EMDB map EMD-38242 and PDB model 8XCG. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



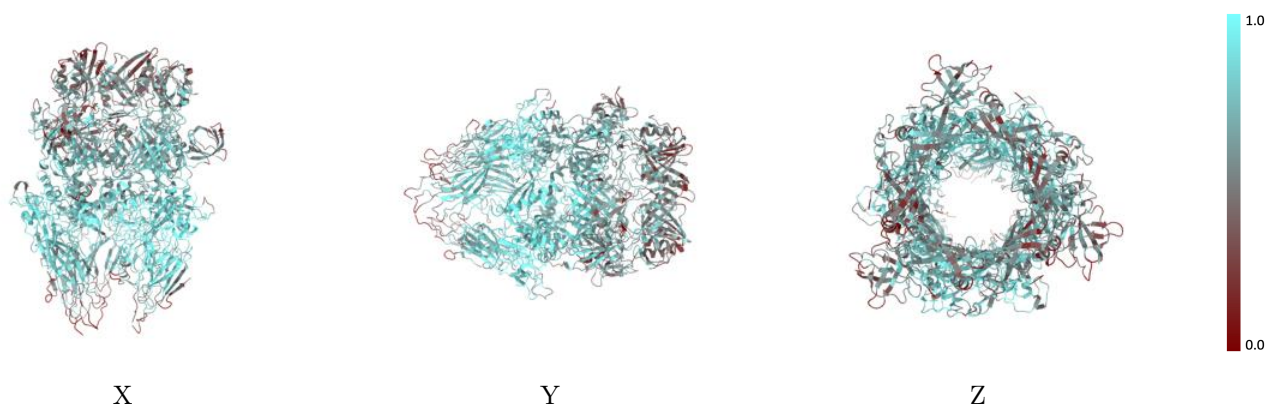
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



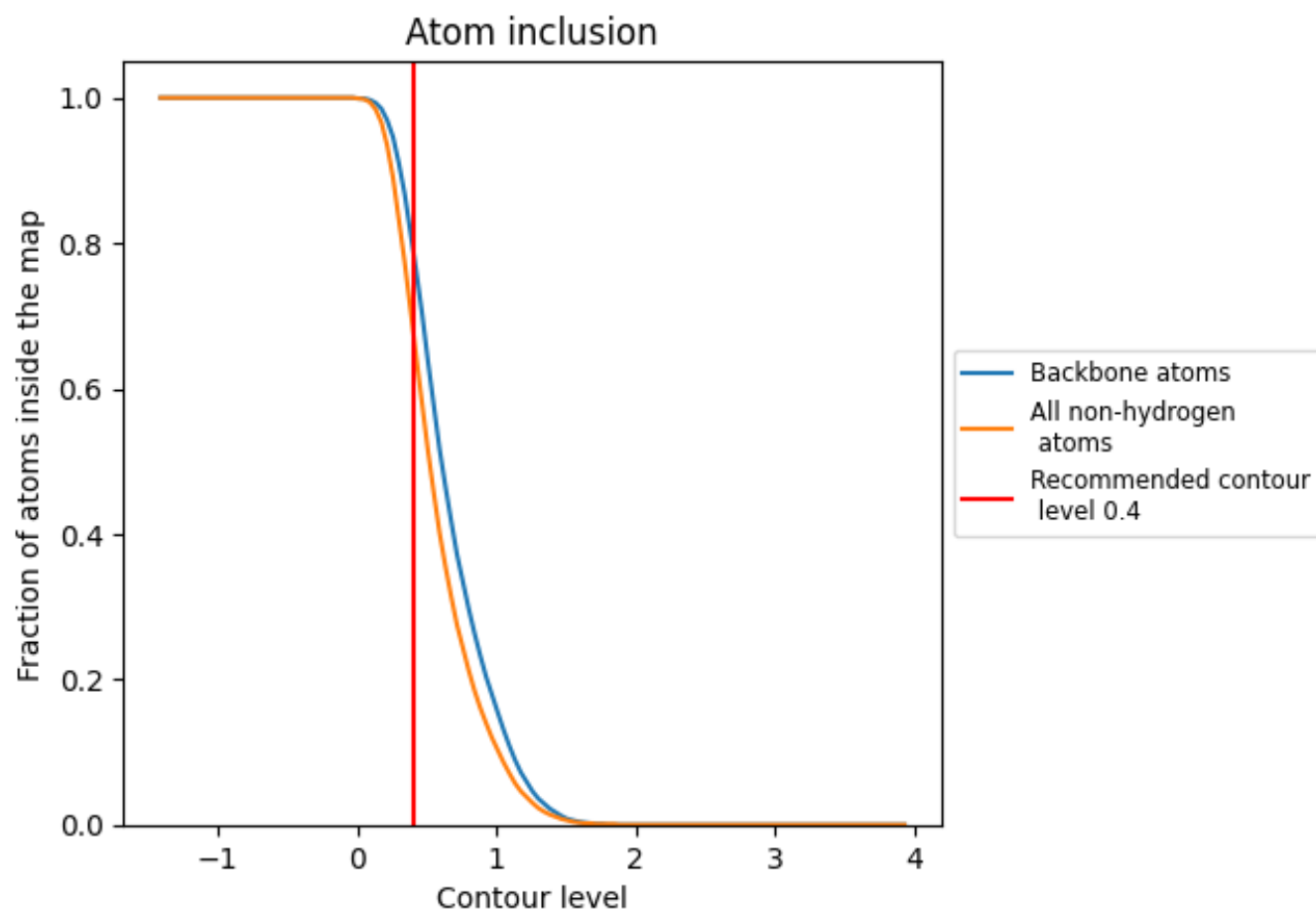
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 68% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6820	0.5000
E	0.5090	0.4760
F	0.7700	0.5160
I	0.6750	0.4860
J	0.6920	0.5020
K	0.5150	0.4620
L	0.7260	0.5140
M	0.5450	0.4740
N	0.7200	0.5200
P	0.6650	0.4990
Y	0.4960	0.4590
Z	0.7060	0.5010
e	0.5170	0.4720
f	0.7440	0.5130
h	0.6400	0.4780
m	0.5860	0.4830

