



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 09:04 AM EST

PDB ID : 3JBH
EMDB ID : EMD-1950
Title : TWO HEAVY MEROMYOSIN INTERACTING-HEADS MOTIFS FLEXIBLE DOCKED INTO TARANTULA THICK FILAMENT 3D-MAP ALLOWS IN DEPTH STUDY OF INTRA- AND INTERMOLECULAR INTERACTIONS
Authors : Alamo, L.; Qi, D.; Wriggers, W.; Pinto, A.; Zhu, J.; Bilbao, A.; Gillilan, R.E.; Hu, S.; Padron, R.
Deposited on : 2015-09-01
Resolution : 20.00 Å (reported)
Based on initial model : 3DTP

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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

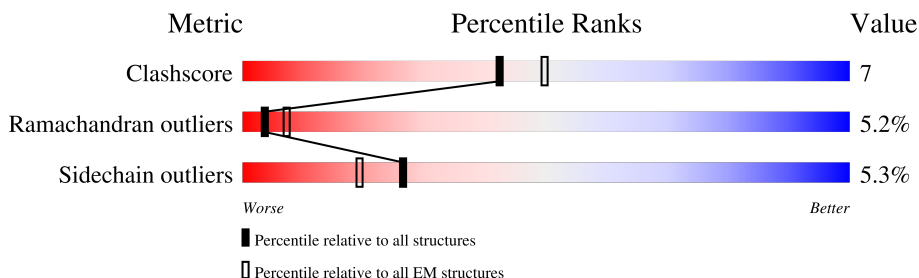
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 20.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1953	
1	B	1953	
1	G	1953	
1	H	1953	
2	C	156	
2	D	156	
2	I	156	
2	J	156	

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Mol	Chain	Length	Quality of chain
3	E	196	<div><div></div><div>73%24%</div><div></div></div>
3	F	196	<div><div>5%</div><div>64%29%6%</div><div></div></div>
3	K	196	<div><div></div><div>78%19%</div><div></div></div>
3	L	196	<div><div>5%</div><div>63%28%7%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 41968 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 MYOSIN 2 HEAVY CHAIN STRIATED MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	962	Total	C	N	O	S	0	0
			7721	4907	1334	1450	30		
1	B	964	Total	C	N	O	S	0	0
			7739	4918	1338	1453	30		
1	G	962	Total	C	N	O	S	0	0
			7721	4907	1334	1450	30		
1	H	964	Total	C	N	O	S	0	0
			7739	4918	1338	1453	30		

- Molecule 2 is a protein called MYOSIN 2 ESSENTIAL LIGHT CHAIN STRIATED MUSCLE.

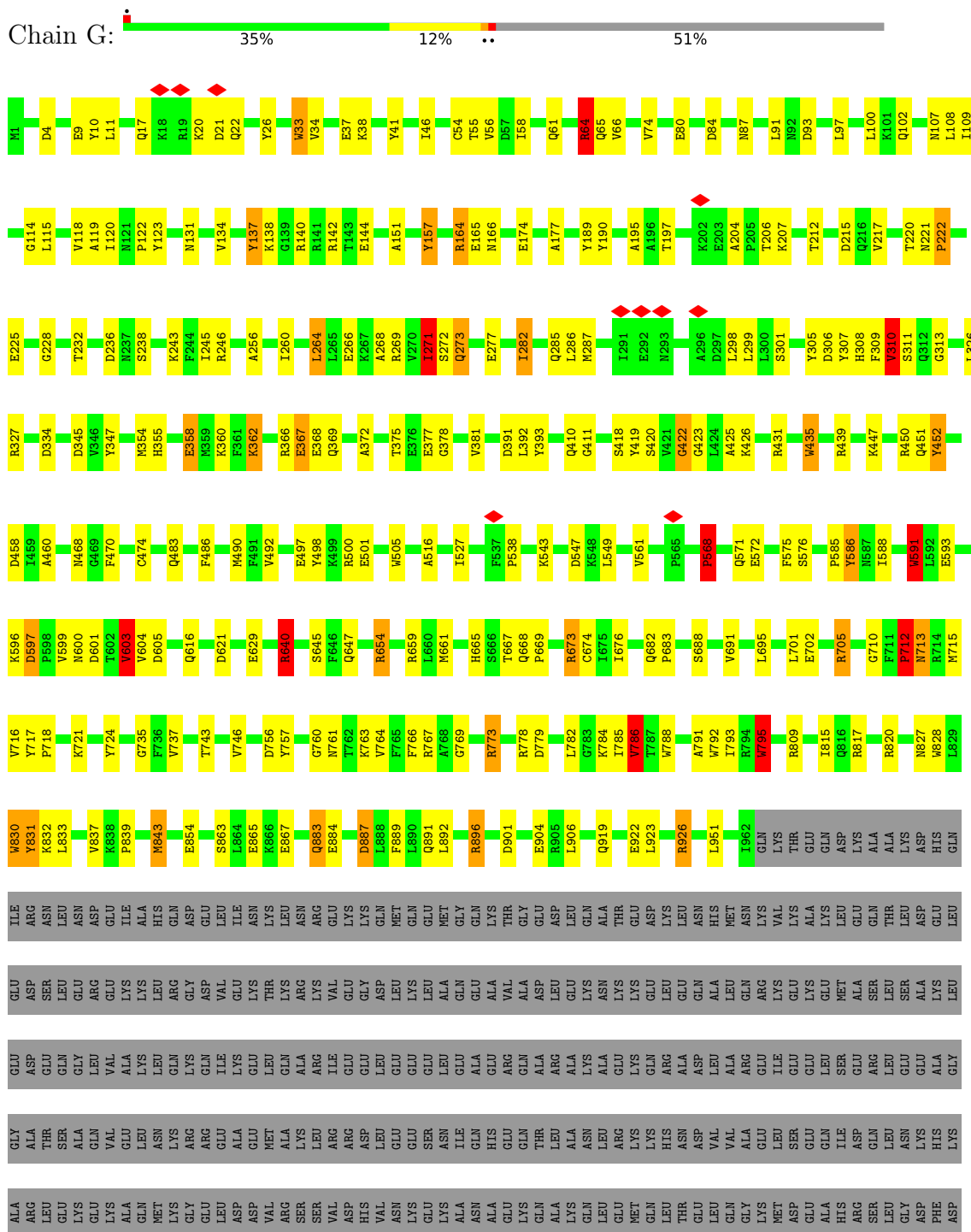
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	156	Total	C	N	O	S	0	0
			1233	779	199	247	8		
2	D	156	Total	C	N	O	S	0	0
			1233	779	199	247	8		
2	I	156	Total	C	N	O	S	0	0
			1233	779	199	247	8		
2	J	156	Total	C	N	O	S	0	0
			1233	779	199	247	8		

- Molecule 3 is a protein called MYOSIN 2 REGULATORY LIGHT CHAIN STRIATED MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	196	Total	C	N	O	S	0	0
			1529	952	257	314	6		
3	F	196	Total	C	N	O	S	0	0
			1529	952	257	314	6		
3	K	196	Total	C	N	O	S	0	0
			1529	952	257	314	6		
3	L	196	Total	C	N	O	S	0	0
			1529	952	257	314	6		

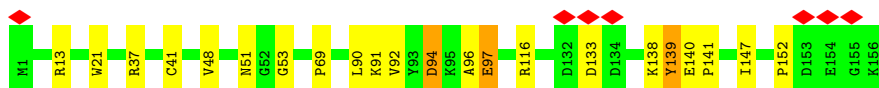
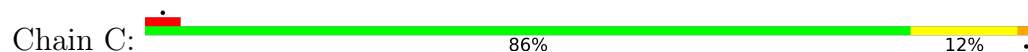
W435	R439	L440	D447	N441	T446	K447	Q448	K449	R450	Q451	Y452	F453	I454	G455	V456	E463	E480	K481	H488	F491	V492	L493	E494	Q495	E496	E497	Y498	K499	R500	E501	D504	W505	C517	I518	E519	L520	I521	K523	P524	M525	G526	I527	L528	S529	I530	L531	E534	S535	M536	F537

- Molecule 1: MYOSIN 2 HEAVY CHAIN STRIATED MUSCLE

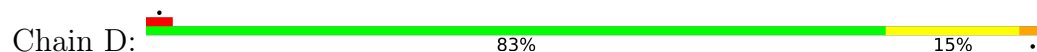




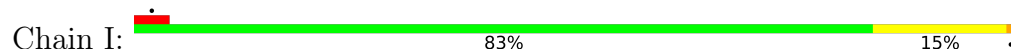
- Molecule 2: MYOSIN 2 ESSENTIAL LIGHT CHAIN STRIATED MUSCLE



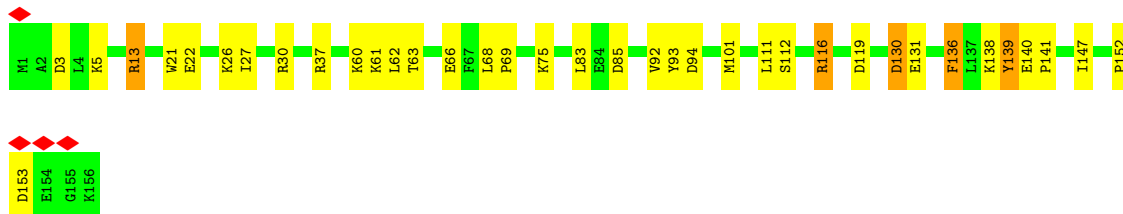
- Molecule 2: MYOSIN 2 ESSENTIAL LIGHT CHAIN STRIATED MUSCLE



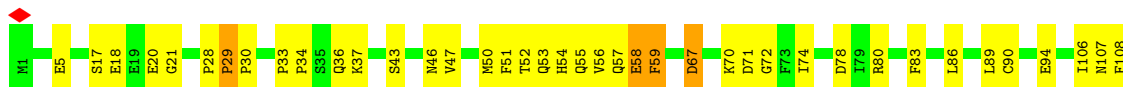
- Molecule 2: MYOSIN 2 ESSENTIAL LIGHT CHAIN STRIATED MUSCLE



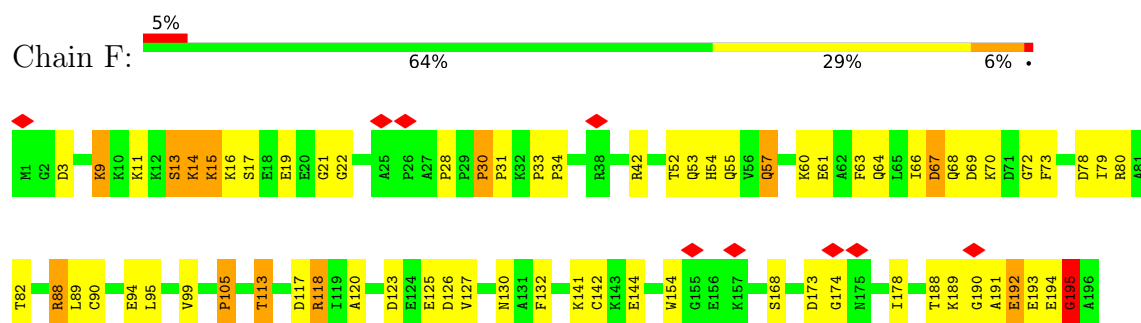
- Molecule 2: MYOSIN 2 ESSENTIAL LIGHT CHAIN STRIATED MUSCLE



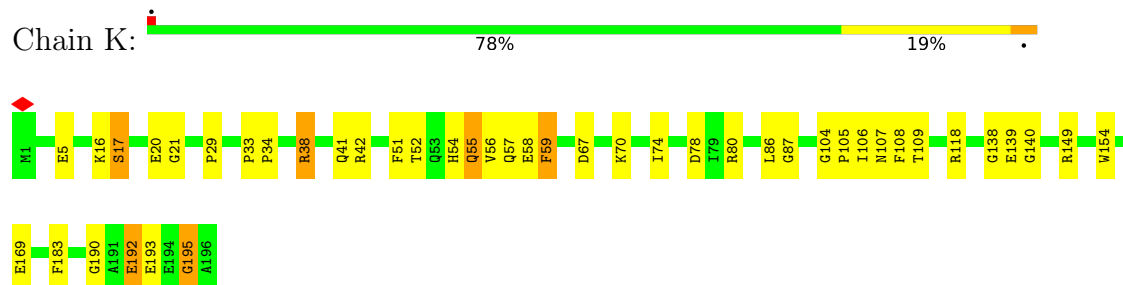
- Molecule 3: MYOSIN 2 REGULATORY LIGHT CHAIN STRIATED MUSCLE



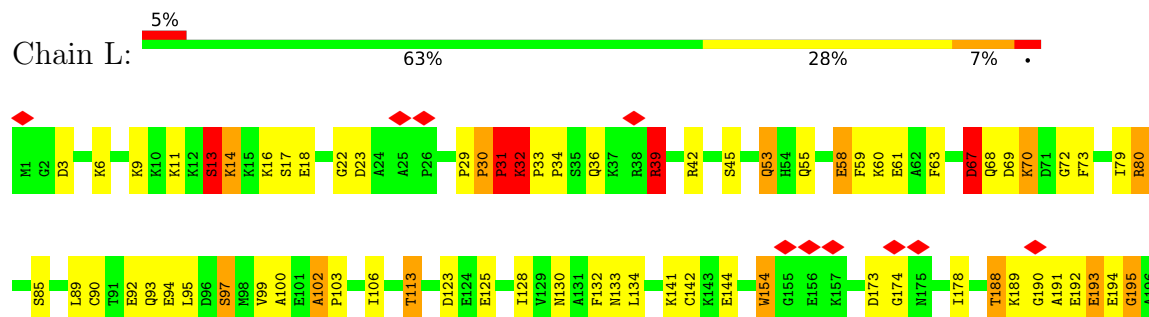
- Molecule 3: MYOSIN 2 REGULATORY LIGHT CHAIN STRIATED MUSCLE



• Molecule 3: MYOSIN 2 REGULATORY LIGHT CHAIN STRIATED MUSCLE



• Molecule 3: MYOSIN 2 REGULATORY LIGHT CHAIN STRIATED MUSCLE



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=30°, rise=100 Å, axial sym=C4	Depositor
Number of segments used	Not provided	
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI/PHILIPS CM120T	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	1950	Depositor
Maximum defocus (nm)	1950	Depositor
Magnification	35000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	247.077	Depositor
Minimum map value	-0.037	Depositor
Average map value	10.023	Depositor
Map value standard deviation	28.567	Depositor
Recommended contour level	25.0	Depositor
Map size (Å)	620, 620, 620.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.48, 2.48, 2.482	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	0.65	0/7867	1.36	93/10591 (0.9%)
1	B	0.64	0/7885	1.35	68/10614 (0.6%)
1	G	0.64	0/7867	1.33	75/10591 (0.7%)
1	H	0.64	0/7885	1.34	64/10614 (0.6%)
2	C	0.66	0/1251	1.20	6/1674 (0.4%)
2	D	0.66	0/1251	1.19	8/1674 (0.5%)
2	I	0.64	0/1251	1.21	9/1674 (0.5%)
2	J	0.65	0/1251	1.21	7/1674 (0.4%)
3	E	0.64	0/1554	1.20	10/2081 (0.5%)
3	F	0.64	0/1554	1.30	11/2081 (0.5%)
3	K	0.65	0/1554	1.24	9/2081 (0.4%)
3	L	0.69	0/1554	1.40	17/2081 (0.8%)
All	All	0.65	0/42724	1.32	377/57430 (0.7%)

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	32
1	B	0	20
1	G	0	25
1	H	0	19
2	D	0	1
2	I	0	1
2	J	0	4
3	E	0	1
3	F	0	3
3	K	0	2
3	L	0	8
All	All	0	116

There are no bond length outliers.

All (377) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	PRO	CA-N-CD	-13.39	92.75	111.50
1	B	380	ARG	NE-CZ-NH1	-12.71	113.94	120.30
1	G	140	ARG	NE-CZ-NH1	-10.79	114.91	120.30
1	B	654	ARG	NE-CZ-NH1	-10.67	114.97	120.30
1	G	367	GLU	CA-C-N	10.62	140.56	117.20
1	G	367	GLU	O-C-N	-10.30	106.22	122.70
1	H	64	ARG	NE-CZ-NH1	-10.23	115.18	120.30
1	G	64	ARG	NE-CZ-NH1	-10.13	115.24	120.30
1	G	778	ARG	NE-CZ-NH1	-9.87	115.36	120.30
1	A	367	GLU	CA-C-N	9.85	138.87	117.20
1	B	12	TYR	CB-CG-CD2	-9.84	115.10	121.00
3	L	39	ARG	NE-CZ-NH1	-9.62	115.49	120.30
1	H	929	ARG	NE-CZ-NH1	-9.50	115.55	120.30
1	A	367	GLU	O-C-N	-9.49	107.52	122.70
1	H	364	ARG	NE-CZ-NH1	-9.40	115.60	120.30
1	A	364	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	A	365	PRO	N-CA-C	9.18	135.98	112.10
1	B	439	ARG	NE-CZ-NH1	-9.11	115.74	120.30
1	A	140	ARG	NE-CZ-NH1	-9.09	115.76	120.30
1	G	310	VAL	CA-C-N	9.03	137.06	117.20
3	E	154	TRP	CD1-CG-CD2	9.02	113.51	106.30
1	B	929	ARG	NE-CZ-NH1	-8.99	115.80	120.30
1	A	505	TRP	CD1-CG-CD2	8.94	113.45	106.30
1	G	505	TRP	CD1-CG-CD2	8.93	113.44	106.30
1	G	310	VAL	O-C-N	-8.91	108.45	122.70
1	H	654	ARG	NE-CZ-NH1	-8.85	115.87	120.30
2	C	21	TRP	CD1-CG-CD2	8.84	113.37	106.30
1	B	140	ARG	NE-CZ-NH1	-8.79	115.91	120.30
1	G	788	TRP	CD1-CG-CD2	8.72	113.28	106.30
1	A	306	ASP	N-CA-C	8.62	134.27	111.00
1	A	591	TRP	CD1-CG-CD2	8.57	113.16	106.30
1	H	929	ARG	NE-CZ-NH2	8.57	124.58	120.30
1	B	794	ARG	NE-CZ-NH1	-8.56	116.02	120.30
3	L	13	SER	O-C-N	-8.55	109.02	122.70
3	K	118	ARG	NE-CZ-NH1	-8.52	116.04	120.30
1	G	206	THR	CA-C-N	8.49	135.87	117.20
1	A	788	TRP	CD1-CG-CD2	8.48	113.08	106.30
1	A	362	LYS	C-N-CA	8.46	142.85	121.70
3	L	154	TRP	CD1-CG-CD2	8.46	113.07	106.30
1	H	828	TRP	CD1-CG-CD2	8.44	113.05	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	21	TRP	CD1-CG-CD2	8.43	113.04	106.30
1	H	565	PRO	N-CA-C	8.39	133.91	112.10
1	B	830	TRP	CD1-CG-CD2	8.38	113.00	106.30
3	E	118	ARG	NE-CZ-NH2	8.36	124.48	120.30
1	A	778	ARG	NE-CZ-NH1	-8.35	116.13	120.30
1	A	788	TRP	CE2-CD2-CG	-8.33	100.64	107.30
2	J	13	ARG	NE-CZ-NH1	-8.33	116.14	120.30
1	H	830	TRP	CD1-CG-CD2	8.32	112.95	106.30
1	A	505	TRP	CE2-CD2-CG	-8.26	100.69	107.30
1	B	103	ARG	NE-CZ-NH2	8.21	124.40	120.30
1	A	206	THR	CA-C-N	8.20	135.24	117.20
1	B	795	TRP	CD1-CG-CD2	8.19	112.85	106.30
1	H	500	ARG	NE-CZ-NH2	8.18	124.39	120.30
1	B	565	PRO	N-CA-C	8.17	133.34	112.10
1	G	505	TRP	CE2-CD2-CG	-8.14	100.78	107.30
1	G	788	TRP	CE2-CD2-CG	-8.13	100.79	107.30
1	G	673	ARG	NE-CZ-NH1	-8.11	116.24	120.30
1	H	788	TRP	CD1-CG-CD2	8.11	112.78	106.30
1	G	591	TRP	CD1-CG-CD2	8.09	112.77	106.30
1	H	591	TRP	CD1-CG-CD2	8.09	112.77	106.30
1	B	640	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	A	828	TRP	CD1-CG-CD2	8.08	112.77	106.30
1	B	828	TRP	CD1-CG-CD2	8.08	112.76	106.30
3	E	154	TRP	CE2-CD2-CG	-8.05	100.86	107.30
1	A	828	TRP	CE2-CD2-CG	-8.04	100.87	107.30
1	A	435	TRP	CD1-CG-CD2	8.03	112.72	106.30
1	H	64	ARG	NE-CZ-NH2	8.00	124.30	120.30
2	I	37	ARG	NE-CZ-NH1	-8.00	116.30	120.30
3	K	154	TRP	CD1-CG-CD2	7.99	112.69	106.30
2	C	21	TRP	CE2-CD2-CG	-7.99	100.91	107.30
1	H	830	TRP	CE2-CD2-CG	-7.97	100.92	107.30
1	G	435	TRP	CD1-CG-CD2	7.95	112.66	106.30
3	F	154	TRP	CD1-CG-CD2	7.93	112.64	106.30
1	B	33	TRP	CE2-CD2-CG	-7.92	100.96	107.30
1	A	311	SER	N-CA-C	7.92	132.37	111.00
1	H	795	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	G	140	ARG	NE-CZ-NH2	7.84	124.22	120.30
1	G	568	PRO	CA-N-CD	-7.83	100.54	111.50
1	H	33	TRP	CD1-CG-CD2	7.81	112.55	106.30
2	C	13	ARG	NE-CZ-NH2	7.77	124.19	120.30
1	A	33	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	G	206	THR	O-C-N	-7.68	110.42	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	792	TRP	CD1-CG-CD2	7.68	112.44	106.30
1	G	792	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	B	788	TRP	CD1-CG-CD2	7.66	112.43	106.30
1	H	435	TRP	CD1-CG-CD2	7.66	112.43	106.30
1	B	830	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	H	505	TRP	CD1-CG-CD2	7.65	112.42	106.30
2	J	21	TRP	CD1-CG-CD2	7.65	112.42	106.30
3	L	154	TRP	CE2-CD2-CG	-7.64	101.18	107.30
1	A	591	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	B	792	TRP	CD1-CG-CD2	7.64	112.41	106.30
1	G	828	TRP	CD1-CG-CD2	7.64	112.41	106.30
1	H	33	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	H	591	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	G	828	TRP	CE2-CD2-CG	-7.62	101.20	107.30
2	I	21	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	B	33	TRP	CD1-CG-CD2	7.61	112.38	106.30
1	B	505	TRP	CD1-CG-CD2	7.61	112.38	106.30
1	G	33	TRP	CD1-CG-CD2	7.59	112.38	106.30
1	G	268	ALA	CA-C-N	7.57	133.85	117.20
1	B	435	TRP	CD1-CG-CD2	7.54	112.33	106.30
1	A	363	GLN	N-CA-CB	-7.53	97.05	110.60
3	K	118	ARG	NE-CZ-NH2	7.49	124.04	120.30
1	H	788	TRP	CE2-CD2-CG	-7.48	101.31	107.30
1	G	896	ARG	NE-CZ-NH1	-7.48	116.56	120.30
1	H	505	TRP	CE2-CD2-CG	-7.48	101.32	107.30
3	K	154	TRP	CE2-CD2-CG	-7.47	101.32	107.30
1	H	828	TRP	CE2-CD2-CG	-7.47	101.33	107.30
1	A	206	THR	O-C-N	-7.47	110.75	122.70
3	F	154	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	B	795	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	B	809	ARG	NE-CZ-NH1	-7.42	116.59	120.30
2	D	21	TRP	CE2-CD2-CG	-7.42	101.37	107.30
1	B	792	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	B	505	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	A	364	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	B	591	TRP	CD1-CG-CD2	7.39	112.21	106.30
1	A	640	ARG	NE-CZ-NH1	-7.37	116.62	120.30
1	G	435	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	A	500	ARG	NE-CZ-NH2	7.35	123.97	120.30
1	A	896	ARG	NE-CZ-NH1	-7.33	116.64	120.30
1	A	792	TRP	CD1-CG-CD2	7.31	112.15	106.30
1	B	788	TRP	CE2-CD2-CG	-7.30	101.46	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	13	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	A	435	TRP	CE2-CD2-CG	-7.27	101.48	107.30
1	B	828	TRP	CE2-CD2-CG	-7.27	101.49	107.30
1	G	450	ARG	NE-CZ-NH1	-7.26	116.67	120.30
1	A	673	ARG	NE-CZ-NH1	-7.26	116.67	120.30
1	H	795	TRP	CE2-CD2-CG	-7.25	101.50	107.30
2	J	21	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	G	591	TRP	CE2-CD2-CG	-7.23	101.52	107.30
1	B	591	TRP	CE2-CD2-CG	-7.22	101.52	107.30
1	G	926	ARG	NE-CZ-NH2	7.22	123.91	120.30
1	A	363	GLN	CA-CB-CG	7.22	129.29	113.40
1	A	654	ARG	NE-CZ-NH2	7.21	123.91	120.30
3	E	192	GLU	O-C-N	-7.21	111.17	122.70
1	H	792	TRP	CE2-CD2-CG	-7.21	101.54	107.30
1	G	654	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	G	268	ALA	O-C-N	-7.19	111.19	122.70
3	L	195	GLY	O-C-N	-7.19	111.20	122.70
1	A	792	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	H	794	ARG	NE-CZ-NH1	-7.15	116.73	120.30
3	K	192	GLU	O-C-N	-7.14	111.27	122.70
1	A	268	ALA	CA-C-N	7.13	132.89	117.20
1	H	435	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	A	33	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	G	593	GLU	CA-CB-CG	7.12	129.06	113.40
1	G	830	TRP	CD1-CG-CD2	7.11	111.99	106.30
2	D	21	TRP	CD1-CG-CD2	7.11	111.99	106.30
2	D	134	ASP	CA-C-N	7.09	130.38	116.20
1	G	795	TRP	CD1-CG-CD2	7.08	111.96	106.30
1	G	795	TRP	CE2-CD2-CG	-7.06	101.65	107.30
2	D	134	ASP	O-C-N	-7.05	111.21	123.20
1	A	830	TRP	CD1-CG-CD2	7.04	111.94	106.30
3	L	13	SER	CA-C-N	7.01	132.62	117.20
1	A	794	ARG	NE-CZ-NH1	-6.99	116.81	120.30
1	G	792	TRP	CE2-CD2-CG	-6.99	101.71	107.30
1	B	380	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	A	795	TRP	CE2-CD2-CG	-6.96	101.73	107.30
1	G	33	TRP	CE2-CD2-CG	-6.93	101.75	107.30
1	G	830	TRP	CE2-CD2-CG	-6.89	101.79	107.30
1	B	435	TRP	CE2-CD2-CG	-6.88	101.79	107.30
3	L	195	GLY	CA-C-N	6.86	132.28	117.20
1	H	12	TYR	CB-CG-CD2	-6.85	116.89	121.00
1	A	365	PRO	CA-C-N	-6.84	102.15	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	42	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	A	830	TRP	CE2-CD2-CG	-6.83	101.83	107.30
1	B	64	ARG	NE-CZ-NH1	-6.79	116.91	120.30
1	B	872	LYS	CG-CD-CE	6.78	132.24	111.90
1	A	828	TRP	CB-CG-CD1	-6.73	118.25	127.00
1	G	640	ARG	NE-CZ-NH1	-6.71	116.94	120.30
1	A	364	ARG	CD-NE-CZ	-6.71	114.21	123.60
1	A	312	GLN	N-CA-C	6.70	129.08	111.00
1	H	364	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	G	450	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	B	640	ARG	NE-CZ-NH1	6.61	123.61	120.30
2	J	37	ARG	NE-CZ-NH1	-6.61	117.00	120.30
1	A	767	ARG	NE-CZ-NH2	6.61	123.60	120.30
1	A	788	TRP	CG-CD2-CE3	6.60	139.84	133.90
1	H	439	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	B	33	TRP	CB-CG-CD1	-6.56	118.47	127.00
1	B	439	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	A	781	ARG	NE-CZ-NH1	-6.55	117.03	120.30
1	A	364	ARG	N-CA-C	6.54	128.66	111.00
1	A	795	TRP	CD1-CG-CD2	6.49	111.49	106.30
1	A	673	ARG	NE-CZ-NH2	6.47	123.53	120.30
1	A	603	VAL	N-CA-C	6.47	128.46	111.00
1	G	809	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	A	313	GLY	O-C-N	-6.43	112.42	122.70
3	K	195	GLY	O-C-N	-6.39	112.48	122.70
3	F	14	LYS	N-CA-C	6.37	128.19	111.00
1	B	708	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	B	708	ARG	NE-CZ-NH2	6.30	123.45	120.30
3	E	192	GLU	CA-C-N	6.30	131.06	117.20
1	A	268	ALA	O-C-N	-6.29	112.63	122.70
1	A	451	GLN	O-C-N	-6.29	112.63	122.70
1	G	422	GLY	CA-C-N	6.26	128.72	116.20
3	L	31	PRO	N-CD-CG	-6.26	93.81	103.20
1	H	280	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	A	788	TRP	CB-CG-CD1	-6.25	118.87	127.00
1	G	712	PRO	N-CA-C	6.24	128.33	112.10
1	A	306	ASP	CA-C-N	-6.23	103.49	117.20
1	G	157	TYR	CB-CG-CD2	-6.22	117.27	121.00
1	A	240	ARG	NE-CZ-NH2	6.19	123.40	120.30
2	J	30	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	B	364	ARG	NE-CZ-NH2	6.18	123.39	120.30
3	F	88	ARG	NE-CZ-NH2	6.17	123.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	192	GLU	CA-C-N	6.14	130.71	117.20
1	A	363	GLN	N-CA-C	6.13	127.55	111.00
1	A	368	GLU	N-CA-C	6.11	127.51	111.00
1	B	500	ARG	NE-CZ-NH1	-6.11	117.24	120.30
1	G	788	TRP	CG-CD2-CE3	6.09	139.38	133.90
1	B	500	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	G	705	ARG	NE-CZ-NH1	-6.07	117.27	120.30
2	D	127	ARG	NE-CZ-NH2	6.05	123.32	120.30
1	B	659	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	G	788	TRP	CB-CG-CD1	-6.02	119.18	127.00
1	H	796	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	A	596	LYS	CA-CB-CG	6.01	126.63	113.40
1	H	380	ARG	NE-CZ-NH1	-6.01	117.30	120.30
1	A	831	TYR	CB-CG-CD2	-6.00	117.40	121.00
1	B	641	LYS	O-C-N	-6.00	113.11	122.70
1	H	33	TRP	CB-CG-CD1	-5.99	119.21	127.00
1	B	905	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	G	313	GLY	O-C-N	-5.99	113.12	122.70
1	H	871	ARG	NE-CZ-NH1	-5.98	117.31	120.30
3	L	31	PRO	N-CA-CB	-5.97	96.04	102.60
3	K	149	ARG	NE-CZ-NH1	-5.95	117.32	120.30
1	B	642	LYS	CA-C-N	5.93	128.07	116.20
1	H	773	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	G	828	TRP	CB-CG-CD1	-5.92	119.30	127.00
1	A	828	TRP	CG-CD2-CE3	5.92	139.23	133.90
1	H	164	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	B	941	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	A	712	PRO	N-CA-C	5.87	127.36	112.10
1	G	596	LYS	CA-CB-CG	5.86	126.28	113.40
1	A	373	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	498	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	A	64	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	A	103	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	G	498	TYR	CB-CG-CD2	-5.81	117.51	121.00
1	H	412	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	B	33	TRP	CG-CD2-CE3	5.81	139.13	133.90
1	B	103	ARG	NE-CZ-NH1	-5.81	117.40	120.30
1	B	452	TYR	CB-CG-CD2	-5.80	117.52	121.00
1	A	778	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	A	313	GLY	CA-C-N	5.79	129.95	117.20
1	B	926	ARG	NE-CZ-NH2	5.77	123.19	120.30
1	G	603	VAL	N-CA-C	5.75	126.54	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	116	ARG	NE-CZ-NH1	-5.75	117.43	120.30
3	K	42	ARG	NE-CZ-NH1	-5.75	117.43	120.30
3	F	13	SER	O-C-N	-5.73	113.53	122.70
1	H	673	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	A	568	PRO	CA-N-CD	-5.72	103.49	111.50
1	A	795	TRP	CB-CG-CD1	-5.72	119.56	127.00
1	B	269	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	G	640	ARG	NE-CZ-NH2	5.71	123.16	120.30
1	H	673	ARG	N-CA-CB	-5.71	100.32	110.60
3	L	67	ASP	N-CA-C	5.71	126.40	111.00
2	D	57	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	A	505	TRP	CG-CD2-CE3	5.68	139.02	133.90
3	E	118	ARG	NE-CZ-NH1	-5.68	117.46	120.30
3	F	195	GLY	O-C-N	-5.68	113.61	122.70
1	A	431	ARG	NE-CZ-NH2	5.67	123.13	120.30
1	A	773	ARG	NE-CZ-NH2	5.67	123.13	120.30
1	H	673	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	H	767	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	B	210	LYS	O-C-N	-5.63	113.69	122.70
3	E	195	GLY	O-C-N	-5.63	113.69	122.70
1	H	565	PRO	CA-N-CD	-5.63	103.62	111.50
1	G	505	TRP	CG-CD2-CE3	5.61	138.95	133.90
1	H	830	TRP	CG-CD2-CE3	5.58	138.92	133.90
1	H	598	PRO	N-CA-C	5.57	126.59	112.10
1	G	820	ARG	NE-CZ-NH1	-5.57	117.51	120.30
1	H	33	TRP	CG-CD2-CE3	5.57	138.91	133.90
1	A	871	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	G	33	TRP	CB-CG-CD1	-5.56	119.77	127.00
1	G	142	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	B	12	TYR	CB-CG-CD1	5.55	124.33	121.00
1	G	887	ASP	CB-CG-OD1	5.55	123.30	118.30
1	H	830	TRP	CB-CG-CD1	-5.55	119.78	127.00
1	H	724	TYR	CB-CG-CD2	-5.54	117.68	121.00
1	B	872	LYS	CB-CG-CD	5.52	125.96	111.60
2	C	21	TRP	CG-CD1-NE1	-5.52	104.58	110.10
2	C	21	TRP	CG-CD2-CE3	5.51	138.85	133.90
3	F	195	GLY	CA-C-N	5.51	129.32	117.20
1	H	141	ARG	NE-CZ-NH2	5.49	123.04	120.30
1	A	375	THR	CA-C-N	5.48	129.25	117.20
1	G	505	TRP	CG-CD1-NE1	-5.48	104.62	110.10
1	G	788	TRP	CG-CD1-NE1	-5.47	104.63	110.10
3	E	154	TRP	CG-CD1-NE1	-5.44	104.66	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	828	TRP	CG-CD2-CE3	5.44	138.80	133.90
1	A	809	ARG	NE-CZ-NH2	5.43	123.01	120.30
3	L	31	PRO	O-C-N	-5.42	114.02	122.70
2	D	13	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	G	313	GLY	CA-C-N	5.41	129.10	117.20
1	H	659	ARG	NE-CZ-NH2	5.41	123.00	120.30
3	E	154	TRP	CG-CD2-CE3	5.40	138.76	133.90
2	I	139	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	B	565	PRO	CA-N-CD	-5.39	103.95	111.50
1	H	137	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	B	280	TYR	CB-CG-CD2	-5.38	117.77	121.00
2	I	21	TRP	CB-CG-CD1	-5.37	120.02	127.00
1	G	64	ARG	NE-CZ-NH2	5.37	122.99	120.30
2	D	37	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	G	786	VAL	CA-CB-CG2	5.36	118.93	110.90
3	L	17	SER	N-CA-C	5.34	125.43	111.00
1	A	505	TRP	CG-CD1-NE1	-5.33	104.77	110.10
1	H	439	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	B	637	GLY	CA-C-N	5.32	126.85	116.20
3	E	154	TRP	CB-CG-CD1	-5.32	120.08	127.00
1	H	140	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	A	505	TRP	CB-CG-CD1	-5.30	120.11	127.00
1	A	189	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	A	360	LYS	O-C-N	-5.30	114.22	122.70
1	G	327	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	B	830	TRP	CB-CG-CD1	-5.29	120.12	127.00
1	H	809	ARG	NE-CZ-NH1	-5.29	117.65	120.30
3	F	67	ASP	N-CA-C	5.28	125.27	111.00
1	G	597	ASP	N-CA-C	5.28	125.27	111.00
3	L	17	SER	O-C-N	-5.28	114.26	122.70
3	L	154	TRP	CG-CD2-CE3	5.27	138.64	133.90
1	A	207	LYS	N-CA-CB	5.27	120.08	110.60
1	A	367	GLU	C-N-CA	5.27	134.87	121.70
1	A	640	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	G	431	ARG	NE-CZ-NH2	5.25	122.93	120.30
1	B	210	LYS	CA-C-N	5.25	128.75	117.20
1	G	596	LYS	N-CA-CB	-5.24	101.17	110.60
1	H	19	ARG	NE-CZ-NH1	-5.24	117.68	120.30
3	L	154	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	A	591	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	H	86	SER	N-CA-C	5.22	125.09	111.00
1	G	773	ARG	NE-CZ-NH2	5.21	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	16	LYS	O-C-N	-5.20	114.38	122.70
1	B	637	GLY	O-C-N	-5.20	114.36	123.20
2	C	21	TRP	CB-CG-CD1	-5.20	120.24	127.00
1	H	637	GLY	CA-C-N	5.20	126.60	116.20
1	H	771	LEU	CA-CB-CG	5.20	127.25	115.30
1	G	820	ARG	NE-CZ-NH2	5.19	122.90	120.30
2	I	156	LYS	CB-CG-CD	-5.19	98.11	111.60
1	H	453	PHE	N-CA-C	5.18	124.98	111.00
3	L	39	ARG	NE-CZ-NH2	5.16	122.88	120.30
2	I	21	TRP	CG-CD2-CE3	5.15	138.54	133.90
1	B	828	TRP	CG-CD1-NE1	-5.14	104.95	110.10
1	A	450	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	B	164	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	A	795	TRP	CG-CD2-CE3	5.13	138.52	133.90
1	H	28	GLY	O-C-N	-5.12	114.51	122.70
1	H	234	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	A	788	TRP	CG-CD1-NE1	-5.10	105.00	110.10
1	B	146	PRO	N-CA-CB	-5.10	96.99	102.60
1	G	422	GLY	O-C-N	-5.10	114.53	123.20
1	G	659	ARG	NE-CZ-NH2	5.09	122.84	120.30
2	I	21	TRP	CG-CD1-NE1	-5.09	105.01	110.10
1	A	365	PRO	CA-CB-CG	-5.09	94.33	104.00
1	G	246	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	A	142	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	B	132	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	33	TRP	CB-CG-CD1	-5.07	120.41	127.00
1	A	596	LYS	N-CA-CB	-5.07	101.48	110.60
3	F	154	TRP	CG-CD2-CE3	5.06	138.46	133.90
1	A	364	ARG	CA-C-N	5.06	131.26	117.10
1	B	870	VAL	CA-C-N	5.05	128.32	117.20
1	G	591	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	H	619	PHE	N-CA-C	5.05	124.64	111.00
1	H	828	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	H	505	TRP	CG-CD2-CE3	5.05	138.44	133.90
1	B	149	LEU	N-CA-C	5.04	124.60	111.00
1	G	137	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	B	141	ARG	NE-CZ-NH2	5.03	122.81	120.30
3	F	118	ARG	NE-CZ-NH1	-5.03	117.79	120.30
1	B	830	TRP	CG-CD1-NE1	-5.01	105.09	110.10
1	B	505	TRP	CG-CD2-CE3	5.01	138.41	133.90
1	A	140	ARG	NE-CZ-NH2	5.01	122.81	120.30
2	J	139	TYR	CB-CG-CD1	-5.00	118.00	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	367	GLU	C-N-CA	5.00	134.21	121.70

There are no chirality outliers.

All (116) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	TYR	Sidechain
1	A	142	ARG	Sidechain
1	A	157	TYR	Sidechain
1	A	190	TYR	Sidechain
1	A	269	ARG	Sidechain
1	A	272	SER	Peptide
1	A	280	TYR	Sidechain
1	A	307	TYR	Sidechain,Peptide
1	A	310	VAL	Peptide
1	A	361	PHE	Sidechain
1	A	363	GLN	Sidechain,Peptide,Mainchain
1	A	364	ARG	Sidechain
1	A	366	ARG	Sidechain,Peptide
1	A	393	TYR	Sidechain
1	A	41	TYR	Sidechain
1	A	410	GLN	Peptide
1	A	412	ARG	Sidechain
1	A	418	SER	Peptide
1	A	567	LYS	Peptide
1	A	586	TYR	Sidechain
1	A	64	ARG	Sidechain
1	A	640	ARG	Sidechain
1	A	708	ARG	Sidechain
1	A	724	TYR	Sidechain
1	A	757	TYR	Sidechain
1	A	796	TYR	Sidechain
1	A	831	TYR	Sidechain
1	A	871	ARG	Sidechain
1	B	103	ARG	Sidechain
1	B	190	TYR	Sidechain
1	B	26	TYR	Sidechain
1	B	278	ARG	Sidechain
1	B	366	ARG	Sidechain
1	B	41	TYR	Sidechain
1	B	419	TYR	Sidechain
1	B	450	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	526	GLY	Peptide
1	B	621	ASP	Peptide
1	B	627	ALA	Peptide
1	B	639	GLY	Peptide
1	B	645	SER	Peptide
1	B	654	ARG	Sidechain
1	B	659	ARG	Sidechain
1	B	673	ARG	Sidechain
1	B	708	ARG	Sidechain
1	B	714	ARG	Sidechain
1	B	867	GLU	Peptide
1	B	941	ARG	Sidechain
2	D	111	LEU	Peptide
3	E	80	ARG	Sidechain
3	F	113	THR	Peptide
3	F	80	ARG	Sidechain
3	F	9	LYS	Peptide
1	G	10	TYR	Sidechain
1	G	123	TYR	Sidechain
1	G	157	TYR	Sidechain
1	G	164	ARG	Sidechain
1	G	190	TYR	Sidechain
1	G	272	SER	Peptide
1	G	273	GLN	Peptide
1	G	305	TYR	Sidechain,Peptide
1	G	307	TYR	Sidechain
1	G	347	TYR	Sidechain
1	G	366	ARG	Peptide
1	G	41	TYR	Sidechain
1	G	410	GLN	Peptide
1	G	418	SER	Peptide
1	G	452	TYR	Sidechain
1	G	586	TYR	Sidechain
1	G	64	ARG	Sidechain
1	G	640	ARG	Sidechain
1	G	654	ARG	Sidechain
1	G	724	TYR	Sidechain
1	G	757	TYR	Sidechain
1	G	817	ARG	Sidechain
1	G	831	TYR	Sidechain
1	G	926	ARG	Sidechain
1	H	110	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	H	112	TYR	Sidechain
1	H	140	ARG	Sidechain
1	H	142	ARG	Sidechain
1	H	164	ARG	Sidechain
1	H	26	TYR	Sidechain
1	H	278	ARG	Sidechain
1	H	347	TYR	Sidechain
1	H	419	TYR	Sidechain
1	H	462	PHE	Sidechain
1	H	571	GLN	Peptide
1	H	621	ASP	Peptide
1	H	627	ALA	Peptide
1	H	647	GLN	Peptide
1	H	654	ARG	Sidechain
1	H	673	ARG	Sidechain
1	H	767	ARG	Sidechain
1	H	79	TYR	Sidechain
1	H	941	ARG	Sidechain
2	I	93	TYR	Sidechain
2	J	111	LEU	Peptide
2	J	116	ARG	Sidechain
2	J	13	ARG	Sidechain
2	J	136	PHE	Peptide
3	K	38	ARG	Sidechain
3	K	80	ARG	Sidechain
3	L	113	THR	Peptide
3	L	29	PRO	Peptide
3	L	30	PRO	Mainchain
3	L	31	PRO	Peptide
3	L	32	LYS	Mainchain,Peptide
3	L	39	ARG	Peptide
3	L	80	ARG	Sidechain

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	7721	0	7778	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7739	0	7799	165	0
1	G	7721	0	7778	108	0
1	H	7739	0	7799	130	0
2	C	1233	0	1227	9	0
2	D	1233	0	1227	9	0
2	I	1233	0	1227	10	0
2	J	1233	0	1227	14	0
3	E	1529	0	1491	27	0
3	F	1529	0	1491	28	0
3	K	1529	0	1491	23	0
3	L	1529	0	1491	47	0
All	All	41968	0	42026	606	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 7.

All (606) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:LYS:HE3	1:B:642:LYS:NZ	1.21	1.52
1:B:641:LYS:CE	1:B:642:LYS:NZ	2.16	1.08
1:A:364:ARG:HA	3:L:31:PRO:HG2	1.42	1.00
1:B:641:LYS:CE	1:B:642:LYS:HZ1	1.70	0.99
1:A:364:ARG:HA	3:L:31:PRO:CG	1.95	0.94
1:A:449:LYS:HD3	1:B:405:ASN:OD1	1.72	0.90
1:B:641:LYS:HE3	1:B:642:LYS:HZ2	1.07	0.90
1:B:635:LYS:HE3	1:B:904:GLU:HA	1.55	0.87
1:H:175:SER:HB2	1:H:463:GLU:HA	1.56	0.87
1:B:641:LYS:HE3	1:B:642:LYS:HZ1	1.01	0.80
1:A:369:GLN:HA	1:A:417:VAL:HG21	1.64	0.80
1:A:500:ARG:HG3	1:B:366:ARG:HB2	1.64	0.79
1:B:174:GLU:HB3	1:B:676:ILE:HD12	1.65	0.79
3:L:22:GLY:HA3	3:L:94:GLU:HG3	1.66	0.78
1:H:135:GLN:HG3	1:H:199:LYS:HE3	1.66	0.77
2:I:100:THR:HB	2:I:136:PHE:HB3	1.65	0.77
3:F:173:ASP:HB3	3:F:178:ILE:HG13	1.66	0.77
1:B:267:LYS:HD3	1:B:430:ASP:HB2	1.67	0.77
1:A:58:ILE:HB	1:A:61:GLN:HB2	1.68	0.76
1:A:833:LEU:HA	3:E:192:GLU:HG3	1.68	0.76
3:L:97:SER:HA	3:L:100:ALA:HB2	1.68	0.76
1:A:206:THR:HB	1:A:207:LYS:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:LYS:HE3	1:B:642:LYS:CE	2.17	0.75
3:E:51:PHE:HB3	3:E:56:VAL:HG21	1.67	0.75
1:G:58:ILE:HB	1:G:61:GLN:HB2	1.69	0.74
3:L:130:ASN:HA	3:L:133:ASN:HB3	1.69	0.74
3:E:192:GLU:HG2	3:E:193:GLU:HA	1.70	0.74
1:B:642:LYS:HE2	1:B:903:GLU:OE1	1.87	0.73
3:L:173:ASP:HB3	3:L:178:ILE:HG13	1.68	0.73
1:A:879:VAL:HG12	1:B:450:ARG:HB2	1.69	0.73
1:H:561:VAL:HB	1:H:576:SER:HB2	1.71	0.72
1:G:833:LEU:HA	3:K:192:GLU:HG3	1.73	0.70
2:I:101:MET:SD	2:I:139:TYR:HB3	2.31	0.70
1:B:902:VAL:HA	1:B:905:ARG:HB2	1.73	0.70
1:H:431:ARG:NH2	1:H:619:PHE:HA	2.07	0.70
2:J:26:LYS:HD2	2:J:61:LYS:HD3	1.73	0.69
1:A:449:LYS:HA	1:A:449:LYS:HE2	1.73	0.69
1:A:271:ILE:HD12	1:A:419:TYR:HA	1.75	0.69
1:G:716:VAL:HG12	1:G:763:LYS:HE2	1.75	0.69
1:H:597:ASP:HB3	1:H:646:PHE:HD2	1.58	0.68
1:B:7:PRO:HA	1:B:12:TYR:HE2	1.58	0.68
3:F:117:ASP:HA	3:F:120:ALA:HB3	1.76	0.67
1:B:13:ILE:HB	1:B:108:LEU:HD22	1.77	0.67
1:B:541:THR:HA	1:B:592:LEU:HD11	1.77	0.67
1:B:641:LYS:CE	1:B:642:LYS:HZ2	1.95	0.67
1:A:37:GLU:HB2	1:A:38:LYS:HD3	1.77	0.67
1:G:779:ASP:HA	1:G:782:LEU:HB2	1.77	0.67
1:A:34:VAL:HG11	1:A:58:ILE:HD12	1.75	0.67
1:G:367:GLU:HB2	1:G:369:GLN:H	1.61	0.66
1:A:309:PHE:HB2	3:L:18:GLU:HG3	1.77	0.66
1:A:772:GLY:HA2	1:A:775:GLU:HG3	1.78	0.65
1:B:175:SER:HB2	1:B:463:GLU:HA	1.76	0.65
1:A:364:ARG:HD2	1:A:371:GLU:H	1.62	0.65
3:K:51:PHE:HB2	3:L:61:GLU:HG2	1.79	0.65
1:H:244:PHE:O	1:H:260:ILE:HA	1.97	0.65
1:A:539:LYS:HD2	2:J:3:ASP:HB2	1.78	0.64
1:A:366:ARG:HA	3:L:39:ARG:HB2	1.78	0.64
1:B:716:VAL:HG13	1:B:718:PRO:HD2	1.79	0.64
1:B:431:ARG:NH2	1:B:619:PHE:HA	2.13	0.64
1:B:388:ASN:HB3	1:B:391:ASP:HB2	1.80	0.64
1:B:423:GLY:HA2	1:B:426:LYS:HE2	1.79	0.64
1:G:645:SER:HB3	1:G:647:GLN:HG3	1.80	0.64
1:A:100:LEU:HB3	1:A:120:ILE:HD11	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:THR:HA	1:B:746:VAL:HG22	1.81	0.63
1:B:635:LYS:HB3	1:B:642:LYS:CD	2.28	0.62
1:B:97:LEU:HD11	1:B:692:MET:HA	1.81	0.62
1:A:712:PRO:HD2	1:A:767:ARG:HA	1.81	0.62
1:G:500:ARG:HG3	1:H:366:ARG:HB2	1.81	0.62
1:A:364:ARG:HA	3:L:31:PRO:HG3	1.80	0.62
2:D:34:ASP:HA	2:D:37:ARG:HD2	1.81	0.62
1:G:34:VAL:HG11	1:G:58:ILE:HD12	1.82	0.62
1:A:762:THR:HG21	1:B:371:GLU:HB3	1.81	0.62
1:H:131:ASN:O	1:H:135:GLN:HB2	2.00	0.62
1:H:356:LEU:HD22	1:H:425:ALA:HB2	1.82	0.62
1:B:635:LYS:HB3	1:B:642:LYS:HD3	1.80	0.61
1:B:833:LEU:HD23	3:F:192:GLU:HG2	1.82	0.61
1:B:904:GLU:O	1:B:908:LYS:HB2	2.01	0.61
1:H:231:LYS:HB3	1:H:278:ARG:H	1.66	0.61
1:H:231:LYS:HG3	1:H:236:ASP:HA	1.83	0.61
1:A:399:PRO:O	1:A:409:THR:HA	2.01	0.61
1:G:166:ASN:ND2	1:G:667:THR:HG22	2.16	0.61
1:H:13:ILE:HB	1:H:108:LEU:HD22	1.83	0.60
1:H:171:ILE:HG12	1:H:672:VAL:HB	1.82	0.60
1:G:884:GLU:HA	1:G:887:ASP:HB2	1.82	0.60
1:G:309:PHE:HB2	1:G:362:LYS:HE3	1.84	0.60
1:H:211:ALA:HB3	1:H:214:GLU:HG2	1.82	0.60
3:E:109:THR:HG23	3:F:70:LYS:HD3	1.84	0.60
1:G:46:ILE:HG23	1:G:54:CYS:SG	2.41	0.60
1:B:431:ARG:HH22	1:B:619:PHE:HA	1.66	0.60
3:L:69:ASP:HB2	3:L:73:PHE:HB2	1.83	0.60
1:B:481:LYS:HD3	1:B:520:LEU:HA	1.84	0.60
1:G:785:ILE:HG23	1:G:786:VAL:HG23	1.83	0.60
1:G:37:GLU:HB2	1:G:38:LYS:HD3	1.82	0.59
1:H:84:ASP:HA	1:H:112:TYR:HB2	1.84	0.59
1:B:84:ASP:HA	1:B:112:TYR:HB2	1.84	0.59
1:B:142:ARG:HG2	1:B:145:VAL:HB	1.85	0.59
1:B:640:ARG:NH1	1:B:896:ARG:HG3	2.17	0.59
1:G:791:ALA:HB2	2:I:44:THR:HG22	1.85	0.59
1:H:498:TYR:HB3	1:H:503:ILE:HG12	1.83	0.59
1:H:743:THR:HA	1:H:746:VAL:HG22	1.83	0.59
1:A:256:ALA:HB1	1:A:447:LYS:HG3	1.84	0.58
1:G:287:MET:SD	1:G:360:LYS:HE2	2.43	0.58
1:H:141:ARG:NH1	1:H:776:GLU:HA	2.18	0.58
1:B:493:LEU:HA	1:B:496:GLU:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:114:GLY:HA2	1:H:712:PRO:HG3	1.85	0.58
1:A:109:ILE:HG21	1:A:122:PRO:HD3	1.86	0.58
1:A:884:GLU:HA	1:A:887:ASP:HB2	1.86	0.58
2:I:131:GLU:HG2	2:I:137:LEU:HD11	1.85	0.58
1:G:118:VAL:HG12	1:G:673:ARG:HB3	1.85	0.58
1:G:243:LYS:HB3	1:G:458:ASP:HB3	1.84	0.58
1:G:713:ASN:HB2	1:G:766:PHE:HB2	1.85	0.58
1:H:635:LYS:HB2	1:H:643:GLY:H	1.69	0.58
1:A:923:LEU:HD23	1:A:926:ARG:HH11	1.69	0.58
1:B:210:LYS:HB3	1:B:211:ALA:HA	1.86	0.58
3:K:20:GLU:HG3	3:K:109:THR:HG21	1.86	0.57
1:A:785:ILE:HG23	1:A:786:VAL:HG23	1.86	0.57
1:B:141:ARG:NH1	1:B:776:GLU:HA	2.19	0.57
1:H:546:GLN:HE22	1:H:575:PHE:HB3	1.69	0.57
3:K:109:THR:HG23	3:L:70:LYS:HD3	1.86	0.57
1:B:157:TYR:HB2	1:B:190:TYR:HE2	1.68	0.57
1:A:308:HIS:HA	3:L:13:SER:HB3	1.86	0.57
1:H:250:GLY:HA2	1:H:450:ARG:HB3	1.86	0.57
1:B:832:LYS:HD3	3:F:191:ALA:HB3	1.86	0.57
1:B:836:LYS:HB3	3:E:46:ASN:HB3	1.86	0.57
1:H:632:GLY:H	1:H:644:ALA:HB2	1.68	0.57
1:B:356:LEU:HD21	1:B:421:VAL:O	2.05	0.57
1:H:356:LEU:HD21	1:H:421:VAL:O	2.05	0.57
1:H:267:LYS:HD3	1:H:430:ASP:HB2	1.88	0.56
1:H:423:GLY:HA2	1:H:426:LYS:HE2	1.87	0.56
3:K:192:GLU:HG2	3:K:193:GLU:HA	1.87	0.56
1:B:168:SER:OG	1:B:669:PRO:HA	2.06	0.56
1:H:726:ILE:HG12	1:H:785:ILE:HB	1.86	0.56
1:B:231:LYS:HG3	1:B:236:ASP:HA	1.87	0.56
3:E:30:PRO:HB3	3:E:37:LYS:HD3	1.87	0.56
1:B:864:LEU:O	1:B:868:GLU:HG2	2.06	0.56
1:H:541:THR:HA	1:H:592:LEU:HD11	1.88	0.56
3:K:41:GLN:HG2	3:L:194:GLU:HG3	1.88	0.56
3:F:132:PHE:HB3	3:F:142:CYS:SG	2.45	0.55
1:H:457:LEU:HD23	1:H:482:LEU:HD13	1.88	0.55
1:A:906:LEU:HD13	1:B:906:LEU:HA	1.87	0.55
1:H:295:LYS:HA	1:H:300:LEU:HD12	1.87	0.55
1:H:480:GLU:HG2	1:H:518:ILE:HG12	1.87	0.55
1:B:871:ARG:HB3	1:B:872:LYS:HD3	1.89	0.55
1:G:743:THR:HA	1:G:746:VAL:HG12	1.88	0.55
1:A:832:LYS:O	3:E:192:GLU:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:LYS:CE	1:B:903:GLU:OE1	2.55	0.55
1:H:138:LYS:HA	1:H:193:VAL:HG13	1.89	0.55
1:B:91:LEU:HD23	1:B:705:ARG:HG2	1.89	0.55
1:G:712:PRO:HD2	1:G:767:ARG:HA	1.89	0.55
1:B:219:GLN:HB3	1:B:332:ALA:HB1	1.89	0.54
2:D:140:GLU:HB3	2:D:141:PRO:HD3	1.87	0.54
1:A:570:GLN:HE21	2:J:26:LYS:HG3	1.71	0.54
1:B:83:GLU:HG3	1:B:84:ASP:H	1.72	0.54
1:H:542:ASP:HB3	1:H:588:ILE:HG22	1.89	0.54
1:A:874:ILE:HD12	1:B:871:ARG:HD2	1.90	0.54
1:B:740:LYS:O	1:B:743:THR:HG22	2.07	0.54
1:B:868:GLU:HG3	1:B:869:LYS:HD2	1.90	0.54
1:A:118:VAL:HA	1:A:673:ARG:O	2.07	0.54
1:A:593:GLU:HG2	1:A:598:PRO:HB3	1.89	0.54
1:H:231:LYS:HB3	1:H:278:ARG:HB2	1.89	0.54
1:G:134:VAL:HG13	1:G:189:TYR:HE1	1.73	0.54
1:B:635:LYS:CE	1:B:904:GLU:HA	2.34	0.54
1:H:732:VAL:HG11	1:H:742:VAL:HG23	1.89	0.54
1:A:33:TRP:HB2	1:A:72:GLN:HB2	1.90	0.54
1:A:711:PHE:HB3	1:A:765:PHE:HB3	1.89	0.54
1:G:451:GLN:HB3	1:G:452:TYR:HA	1.90	0.54
1:B:146:PRO:HB2	1:B:147:PRO:HD2	1.91	0.53
1:B:811:ALA:HA	3:F:127:VAL:HG13	1.91	0.53
1:A:134:VAL:HG13	1:A:189:TYR:HE1	1.73	0.53
1:B:673:ARG:HH21	1:B:673:ARG:HB3	1.72	0.53
1:G:100:LEU:HB3	1:G:120:ILE:HD11	1.90	0.53
1:H:832:LYS:HD3	3:L:191:ALA:HB3	1.90	0.53
3:E:74:ILE:HG23	3:E:78:ASP:HB2	1.91	0.53
3:K:74:ILE:HG23	3:K:78:ASP:HB2	1.91	0.53
1:A:599:VAL:HG11	1:A:604:VAL:HG23	1.91	0.53
1:B:732:VAL:HG11	1:B:742:VAL:HG23	1.89	0.53
1:G:256:ALA:HB1	1:G:447:LYS:HG3	1.91	0.53
1:G:951:LEU:HD11	1:H:952:LYS:HE3	1.90	0.53
1:H:747:LEU:HB3	1:H:752:LEU:HD23	1.90	0.53
2:I:94:ASP:HB2	2:I:139:TYR:HE2	1.73	0.53
3:L:58:GLU:HA	3:L:61:GLU:HB2	1.91	0.52
1:G:599:VAL:HG22	1:G:603:VAL:HG23	1.91	0.52
1:H:15:MET:SD	1:H:82:CYS:HA	2.50	0.52
1:H:157:TYR:HB2	1:H:190:TYR:HE2	1.74	0.52
3:K:51:PHE:HB3	3:K:56:VAL:HG21	1.91	0.52
1:G:245:ILE:HG23	1:G:260:ILE:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:354:MET:SD	1:G:358:GLU:HG3	2.49	0.52
1:A:721:LYS:NZ	1:B:379:GLU:OE1	2.34	0.52
1:H:330:ASP:CG	1:H:343:LYS:HZ1	2.12	0.52
1:A:837:VAL:HG21	3:E:86:LEU:HA	1.91	0.52
1:B:154:ASP:HA	1:B:189:TYR:CZ	2.45	0.52
1:H:265:LEU:HD23	1:H:430:ASP:HA	1.91	0.52
1:G:422:GLY:HA2	1:G:425:ALA:H	1.75	0.52
3:L:132:PHE:HB3	3:L:142:CYS:SG	2.49	0.52
1:G:84:ASP:HB3	1:G:87:ASN:HD22	1.74	0.52
1:H:54:CYS:SG	1:H:56:VAL:HG23	2.49	0.52
1:H:356:LEU:HD11	1:H:424:LEU:HB3	1.91	0.52
1:H:677:PRO:HB2	1:H:686:ILE:HA	1.92	0.52
2:J:27:ILE:HG13	2:J:62:LEU:HB2	1.91	0.52
1:B:175:SER:HB3	1:B:234:ARG:NH2	2.24	0.51
1:B:169:MET:HB3	1:B:456:VAL:HG22	1.92	0.51
1:H:167:GLN:NE2	1:H:668:GLN:HB3	2.25	0.51
1:H:166:ASN:HB3	1:H:667:THR:HG22	1.93	0.51
1:B:271:ILE:HA	1:B:309:PHE:CE1	2.46	0.51
1:H:119:ALA:O	1:H:674:CYS:HA	2.10	0.51
1:H:145:VAL:HG12	1:H:151:ALA:HB2	1.93	0.51
1:H:146:PRO:HB2	1:H:147:PRO:HD2	1.92	0.51
1:H:724:TYR:HE2	1:H:747:LEU:HD23	1.74	0.51
1:B:5:PRO:HG3	1:B:769:GLY:HA2	1.92	0.51
2:D:41:CYS:O	2:D:43:PRO:HD3	2.10	0.51
1:B:138:LYS:HA	1:B:193:VAL:HG13	1.93	0.51
1:B:930:GLU:HA	1:B:933:ALA:HB3	1.91	0.51
1:H:283:PHE:HB3	1:H:354:MET:SD	2.51	0.51
1:H:144:GLU:O	1:H:146:PRO:HD3	2.11	0.50
1:H:237:ASN:OD1	1:H:281:HIS:HE1	1.94	0.50
3:F:69:ASP:HB2	3:F:73:PHE:HB2	1.94	0.50
1:H:493:LEU:HA	1:H:496:GLU:HB2	1.93	0.50
1:A:55:THR:HA	1:A:65:GLN:HA	1.93	0.50
1:A:309:PHE:CE2	3:L:31:PRO:N	2.80	0.50
1:A:830:TRP:HA	3:E:195:GLY:HA3	1.94	0.50
1:B:726:ILE:HG12	1:B:785:ILE:HB	1.93	0.50
2:C:48:VAL:HG12	2:C:53:GLY:HA3	1.93	0.50
1:H:521:ILE:HB	1:H:524:PRO:HD2	1.94	0.50
2:J:140:GLU:HB3	2:J:141:PRO:HD3	1.93	0.50
3:L:6:LYS:HD3	3:L:9:LYS:O	2.11	0.50
1:G:435:TRP:O	1:G:439:ARG:HG2	2.12	0.50
1:H:240:ARG:HB3	1:H:266:GLU:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ARG:HD2	1:B:315:ILE:O	2.12	0.50
1:A:170:LEU:HD13	1:A:482:LEU:HD11	1.94	0.50
1:G:883:GLN:OE1	1:H:450:ARG:HG3	2.12	0.50
3:L:59:PHE:O	3:L:63:PHE:HB2	2.11	0.50
1:A:892:LEU:HD22	1:A:896:ARG:HH22	1.76	0.49
1:H:169:MET:O	1:H:456:VAL:HA	2.11	0.49
3:L:92:GLU:HA	3:L:95:LEU:HG	1.93	0.49
1:G:795:TRP:HZ3	2:I:40:ASP:HA	1.77	0.49
1:A:875:GLU:O	1:A:879:VAL:HG23	2.13	0.49
1:B:497:GLU:HG2	1:B:668:GLN:HG3	1.94	0.49
1:B:636:GLY:H	1:B:643:GLY:HA3	1.78	0.49
1:G:310:VAL:HB	1:G:311:SER:HA	1.94	0.49
1:A:690:LEU:O	1:A:694:GLN:HG3	2.12	0.49
1:B:635:LYS:HE3	1:B:904:GLU:CA	2.34	0.49
3:F:22:GLY:HA3	3:F:94:GLU:HG2	1.94	0.49
1:H:167:GLN:HE22	1:H:668:GLN:HB3	1.78	0.49
1:H:721:LYS:HB3	2:J:92:VAL:HG12	1.95	0.49
2:J:68:LEU:HB2	2:J:69:PRO:HD3	1.95	0.49
2:I:103:ALA:HB2	2:I:137:LEU:HD13	1.95	0.49
3:E:51:PHE:HB2	3:F:61:GLU:HG2	1.95	0.49
3:F:188:THR:HG22	3:F:189:LYS:H	1.78	0.48
1:G:84:ASP:HB3	1:G:87:ASN:ND2	2.27	0.48
1:A:451:GLN:HB3	1:A:452:TYR:HA	1.95	0.48
1:A:716:VAL:HG21	1:B:390:ALA:HA	1.93	0.48
1:H:97:LEU:HD12	1:H:695:LEU:HD12	1.94	0.48
3:E:67:ASP:O	3:E:70:LYS:NZ	2.47	0.48
1:G:285:GLN:NE2	1:G:326:LEU:HB2	2.27	0.48
1:H:484:GLN:HA	1:H:484:GLN:OE1	2.13	0.48
3:K:67:ASP:O	3:K:70:LYS:NZ	2.46	0.48
1:A:435:TRP:O	1:A:439:ARG:HG2	2.14	0.48
1:B:248:HIS:HA	1:B:452:TYR:O	2.14	0.48
1:H:930:GLU:HA	1:H:933:ALA:HB3	1.95	0.48
1:H:109:ILE:HG23	1:H:120:ILE:O	2.14	0.48
1:H:210:LYS:HB3	1:H:211:ALA:HA	1.95	0.48
1:H:714:ARG:HA	1:H:764:VAL:O	2.13	0.48
1:A:372:ALA:HB3	1:A:377:GLU:HA	1.96	0.48
1:G:221:ASN:HB3	1:G:222:PRO:HD3	1.96	0.48
1:G:863:SER:O	1:G:867:GLU:HG2	2.14	0.48
1:A:134:VAL:HG11	1:A:192:ASN:OD1	2.14	0.48
1:A:461:GLY:HA2	1:A:479:ASN:OD1	2.14	0.48
1:G:588:ILE:O	1:G:591:TRP:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:171:ILE:HA	1:H:672:VAL:O	2.13	0.48
1:G:109:ILE:HG21	1:G:122:PRO:HD3	1.95	0.47
1:B:419:TYR:OH	1:B:426:LYS:NZ	2.47	0.47
3:E:20:GLU:HG3	3:E:109:THR:HG21	1.95	0.47
1:B:244:PHE:O	1:B:260:ILE:HA	2.14	0.47
3:F:33:PRO:HA	3:F:34:PRO:HD3	1.83	0.47
1:G:119:ALA:O	1:G:674:CYS:HA	2.13	0.47
1:A:232:THR:O	1:A:236:ASP:HA	2.14	0.47
1:A:789:LEU:O	1:A:793:ILE:HG13	2.15	0.47
1:B:356:LEU:HD22	1:B:425:ALA:HB2	1.95	0.47
2:J:136:PHE:O	2:J:138:LYS:NZ	2.43	0.47
1:A:119:ALA:O	1:A:674:CYS:HA	2.14	0.47
1:B:530:ILE:HG12	1:B:548:LYS:HB2	1.95	0.47
1:G:56:VAL:HG22	1:G:64:ARG:O	2.13	0.47
1:H:169:MET:HB3	1:H:456:VAL:HG22	1.96	0.47
1:H:563:PRO:HB2	1:H:566:PRO:HD2	1.95	0.47
1:B:141:ARG:HH12	1:B:779:ASP:CG	2.18	0.47
1:H:817:ARG:NH2	3:L:123:ASP:OD2	2.48	0.47
1:A:55:THR:HG22	1:A:65:GLN:HB3	1.96	0.47
1:B:157:TYR:HA	1:B:160:MET:HG2	1.97	0.47
1:B:711:PHE:HA	1:B:712:PRO:HD3	1.72	0.47
3:F:126:ASP:O	3:F:130:ASN:HB2	2.15	0.47
1:H:894:SER:HA	1:H:897:SER:OG	2.15	0.47
3:K:52:THR:HB	3:K:55:GLN:HE21	1.80	0.47
1:A:662:ALA:O	1:A:665:HIS:HB2	2.15	0.47
1:B:526:GLY:CA	1:B:654:ARG:HD3	2.45	0.47
1:A:353:CYS:SG	1:A:428:MET:SD	3.13	0.47
1:A:420:SER:O	1:A:423:GLY:HA3	2.14	0.47
1:A:867:GLU:OE1	1:B:872:LYS:HD2	2.15	0.47
1:H:278:ARG:HD2	1:H:315:ILE:O	2.15	0.47
1:A:272:SER:HB2	1:A:418:SER:HB2	1.97	0.47
1:G:107:ASN:O	1:G:109:ILE:HG23	2.15	0.47
1:H:141:ARG:HH12	1:H:779:ASP:CG	2.18	0.47
1:B:242:GLY:O	1:B:262:THR:HA	2.15	0.46
1:H:33:TRP:HB2	1:H:72:GLN:HB2	1.96	0.46
2:J:60:LYS:HZ1	2:J:66:GLU:CD	2.18	0.46
1:B:142:ARG:HH11	1:B:151:ALA:HB1	1.80	0.46
1:A:6:ASP:OD1	1:A:7:PRO:HD3	2.14	0.46
1:A:362:LYS:H	3:L:32:LYS:HE3	1.80	0.46
1:B:640:ARG:HH12	1:B:896:ARG:HG3	1.79	0.46
3:F:79:ILE:HG21	3:F:99:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:141:LYS:NZ	3:F:173:ASP:O	2.46	0.46
1:G:80:GLU:HG3	1:G:102:GLN:HE22	1.79	0.46
1:H:215:ASP:O	1:H:219:GLN:HG2	2.14	0.46
3:L:79:ILE:HG13	3:L:99:VAL:HG13	1.96	0.46
1:A:571:GLN:HG2	1:A:572:GLU:HB2	1.95	0.46
1:A:836:LYS:HB2	3:E:192:GLU:HB3	1.98	0.46
1:B:7:PRO:HA	1:B:12:TYR:CE2	2.44	0.46
1:B:256:ALA:O	1:B:446:THR:HA	2.15	0.46
3:E:192:GLU:CG	3:E:193:GLU:HA	2.43	0.46
1:G:571:GLN:HG2	1:G:572:GLU:HB2	1.97	0.46
1:H:192:ASN:HA	1:H:197:THR:HG21	1.98	0.46
1:H:845:LYS:HE2	1:H:848:ASP:HB3	1.97	0.46
2:J:83:LEU:HD21	2:J:147:ILE:HG21	1.96	0.46
1:A:575:PHE:HD2	1:A:588:ILE:HD11	1.80	0.46
3:F:30:PRO:HA	3:F:31:PRO:HD2	1.84	0.46
1:A:309:PHE:HD2	3:L:18:GLU:HG3	1.80	0.46
1:A:713:ASN:HB2	1:A:766:PHE:HB2	1.97	0.46
1:H:142:ARG:HD3	1:H:713:ASN:OD1	2.14	0.46
1:B:168:SER:O	1:B:670:HIS:HB2	2.15	0.46
3:F:54:HIS:HB2	3:F:57:GLN:OE1	2.16	0.46
1:H:248:HIS:HA	1:H:452:TYR:O	2.16	0.46
1:H:402:LYS:HE2	1:H:405:ASN:HA	1.97	0.46
2:I:90:LEU:HD22	2:I:139:TYR:HB2	1.98	0.46
1:B:546:GLN:HE22	1:B:575:PHE:HB3	1.80	0.46
1:G:378:GLY:HA2	1:G:381:VAL:HG23	1.97	0.46
3:K:33:PRO:HA	3:K:34:PRO:HD3	1.83	0.46
1:G:164:ARG:O	1:H:400:LYS:HE3	2.16	0.46
1:H:358:GLU:HB2	1:H:377:GLU:HB3	1.97	0.46
1:A:137:TYR:O	1:A:140:ARG:HG2	2.15	0.46
1:A:629:GLU:HB2	1:A:640:ARG:HA	1.98	0.46
1:B:104:TYR:HE2	1:B:686:ILE:HB	1.80	0.46
1:B:231:LYS:HB3	1:B:278:ARG:HB2	1.98	0.46
1:H:103:ARG:HG2	1:H:111:THR:OG1	2.15	0.46
3:K:107:ASN:OD1	3:K:109:THR:HB	2.16	0.46
1:B:168:SER:HA	1:B:455:GLY:O	2.16	0.45
1:B:845:LYS:HE2	1:B:848:ASP:HB3	1.98	0.45
3:E:153:THR:O	3:E:157:LYS:NZ	2.44	0.45
1:G:273:GLN:HG2	1:G:277:GLU:HB2	1.99	0.45
1:G:691:VAL:O	1:G:695:LEU:HG	2.16	0.45
1:H:17:GLN:NE2	1:H:81:LYS:HB2	2.31	0.45
1:H:131:ASN:ND2	1:H:207:LYS:HD3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:193:GLU:HB2	3:L:194:GLU:H	1.70	0.45
1:G:174:GLU:HB2	1:G:676:ILE:HD11	1.98	0.45
1:B:142:ARG:NH1	1:B:151:ALA:HB1	2.32	0.45
1:B:423:GLY:O	1:B:426:LYS:HG2	2.16	0.45
1:B:701:LEU:HG	1:B:705:ARG:HH21	1.81	0.45
1:B:953:LYS:NZ	1:B:957:ASP:OD2	2.49	0.45
1:G:115:LEU:HD23	1:G:490:MET:SD	2.56	0.45
3:L:90:CYS:SG	3:L:95:LEU:HD23	2.57	0.45
1:B:504:ASP:HB3	1:B:758:ARG:HD2	1.99	0.45
1:B:567:LYS:HB3	1:B:568:PRO:HD3	1.99	0.45
1:G:93:ASP:HB3	1:G:701:LEU:HD22	1.98	0.45
1:H:132:ARG:HB2	1:H:204:ALA:HB1	1.98	0.45
2:C:90:LEU:HD22	2:C:139:TYR:HB2	1.98	0.45
1:G:264:LEU:HD22	1:G:474:CYS:HB2	1.98	0.45
1:A:46:ILE:HG23	1:A:54:CYS:SG	2.57	0.45
1:A:309:PHE:HE2	3:L:31:PRO:HD2	1.82	0.45
1:A:364:ARG:C	3:L:31:PRO:HG2	2.37	0.45
1:G:355:HIS:HB3	1:G:381:VAL:HG22	1.99	0.45
3:K:192:GLU:CG	3:K:193:GLU:HA	2.46	0.45
1:B:141:ARG:NH2	2:D:112:SER:O	2.50	0.45
1:G:891:GLN:HE21	1:G:891:GLN:HA	1.82	0.45
3:K:57:GLN:HB3	3:L:60:LYS:NZ	2.32	0.45
1:A:565:PRO:HA	1:A:566:PRO:HD2	1.86	0.45
1:G:137:TYR:HE2	1:G:151:ALA:HB2	1.82	0.45
1:B:868:GLU:HA	1:B:872:LYS:HG2	1.99	0.45
2:C:37:ARG:HA	2:C:41:CYS:O	2.17	0.45
1:H:953:LYS:NZ	1:H:957:ASP:OD2	2.50	0.45
1:A:375:THR:HA	1:A:377:GLU:HG3	1.99	0.44
1:A:947:GLU:HB3	1:B:948:ILE:HD11	2.00	0.44
1:B:817:ARG:NH2	3:F:123:ASP:OD2	2.50	0.44
1:G:91:LEU:HD13	1:G:705:ARG:HG2	1.98	0.44
1:G:420:SER:O	1:G:423:GLY:HA3	2.18	0.44
1:H:119:ALA:HB3	1:H:674:CYS:SG	2.57	0.44
1:H:167:GLN:O	1:H:454:ILE:HA	2.17	0.44
1:B:142:ARG:HD3	1:B:713:ASN:OD1	2.17	0.44
1:B:522:GLU:OE2	1:B:658:ASN:HB2	2.18	0.44
1:H:647:GLN:OE1	1:H:648:THR:HA	2.17	0.44
1:H:702:GLU:HG3	1:H:705:ARG:NH1	2.33	0.44
1:A:561:VAL:HB	1:A:576:SER:HB2	1.99	0.44
1:A:367:GLU:HB3	1:A:368:GLU:HB2	1.99	0.44
1:G:367:GLU:HB3	1:G:368:GLU:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:422:GLY:O	1:G:426:LYS:HB2	2.18	0.44
1:G:832:LYS:O	3:K:192:GLU:HA	2.17	0.44
1:G:901:ASP:HB3	1:H:523:LYS:HD3	2.00	0.44
1:A:795:TRP:HA	2:C:37:ARG:HD3	1.99	0.44
1:B:790:GLN:O	1:B:794:ARG:HG2	2.18	0.44
3:F:11:LYS:HE3	3:F:11:LYS:HB2	1.81	0.44
1:G:837:VAL:HG21	3:K:86:LEU:HA	1.99	0.44
1:B:495:GLN:HA	1:B:498:TYR:CD1	2.53	0.44
1:B:926:ARG:HG2	1:B:929:ARG:HD2	1.98	0.44
3:F:66:ILE:HG23	3:F:82:THR:HG21	1.99	0.44
1:H:246:ARG:O	1:H:258:ALA:HA	2.18	0.44
1:H:601:ASP:HB3	1:H:629:GLU:HG2	2.00	0.44
1:A:468:ASN:HB2	1:A:585:PRO:O	2.18	0.44
1:B:521:ILE:HB	1:B:524:PRO:HD2	1.99	0.44
2:C:138:LYS:O	2:C:141:PRO:HD2	2.17	0.44
1:G:222:PRO:HA	1:G:225:GLU:HB2	2.00	0.44
1:G:682:GLN:HA	1:G:683:PRO:HD2	1.90	0.44
1:G:815:ILE:HD11	3:K:183:PHE:HE1	1.81	0.44
1:A:716:VAL:HG12	1:A:763:LYS:HE2	2.00	0.44
1:A:757:TYR:HB3	1:A:770:VAL:HG11	2.00	0.44
1:B:563:PRO:HB2	1:B:566:PRO:HD2	2.00	0.44
1:B:868:GLU:CA	1:B:872:LYS:HG2	2.48	0.44
1:G:232:THR:OG1	1:G:238:SER:HB3	2.17	0.44
1:A:134:VAL:HG13	1:A:189:TYR:CE1	2.51	0.44
1:A:832:LYS:HB3	3:E:191:ALA:O	2.18	0.44
1:B:714:ARG:HA	1:B:764:VAL:O	2.18	0.44
1:B:836:LYS:HD2	1:B:836:LYS:O	2.18	0.44
1:G:561:VAL:HB	1:G:576:SER:HB2	2.00	0.44
1:H:141:ARG:HH11	1:H:776:GLU:HA	1.83	0.44
3:L:11:LYS:HB2	3:L:11:LYS:HE3	1.75	0.44
1:B:488:HIS:O	1:B:492:VAL:HB	2.18	0.43
1:G:830:TRP:HA	3:K:195:GLY:HA3	1.98	0.43
1:H:159:ALA:HB2	1:H:714:ARG:O	2.18	0.43
1:H:400:LYS:HA	1:H:400:LYS:HD3	1.84	0.43
1:A:268:ALA:N	1:A:269:ARG:HB2	2.34	0.43
1:B:246:ARG:HA	1:B:454:ILE:O	2.17	0.43
1:B:723:ARG:HD2	2:D:112:SER:HB2	2.00	0.43
1:G:717:TYR:CE1	1:G:764:VAL:HB	2.53	0.43
1:H:668:GLN:OE1	1:H:763:LYS:NZ	2.51	0.43
1:A:364:ARG:O	3:L:31:PRO:HG2	2.18	0.43
1:A:782:LEU:HA	1:A:785:ILE:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:871:ARG:HB3	1:B:872:LYS:HE2	2.00	0.43
1:H:298:LEU:HA	1:H:384:LEU:HD21	1.99	0.43
2:J:93:TYR:CZ	2:J:101:MET:HA	2.54	0.43
1:A:231:LYS:HA	1:A:236:ASP:O	2.18	0.43
1:A:835:ILE:O	1:A:839:PRO:HD2	2.17	0.43
1:G:164:ARG:HH11	1:H:606:GLN:NE2	2.17	0.43
1:A:85:MET:HA	1:A:88:LEU:HD13	2.01	0.43
1:A:166:ASN:ND2	1:A:667:THR:HG22	2.34	0.43
1:B:869:LYS:O	1:B:873:ASP:HB2	2.19	0.43
1:G:55:THR:HA	1:G:65:GLN:HA	2.01	0.43
1:G:629:GLU:HB2	1:G:640:ARG:HA	2.00	0.43
1:H:5:PRO:HG3	1:H:769:GLY:HA2	2.00	0.43
1:H:331:THR:HA	1:H:334:ASP:OD2	2.18	0.43
2:J:22:GLU:HB3	3:L:154:TRP:HZ2	1.84	0.43
1:A:792:TRP:CZ3	2:C:147:ILE:HA	2.54	0.43
1:A:926:ARG:O	1:A:929:ARG:HB3	2.18	0.43
1:B:523:LYS:O	1:B:527:ILE:HG13	2.18	0.43
1:H:701:LEU:O	1:H:705:ARG:HG3	2.19	0.43
1:A:17:GLN:OE1	1:A:20:LYS:NZ	2.51	0.43
1:A:107:ASN:O	1:A:109:ILE:HG23	2.19	0.43
1:B:233:VAL:HG22	1:B:275:THR:O	2.19	0.43
3:E:90:CYS:HB3	3:E:94:GLU:HB2	2.01	0.43
1:G:17:GLN:OE1	1:G:20:LYS:NZ	2.52	0.43
1:G:661:MET:O	1:G:665:HIS:HD2	2.01	0.43
1:G:843:MET:SD	3:K:57:GLN:HB2	2.59	0.43
1:H:126:PHE:HB3	1:H:128:ILE:HG13	2.00	0.43
3:L:33:PRO:HB2	3:L:34:PRO:CD	2.48	0.43
1:A:599:VAL:HG22	1:A:603:VAL:HG23	2.01	0.43
1:B:31:MET:HB2	1:B:74:VAL:HG11	2.01	0.43
1:B:155:GLY:HA2	1:B:158:SER:OG	2.18	0.43
1:B:701:LEU:HG	1:B:705:ARG:NH2	2.33	0.43
1:G:710:GLY:O	1:G:767:ARG:NH2	2.51	0.43
1:A:557:SER:HA	1:A:558:PRO:HD3	1.87	0.43
1:A:690:LEU:HG	1:A:694:GLN:HE21	1.84	0.43
1:B:119:ALA:O	1:B:674:CYS:HA	2.19	0.43
3:E:28:PRO:HA	3:E:29:PRO:HD3	1.86	0.43
1:G:575:PHE:HD2	1:G:588:ILE:HD11	1.83	0.43
1:A:367:GLU:HB2	1:A:369:GLN:H	1.84	0.43
1:A:923:LEU:HD21	1:B:924:GLN:HG2	2.01	0.43
1:G:377:GLU:HB3	1:G:393:TYR:OH	2.19	0.43
1:H:159:ALA:HA	1:H:715:MET:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:VAL:HG12	1:A:311:SER:HA	2.01	0.42
1:B:240:ARG:HB2	1:B:280:TYR:HE2	1.83	0.42
1:B:531:LEU:HG	1:B:595:ASN:ND2	2.34	0.42
1:B:534:GLU:OE1	1:B:537:PHE:CD1	2.72	0.42
1:B:109:ILE:HG21	1:B:122:PRO:HD3	1.99	0.42
1:B:875:GLU:O	1:B:878:ASN:HB3	2.20	0.42
3:E:33:PRO:HA	3:E:34:PRO:HD3	1.86	0.42
3:E:57:GLN:HB3	3:F:60:LYS:NZ	2.34	0.42
3:L:14:LYS:HD3	3:L:103:PRO:HB2	2.00	0.42
1:B:54:CYS:O	1:B:65:GLN:HA	2.20	0.42
1:B:668:GLN:OE1	1:B:763:LYS:NZ	2.51	0.42
1:H:371:GLU:HG2	1:H:397:VAL:HG21	2.01	0.42
1:B:75:ASN:HA	1:B:76:PRO:HD3	1.89	0.42
1:B:480:GLU:HG2	1:B:518:ILE:HG12	2.02	0.42
1:G:232:THR:O	1:G:236:ASP:HA	2.19	0.42
1:G:195:ALA:HB1	1:G:197:THR:HG23	2.02	0.42
1:H:342:TYR:HA	1:H:345:ASP:HB2	2.01	0.42
1:H:503:ILE:HG22	1:H:760:GLY:HA2	2.01	0.42
3:L:23:ASP:HA	3:L:93:GLN:NE2	2.34	0.42
3:L:102:ALA:HB1	3:L:106:ILE:HD11	2.00	0.42
1:B:654:ARG:HE	1:B:654:ARG:HA	1.84	0.42
1:B:721:LYS:HB3	2:D:92:VAL:HG12	2.02	0.42
3:E:72:GLY:O	3:E:107:ASN:HA	2.20	0.42
1:G:497:GLU:O	1:G:501:GLU:HG2	2.19	0.42
1:A:282:ILE:HA	1:A:285:GLN:OE1	2.19	0.42
1:B:702:GLU:HG3	1:B:705:ARG:NH1	2.34	0.42
1:B:743:THR:HG23	1:B:744:GLU:OE2	2.20	0.42
1:A:80:GLU:HG3	1:A:102:GLN:HE22	1.85	0.42
1:G:468:ASN:HB2	1:G:585:PRO:O	2.20	0.42
3:L:188:THR:HG22	3:L:189:LYS:H	1.83	0.42
1:B:501:GLU:O	1:B:761:ASN:HB2	2.20	0.42
3:F:13:SER:HA	3:F:15:LYS:N	2.35	0.42
1:G:923:LEU:HD13	1:H:923:LEU:HB3	2.02	0.42
1:H:1:MET:HA	1:H:4:ASP:O	2.20	0.42
1:B:716:VAL:HG22	1:B:762:THR:HG22	2.02	0.42
2:D:83:LEU:HD21	2:D:147:ILE:HG21	2.01	0.42
1:G:906:LEU:HD13	1:H:906:LEU:HA	2.01	0.42
1:H:512:LEU:HB3	1:H:580:TYR:OH	2.20	0.42
1:H:711:PHE:HA	1:H:712:PRO:HD3	1.73	0.42
1:A:782:LEU:HD13	2:C:92:VAL:HB	2.01	0.41
1:B:157:TYR:CZ	1:B:161:LEU:HD11	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:134:VAL:HG13	1:G:189:TYR:CE1	2.54	0.41
1:H:142:ARG:HG2	1:H:145:VAL:HB	2.01	0.41
1:A:132:ARG:HG3	1:A:205:PRO:HB2	2.01	0.41
1:A:500:ARG:HD2	1:B:367:GLU:HB3	2.01	0.41
2:D:22:GLU:CD	2:D:61:LYS:HZ3	2.22	0.41
3:E:51:PHE:HA	3:E:56:VAL:HG11	2.01	0.41
3:E:83:PHE:HB3	3:E:89:LEU:HG	2.01	0.41
1:G:97:LEU:HD11	1:G:688:SER:HB3	2.02	0.41
1:G:282:ILE:HA	1:G:285:GLN:OE1	2.20	0.41
1:H:528:LEU:HD12	1:H:529:SER:HB3	2.01	0.41
1:H:804:LYS:HE3	3:L:134:LEU:O	2.21	0.41
1:B:727:LEU:HG	1:B:782:LEU:HD21	2.01	0.41
1:G:667:THR:O	1:G:669:PRO:HD3	2.20	0.41
1:H:654:ARG:HA	1:H:654:ARG:HE	1.85	0.41
3:K:16:LYS:NZ	3:K:17:SER:OG	2.46	0.41
3:K:104:GLY:HA3	3:K:105:PRO:HD3	1.84	0.41
1:A:364:ARG:CB	1:A:369:GLN:O	2.68	0.41
1:B:717:TYR:HE1	1:B:743:THR:HG21	1.85	0.41
3:E:5:GLU:OE2	3:F:90:CYS:HB3	2.20	0.41
1:G:889:PHE:HA	1:G:892:LEU:HD12	2.02	0.41
1:A:181:GLU:OE2	1:A:185:LYS:NZ	2.53	0.41
1:B:402:LYS:NZ	1:B:630:LYS:O	2.46	0.41
2:D:19:TYR:O	2:D:21:TRP:HD1	2.02	0.41
3:E:43:SER:HA	3:F:193:GLU:O	2.20	0.41
1:H:541:THR:HG23	1:H:544:SER:H	1.84	0.41
1:A:406:GLU:HB3	2:J:5:LYS:HG2	2.03	0.41
1:A:501:GLU:O	1:B:364:ARG:NH2	2.54	0.41
1:G:131:ASN:ND2	1:G:204:ALA:O	2.54	0.41
1:G:217:VAL:HA	1:G:220:THR:OG1	2.20	0.41
1:G:271:ILE:HD12	1:G:419:TYR:HA	2.02	0.41
1:G:718:PRO:HG2	1:H:389:ALA:HB1	2.02	0.41
1:H:530:ILE:HG12	1:H:548:LYS:HB2	2.02	0.41
3:L:30:PRO:HA	3:L:31:PRO:HD3	1.84	0.41
1:A:309:PHE:CD2	3:L:18:GLU:HG3	2.55	0.41
1:A:715:MET:O	1:A:763:LYS:HD2	2.20	0.41
1:A:779:ASP:HA	1:A:782:LEU:HB2	2.02	0.41
1:B:829:LEU:O	3:F:195:GLY:HA3	2.21	0.41
1:G:715:MET:O	1:G:763:LYS:HD2	2.20	0.41
1:G:769:GLY:O	1:G:773:ARG:N	2.54	0.41
1:G:843:MET:HG2	3:L:53:GLN:O	2.20	0.41
1:A:883:GLN:NE2	1:B:451:GLN:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:PHE:HD1	1:B:309:PHE:HA	1.79	0.41
1:B:400:LYS:HD3	1:B:400:LYS:HA	1.91	0.41
2:C:94:ASP:HB2	2:C:139:TYR:HE2	1.86	0.41
1:G:33:TRP:HE1	1:G:74:VAL:HA	1.86	0.41
1:G:372:ALA:HB3	1:G:377:GLU:HG2	2.03	0.41
1:G:815:ILE:HD13	1:G:815:ILE:HA	1.95	0.41
1:H:110:TYR:OH	1:H:185:LYS:NZ	2.51	0.41
1:H:234:ARG:NH2	1:H:676:ILE:HD13	2.35	0.41
1:H:300:LEU:HA	1:H:307:TYR:OH	2.20	0.41
1:H:523:LYS:HE2	1:H:523:LYS:HB3	1.89	0.41
1:A:11:LEU:HD11	1:A:148:HIS:HB2	2.02	0.41
1:A:364:ARG:HG3	3:L:36:GLN:HG3	2.03	0.41
1:A:369:GLN:HG2	1:A:417:VAL:HG11	2.03	0.41
1:A:710:GLY:O	1:A:767:ARG:NH2	2.54	0.41
1:B:9:GLU:CD	1:B:132:ARG:HH11	2.25	0.41
1:B:230:ALA:HB1	1:B:278:ARG:O	2.21	0.41
1:B:260:ILE:H	1:B:441:ASN:ND2	2.19	0.41
1:B:491:PHE:O	1:B:495:GLN:HG2	2.20	0.41
1:G:286:LEU:HD11	1:G:298:LEU:HD22	2.02	0.41
1:G:483:GLN:O	1:G:486:PHE:HB3	2.20	0.41
1:G:919:GLN:HA	1:G:922:GLU:HG2	2.01	0.41
3:K:5:GLU:OE2	3:L:90:CYS:HB3	2.21	0.41
1:B:612:ASN:O	1:B:614:LEU:N	2.54	0.41
3:L:141:LYS:NZ	3:L:173:ASP:O	2.47	0.41
1:A:364:ARG:HH11	3:L:33:PRO:HD3	1.85	0.40
1:B:283:PHE:HB3	1:B:354:MET:SD	2.60	0.40
3:E:33:PRO:HB2	3:E:36:GLN:NE2	2.36	0.40
1:G:892:LEU:HD22	1:G:896:ARG:HH22	1.86	0.40
1:B:163:ASN:HD21	1:B:165:GLU:HB3	1.87	0.40
1:B:169:MET:O	1:B:456:VAL:HA	2.21	0.40
3:F:9:LYS:O	3:F:13:SER:HB3	2.21	0.40
1:H:175:SER:HB3	1:H:234:ARG:NH2	2.36	0.40
1:H:635:LYS:HB2	1:H:643:GLY:N	2.36	0.40
1:H:723:ARG:HD2	2:J:112:SER:HB2	2.03	0.40
2:I:143:VAL:O	2:I:146:ILE:HB	2.22	0.40
2:C:91:LYS:HD3	2:C:97:GLU:HG2	2.03	0.40
1:G:527:ILE:HG23	1:G:549:LEU:HD11	2.04	0.40
1:G:793:ILE:HG23	2:I:125:ILE:HD12	2.02	0.40
3:K:41:GLN:HA	3:L:85:SER:O	2.21	0.40
1:A:41:TYR:HD1	1:A:97:LEU:HD22	1.87	0.40
1:A:922:GLU:HG3	1:A:923:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:HIS:ND1	1:B:453:PHE:HB3	2.37	0.40
1:B:309:PHE:CD1	1:B:357:GLY:HA3	2.57	0.40
1:B:330:ASP:CG	1:B:343:LYS:HZ1	2.24	0.40
1:B:715:MET:O	1:B:763:LYS:HA	2.21	0.40
3:F:68:GLN:OE1	3:F:78:ASP:HB2	2.21	0.40
1:H:162:ALA:O	1:H:164:ARG:NH2	2.55	0.40
1:B:41:TYR:HD1	1:B:97:LEU:HD22	1.86	0.40
1:B:831:TYR:HD2	3:F:194:GLU:HB3	1.86	0.40
1:G:599:VAL:HG11	1:G:604:VAL:HG23	2.04	0.40
1:H:7:PRO:HA	1:H:12:TYR:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	960/1953 (49%)	772 (80%)	149 (16%)	39 (4%)	3	23
1	B	962/1953 (49%)	779 (81%)	128 (13%)	55 (6%)	1	18
1	G	960/1953 (49%)	783 (82%)	136 (14%)	41 (4%)	2	22
1	H	962/1953 (49%)	779 (81%)	125 (13%)	58 (6%)	1	17
2	C	154/156 (99%)	137 (89%)	13 (8%)	4 (3%)	5	31
2	D	154/156 (99%)	139 (90%)	11 (7%)	4 (3%)	5	31
2	I	154/156 (99%)	135 (88%)	16 (10%)	3 (2%)	8	38
2	J	154/156 (99%)	131 (85%)	19 (12%)	4 (3%)	5	31
3	E	194/196 (99%)	139 (72%)	40 (21%)	15 (8%)	1	13
3	F	194/196 (99%)	136 (70%)	41 (21%)	17 (9%)	1	11
3	K	194/196 (99%)	144 (74%)	37 (19%)	13 (7%)	1	15
3	L	194/196 (99%)	129 (66%)	46 (24%)	19 (10%)	0	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5236/9220 (57%)	4203 (80%)	761 (14%)	272 (5%)	4	19

All (272) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	22	GLN
1	A	138	LYS
1	A	269	ARG
1	A	310	VAL
1	A	311	SER
1	A	363	GLN
1	A	365	PRO
1	A	393	TYR
1	A	394	LYS
1	A	568	PRO
1	A	603	VAL
1	A	845	LYS
1	B	68	LYS
1	B	86	SER
1	B	142	ARG
1	B	149	LEU
1	B	178	GLY
1	B	205	PRO
1	B	367	GLU
1	B	565	PRO
1	B	613	LYS
1	B	621	ASP
1	B	646	PHE
1	B	680	LEU
1	B	725	THR
1	B	733	PRO
1	B	869	LYS
2	D	152	PRO
3	E	17	SER
3	E	47	VAL
3	E	50	MET
3	F	14	LYS
3	F	15	LYS
3	F	53	GLN
3	F	105	PRO
3	F	125	GLU

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Mol	Chain	Res	Type
3	F	144	GLU
1	G	22	GLN
1	G	138	LYS
1	G	177	ALA
1	G	264	LEU
1	G	282	ILE
1	G	358	GLU
1	G	568	PRO
1	G	601	ASP
1	G	603	VAL
1	G	843	MET
1	H	21	ASP
1	H	68	LYS
1	H	86	SER
1	H	142	ARG
1	H	205	PRO
1	H	307	TYR
1	H	367	GLU
1	H	565	PRO
1	H	622	HIS
1	H	645	SER
1	H	680	LEU
1	H	725	THR
1	H	733	PRO
1	H	752	LEU
1	H	842	THR
2	I	97	GLU
3	K	17	SER
3	L	13	SER
3	L	16	LYS
3	L	31	PRO
3	L	32	LYS
3	L	53	GLN
3	L	58	GLU
3	L	67	ASP
3	L	125	GLU
3	L	144	GLU
1	A	271	ILE
1	A	366	ARG
1	A	460	ALA
1	A	621	ASP
1	A	737	VAL

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Mol	Chain	Res	Type
1	A	831	TYR
1	A	843	MET
1	B	14	SER
1	B	274	GLN
1	B	312	GLN
1	B	446	THR
1	B	447	LYS
1	B	451	GLN
1	B	517	CYS
1	B	535	SER
1	B	645	SER
1	B	752	LEU
1	B	834	TYR
1	B	842	THR
1	B	844	ALA
1	B	870	VAL
2	C	97	GLU
2	C	152	PRO
3	E	55	GLN
3	E	59	PHE
3	E	139	GLU
3	F	63	PHE
3	F	174	GLY
3	F	195	GLY
1	G	269	ARG
1	G	271	ILE
1	G	308	HIS
1	G	516	ALA
1	G	621	ASP
1	G	712	PRO
1	G	735	GLY
1	G	737	VAL
1	G	831	TYR
1	H	3	GLU
1	H	11	LEU
1	H	178	GLY
1	H	356	LEU
1	H	580	TYR
1	H	613	LYS
1	H	621	ASP
1	H	646	PHE
1	H	648	THR

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Mol	Chain	Res	Type
1	H	738	ASP
1	H	804	LYS
1	H	834	TYR
3	K	55	GLN
3	K	59	PHE
3	K	169	GLU
3	L	174	GLY
3	L	195	GLY
1	A	11	LEU
1	A	177	ALA
1	A	228	GLY
1	A	270	VAL
1	A	299	LEU
1	A	367	GLU
1	A	392	LEU
1	A	597	ASP
1	A	712	PRO
1	A	784	LYS
1	B	3	GLU
1	B	77	PRO
1	B	292	GLU
1	B	448	GLN
1	B	529	SER
1	B	567	LYS
1	B	630	LYS
1	B	751	GLN
2	C	96	ALA
2	C	116	ARG
3	E	53	GLN
3	E	58	GLU
3	E	169	GLU
3	F	72	GLY
1	G	11	LEU
1	G	108	LEU
1	G	114	GLY
1	G	144	GLU
1	G	207	LYS
1	G	310	VAL
1	H	14	SER
1	H	57	ASP
1	H	109	ILE
1	H	446	THR

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Mol	Chain	Res	Type
1	H	529	SER
1	H	567	LYS
1	H	573	ALA
1	H	751	GLN
1	H	844	ALA
2	J	152	PRO
3	K	139	GLU
3	L	72	GLY
3	L	192	GLU
1	A	207	LYS
1	A	827	ASN
1	B	20	LYS
1	B	57	ASP
1	B	601	ASP
1	B	804	LYS
1	B	871	ARG
3	E	106	ILE
3	F	28	PRO
3	F	57	GLN
3	F	95	LEU
3	F	192	GLU
1	G	9	GLU
1	G	392	LEU
1	G	460	ALA
1	G	784	LYS
1	G	827	ASN
1	H	137	TYR
1	H	200	PRO
1	H	251	PRO
1	H	375	THR
1	H	639	GLY
1	H	803	LYS
2	I	116	ARG
2	J	130	ASP
3	L	70	LYS
3	L	80	ARG
3	L	188	THR
3	L	190	GLY
1	A	735	GLY
1	B	618	ILE
2	D	40	ASP
3	E	21	GLY

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Mol	Chain	Res	Type
3	E	67	ASP
3	F	88	ARG
1	G	299	LEU
1	G	301	SER
1	G	375	THR
1	G	411	GLY
1	H	5	PRO
1	H	90	TYR
1	H	175	SER
1	H	491	PHE
1	H	597	ASP
1	H	707	CYS
2	J	75	LYS
2	J	131	GLU
3	K	138	GLY
3	L	14	LYS
1	A	719	ASP
1	B	200	PRO
1	B	251	PRO
1	B	375	THR
1	B	629	GLU
1	B	734	LYS
2	D	43	PRO
3	F	190	GLY
1	G	597	ASP
1	H	618	ILE
1	H	833	LEU
2	I	152	PRO
3	K	21	GLY
3	K	38	ARG
3	L	102	ALA
1	A	66	VAL
1	A	282	ILE
1	B	846	VAL
2	D	135	GLY
3	E	29	PRO
3	E	138	GLY
1	H	58	ILE
1	H	492	VAL
3	K	106	ILE
1	G	228	GLY
1	G	839	PRO

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Mol	Chain	Res	Type
1	H	198	PRO
1	H	599	VAL
3	K	140	GLY
1	B	404	GLY
1	G	492	VAL
1	G	760	GLY
1	H	511	GLY
3	K	29	PRO
3	K	87	GLY
3	K	190	GLY
1	A	364	ARG
1	A	760	GLY
1	A	839	PRO
1	B	58	ILE
1	B	634	GLY
1	B	639	GLY
3	F	21	GLY
1	G	66	VAL
1	H	564	LYS
1	H	631	GLY
1	B	198	PRO
1	B	750	ILE
3	E	140	GLY
1	G	786	VAL
1	H	750	ILE

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	833/1689 (49%)	792 (95%)	41 (5%)	25	50
1	B	835/1689 (49%)	780 (93%)	55 (7%)	16	41
1	G	833/1689 (49%)	798 (96%)	35 (4%)	30	54
1	H	835/1689 (49%)	785 (94%)	50 (6%)	19	44
2	C	132/132 (100%)	126 (96%)	6 (4%)	27	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	132/132 (100%)	126 (96%)	6 (4%)	27	52
2	I	132/132 (100%)	127 (96%)	5 (4%)	33	57
2	J	132/132 (100%)	125 (95%)	7 (5%)	22	47
3	E	164/164 (100%)	157 (96%)	7 (4%)	29	53
3	F	164/164 (100%)	150 (92%)	14 (8%)	10	33
3	K	164/164 (100%)	160 (98%)	4 (2%)	49	69
3	L	164/164 (100%)	154 (94%)	10 (6%)	18	44
All	All	4520/7940 (57%)	4280 (95%)	240 (5%)	26	47

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASP
1	A	63	SER
1	A	145	VAL
1	A	172	THR
1	A	175	SER
1	A	222	PRO
1	A	266	GLU
1	A	271	ILE
1	A	281	HIS
1	A	308	HIS
1	A	309	PHE
1	A	312	GLN
1	A	334	ASP
1	A	345	ASP
1	A	362	LYS
1	A	363	GLN
1	A	365	PRO
1	A	388	ASN
1	A	397	VAL
1	A	418	SER
1	A	470	PHE
1	A	543	LYS
1	A	547	ASP
1	A	568	PRO
1	A	572	GLU
1	A	586	TYR
1	A	591	TRP
1	A	600	ASN

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Mol	Chain	Res	Type
1	A	616	GLN
1	A	693	HIS
1	A	696	THR
1	A	761	ASN
1	A	795	TRP
1	A	815	ILE
1	A	854	GLU
1	A	868	GLU
1	A	871	ARG
1	A	872	LYS
1	A	875	GLU
1	A	887	ASP
1	A	932	ASP
1	B	4	ASP
1	B	12	TYR
1	B	87	ASN
1	B	91	LEU
1	B	93	ASP
1	B	103	ARG
1	B	129	TYR
1	B	134	VAL
1	B	141	ARG
1	B	146	PRO
1	B	163	ASN
1	B	172	THR
1	B	174	GLU
1	B	180	THR
1	B	192	ASN
1	B	198	PRO
1	B	203	GLU
1	B	222	PRO
1	B	302	ASP
1	B	309	PHE
1	B	341	GLU
1	B	393	TYR
1	B	405	ASN
1	B	413	ASN
1	B	415	THR
1	B	417	VAL
1	B	448	GLN
1	B	524	PRO
1	B	565	PRO

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Mol	Chain	Res	Type
1	B	593	GLU
1	B	608	LYS
1	B	622	HIS
1	B	647	GLN
1	B	648	THR
1	B	654	ARG
1	B	668	GLN
1	B	681	LYS
1	B	708	ARG
1	B	716	VAL
1	B	718	PRO
1	B	758	ARG
1	B	771	LEU
1	B	776	GLU
1	B	826	ARG
1	B	827	ASN
1	B	836	LYS
1	B	838	LYS
1	B	843	MET
1	B	862	GLU
1	B	867	GLU
1	B	872	LYS
1	B	873	ASP
1	B	887	ASP
1	B	896	ARG
1	B	954	GLU
2	C	51	ASN
2	C	69	PRO
2	C	94	ASP
2	C	133	ASP
2	C	139	TYR
2	C	140	GLU
2	D	85	ASP
2	D	94	ASP
2	D	119	ASP
2	D	130	ASP
2	D	134	ASP
2	D	139	TYR
3	E	18	GLU
3	E	52	THR
3	E	54	HIS
3	E	58	GLU

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Mol	Chain	Res	Type
3	E	59	PHE
3	E	71	ASP
3	E	108	PHE
3	F	3	ASP
3	F	17	SER
3	F	19	GLU
3	F	30	PRO
3	F	42	ARG
3	F	52	THR
3	F	55	GLN
3	F	64	GLN
3	F	67	ASP
3	F	89	LEU
3	F	105	PRO
3	F	113	THR
3	F	118	ARG
3	F	168	SER
1	G	4	ASP
1	G	21	ASP
1	G	26	TYR
1	G	165	GLU
1	G	212	THR
1	G	215	ASP
1	G	222	PRO
1	G	266	GLU
1	G	271	ILE
1	G	306	ASP
1	G	334	ASP
1	G	345	ASP
1	G	362	LYS
1	G	391	ASP
1	G	470	PHE
1	G	538	PRO
1	G	543	LYS
1	G	547	ASP
1	G	568	PRO
1	G	586	TYR
1	G	591	TRP
1	G	600	ASN
1	G	605	ASP
1	G	616	GLN
1	G	668	GLN

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Mol	Chain	Res	Type
1	G	702	GLU
1	G	713	ASN
1	G	721	LYS
1	G	756	ASP
1	G	761	ASN
1	G	795	TRP
1	G	854	GLU
1	G	865	GLU
1	G	883	GLN
1	G	904	GLU
1	H	4	ASP
1	H	12	TYR
1	H	83	GLU
1	H	91	LEU
1	H	92	ASN
1	H	93	ASP
1	H	103	ARG
1	H	134	VAL
1	H	141	ARG
1	H	145	VAL
1	H	146	PRO
1	H	180	THR
1	H	192	ASN
1	H	203	GLU
1	H	222	PRO
1	H	236	ASP
1	H	302	ASP
1	H	341	GLU
1	H	405	ASN
1	H	473	LEU
1	H	522	GLU
1	H	524	PRO
1	H	565	PRO
1	H	571	GLN
1	H	593	GLU
1	H	597	ASP
1	H	601	ASP
1	H	608	LYS
1	H	641	LYS
1	H	642	LYS
1	H	645	SER
1	H	649	VAL

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Mol	Chain	Res	Type
1	H	668	GLN
1	H	681	LYS
1	H	716	VAL
1	H	743	THR
1	H	771	LEU
1	H	794	ARG
1	H	826	ARG
1	H	836	LYS
1	H	838	LYS
1	H	843	MET
1	H	862	GLU
1	H	868	GLU
1	H	887	ASP
1	H	896	ARG
1	H	923	LEU
1	H	925	GLU
1	H	948	ILE
1	H	954	GLU
2	I	42	LYS
2	I	51	ASN
2	I	94	ASP
2	I	119	ASP
2	I	140	GLU
2	J	63	THR
2	J	85	ASP
2	J	94	ASP
2	J	119	ASP
2	J	130	ASP
2	J	139	TYR
2	J	153	ASP
3	K	54	HIS
3	K	58	GLU
3	K	59	PHE
3	K	108	PHE
3	L	3	ASP
3	L	45	SER
3	L	55	GLN
3	L	67	ASP
3	L	68	GLN
3	L	89	LEU
3	L	97	SER
3	L	113	THR

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Mol	Chain	Res	Type
3	L	128	ILE
3	L	193	GLU

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

Mol	Chain	Res	Type
1	A	148	HIS
1	A	281	HIS
1	A	570	GLN
1	A	668	GLN
1	A	921	GLN
1	B	148	HIS
1	B	163	ASN
1	B	441	ASN
1	B	595	ASN
1	B	693	HIS
2	C	51	ASN
2	C	73	GLN
2	D	108	HIS
3	E	54	HIS
3	F	130	ASN
1	G	87	ASN
1	G	281	HIS
1	G	665	HIS
1	G	670	HIS
1	G	891	GLN
1	H	75	ASN
1	H	107	ASN
1	H	192	ASN
1	H	281	HIS
1	H	546	GLN
1	H	616	GLN
1	H	670	HIS
2	I	51	ASN
2	I	73	GLN
3	K	55	GLN
3	L	55	GLN

5.3.3 RNA ⓘ

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 monosaccharides 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.

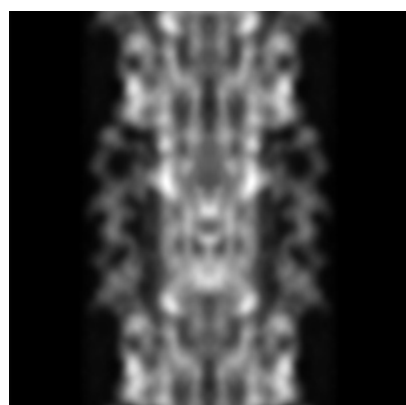
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1950. These allow visual inspection of the internal detail of the map and identification of artifacts.

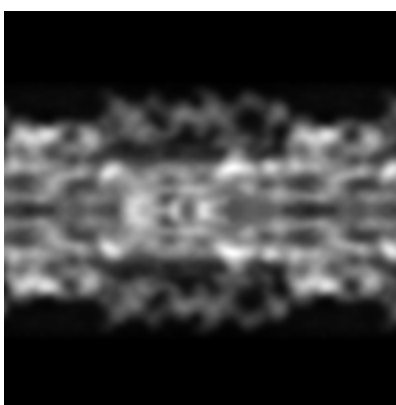
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

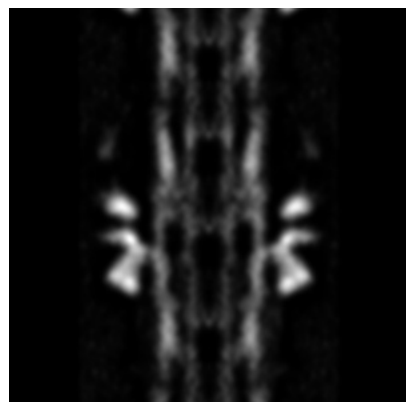


Z

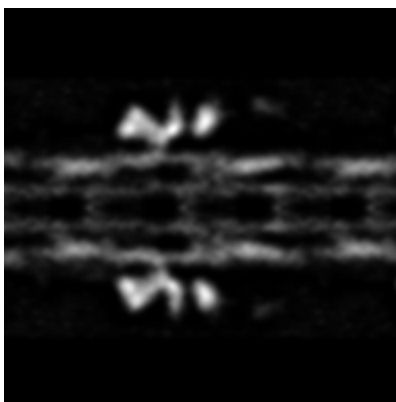
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

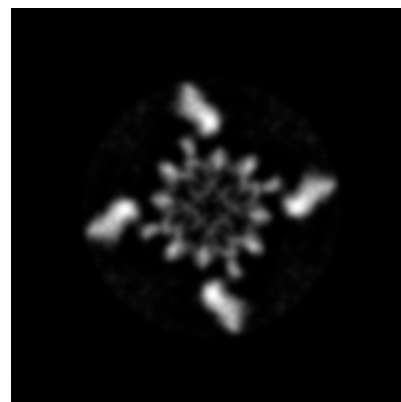
6.2.1 Primary map



X Index: 125



Y Index: 125

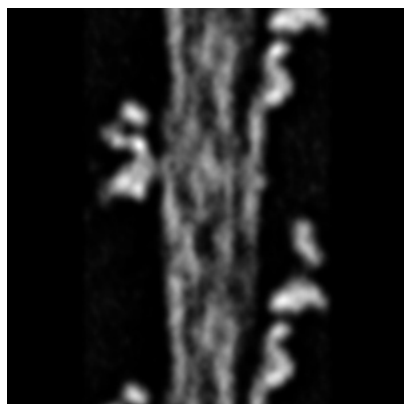


Z Index: 125

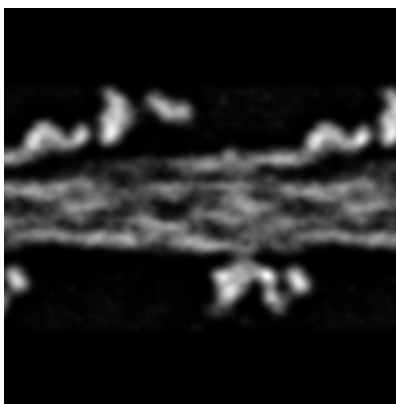
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 150



Y Index: 99



Z Index: 200

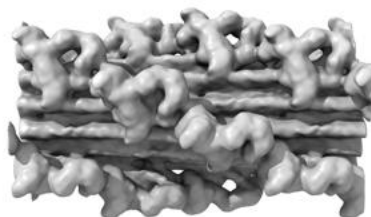
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

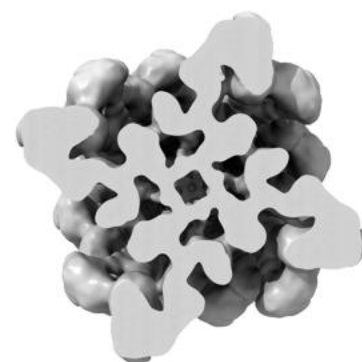
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 25.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

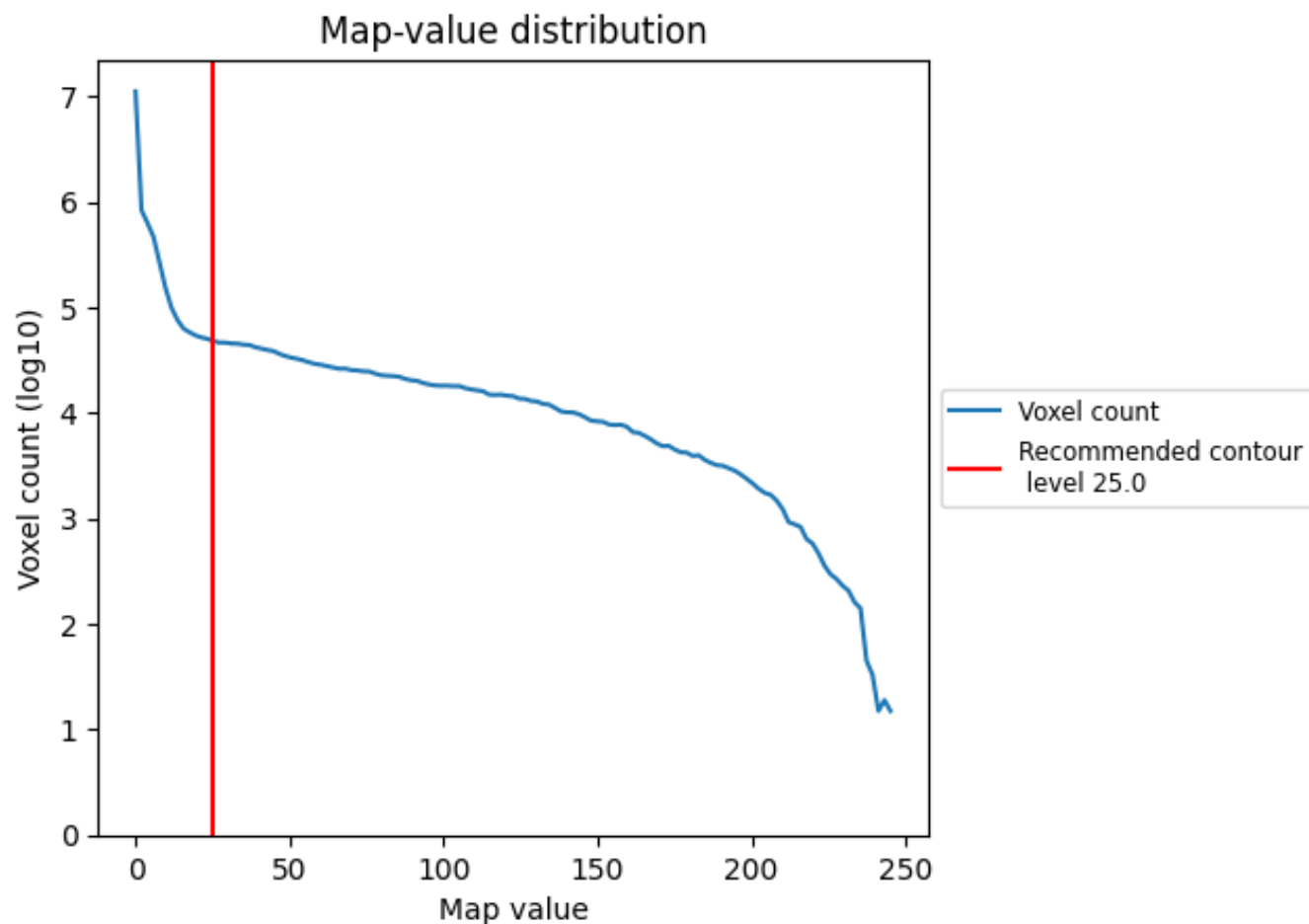
6.5 Mask visualisation

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

7 Map analysis [i](#)

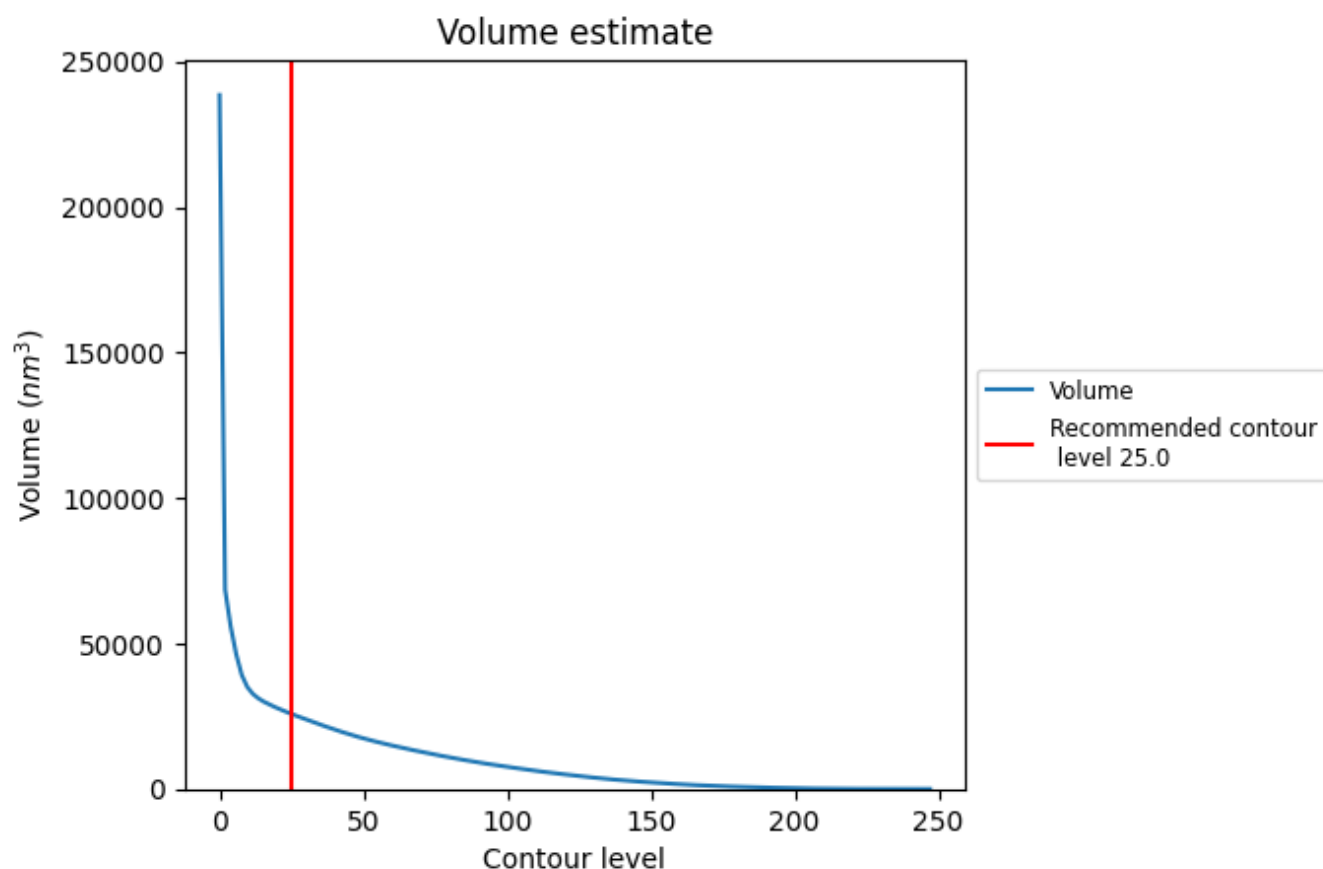
This section contains the results of statistical analysis of the map.

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.

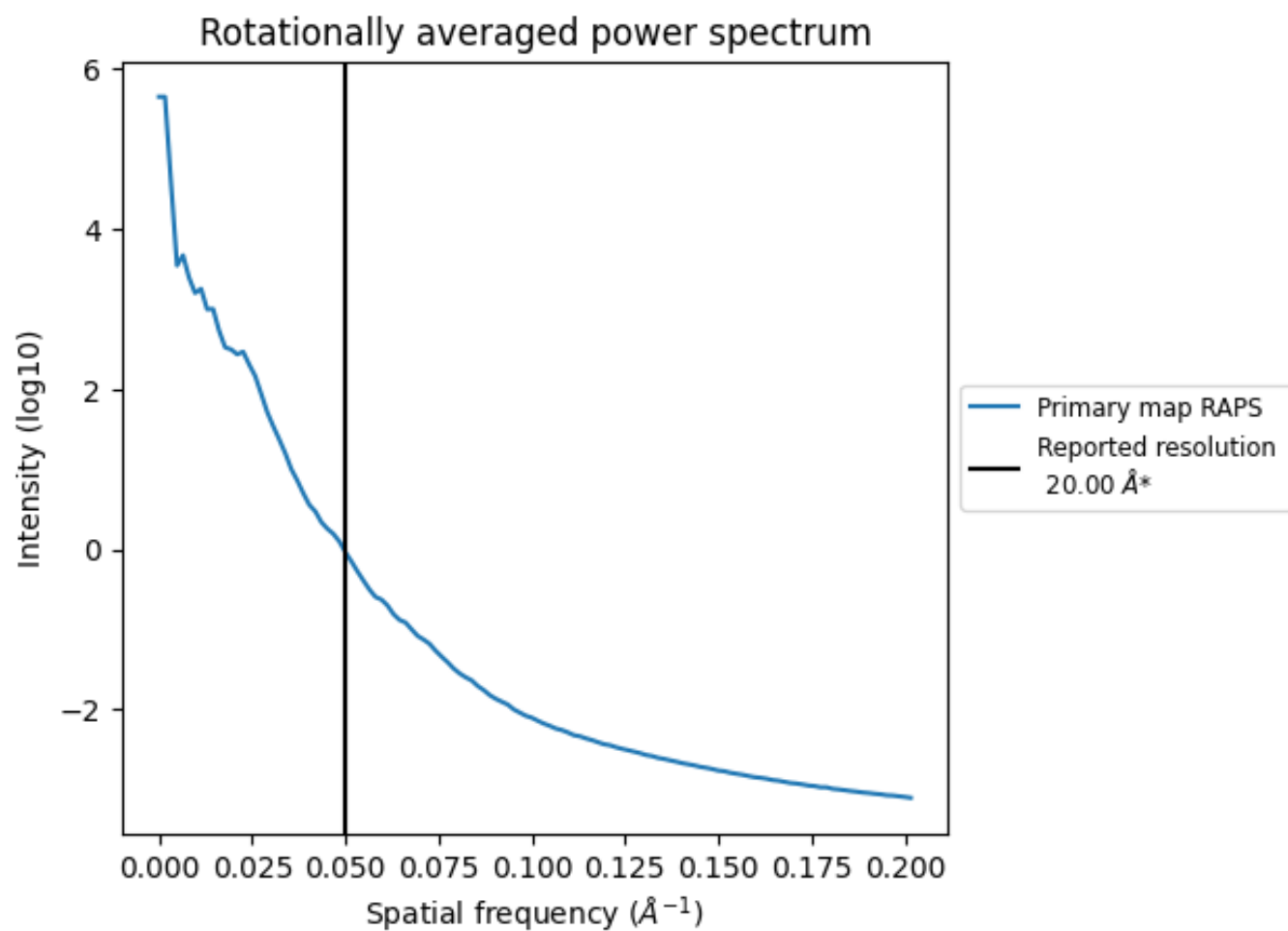
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 25767 nm³; this corresponds to an approximate mass of 23276 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 0.050 Å⁻¹

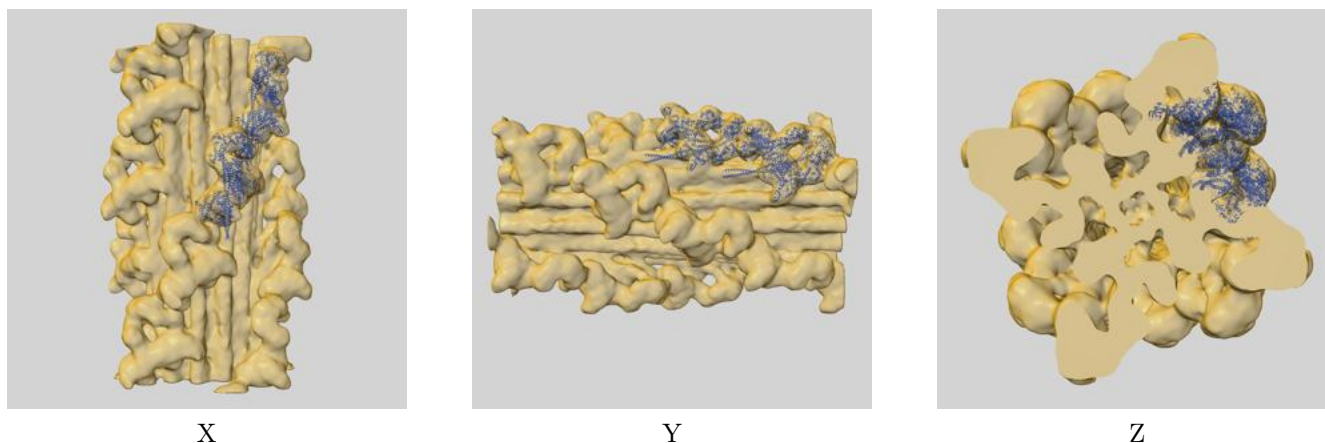
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

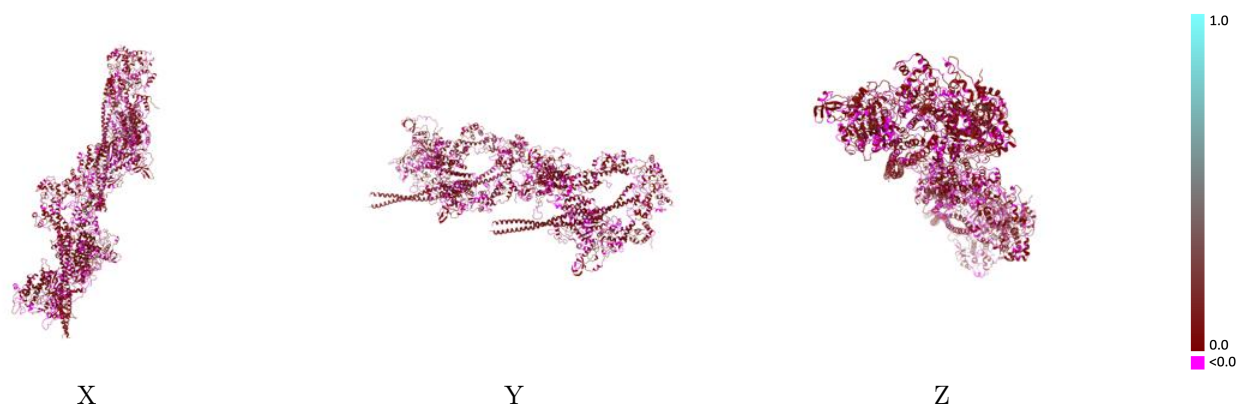
This section contains information regarding the fit between EMDB map EMD-1950 and PDB model 3JBH. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



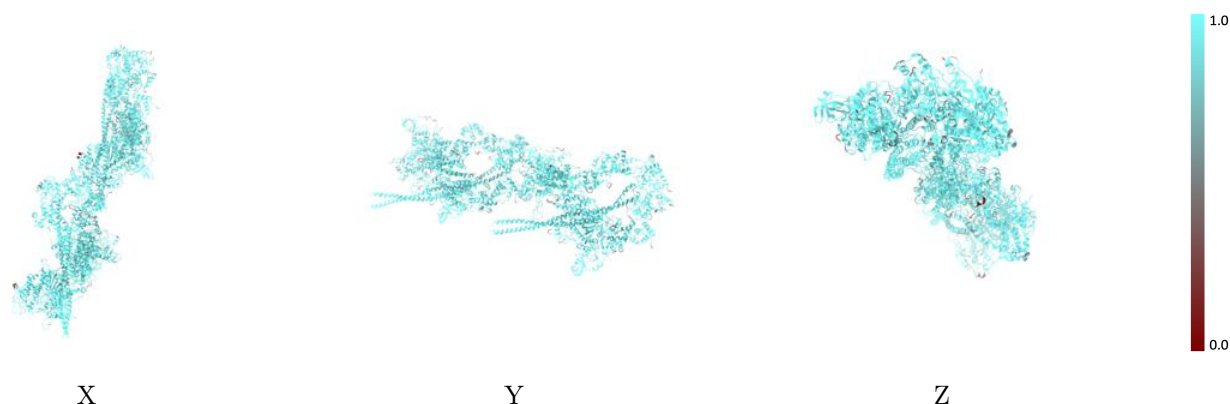
The images above show the 3D surface view of the map at the recommended contour level 25.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



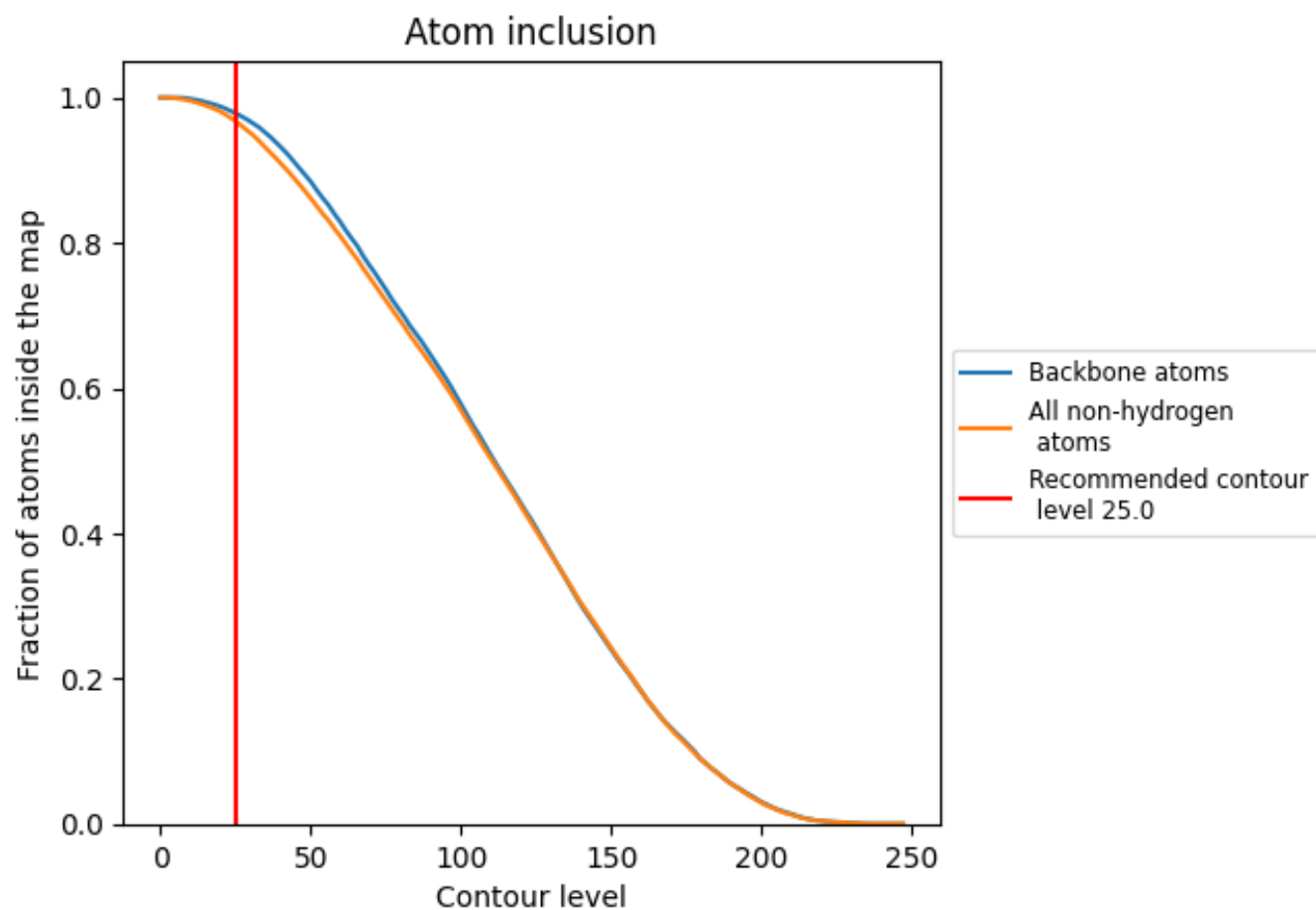
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (25.0).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (25.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9676	<div></div> 0.0440
A	<div></div> 0.9732	<div></div> 0.0440
B	<div></div> 0.9674	<div></div> 0.0430
C	<div></div> 0.9540	<div></div> 0.0530
D	<div></div> 0.9589	<div></div> 0.0410
E	<div></div> 0.9716	<div></div> 0.0430
F	<div></div> 0.9458	<div></div> 0.0440
G	<div></div> 0.9768	<div></div> 0.0460
H	<div></div> 0.9678	<div></div> 0.0430
I	<div></div> 0.9548	<div></div> 0.0520
J	<div></div> 0.9614	<div></div> 0.0380
K	<div></div> 0.9676	<div></div> 0.0440
L	<div></div> 0.9439	<div></div> 0.0440

