



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 06:59 AM UTC

PDB ID : 3JAX / pdb_00003jax
EMDB ID : EMD-6370
Title : Heavy meromyosin from Schistosoma mansoni muscle thick filament by negative stain EM
Authors : Sulbaran, G.; Alamo, L.; Pinto, A.; Marquez, G.; Mendez, F.; Padron, R.; Craig, R.
Deposited on : 2015-07-03
Resolution : 23.00 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:

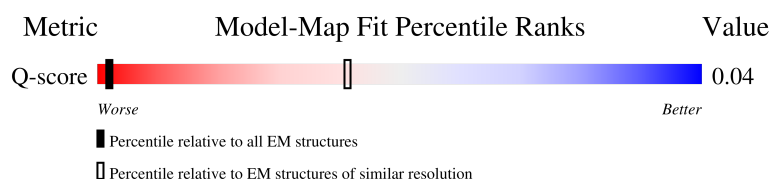
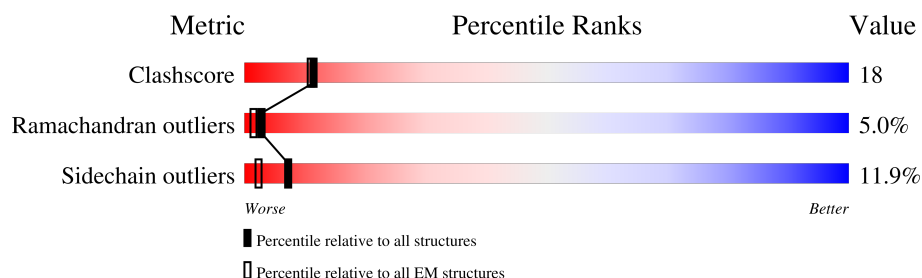
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 23.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	17 (22.90 - 23.50)

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	974	12% 52% 33% 11% ••
1	B	974	6% 44% 37% 12% ••
2	C	151	19% 68% 24% 7% •
2	D	151	38% 45% 12% ••

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Mol	Chain	Length	Quality of chain
3	E	196	35% 54% 34% 10%
3	F	196	5% 38% 34% 17% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25293 atoms, of which 4713 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.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	938	Total	C	H	N	O	S	0	0
			9360	4819	1759	1312	1432	38		
1	B	940	Total	C	H	N	O	S	0	0
			9379	4828	1764	1315	1434	38		

- Molecule 2 is a protein called smooth muscle myosin essential light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	148	Total	C	H	N	O	S	0	0
			1411	722	251	193	234	11		
2	D	148	Total	C	H	N	O	S	0	0
			1411	722	251	193	234	11		

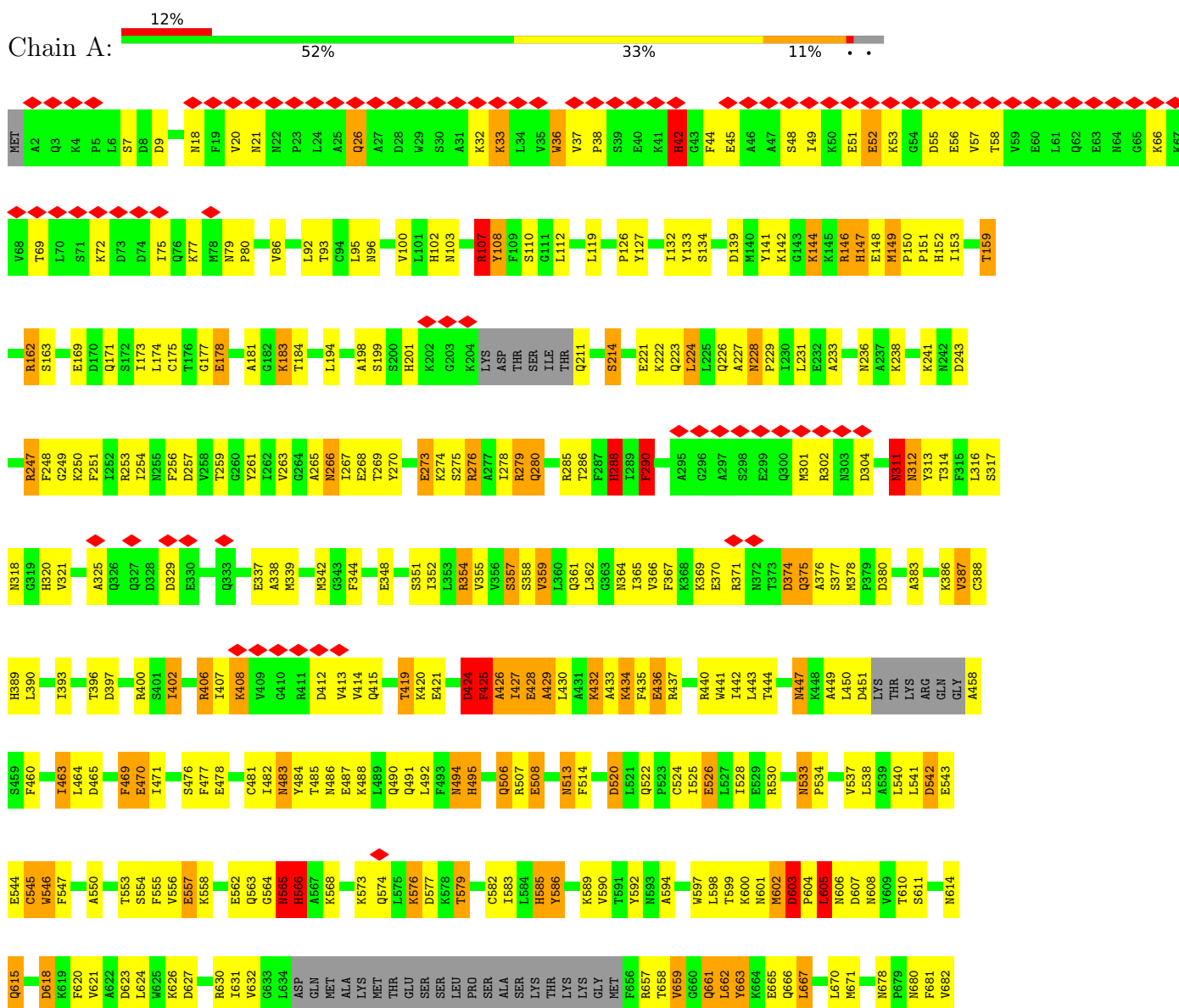
- Molecule 3 is a protein called myosin regulatory light chain.

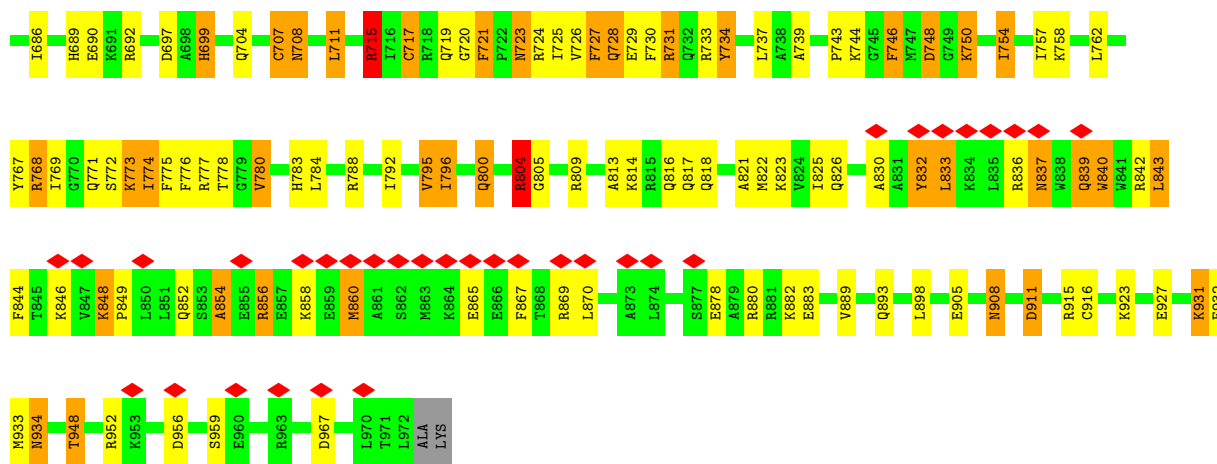
Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	196	Total	C	H	N	O	S	0	0
			1866	948	344	259	309	6		
3	F	196	Total	C	H	N	O	S	0	0
			1866	948	344	259	309	6		

3 Residue-property plots

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

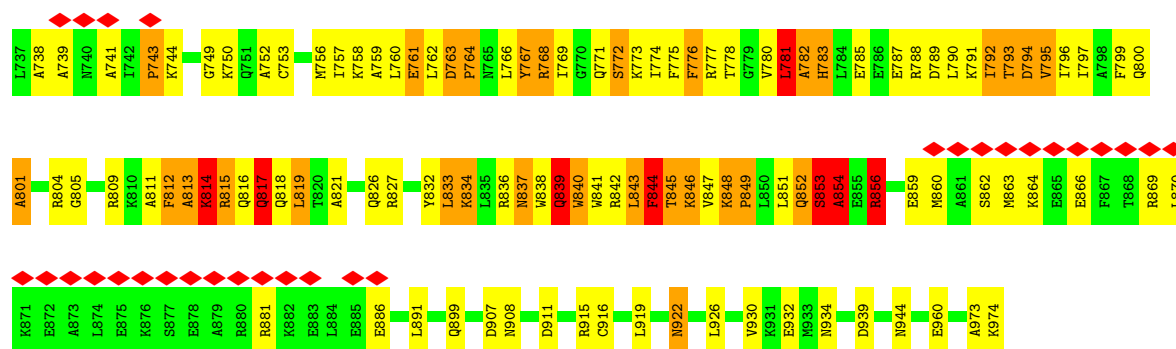
- Molecule 1: myosin 2 heavy chain



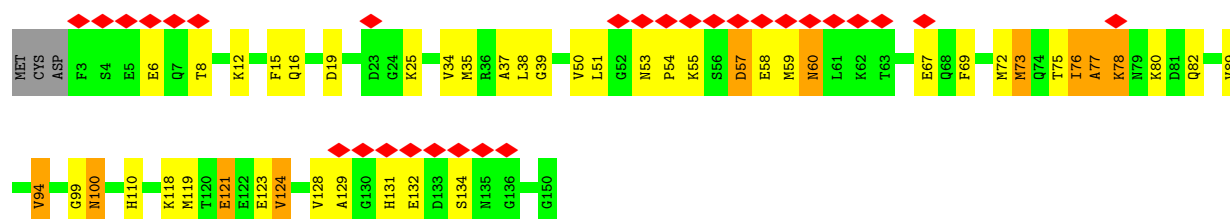


• Molecule 1: myosin 2 heavy chain

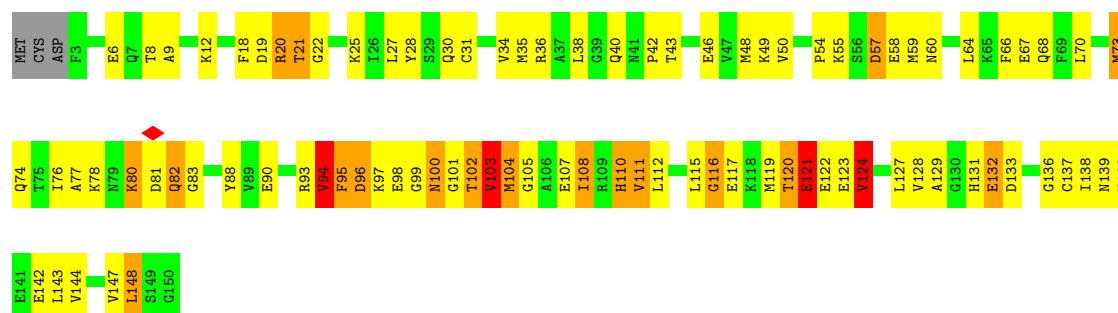




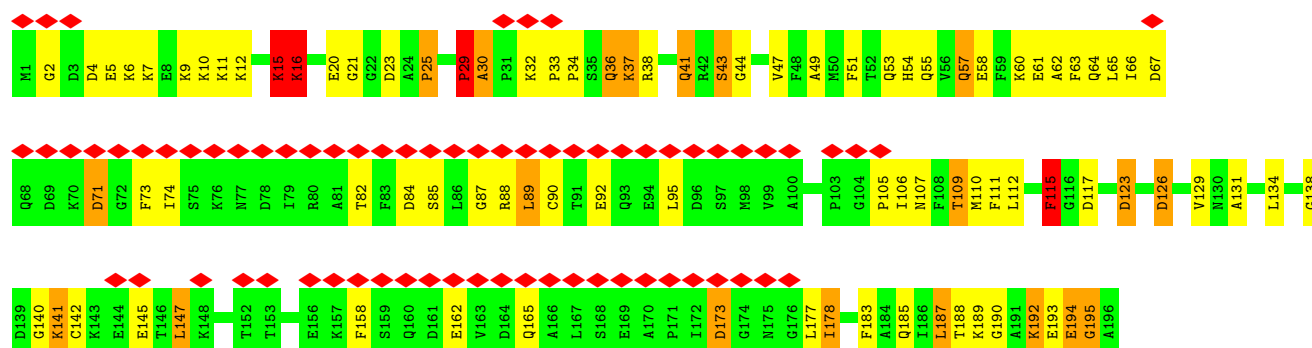
• Molecule 2: smooth muscle myosin essential light chain



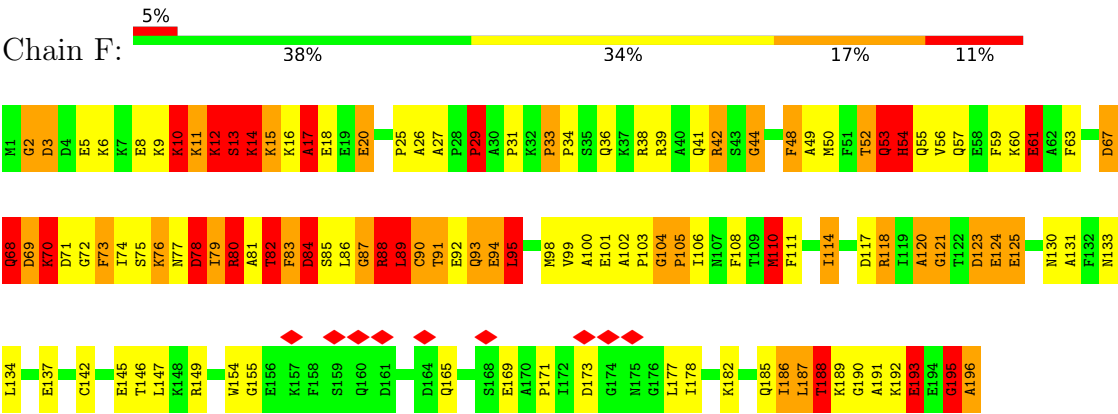
• Molecule 2: smooth muscle myosin essential light chain



• Molecule 3: myosin regulatory light chain



● Molecule 3: myosin regulatory light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=30°, rise=145 Å, axial sym=C4	Depositor
Number of segments used	9500	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI/PHILIPS CM120T	Depositor
Voltage (kV)	80	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	42000	Depositor
Image detector	TVIPS TEMCAM-F224 (2k x 2k)	Depositor
Maximum map value	36.991	Depositor
Minimum map value	-0.168	Depositor
Average map value	1.011	Depositor
Map value standard deviation	3.858	Depositor
Recommended contour level	6	Depositor
Map size (Å)	746.69995, 746.69995, 746.69995	wwPDB
Map dimensions	131, 131, 131	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	5.7, 5.7, 5.7	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	0.74	15/7730 (0.2%)	1.74	163/10402 (1.6%)
1	B	0.75	15/7744 (0.2%)	1.77	180/10420 (1.7%)
2	C	0.67	2/1175 (0.2%)	1.60	12/1575 (0.8%)
2	D	0.71	2/1175 (0.2%)	1.73	24/1575 (1.5%)
3	E	0.69	1/1546 (0.1%)	1.73	30/2071 (1.4%)
3	F	0.76	2/1546 (0.1%)	1.94	55/2071 (2.7%)
All	All	0.74	37/20916 (0.2%)	1.76	464/28114 (1.7%)

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	22
1	B	0	31
2	D	0	7
3	E	0	3
3	F	0	16
All	All	0	79

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	495	HIS	CD2-NE2	-6.95	1.30	1.37
1	B	783	HIS	CD2-NE2	-6.91	1.30	1.37
1	A	566	HIS	CD2-NE2	-6.90	1.30	1.37
1	B	585	HIS	CD2-NE2	-6.89	1.30	1.37
1	B	389	HIS	CD2-NE2	-6.84	1.30	1.37
1	A	689	HIS	CD2-NE2	-6.82	1.30	1.37
1	B	689	HIS	CD2-NE2	-6.78	1.30	1.37
1	A	42	HIS	CD2-NE2	-6.76	1.30	1.37
1	A	495	HIS	CD2-NE2	-6.71	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	389	HIS	CD2-NE2	-6.70	1.30	1.37
1	A	201	HIS	CD2-NE2	-6.65	1.30	1.37
1	A	288	HIS	CD2-NE2	-6.65	1.30	1.37
1	A	585	HIS	CD2-NE2	-6.62	1.30	1.37
3	F	54	HIS	CD2-NE2	-6.61	1.30	1.37
1	B	42	HIS	CD2-NE2	-6.54	1.30	1.37
2	C	110	HIS	CD2-NE2	-6.50	1.30	1.37
1	A	783	HIS	CD2-NE2	-6.44	1.30	1.37
1	B	288	HIS	CD2-NE2	-6.41	1.30	1.37
1	B	152	HIS	CD2-NE2	-6.30	1.30	1.37
1	B	699	HIS	CD2-NE2	-6.29	1.30	1.37
1	B	566	HIS	CD2-NE2	-6.24	1.30	1.37
1	B	320	HIS	CD2-NE2	-6.19	1.31	1.37
1	B	201	HIS	CD2-NE2	-6.16	1.31	1.37
1	A	699	HIS	CD2-NE2	-6.16	1.31	1.37
1	A	102	HIS	CD2-NE2	-6.15	1.31	1.37
2	D	110	HIS	CD2-NE2	-6.12	1.31	1.37
1	B	147	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	147	HIS	CD2-NE2	-6.06	1.31	1.37
2	C	131	HIS	CD2-NE2	-6.05	1.31	1.37
2	D	131	HIS	CD2-NE2	-6.04	1.31	1.37
1	B	102	HIS	CD2-NE2	-6.00	1.31	1.37
3	E	54	HIS	CD2-NE2	-5.96	1.31	1.37
1	A	320	HIS	CD2-NE2	-5.94	1.31	1.37
1	A	152	HIS	CD2-NE2	-5.82	1.31	1.37
3	F	54	HIS	CG-ND1	-5.26	1.32	1.38
1	A	288	HIS	CG-ND1	-5.11	1.32	1.38
1	B	152	HIS	CG-ND1	-5.07	1.32	1.38

All (464) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	ASN	N-CA-C	11.42	129.38	113.16
3	F	73	PHE	CA-CB-CG	11.02	124.82	113.80
1	A	603	ASP	CA-CB-CG	10.89	123.49	112.60
1	A	602	MET	N-CA-C	10.87	123.20	111.36
1	A	621	VAL	N-CA-C	10.85	121.14	111.81
2	D	104	MET	N-CA-C	10.26	123.92	109.15
1	B	167	ASP	CA-CB-CG	10.24	122.84	112.60
3	F	54	HIS	CA-CB-CG	9.82	123.62	113.80
1	B	697	ASP	CA-CB-CG	9.73	122.33	112.60
1	A	425	PHE	CA-C-O	-9.59	110.83	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	PHE	CA-CB-CG	9.56	123.36	113.80
1	A	934	ASN	CA-CB-CG	9.45	122.05	112.60
1	A	227	ALA	N-CA-C	9.38	125.56	112.04
1	A	566	HIS	CB-CG-CD2	-9.32	119.08	131.20
1	A	425	PHE	N-CA-CB	9.19	123.15	110.10
1	A	428	GLU	CA-CB-CG	9.13	132.36	114.10
1	A	659	VAL	CB-CA-C	-9.07	100.16	112.04
1	B	499	ILE	N-CA-C	9.05	118.93	110.42
1	A	659	VAL	N-CA-CB	9.02	123.51	110.52
3	F	89	LEU	N-CA-C	8.98	120.51	108.38
1	B	196	VAL	CB-CA-C	8.87	120.68	110.93
1	A	428	GLU	N-CA-CB	8.80	123.00	110.07
3	E	192	LYS	O-C-N	-8.66	112.21	123.21
1	B	90	ALA	N-CA-C	8.48	120.45	111.03
1	B	394	ASN	CA-C-O	8.42	129.31	120.30
1	B	585	HIS	CB-CG-CD2	-8.35	120.35	131.20
1	B	228	ASN	OD1-CG-ND2	-8.34	114.26	122.60
1	B	934	ASN	CA-CB-CG	8.34	120.94	112.60
3	E	36	GLN	N-CA-C	8.21	120.23	111.28
1	B	529	GLU	N-CA-C	8.21	123.38	113.12
1	A	387	VAL	N-CA-C	8.20	118.25	110.30
3	F	195	GLY	O-C-N	-8.13	112.12	122.70
1	A	107	ARG	NE-CZ-NH2	-8.12	111.89	119.20
1	A	665	GLU	N-CA-C	8.11	121.14	111.33
3	E	187	LEU	N-CA-C	8.09	120.72	110.61
1	A	566	HIS	CB-CG-ND1	8.05	134.78	122.70
1	A	908	ASN	CA-CB-CG	7.96	120.56	112.60
1	B	303	ASN	CA-CB-CG	7.96	120.56	112.60
1	B	856	ARG	N-CA-C	7.93	127.69	110.80
1	A	618	ASP	CA-CB-CG	7.91	120.51	112.60
1	A	42	HIS	CB-CG-CD2	-7.91	120.92	131.20
1	A	795	VAL	N-CA-C	7.90	125.78	109.34
3	F	88	ARG	N-CA-C	7.88	115.24	108.78
1	B	424	ASP	CA-CB-CG	7.87	120.47	112.60
1	A	338	ALA	N-CA-C	7.84	121.79	111.75
1	A	839	GLN	OE1-CD-NE2	-7.83	114.77	122.60
3	F	14	LYS	N-CA-C	7.82	132.91	111.00
1	A	447	ASN	OD1-CG-ND2	-7.79	114.81	122.60
1	B	152	HIS	CA-CB-CG	7.75	121.55	113.80
1	B	608	ASN	OD1-CG-ND2	-7.73	114.87	122.60
1	B	178	GLU	N-CA-C	7.62	121.26	109.60
1	A	389	HIS	CB-CG-CD2	-7.54	121.39	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	66	PHE	N-CA-C	7.47	119.06	111.07
1	A	661	GLN	OE1-CD-NE2	-7.45	115.15	122.60
1	A	883	GLU	N-CA-C	7.44	119.47	111.36
3	F	91	THR	O-C-N	-7.44	114.63	123.03
1	A	464	LEU	N-CA-C	7.43	120.66	107.80
3	E	16	LYS	CA-CB-CG	7.42	128.94	114.10
1	A	483	ASN	OD1-CG-ND2	-7.39	115.20	122.60
1	B	661	GLN	OE1-CD-NE2	-7.36	115.25	122.60
1	A	783	HIS	CB-CG-CD2	-7.32	121.68	131.20
3	F	187	LEU	N-CA-C	7.32	126.38	110.80
2	D	96	ASP	N-CA-C	7.31	121.89	113.19
1	A	226	GLN	N-CA-C	7.30	122.02	110.70
3	F	188	THR	N-CA-C	7.26	126.28	110.80
1	A	795	VAL	O-C-N	-7.18	113.60	122.57
1	B	838	TRP	N-CA-C	7.18	120.11	108.34
1	B	389	HIS	CB-CG-CD2	-7.17	121.87	131.20
2	C	124	VAL	N-CA-C	7.15	117.94	110.72
1	B	845	THR	N-CA-C	7.13	122.86	113.30
1	B	837	ASN	OD1-CG-ND2	-7.10	115.50	122.60
1	B	150	PRO	N-CA-C	7.04	119.29	110.70
3	F	91	THR	CA-C-O	-7.03	113.09	121.66
1	B	136	LYS	N-CA-C	-7.02	103.55	111.14
1	A	9	ASP	CA-CB-CG	7.01	119.61	112.60
1	A	318	ASN	CA-CB-CG	7.00	119.60	112.60
1	A	228	ASN	OD1-CG-ND2	-6.95	115.65	122.60
3	E	16	LYS	N-CA-CB	6.89	122.13	110.49
1	B	782	ALA	N-CA-CB	-6.85	100.47	110.40
1	B	627	ASP	CA-CB-CG	6.85	119.45	112.60
1	B	501	GLU	N-CA-C	-6.83	103.29	111.69
1	B	149	MET	CA-C-N	6.82	127.40	120.38
1	B	149	MET	C-N-CA	6.82	127.40	120.38
3	E	23	ASP	CA-CB-CG	6.78	119.38	112.60
3	E	123	ASP	CA-CB-CG	6.78	119.38	112.60
1	A	697	ASP	CA-CB-CG	6.77	119.37	112.60
2	D	133	ASP	CA-CB-CG	6.75	119.35	112.60
1	B	719	GLN	OE1-CD-NE2	-6.74	115.86	122.60
1	B	839	GLN	N-CA-C	6.71	125.10	110.80
1	B	394	ASN	OD1-CG-ND2	-6.69	115.91	122.60
2	D	129	ALA	N-CA-C	6.68	120.17	110.42
1	A	42	HIS	CB-CG-ND1	6.67	132.70	122.70
1	A	893	GLN	OE1-CD-NE2	-6.63	115.97	122.60
3	F	53	GLN	OE1-CD-NE2	-6.62	115.98	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	193	GLU	N-CA-C	6.62	121.48	113.41
3	F	10	LYS	N-CA-C	-6.60	105.38	113.50
3	E	25	PRO	N-CA-C	6.60	120.76	110.80
2	D	94	VAL	CA-CB-CG1	6.58	121.58	110.40
1	B	513	ASN	CA-CB-CG	6.58	119.18	112.60
3	F	79	ILE	N-CA-C	-6.55	106.41	112.96
1	B	463	ILE	O-C-N	-6.54	116.00	123.00
2	C	118	LYS	N-CA-C	6.53	119.49	110.35
1	B	394	ASN	CA-CB-CG	-6.53	106.07	112.60
1	B	973	ALA	N-CA-C	6.51	119.21	110.35
1	A	159	THR	CA-CB-OG1	-6.51	99.83	109.60
1	A	248	PHE	N-CA-C	6.50	118.95	109.07
1	B	329	ASP	CA-CB-CG	6.49	119.09	112.60
1	A	266	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	A	470	GLU	N-CA-C	6.48	119.56	109.52
1	B	148	GLU	N-CA-C	-6.48	105.53	113.50
1	A	513	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	A	276	ARG	N-CA-C	6.46	120.26	112.38
1	A	911	ASP	CA-CB-CG	6.46	119.06	112.60
3	F	169	GLU	N-CA-C	6.45	119.31	111.82
2	D	94	VAL	N-CA-C	6.45	122.75	109.34
1	B	147	HIS	CA-CB-CG	6.43	120.23	113.80
1	A	967	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	627	ASP	CA-CB-CG	6.43	119.03	112.60
2	D	110	HIS	CB-CG-CD2	-6.42	122.86	131.20
2	D	68	GLN	N-CA-C	-6.42	105.34	113.43
1	A	565	ASN	OD1-CG-ND2	-6.41	116.19	122.60
1	B	79	ASN	CA-C-N	6.39	124.32	119.66
1	B	79	ASN	C-N-CA	6.39	124.32	119.66
1	B	812	PHE	N-CA-C	6.39	118.77	111.11
1	A	288	HIS	CA-CB-CG	6.38	120.18	113.80
1	B	585	HIS	CB-CG-ND1	6.37	132.25	122.70
3	E	109	THR	CA-C-O	-6.35	114.13	120.80
1	A	748	ASP	CA-CB-CG	6.35	118.95	112.60
1	B	495	HIS	CB-CG-CD2	-6.34	122.96	131.20
1	B	781	LEU	CA-C-O	6.34	129.57	120.51
1	B	150	PRO	N-CA-CB	-6.34	96.93	103.08
1	B	565	ASN	OD1-CG-ND2	-6.34	116.26	122.60
1	A	659	VAL	N-CA-C	-6.32	104.69	110.82
3	E	117	ASP	CA-CB-CG	6.32	118.92	112.60
3	F	54	HIS	N-CA-CB	6.31	121.16	110.49
1	B	783	HIS	CA-CB-CG	-6.31	107.49	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	PRO	N-CA-C	6.31	125.46	112.47
1	B	288	HIS	CA-CB-CG	6.30	120.11	113.80
2	C	16	GLN	OE1-CD-NE2	-6.28	116.32	122.60
2	D	93	ARG	N-CA-C	-6.27	104.73	112.38
1	A	666	GLN	OE1-CD-NE2	-6.26	116.34	122.60
1	B	818	GLN	N-CA-C	6.26	120.48	112.34
1	A	520	ASP	N-CA-C	-6.25	96.94	107.99
1	A	389	HIS	CB-CG-ND1	6.23	132.05	122.70
3	F	79	ILE	CB-CA-C	6.22	116.54	111.06
3	E	88	ARG	N-CA-C	6.21	118.56	108.63
2	C	128	VAL	N-CA-C	6.21	117.22	111.45
1	B	442	ILE	N-CA-C	6.20	116.31	110.30
1	A	678	ASN	OD1-CG-ND2	-6.20	116.40	122.60
3	E	15	LYS	N-CA-C	6.19	122.25	113.02
1	B	287	PHE	CA-C-N	6.19	130.10	120.82
1	B	287	PHE	C-N-CA	6.19	130.10	120.82
1	B	18	ASN	OD1-CG-ND2	-6.19	116.41	122.60
2	C	100	ASN	N-CA-C	6.18	123.97	110.80
1	A	153	ILE	N-CA-C	6.17	122.18	109.34
1	A	730	PHE	CA-CB-CG	-6.17	107.63	113.80
3	F	76	LYS	N-CA-CB	6.17	119.13	109.94
1	B	394	ASN	N-CA-C	6.16	118.44	108.41
2	D	100	ASN	N-CA-C	6.15	120.79	113.16
1	A	279	ARG	CA-CB-CG	6.15	126.39	114.10
1	A	228	ASN	CB-CG-ND2	6.12	125.59	116.40
1	A	290	PHE	CA-CB-CG	6.12	119.92	113.80
1	B	812	PHE	CA-CB-CG	6.12	119.92	113.80
1	B	699	HIS	CB-CG-CD2	-6.12	123.25	131.20
1	B	464	LEU	N-CA-C	6.11	120.69	107.49
3	F	196	ALA	N-CA-C	6.11	128.10	111.00
1	A	494	ASN	OD1-CG-ND2	-6.09	116.50	122.60
1	B	484	TYR	CA-CB-CG	6.08	124.85	113.90
1	A	542	ASP	CA-CB-CG	6.07	118.67	112.60
1	B	384	ALA	N-CA-C	6.07	118.86	111.82
1	A	783	HIS	CB-CG-ND1	6.05	131.78	122.70
1	B	854	ALA	N-CA-C	6.05	123.68	110.80
3	E	30	ALA	N-CA-C	6.05	123.17	109.81
1	B	725	ILE	O-C-N	-6.04	115.02	122.57
1	A	273	GLU	N-CA-CB	6.04	120.70	110.49
3	E	67	ASP	CA-CB-CG	6.02	118.62	112.60
1	A	513	ASN	CB-CG-ND2	6.02	125.43	116.40
1	B	15	VAL	N-CA-CB	6.01	120.23	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	ALA	N-CA-C	6.01	119.45	111.75
2	D	110	HIS	CA-CB-CG	-6.01	107.78	113.80
1	B	727	PHE	CA-CB-CG	6.01	119.81	113.80
3	E	63	PHE	N-CA-C	-5.98	104.84	111.36
1	B	736	ILE	N-CA-CB	-5.97	104.55	112.26
1	B	608	ASN	N-CA-C	5.96	118.29	111.02
1	A	594	ALA	N-CA-C	5.95	120.54	113.28
1	B	681	PHE	N-CA-C	5.95	119.24	109.72
3	F	94	GLU	CA-CB-CG	5.95	126.00	114.10
3	F	18	GLU	N-CA-C	5.95	118.72	111.82
2	D	19	ASP	CA-CB-CG	5.94	118.54	112.60
1	B	103	ASN	OD1-CG-ND2	-5.94	116.66	122.60
1	A	419	THR	CA-C-O	-5.93	115.78	122.01
3	E	195	GLY	O-C-N	-5.93	114.99	122.70
3	F	25	PRO	N-CA-C	5.93	121.45	111.32
1	A	248	PHE	O-C-N	-5.91	116.51	123.25
1	B	396	THR	CA-C-O	5.91	127.22	120.90
3	F	186	ILE	O-C-N	-5.91	115.18	122.57
3	F	114	ILE	N-CA-CB	5.90	120.96	111.23
1	B	801	ALA	N-CA-C	5.89	117.70	111.28
1	B	276	ARG	N-CA-C	5.89	118.48	111.71
1	A	177	GLY	CA-C-O	-5.88	118.17	122.23
1	A	201	HIS	CB-CG-CD2	-5.86	123.58	131.20
1	B	922	ASN	CA-CB-CG	5.86	118.46	112.60
1	B	944	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	A	465	ASP	CA-CB-CG	5.85	118.45	112.60
2	D	103	VAL	N-CA-C	5.85	117.85	108.85
3	F	70	LYS	N-CA-C	5.85	123.25	110.80
1	B	374	ASP	CA-CB-CG	-5.84	106.76	112.60
1	B	117	SER	N-CA-C	-5.83	102.96	111.30
1	B	14	PHE	CB-CA-C	-5.83	99.64	109.50
3	F	78	ASP	O-C-N	-5.83	114.86	122.20
1	A	80	PRO	N-CA-C	5.82	117.80	110.70
3	E	109	THR	CA-CB-OG1	-5.81	100.88	109.60
1	B	908	ASN	CA-CB-CG	5.81	118.41	112.60
1	A	147	HIS	CA-CB-CG	5.80	119.60	113.80
1	B	731	ARG	CA-C-O	5.79	126.74	120.55
1	A	726	VAL	O-C-N	-5.79	115.34	122.57
3	F	61	GLU	CB-CG-CD	5.77	122.40	112.60
1	A	52	GLU	N-CA-C	5.76	117.85	108.63
1	A	325	ALA	N-CA-C	5.76	119.50	111.90
1	B	228	ASN	CB-CG-ND2	5.75	125.03	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	476	SER	CA-C-O	-5.75	115.01	121.05
3	F	20	GLU	N-CA-C	5.74	119.10	111.75
3	F	82	THR	CA-CB-CG2	5.74	120.26	110.50
2	C	60	ASN	OD1-CG-ND2	-5.74	116.86	122.60
3	F	82	THR	N-CA-C	5.73	123.01	110.80
1	B	394	ASN	N-CA-CB	5.72	119.58	110.65
1	A	406	ARG	N-CA-C	-5.72	101.64	109.71
1	B	490	GLN	N-CA-C	-5.71	104.96	111.07
3	F	79	ILE	CA-C-O	5.71	124.08	119.29
1	B	736	ILE	CB-CA-C	5.71	118.28	111.20
1	B	266	ASN	OD1-CG-ND2	-5.69	116.91	122.60
3	F	185	GLN	OE1-CD-NE2	-5.69	116.91	122.60
1	B	151	PRO	N-CA-C	5.69	124.19	112.47
2	D	142	GLU	N-CA-C	5.68	120.35	112.45
2	D	77	ALA	N-CA-C	5.67	122.88	110.80
1	A	311	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	B	379	PRO	N-CA-C	5.67	124.14	112.47
3	F	54	HIS	N-CA-C	5.66	122.85	110.80
3	E	57	GLN	O-C-N	5.65	128.13	122.08
2	C	89	VAL	N-CA-CB	5.64	116.77	110.51
1	B	732	GLN	N-CA-C	-5.64	101.16	109.62
1	A	731	ARG	N-CA-C	5.63	118.15	111.33
1	B	362	LEU	N-CA-C	5.63	122.80	110.80
1	A	86	VAL	N-CA-C	5.63	121.05	109.34
1	B	783	HIS	CB-CG-CD2	-5.63	123.88	131.20
1	B	103	ASN	N-CA-C	5.63	119.76	113.01
2	D	82	GLN	OE1-CD-NE2	-5.61	116.99	122.60
3	F	68	GLN	CA-C-N	-5.61	114.82	123.17
3	F	68	GLN	C-N-CA	-5.61	114.82	123.17
1	B	486	ASN	OD1-CG-ND2	-5.60	117.00	122.60
3	E	111	PHE	CA-CB-CG	5.60	119.40	113.80
3	F	53	GLN	CG-CD-NE2	5.60	124.80	116.40
1	A	585	HIS	CB-CG-CD2	-5.59	123.93	131.20
1	A	708	ASN	CA-CB-CG	5.59	118.19	112.60
1	B	192	GLN	OE1-CD-NE2	-5.59	117.01	122.60
3	E	74	ILE	CA-C-O	5.58	125.91	120.27
1	A	659	VAL	CA-CB-CG2	5.58	119.89	110.40
2	D	139	ASN	OD1-CG-ND2	-5.58	117.02	122.60
1	B	718	ARG	CA-CB-CG	5.57	125.25	114.10
2	C	57	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	545	CYS	N-CA-C	-5.57	105.12	111.14
1	A	513	ASN	CA-CB-CG	5.57	118.17	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	77	ALA	N-CA-C	5.57	122.65	110.80
1	A	796	ILE	CA-CB-CG1	5.56	119.85	110.40
1	A	804	ARG	NE-CZ-NH2	5.56	124.20	119.20
3	E	54	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	B	483	ASN	OD1-CG-ND2	-5.55	117.05	122.60
1	B	170	ASP	N-CA-C	5.55	118.33	110.50
1	B	689	HIS	CB-CG-CD2	-5.55	123.99	131.20
1	A	618	ASP	N-CA-C	5.54	117.67	110.53
1	A	774	ILE	N-CA-CB	5.53	117.38	111.46
1	B	469	PHE	CA-C-O	5.53	128.42	120.51
1	B	934	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	B	441	TRP	CB-CG-CD1	-5.53	118.61	126.90
1	B	37	VAL	CA-C-N	5.53	125.54	119.90
1	B	37	VAL	C-N-CA	5.53	125.54	119.90
1	A	147	HIS	CB-CG-CD2	-5.52	124.02	131.20
1	A	750	LYS	CA-CB-CG	5.52	125.14	114.10
3	E	57	GLN	OE1-CD-NE2	-5.52	117.08	122.60
1	A	415	GLN	N-CA-C	-5.51	100.26	109.24
1	A	661	GLN	CG-CD-NE2	5.51	124.66	116.40
1	A	739	ALA	N-CA-C	5.51	119.50	112.34
1	A	878	GLU	N-CA-C	5.50	117.09	111.14
2	D	94	VAL	O-C-N	-5.50	115.69	122.57
1	A	800	GLN	OE1-CD-NE2	-5.50	117.10	122.60
3	F	87	GLY	O-C-N	-5.50	115.55	122.70
1	B	771	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	A	469	PHE	CA-CB-CG	5.49	119.29	113.80
1	A	329	ASP	CA-CB-CG	5.47	118.07	112.60
1	B	513	ASN	OD1-CG-ND2	-5.47	117.13	122.60
1	B	844	PHE	CA-CB-CG	5.47	119.27	113.80
1	B	303	ASN	OD1-CG-ND2	-5.47	117.13	122.60
1	B	150	PRO	CA-C-N	5.47	126.67	119.84
1	B	150	PRO	C-N-CA	5.47	126.67	119.84
1	B	419	THR	CA-C-O	-5.47	115.66	121.94
1	B	732	GLN	CG-CD-NE2	5.46	124.60	116.40
1	B	827	ARG	CB-CA-C	-5.46	102.08	110.81
1	A	36	TRP	CG-CD2-CE3	5.46	139.35	133.90
1	A	184	THR	CA-C-O	5.45	126.54	120.82
1	B	683	ARG	CD-NE-CZ	-5.45	116.78	124.40
2	D	148	LEU	N-CA-C	5.44	119.76	113.18
1	B	678	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	B	720	GLY	O-C-N	-5.43	118.86	123.59
1	A	279	ARG	O-C-N	-5.43	115.37	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	719	GLN	CG-CD-NE2	5.42	124.54	116.40
1	B	312	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	B	299	GLU	N-CA-C	5.42	118.68	111.75
1	A	566	HIS	CA-CB-CG	5.41	119.21	113.80
1	B	727	PHE	N-CA-C	5.41	117.87	111.33
1	B	795	VAL	CA-C-O	-5.41	114.93	120.71
1	B	814	LYS	N-CA-C	5.40	122.31	110.80
3	E	71	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	931	LYS	CA-C-O	-5.40	115.34	120.90
1	B	827	ARG	CA-CB-CG	5.40	124.90	114.10
1	A	149	MET	CA-C-N	5.39	125.94	120.38
1	A	149	MET	C-N-CA	5.39	125.94	120.38
1	A	602	MET	CA-C-O	-5.39	114.70	120.42
1	A	721	PHE	CA-C-N	5.39	124.85	119.24
1	A	721	PHE	C-N-CA	5.39	124.85	119.24
3	E	165	GLN	OE1-CD-NE2	-5.38	117.22	122.60
3	F	93	GLN	N-CA-CB	-5.38	102.18	109.98
1	A	436	GLU	CA-C-O	-5.38	114.05	120.56
1	A	680	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	A	495	HIS	CB-CG-CD2	-5.38	124.21	131.20
1	A	689	HIS	CB-CG-CD2	-5.37	124.22	131.20
1	B	441	TRP	CE2-CD2-CG	-5.37	100.75	107.20
1	B	498	PHE	CA-CB-CG	5.36	119.16	113.80
1	A	80	PRO	CA-C-N	5.35	125.67	119.47
1	A	80	PRO	C-N-CA	5.35	125.67	119.47
1	A	337	GLU	N-CA-C	5.35	117.19	111.36
1	B	708	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	B	376	ALA	N-CA-C	5.34	118.82	110.32
3	E	185	GLN	OE1-CD-NE2	-5.34	117.26	122.60
3	F	123	ASP	N-CA-C	5.34	122.18	110.80
1	B	133	TYR	N-CA-C	-5.34	98.56	107.80
1	B	320	HIS	N-CA-C	-5.33	98.53	108.02
1	B	678	ASN	CA-C-N	5.33	125.24	119.85
1	B	678	ASN	C-N-CA	5.33	125.24	119.85
1	B	36	TRP	CE2-CD2-CG	-5.33	100.80	107.20
3	E	126	ASP	N-CA-C	5.33	117.83	111.71
1	A	728	GLN	CA-C-O	5.32	125.83	119.60
1	B	406	ARG	CA-CB-CG	5.32	124.74	114.10
3	E	89	LEU	N-CA-C	5.32	118.15	110.28
1	A	377	SER	N-CA-C	5.31	117.06	109.14
1	A	795	VAL	CA-CB-CG1	5.31	119.43	110.40
1	B	311	ASN	CA-CB-CG	5.31	117.91	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	468	GLY	N-CA-C	5.30	118.84	111.10
2	D	57	ASP	CA-CB-CG	5.30	117.90	112.60
2	D	103	VAL	N-CA-CB	-5.29	100.96	111.91
1	B	167	ASP	N-CA-C	5.29	117.96	111.82
3	F	125	GLU	N-CA-C	5.29	122.07	110.80
1	B	730	PHE	N-CA-C	5.28	118.51	111.75
2	C	19	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	250	LYS	N-CA-C	5.28	122.05	110.80
1	A	606	ASN	CA-CB-CG	5.28	117.88	112.60
1	B	147	HIS	CA-C-O	5.28	125.92	119.64
1	A	37	VAL	CA-C-N	5.27	125.19	119.76
1	A	37	VAL	C-N-CA	5.27	125.19	119.76
1	B	811	ALA	N-CA-C	5.27	119.81	113.17
1	B	327	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	B	840	TRP	CE2-CD2-CG	-5.27	100.88	107.20
1	B	389	HIS	CB-CG-ND1	5.26	130.60	122.70
1	B	441	TRP	CG-CD2-CE3	5.26	139.16	133.90
1	B	542	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	104	LEU	CA-C-N	5.26	127.64	120.54
1	B	104	LEU	C-N-CA	5.26	127.64	120.54
3	F	83	PHE	CA-CB-CG	-5.25	108.55	113.80
1	B	186	ASN	OD1-CG-ND2	-5.24	117.36	122.60
3	F	68	GLN	CB-CA-C	-5.23	101.86	110.08
1	A	146	ARG	N-CA-C	5.23	116.98	111.28
2	D	124	VAL	N-CA-CB	5.23	116.32	110.62
3	F	26	ALA	N-CA-C	5.22	118.53	111.17
3	F	41	GLN	CG-CD-NE2	5.22	124.22	116.40
1	B	394	ASN	O-C-N	5.21	129.32	123.27
1	B	674	LEU	N-CA-C	5.21	118.42	111.75
3	F	13	SER	O-C-N	-5.21	115.66	122.59
1	B	463	ILE	CA-C-O	-5.21	115.24	121.28
1	A	441	TRP	CE2-CD2-CG	-5.21	100.95	107.20
1	B	732	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	B	326	GLN	N-CA-C	-5.20	100.22	109.06
1	B	373	THR	N-CA-C	-5.20	107.00	113.55
1	A	428	GLU	CB-CA-C	5.19	119.43	110.86
1	A	837	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	A	408	LYS	CA-CB-CG	5.18	124.46	114.10
1	A	557	GLU	CB-CG-CD	5.18	121.41	112.60
1	A	224	LEU	N-CA-C	5.17	121.82	110.80
1	B	535	PRO	N-CA-C	5.17	119.44	111.21
1	B	666	GLN	OE1-CD-NE2	-5.17	117.43	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	PRO	N-CA-C	5.17	119.20	111.14
1	A	18	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	A	194	LEU	N-CA-C	5.17	116.91	111.28
1	A	263	VAL	CA-C-O	-5.17	116.20	120.80
1	A	597	TRP	CE2-CD2-CG	-5.17	101.00	107.20
1	A	20	VAL	N-CA-C	5.16	115.40	108.17
1	B	277	ALA	N-CA-C	5.16	119.05	112.34
1	A	708	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	A	214	SER	N-CA-C	5.16	118.03	109.46
1	A	424	ASP	O-C-N	-5.16	114.15	122.41
1	B	21	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	A	723	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	A	150	PRO	N-CA-C	5.15	116.98	110.70
1	A	780	VAL	N-CA-C	5.15	120.06	109.34
1	B	512	TRP	CB-CG-CD1	-5.15	119.17	126.90
2	C	124	VAL	CA-C-O	-5.15	115.39	120.85
3	F	67	ASP	N-CA-C	5.15	121.77	110.80
1	A	183	LYS	N-CA-C	5.15	118.02	111.69
1	A	36	TRP	CE2-CD2-CG	-5.14	101.03	107.20
1	A	380	ASP	N-CA-C	5.14	116.80	108.26
3	F	39	ARG	N-CA-C	-5.14	107.66	114.04
1	B	726	VAL	N-CA-C	5.13	115.62	108.84
1	A	463	ILE	O-C-N	-5.13	117.35	123.05
1	B	248	PHE	N-CA-C	-5.13	99.98	108.75
1	A	26	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	B	546	TRP	CE2-CD2-CG	-5.12	101.05	107.20
1	A	727	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	565	ASN	CA-CB-CG	5.11	117.71	112.60
3	E	115	PHE	N-CA-C	5.11	116.54	111.07
1	B	565	ASN	CA-CB-CG	5.11	117.71	112.60
1	B	795	VAL	N-CA-C	5.11	116.57	111.00
2	D	124	VAL	CA-CB-CG2	5.11	119.09	110.40
3	E	29	PRO	N-CA-CB	-5.11	97.89	103.25
1	B	77	LYS	N-CA-C	5.10	121.67	110.80
1	B	378	MET	CA-C-N	5.10	126.21	119.84
1	B	378	MET	C-N-CA	5.10	126.21	119.84
1	A	42	HIS	CA-CB-CG	5.10	118.90	113.80
1	A	508	GLU	N-CA-C	5.09	121.65	110.80
1	B	567	ALA	N-CA-C	5.09	121.65	110.80
3	F	84	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	318	ASN	CA-CB-CG	5.09	117.69	112.60
1	B	333	GLN	OE1-CD-NE2	-5.09	117.51	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	468	GLY	O-C-N	5.09	128.33	123.65
1	A	911	ASP	CB-CA-C	-5.08	102.30	110.74
1	B	36	TRP	CB-CG-CD1	-5.08	119.28	126.90
1	B	763	ASP	CA-C-N	5.08	126.19	119.84
1	B	763	ASP	C-N-CA	5.08	126.19	119.84
1	A	948	THR	CA-CB-OG1	-5.08	101.98	109.60
1	B	78	MET	N-CA-C	5.08	117.23	110.53
3	F	94	GLU	CB-CA-C	-5.08	103.40	111.17
1	A	169	GLU	N-CA-C	-5.08	102.77	110.28
1	A	715	ARG	N-CA-C	5.07	117.54	111.71
1	A	184	THR	N-CA-CB	-5.07	102.66	110.01
1	B	36	TRP	CG-CD2-CE3	5.07	138.97	133.90
3	E	43	SER	N-CA-C	5.07	121.59	110.80
1	B	372	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	B	512	TRP	CE2-CD2-CG	-5.06	101.13	107.20
3	F	104	GLY	CA-C-N	5.05	126.16	119.84
3	F	104	GLY	C-N-CA	5.05	126.16	119.84
1	B	398	PHE	CA-CB-CG	5.05	118.85	113.80
3	F	49	ALA	N-CA-C	5.04	117.61	110.50
3	F	173	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	290	PHE	CA-CB-CG	5.04	118.84	113.80
1	A	840	TRP	CE2-CD2-CG	-5.03	101.16	107.20
1	B	838	TRP	CE2-CD2-CG	-5.03	101.16	107.20
3	F	12	LYS	N-CA-C	5.03	121.51	110.80
1	A	266	ASN	CB-CG-ND2	5.03	123.94	116.40
1	B	618	ASP	CA-CB-CG	5.03	117.63	112.60
2	C	129	ALA	N-CA-C	5.03	117.33	110.24
1	B	841	TRP	CE2-CD2-CG	-5.03	101.17	107.20
3	F	67	ASP	CA-CB-CG	5.02	117.62	112.60
1	B	566	HIS	CB-CG-CD2	-5.02	124.68	131.20
1	B	281	ALA	N-CA-C	5.01	116.41	110.19
1	A	144	LYS	CA-C-O	5.01	125.89	120.43
1	A	546	TRP	CE2-CD2-CG	-5.00	101.19	107.20
1	A	312	ASN	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (79) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ARG	Sidechain
1	A	108	TYR	Sidechain
1	A	127	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	133	TYR	Sidechain
1	A	249	GLY	Peptide
1	A	270	TYR	Sidechain
1	A	276	ARG	Sidechain
1	A	313	TYR	Sidechain
1	A	354	ARG	Sidechain
1	A	359	VAL	Peptide
1	A	362	LEU	Peptide
1	A	424	ASP	Peptide
1	A	427	ILE	Peptide
1	A	432	LYS	Peptide
1	A	663	TYR	Sidechain
1	A	715	ARG	Sidechain
1	A	734	TYR	Sidechain
1	A	746	PHE	Sidechain
1	A	768	ARG	Sidechain
1	A	773	LYS	Peptide
1	A	804	ARG	Sidechain
1	A	832	TYR	Sidechain
1	B	116	TYR	Sidechain
1	B	127	TYR	Sidechain
1	B	141	TYR	Sidechain
1	B	146	ARG	Sidechain
1	B	193	TYR	Sidechain
1	B	211	GLN	Peptide
1	B	270	TYR	Sidechain
1	B	276	ARG	Sidechain
1	B	302	ARG	Sidechain
1	B	313	TYR	Sidechain
1	B	372	ASN	Peptide
1	B	377	SER	Peptide
1	B	467	ALA	Peptide
1	B	630	ARG	Sidechain
1	B	657	ARG	Sidechain
1	B	683	ARG	Peptide
1	B	691	LYS	Peptide
1	B	719	GLN	Peptide
1	B	733	ARG	Sidechain
1	B	734	TYR	Sidechain
1	B	767	TYR	Sidechain
1	B	768	ARG	Sidechain
1	B	776	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	B	781	LEU	Peptide
1	B	792	ILE	Peptide
1	B	815	ARG	Sidechain
1	B	817	GLN	Peptide
1	B	832	TYR	Sidechain
1	B	844	PHE	Peptide
1	B	848	LYS	Peptide
1	B	915	ARG	Sidechain
2	D	120	THR	Peptide
2	D	20	ARG	Sidechain
2	D	28	TYR	Sidechain
2	D	36	ARG	Sidechain
2	D	67	GLU	Peptide
2	D	95	PHE	Sidechain
2	D	99	GLY	Peptide
3	E	138	GLY	Peptide
3	E	21	GLY	Peptide
3	E	25	PRO	Peptide
3	F	10	LYS	Peptide
3	F	101	GLU	Peptide
3	F	17	ALA	Peptide
3	F	2	GLY	Peptide
3	F	38	ARG	Sidechain
3	F	52	THR	Peptide
3	F	53	GLN	Peptide
3	F	54	HIS	Peptide
3	F	68	GLN	Peptide
3	F	69	ASP	Peptide
3	F	70	LYS	Peptide
3	F	71	ASP	Peptide
3	F	78	ASP	Peptide
3	F	80	ARG	Peptide
3	F	88	ARG	Peptide
3	F	89	LEU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7601	1759	7638	238	0
1	B	7615	1764	7656	342	0
2	C	1160	251	1126	18	0
2	D	1160	251	1126	62	0
3	E	1522	344	1492	59	0
3	F	1522	344	1492	110	0
All	All	20580	4713	20530	736	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (736) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:12:LYS:HA	3:F:68:GLN:HG3	1.41	0.99
1:B:238:LYS:HB3	1:B:285:ARG:HB2	1.43	0.98
1:B:375:GLN:HA	1:B:419:THR:HA	1.43	0.98
1:B:178:GLU:HA	1:B:469:PHE:HB3	1.42	0.98
1:A:273:GLU:HA	1:A:478:GLU:HG2	1.46	0.97
3:F:88:ARG:HD2	3:F:89:LEU:HB2	1.45	0.97
1:B:856:ARG:HA	1:B:859:GLU:HB2	1.47	0.96
1:A:728:GLN:HG3	1:B:395:VAL:HB	1.46	0.96
1:A:33:LYS:HB3	1:A:49:ILE:HB	1.52	0.91
1:B:118:GLY:HA3	1:B:717:CYS:HB3	1.54	0.90
1:B:122:VAL:HA	1:B:683:ARG:HB2	1.52	0.90
1:B:147:HIS:HB3	1:B:782:ALA:HB3	1.54	0.89
3:E:9:LYS:HD3	3:F:81:ALA:HA	1.58	0.86
1:A:238:LYS:HB3	1:A:285:ARG:HB2	1.61	0.83
1:A:367:PHE:HB2	1:A:424:ASP:HB2	1.60	0.83
1:A:487:GLU:HG3	1:A:525:ILE:HG12	1.58	0.83
1:B:729:GLU:HG2	2:D:107:GLU:HG2	1.60	0.81
1:B:732:GLN:HB3	2:D:94:VAL:HA	1.63	0.80
3:E:142:CYS:HB3	3:E:147:LEU:HD21	1.63	0.80
1:B:123:VAL:HG21	1:B:682:VAL:HG12	1.62	0.80
1:B:731:ARG:HB2	1:B:753:CYS:HB2	1.63	0.80
1:B:736:ILE:HG12	1:B:795:VAL:HB	1.63	0.80
3:F:3:ASP:HA	3:F:6:LYS:HB2	1.66	0.78
1:A:822:MET:HA	1:A:825:ILE:HD12	1.65	0.77
3:E:57:GLN:HG3	3:E:58:GLU:HG3	1.65	0.77
1:B:3:GLN:HG3	1:B:17:LYS:HD3	1.67	0.75
1:B:727:PHE:HB2	1:B:774:ILE:HB	1.69	0.75
1:B:15:VAL:HG12	1:B:112:LEU:HD13	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:VAL:HG11	1:B:186:ASN:HD21	1.50	0.75
1:B:731:ARG:HD2	1:B:756:MET:HE1	1.68	0.75
3:F:60:LYS:HA	3:F:63:PHE:HB2	1.69	0.74
1:A:231:LEU:HD21	1:A:442:ILE:HG13	1.69	0.74
1:B:33:LYS:HB3	1:B:49:ILE:HB	1.68	0.74
1:A:355:VAL:HA	1:A:358:SER:HB2	1.69	0.73
1:B:524:CYS:HB2	1:B:568:LYS:HD3	1.70	0.72
1:A:428:GLU:HB2	1:A:432:LYS:HE3	1.71	0.72
2:D:83:GLY:HA3	2:D:88:TYR:HE2	1.54	0.72
1:B:801:ALA:HB2	2:D:43:THR:HG22	1.72	0.72
1:A:428:GLU:O	1:A:432:LYS:HG2	1.90	0.72
3:E:6:LYS:HE2	3:E:32:LYS:HA	1.72	0.72
3:F:54:HIS:HB3	3:F:57:GLN:HB2	1.72	0.71
1:A:268:GLU:HA	1:A:443:LEU:HD21	1.73	0.71
1:B:382:THR:HA	1:B:385:GLN:HB3	1.72	0.70
1:A:610:THR:HG21	1:A:631:ILE:HG13	1.73	0.70
2:D:20:ARG:HH21	2:D:27:LEU:HD11	1.54	0.70
1:A:352:ILE:HA	1:A:355:VAL:HB	1.73	0.70
1:A:792:ILE:HD12	2:C:94:VAL:HG13	1.72	0.70
1:A:840:TRP:HA	3:E:195:GLY:HA3	1.73	0.70
1:A:754:ILE:HA	1:A:757:ILE:HB	1.74	0.70
1:B:265:ALA:HB3	1:B:450:LEU:HB3	1.73	0.70
1:A:860:MET:SD	1:B:863:MET:SD	2.90	0.70
1:B:402:ILE:HG12	1:B:427:ILE:HD13	1.74	0.69
3:F:52:THR:HG21	3:F:56:VAL:HB	1.72	0.69
1:B:138:ILE:HG21	1:B:196:VAL:HG13	1.74	0.69
1:B:496:THR:HB	1:B:679:PRO:HG3	1.73	0.69
3:F:11:LYS:HB3	3:F:104:GLY:HA3	1.73	0.69
1:A:491:GLN:HB2	1:A:525:ILE:HD12	1.74	0.69
2:D:119:MET:HB3	2:D:123:GLU:HB2	1.73	0.68
3:F:111:PHE:HA	3:F:114:ILE:HG12	1.75	0.68
1:B:843:LEU:HA	3:F:192:LYS:HA	1.76	0.68
1:A:339:MET:SD	1:A:352:ILE:HG21	2.34	0.68
3:F:15:LYS:HG2	3:F:102:ALA:HA	1.77	0.67
1:A:524:CYS:SG	1:A:585:HIS:HA	2.34	0.67
1:A:424:ASP:HA	1:A:427:ILE:HG22	1.74	0.67
1:B:817:GLN:HB2	3:F:134:LEU:HD13	1.76	0.67
1:B:124:ILE:HG13	1:B:685:ILE:HB	1.74	0.67
2:D:95:PHE:HB2	2:D:103:VAL:HG13	1.77	0.67
1:B:671:MET:SD	1:B:674:LEU:HD12	2.35	0.67
1:B:671:MET:HG3	1:B:675:ARG:NH1	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:ARG:HB3	1:B:881:ARG:HD2	1.77	0.66
2:D:95:PHE:HD1	2:D:107:GLU:HG3	1.61	0.66
3:F:74:ILE:HB	3:F:106:ILE:HB	1.76	0.66
1:B:176:THR:OG1	1:B:683:ARG:HA	1.95	0.66
1:B:763:ASP:HB3	1:B:766:LEU:HD12	1.77	0.66
2:D:54:PRO:HB2	2:D:59:MET:HG2	1.78	0.66
1:B:789:ASP:HB3	2:D:116:GLY:HA2	1.78	0.66
3:F:11:LYS:HA	3:F:103:PRO:O	1.96	0.66
1:B:269:THR:HG22	1:B:443:LEU:HD22	1.77	0.66
3:F:106:ILE:HA	3:F:110:MET:HB3	1.78	0.65
1:A:898:LEU:HD21	1:B:899:GLN:HE21	1.60	0.65
1:A:437:ARG:HA	1:A:440:ARG:HB2	1.77	0.65
1:A:139:ASP:HA	1:A:142:LYS:HB2	1.77	0.65
1:A:768:ARG:HB3	1:A:775:PHE:HB2	1.79	0.65
1:B:76:GLN:HB3	1:B:96:ASN:HD21	1.61	0.65
1:B:393:ILE:HD11	1:B:398:PHE:HD1	1.61	0.65
1:B:704:GLN:HA	1:B:707:CYS:SG	2.36	0.64
3:F:80:ARG:HD2	3:F:95:LEU:HD21	1.80	0.64
1:A:49:ILE:HG23	1:A:57:VAL:HG11	1.79	0.64
1:B:554:SER:HA	1:B:557:GLU:HG2	1.80	0.64
1:B:797:ILE:HG12	2:D:117:GLU:HG2	1.79	0.64
1:B:362:LEU:HD13	1:B:431:ALA:HA	1.78	0.63
2:C:54:PRO:HB3	2:C:58:GLU:HG2	1.80	0.63
3:F:78:ASP:O	3:F:82:THR:HB	1.99	0.63
1:B:610:THR:HG22	1:B:628:VAL:HG22	1.81	0.63
1:B:148:GLU:HG3	1:B:149:MET:HE2	1.80	0.62
1:B:278:ILE:HG12	1:B:432:LYS:HE2	1.81	0.62
2:D:80:LYS:HD2	2:D:81:ASP:H	1.62	0.62
1:A:53:LYS:HB2	1:A:56:GLU:HB2	1.80	0.62
2:D:35:MET:HE1	2:D:76:ILE:HD12	1.80	0.62
1:A:407:ILE:HG13	1:A:414:VAL:HB	1.82	0.62
1:A:658:THR:O	1:A:662:LEU:HB3	1.99	0.62
3:F:68:GLN:NE2	3:F:78:ASP:HB2	2.14	0.62
1:A:485:THR:HG23	1:A:667:LEU:HD11	1.82	0.62
2:C:54:PRO:HB2	2:C:59:MET:HG2	1.81	0.62
1:B:173:ILE:HG12	1:B:680:ASN:HB2	1.82	0.62
2:D:111:VAL:HG13	2:D:115:LEU:HD22	1.82	0.62
3:E:20:GLU:HB3	3:E:110:MET:HE3	1.81	0.61
1:A:737:LEU:HD21	1:A:788:ARG:HA	1.82	0.61
1:B:735:GLU:HA	1:B:756:MET:HE2	1.80	0.61
2:D:35:MET:HE3	2:D:73:MET:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:THR:O	1:B:188:LYS:HE3	2.01	0.61
1:B:859:GLU:HB3	1:B:863:MET:SD	2.41	0.61
2:D:70:LEU:HG	2:D:74:GLN:HE21	1.65	0.61
1:A:447:ASN:HA	1:A:450:LEU:HB2	1.80	0.61
1:B:535:PRO:HB2	1:B:540:LEU:HG	1.82	0.61
1:A:771:GLN:O	1:B:379:PRO:HA	1.99	0.61
3:F:8:GLU:HA	3:F:11:LYS:HD2	1.83	0.61
1:A:667:LEU:O	1:A:671:MET:HB2	2.01	0.61
1:B:503:GLU:HA	1:B:506:GLN:HB2	1.81	0.61
3:E:66:ILE:HA	3:E:82:THR:HG21	1.82	0.61
1:A:425:PHE:CE2	1:A:428:GLU:HG3	2.36	0.60
1:B:223:GLN:HB3	1:B:342:MET:SD	2.41	0.60
1:A:729:GLU:HG3	1:B:396:THR:HB	1.82	0.60
3:F:130:ASN:HA	3:F:133:ASN:HB3	1.82	0.60
1:A:426:ALA:HA	1:A:429:ALA:HB3	1.83	0.60
1:B:266:ASN:HA	1:B:447:ASN:OD1	2.00	0.60
1:A:275:SER:OG	1:A:600:LYS:HE2	2.02	0.60
3:F:13:SER:HA	3:F:15:LYS:N	2.17	0.60
1:B:238:LYS:HD3	1:B:285:ARG:HD3	1.83	0.60
1:B:804:ARG:NH2	2:D:119:MET:SD	2.75	0.60
3:F:44:GLY:O	3:F:120:ALA:HA	2.01	0.60
1:B:146:ARG:HB2	1:B:723:ASN:OD1	2.01	0.59
1:B:510:ILE:HD12	1:B:768:ARG:HG2	1.84	0.59
1:B:49:ILE:HG23	1:B:57:VAL:HG11	1.83	0.59
1:B:735:GLU:HA	1:B:756:MET:CE	2.32	0.59
1:B:845:THR:HB	3:F:189:LYS:HA	1.84	0.59
3:E:4:ASP:HA	3:E:7:LYS:HD2	1.83	0.59
3:F:98:MET:HE3	3:F:98:MET:O	2.02	0.59
1:B:153:ILE:HG12	1:B:186:ASN:O	2.01	0.59
1:B:164:MET:SD	1:B:459:SER:HB2	2.43	0.59
3:E:61:GLU:HA	3:E:64:GLN:OE1	2.03	0.59
1:A:817:GLN:HG3	3:E:134:LEU:HB3	1.84	0.59
1:B:301:MET:HA	1:B:304:ASP:HB2	1.84	0.59
3:F:69:ASP:HB2	3:F:73:PHE:HB2	1.85	0.59
1:A:175:CYS:SG	1:A:682:VAL:HB	2.43	0.59
1:B:437:ARG:HB3	1:B:624:LEU:HB3	1.85	0.59
1:A:911:ASP:HB3	1:A:915:ARG:HH21	1.68	0.58
1:B:483:ASN:HA	1:B:486:ASN:HB2	1.85	0.58
1:A:77:LYS:H	1:A:77:LYS:HD2	1.68	0.58
1:B:852:GLN:O	1:B:853:SER:HB2	2.02	0.58
1:B:354:ARG:HB2	1:B:390:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:793:THR:HA	1:B:797:ILE:HB	1.83	0.58
3:E:37:LYS:HB2	3:F:89:LEU:HD21	1.84	0.58
1:A:492:LEU:HD22	1:A:671:MET:SD	2.43	0.58
1:B:843:LEU:HD13	3:F:196:ALA:HB3	1.85	0.58
1:B:388:CYS:HA	1:B:391:MET:HB2	1.85	0.58
1:A:119:LEU:HB2	1:A:717:CYS:SG	2.43	0.58
1:A:707:CYS:SG	1:A:708:ASN:N	2.77	0.58
2:C:38:LEU:HD12	2:C:73:MET:HG3	1.86	0.57
1:B:727:PHE:HA	1:B:730:PHE:HB2	1.85	0.57
1:A:163:SER:HB3	1:A:171:GLN:NE2	2.18	0.57
1:A:870:LEU:HB3	1:B:870:LEU:HB3	1.86	0.57
1:B:306:LEU:HB3	1:B:386:LYS:HE3	1.87	0.57
3:E:62:ALA:HA	3:E:65:LEU:HB2	1.86	0.57
1:B:223:GLN:HG2	1:B:342:MET:HA	1.87	0.57
1:A:553:THR:HA	1:A:579:THR:HG21	1.87	0.57
1:A:605:LEU:HD21	1:A:662:LEU:HD22	1.87	0.57
1:A:723:ASN:HB2	1:A:776:PHE:HB2	1.87	0.57
3:F:14:LYS:HB3	3:F:103:PRO:HB2	1.87	0.57
1:A:107:ARG:HG2	1:A:112:LEU:HB2	1.85	0.57
1:B:164:MET:HE2	1:B:171:GLN:HG3	1.87	0.57
1:B:614:ASN:HB2	1:B:628:VAL:HG21	1.87	0.57
2:D:42:PRO:HB3	2:D:76:ILE:HG21	1.86	0.57
2:D:104:MET:HB3	2:D:107:GLU:HB3	1.85	0.57
1:A:556:VAL:HB	1:A:579:THR:HG22	1.87	0.56
1:A:290:PHE:HD1	1:A:316:LEU:HD21	1.69	0.56
1:B:576:LYS:HD2	1:B:577:ASP:H	1.70	0.56
1:A:856:ARG:NH2	1:B:856:ARG:HB3	2.20	0.56
1:B:137:ILE:O	1:B:141:TYR:HB2	2.06	0.56
1:B:726:VAL:HA	1:B:773:LYS:HA	1.87	0.56
1:A:576:LYS:HD2	1:A:577:ASP:H	1.70	0.56
1:B:173:ILE:O	1:B:463:ILE:HA	2.06	0.56
3:F:68:GLN:HB2	3:F:78:ASP:CG	2.30	0.56
1:B:502:GLN:HG2	1:B:512:TRP:CD1	2.41	0.56
1:A:573:LYS:H	1:A:573:LYS:HD2	1.70	0.55
1:A:842:ARG:NH1	3:E:194:GLU:HB2	2.21	0.55
1:B:194:LEU:HD12	1:B:198:ALA:HB2	1.87	0.55
1:A:144:LYS:HD2	1:A:148:GLU:HB2	1.89	0.55
1:A:247:ARG:HG3	1:A:273:GLU:HB3	1.88	0.55
1:B:391:MET:HE2	1:B:613:LEU:HD21	1.88	0.55
3:F:9:LYS:HG2	3:F:12:LYS:HB2	1.89	0.55
2:D:18:PHE:HB3	2:D:30:GLN:NE2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:TYR:HE1	1:A:126:PRO:HA	1.71	0.55
1:A:141:TYR:HA	1:A:149:MET:HG3	1.88	0.55
1:B:614:ASN:ND2	1:B:626:LYS:HA	2.21	0.55
1:B:814:LYS:HD3	3:F:137:GLU:HA	1.89	0.55
3:F:117:ASP:HA	3:F:120:ALA:HB3	1.87	0.55
1:A:274:LYS:HB2	1:A:432:LYS:HB2	1.88	0.55
1:B:768:ARG:HB3	1:B:775:PHE:HB2	1.89	0.55
1:B:833:LEU:H	1:B:833:LEU:HD22	1.72	0.55
1:B:306:LEU:HD11	1:B:389:HIS:HD2	1.72	0.54
2:C:35:MET:SD	2:C:76:ILE:HD12	2.47	0.54
1:A:704:GLN:HA	1:A:707:CYS:SG	2.48	0.54
1:B:492:LEU:HD13	1:B:675:ARG:HH21	1.73	0.54
1:B:580:GLU:HB3	1:B:593:ASN:HD22	1.72	0.54
1:B:722:PRO:HD2	1:B:777:ARG:HA	1.88	0.54
1:A:402:ILE:HG12	1:A:427:ILE:HD13	1.90	0.54
1:A:734:TYR:HB3	1:A:737:LEU:HD12	1.89	0.54
1:A:809:ARG:HB3	2:C:37:ALA:HA	1.89	0.54
1:A:178:GLU:O	1:A:183:LYS:NZ	2.41	0.54
1:B:253:ARG:O	1:B:265:ALA:HA	2.08	0.54
1:B:846:LYS:NZ	3:F:191:ALA:HA	2.23	0.54
1:A:266:ASN:HA	1:A:447:ASN:OD1	2.08	0.54
1:A:351:SER:HA	1:A:354:ARG:HG2	1.88	0.54
1:B:323:ILE:HG21	1:B:326:GLN:NE2	2.23	0.54
1:B:610:THR:HG21	1:B:631:ILE:HG13	1.89	0.54
1:B:768:ARG:O	1:B:774:ILE:HA	2.08	0.54
1:B:845:THR:HG21	3:F:188:THR:O	2.08	0.54
1:A:814:LYS:O	1:A:817:GLN:HG2	2.08	0.54
1:B:844:PHE:HB3	1:B:845:THR:HG23	1.90	0.53
3:E:112:LEU:HA	3:E:115:PHE:HB2	1.89	0.53
1:A:253:ARG:O	1:A:265:ALA:HA	2.08	0.53
1:B:101:LEU:HD13	1:B:702:LEU:HD13	1.90	0.53
1:B:788:ARG:HG2	1:B:792:ILE:HG12	1.90	0.53
1:A:491:GLN:HB2	1:A:525:ILE:CD1	2.38	0.53
1:A:818:GLN:O	1:A:821:ALA:HB3	2.09	0.53
1:B:496:THR:HA	1:B:500:LEU:HB2	1.91	0.53
1:B:145:LYS:HB3	1:B:782:ALA:HB1	1.90	0.53
1:B:821:ALA:HB1	3:F:131:ALA:HA	1.89	0.53
1:B:433:ALA:O	1:B:437:ARG:HG2	2.08	0.53
3:F:42:ARG:NH1	3:F:121:GLY:O	2.42	0.53
1:A:728:GLN:HE22	1:B:385:GLN:HG3	1.74	0.53
1:A:800:GLN:O	1:A:804:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:119:MET:HE3	2:D:123:GLU:HB3	1.91	0.53
3:E:16:LYS:HB3	3:F:68:GLN:O	2.08	0.53
3:E:38:ARG:HG2	3:F:88:ARG:HD3	1.90	0.53
1:A:839:GLN:HA	3:E:194:GLU:HG2	1.91	0.53
3:E:90:CYS:HB2	3:E:95:LEU:HG	1.89	0.53
3:F:106:ILE:HD13	3:F:114:ILE:HG21	1.90	0.53
1:A:33:LYS:O	1:A:48:SER:HA	2.09	0.53
2:D:111:VAL:HA	2:D:115:LEU:HD13	1.91	0.53
3:F:8:GLU:O	3:F:11:LYS:HB2	2.09	0.53
3:F:106:ILE:HD13	3:F:114:ILE:HD13	1.91	0.53
1:B:191:ILE:HG23	1:B:224:LEU:HG	1.91	0.53
1:A:528:ILE:HG12	1:A:538:LEU:HG	1.91	0.52
1:B:430:LEU:HD11	1:B:613:LEU:HD11	1.91	0.52
1:A:198:ALA:O	1:A:261:TYR:HA	2.09	0.52
2:C:8:THR:O	2:C:12:LYS:HG3	2.09	0.52
2:C:15:PHE:HD2	2:C:34:VAL:HG11	1.75	0.52
2:D:132:GLU:HB2	2:D:136:GLY:HA2	1.90	0.52
3:E:73:PHE:HA	3:E:107:ASN:HA	1.91	0.52
1:A:830:ALA:HA	1:A:833:LEU:HD22	1.90	0.52
1:B:819:LEU:HD12	2:D:22:GLY:HA2	1.92	0.52
1:B:99:SER:HA	1:B:102:HIS:HB3	1.91	0.52
1:A:433:ALA:HA	1:A:436:GLU:HB2	1.92	0.52
1:A:814:LYS:HE3	3:E:134:LEU:O	2.10	0.52
1:B:172:SER:HA	1:B:462:GLY:O	2.10	0.52
2:D:54:PRO:HB3	2:D:58:GLU:HG2	1.92	0.52
1:A:49:ILE:HD11	1:A:75:ILE:HD12	1.92	0.52
1:A:425:PHE:CD2	1:A:428:GLU:HG3	2.45	0.52
3:E:109:THR:OG1	3:F:70:LYS:HB3	2.10	0.52
1:A:750:LYS:HG3	1:A:769:ILE:HG21	1.91	0.51
1:B:480:LEU:HD23	1:B:481:CYS:SG	2.50	0.51
1:B:764:PRO:HA	1:B:767:TYR:HE2	1.75	0.51
1:B:800:GLN:O	1:B:804:ARG:HG3	2.10	0.51
1:B:247:ARG:HG3	1:B:273:GLU:HB3	1.90	0.51
1:B:466:ILE:HD13	1:B:489:LEU:HD23	1.92	0.51
1:B:674:LEU:HA	1:B:677:THR:OG1	2.09	0.51
1:B:809:ARG:NH2	2:D:40:GLN:O	2.42	0.51
1:A:582:CYS:HA	1:A:590:VAL:O	2.09	0.51
1:B:671:MET:HG3	1:B:675:ARG:HH12	1.76	0.51
3:F:73:PHE:O	3:F:74:ILE:HG13	2.10	0.51
1:A:425:PHE:O	1:A:429:ALA:N	2.44	0.51
1:B:183:LYS:HG2	1:B:466:ILE:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:735:GLU:N	1:B:756:MET:SD	2.84	0.51
3:F:83:PHE:HB3	3:F:88:ARG:O	2.10	0.51
1:A:42:HIS:HD2	1:A:45:GLU:HB3	1.75	0.51
1:A:233:ALA:O	1:A:288:HIS:HB2	2.11	0.51
1:B:545:CYS:SG	1:B:602:MET:HB2	2.51	0.51
3:E:82:THR:HA	3:E:85:SER:OG	2.11	0.51
1:A:767:TYR:CD1	1:A:769:ILE:HG12	2.46	0.51
1:B:222:LYS:O	1:B:226:GLN:HG2	2.11	0.51
1:A:545:CYS:SG	1:A:602:MET:SD	3.02	0.50
1:B:252:ILE:HB	1:B:463:ILE:HB	1.92	0.50
1:B:358:SER:HB3	1:B:390:LEU:HB2	1.94	0.50
1:B:494:ASN:N	1:B:494:ASN:HD22	2.09	0.50
1:B:583:ILE:HG12	1:B:592:TYR:HE2	1.76	0.50
3:F:75:SER:HA	3:F:105:PRO:HA	1.94	0.50
1:A:729:GLU:OE2	1:B:396:THR:HA	2.12	0.50
1:B:148:GLU:O	1:B:150:PRO:HD3	2.12	0.50
1:B:847:VAL:HG12	1:B:851:LEU:HD21	1.94	0.50
3:F:88:ARG:CD	3:F:89:LEU:HB2	2.32	0.50
1:A:507:ARG:HG2	1:B:372:ASN:ND2	2.26	0.50
1:B:150:PRO:O	1:B:155:ALA:HB2	2.10	0.50
1:B:734:TYR:CD2	1:B:788:ARG:HD3	2.47	0.50
2:D:108:ILE:HD12	2:D:128:VAL:HG12	1.94	0.50
3:E:9:LYS:NZ	3:F:80:ARG:HA	2.27	0.50
3:F:69:ASP:CB	3:F:73:PHE:HB2	2.40	0.50
3:F:177:LEU:HD11	3:F:182:LYS:HD2	1.93	0.50
1:B:138:ILE:HG23	1:B:197:VAL:HG23	1.94	0.50
3:F:78:ASP:HA	3:F:81:ALA:HB3	1.94	0.50
1:A:537:VAL:HG13	1:A:555:PHE:HZ	1.76	0.50
1:B:108:TYR:HD1	1:B:113:ILE:HG22	1.77	0.50
1:B:405:PRO:HB3	1:B:606:ASN:HD21	1.76	0.50
1:A:821:ALA:HB1	3:E:131:ALA:HA	1.94	0.49
1:B:511:GLU:O	1:B:768:ARG:NH1	2.45	0.49
1:B:766:LEU:HD13	1:B:780:VAL:HG21	1.94	0.49
1:B:152:HIS:HB3	1:B:155:ALA:H	1.76	0.49
1:A:931:LYS:HA	1:A:934:ASN:HD22	1.76	0.49
1:B:141:TYR:HB3	1:B:193:TYR:HE2	1.77	0.49
1:B:752:ALA:C	1:B:756:MET:HE3	2.38	0.49
1:B:620:PHE:O	1:B:624:LEU:HG	2.13	0.49
3:E:62:ALA:O	3:E:66:ILE:HB	2.12	0.49
1:B:74:ASP:O	1:B:76:GLN:HG3	2.12	0.49
1:A:49:ILE:HG23	1:A:57:VAL:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:PHE:CE1	1:A:427:ILE:HG21	2.47	0.49
1:B:730:PHE:CD1	1:B:774:ILE:HG21	2.47	0.49
1:B:919:LEU:HA	1:B:922:ASN:HB3	1.94	0.49
3:E:141:LYS:HE2	3:E:178:ILE:HB	1.94	0.49
1:A:36:TRP:HA	1:A:45:GLU:O	2.12	0.49
1:A:119:LEU:HD12	1:A:717:CYS:SG	2.52	0.49
1:A:223:GLN:NE2	1:A:449:ALA:HB1	2.28	0.49
1:A:813:ALA:HA	1:A:816:GLN:OE1	2.13	0.49
1:A:848:LYS:H	1:A:849:PRO:HD2	1.77	0.49
1:B:302:ARG:HA	1:B:307:LEU:HD12	1.94	0.49
1:B:851:LEU:HA	3:E:53:GLN:NE2	2.28	0.49
2:D:140:TYR:O	2:D:144:VAL:HG23	2.13	0.49
1:B:141:TYR:HB3	1:B:193:TYR:CE2	2.47	0.49
3:E:51:PHE:HB3	3:F:61:GLU:HG3	1.94	0.49
3:E:60:LYS:HE2	3:F:60:LYS:HD3	1.94	0.49
1:A:889:VAL:HG11	1:B:258:VAL:HG22	1.95	0.48
1:B:178:GLU:O	1:B:183:LYS:NZ	2.46	0.48
1:B:727:PHE:HB3	1:B:772:SER:O	2.13	0.48
1:A:351:SER:HB3	1:A:390:LEU:HD11	1.94	0.48
1:B:805:GLY:O	1:B:809:ARG:HG2	2.13	0.48
1:B:813:ALA:O	1:B:816:GLN:HG2	2.12	0.48
2:C:121:GLU:HA	2:C:124:VAL:HG22	1.95	0.48
1:A:174:LEU:O	1:A:681:PHE:HA	2.13	0.48
2:D:127:LEU:HD11	2:D:147:VAL:HG12	1.96	0.48
3:F:48:PHE:HB2	3:F:56:VAL:HG23	1.96	0.48
1:A:659:VAL:HA	1:A:662:LEU:HD23	1.94	0.48
3:F:79:ILE:HG23	3:F:83:PHE:HB2	1.95	0.48
1:B:732:GLN:CB	2:D:94:VAL:HA	2.38	0.48
1:A:370:GLU:HB2	1:A:376:ALA:HA	1.94	0.48
1:B:364:ASN:HB2	1:B:383:ALA:HA	1.96	0.48
1:B:404:THR:HG22	1:B:417:ALA:HA	1.95	0.48
1:B:785:GLU:CD	1:B:788:ARG:HH21	2.22	0.48
1:A:238:LYS:HG3	1:A:243:ASP:HA	1.95	0.48
1:B:237:ALA:HB3	1:B:247:ARG:HD3	1.96	0.48
1:B:726:VAL:HG13	1:B:772:SER:O	2.14	0.48
1:A:603:ASP:O	1:A:605:LEU:HD22	2.13	0.48
1:B:339:MET:HB3	1:B:344:PHE:HB2	1.96	0.48
3:F:15:LYS:N	3:F:103:PRO:HD2	2.29	0.48
1:A:421:GLU:O	1:A:425:PHE:HB2	2.14	0.47
1:A:522:GLN:O	1:A:526:GLU:HG2	2.14	0.47
1:A:542:ASP:O	1:A:545:CYS:SG	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:923:LYS:HG2	1:B:926:LEU:HD11	1.95	0.47
1:B:727:PHE:CE1	1:B:769:ILE:HD12	2.49	0.47
1:B:290:PHE:HB3	1:B:360:LEU:HD21	1.94	0.47
1:A:367:PHE:O	1:A:420:LYS:HG3	2.13	0.47
1:A:383:ALA:HA	1:A:386:LYS:HD2	1.94	0.47
1:B:7:SER:H	1:B:10:GLU:HB2	1.79	0.47
1:B:178:GLU:CA	1:B:469:PHE:HB3	2.29	0.47
1:B:617:SER:HB2	2:C:99:GLY:HA3	1.94	0.47
1:B:881:ARG:HH11	1:B:881:ARG:HG2	1.78	0.47
1:A:275:SER:CB	1:A:600:LYS:HE2	2.45	0.47
1:A:483:ASN:HB2	1:A:592:TYR:OH	2.14	0.47
1:B:123:VAL:HG11	1:B:186:ASN:ND2	2.24	0.47
2:C:119:MET:HE3	2:C:123:GLU:HB3	1.96	0.47
1:B:854:ALA:O	3:F:55:GLN:HB2	2.14	0.47
1:A:95:LEU:HD22	1:A:100:VAL:HG22	1.97	0.47
1:A:843:LEU:HA	3:E:192:LYS:HA	1.97	0.47
1:A:956:ASP:O	1:A:959:SER:HB3	2.14	0.47
1:B:406:ARG:HB3	1:B:608:ASN:HD21	1.79	0.47
1:B:707:CYS:SG	1:B:708:ASN:N	2.88	0.47
3:E:84:ASP:HB2	3:E:89:LEU:HD21	1.97	0.47
1:B:58:THR:HA	1:B:69:THR:HA	1.97	0.47
1:B:104:LEU:HD12	1:B:710:VAL:HG11	1.97	0.47
1:B:480:LEU:HG	1:B:528:ILE:HD11	1.95	0.47
1:B:783:HIS:CE1	1:B:787:GLU:HG3	2.50	0.47
1:B:789:ASP:OD1	2:D:115:LEU:HA	2.14	0.47
1:A:58:THR:HA	1:A:69:THR:HA	1.96	0.47
1:A:269:THR:O	1:A:440:ARG:NH1	2.47	0.47
1:B:121:CYS:O	1:B:123:VAL:HG23	2.15	0.47
1:B:323:ILE:HG21	1:B:326:GLN:HE21	1.80	0.47
1:A:541:LEU:HA	1:A:544:GLU:HB2	1.97	0.47
1:A:626:LYS:HB2	1:A:626:LYS:HE3	1.74	0.47
2:D:8:THR:HG22	2:D:12:LYS:HE3	1.96	0.47
3:F:90:CYS:HA	3:F:94:GLU:HB2	1.96	0.47
1:A:355:VAL:O	1:A:359:VAL:HG23	2.15	0.46
1:B:815:ARG:O	2:D:18:PHE:HA	2.15	0.46
1:A:236:ASN:O	1:A:288:HIS:HD2	1.98	0.46
1:A:301:MET:HA	1:A:304:ASP:HB2	1.96	0.46
1:A:533:ASN:HB3	1:A:534:PRO:HD2	1.96	0.46
1:B:150:PRO:HB2	1:B:151:PRO:HD2	1.96	0.46
1:B:800:GLN:NE2	2:D:112:LEU:HA	2.29	0.46
1:B:801:ALA:CB	2:D:43:THR:HG22	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:20:GLU:HG2	3:E:110:MET:HB2	1.96	0.46
1:A:524:CYS:SG	1:A:585:HIS:ND1	2.88	0.46
1:A:547:PHE:HB3	1:A:550:ALA:HB2	1.96	0.46
1:A:601:ASN:C	1:A:659:VAL:HG23	2.40	0.46
2:D:80:LYS:HD2	2:D:81:ASP:N	2.28	0.46
3:E:92:GLU:HA	3:E:95:LEU:HD12	1.97	0.46
3:F:2:GLY:O	3:F:5:GLU:HB3	2.15	0.46
1:A:583:ILE:O	1:A:589:LYS:HA	2.14	0.46
1:B:833:LEU:HD23	1:B:834:LYS:NZ	2.30	0.46
2:D:105:GLY:O	2:D:108:ILE:HG22	2.15	0.46
1:B:840:TRP:HB3	3:F:118:ARG:HG2	1.96	0.46
3:E:33:PRO:O	3:E:36:GLN:HG3	2.15	0.46
1:A:256:PHE:O	1:A:458:ALA:N	2.47	0.46
1:B:358:SER:O	1:B:362:LEU:HD12	2.15	0.46
1:B:753:CYS:HA	1:B:756:MET:SD	2.56	0.46
2:C:75:THR:HA	2:C:78:LYS:HZ1	1.80	0.46
2:D:34:VAL:O	2:D:38:LEU:HG	2.14	0.46
1:A:583:ILE:HD11	1:A:592:TYR:HE2	1.79	0.46
1:A:604:PRO:HA	1:A:657:ARG:O	2.16	0.46
1:A:762:LEU:HD11	1:A:784:LEU:HD21	1.98	0.46
1:A:933:MET:HE1	1:B:930:VAL:HG13	1.97	0.46
2:D:40:GLN:HG3	2:D:42:PRO:HG3	1.97	0.46
1:B:135:GLU:HA	1:B:138:ILE:HB	1.97	0.46
1:B:376:ALA:HB3	1:B:420:LYS:HB2	1.98	0.46
1:B:732:GLN:HB3	2:D:94:VAL:C	2.40	0.46
3:F:106:ILE:CD1	3:F:114:ILE:HG21	2.44	0.46
1:B:97:GLU:CD	1:B:706:ARG:HH21	2.24	0.46
1:B:358:SER:OG	1:B:434:LYS:NZ	2.48	0.46
1:B:826:GLN:HE22	3:F:155:GLY:HA3	1.81	0.46
2:C:51:LEU:HD13	2:C:59:MET:SD	2.56	0.46
1:B:846:LYS:O	1:B:849:PRO:HD2	2.15	0.46
2:C:69:PHE:HA	2:C:72:MET:SD	2.56	0.46
1:A:905:GLU:HA	1:A:908:ASN:ND2	2.30	0.45
1:B:218:GLY:O	1:B:222:LYS:NZ	2.50	0.45
1:B:367:PHE:CE1	1:B:378:MET:HB2	2.51	0.45
1:B:497:MET:HA	1:B:501:GLU:HB3	1.97	0.45
1:A:274:LYS:HG3	1:A:432:LYS:HD3	1.97	0.45
1:B:792:ILE:HD12	1:B:796:ILE:HB	1.97	0.45
1:B:839:GLN:OE1	3:F:88:ARG:HB3	2.15	0.45
1:B:842:ARG:HB2	3:F:191:ALA:CB	2.45	0.45
1:A:630:ARG:NH1	1:A:662:LEU:HB2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LYS:HA	1:B:75:ILE:HG12	1.98	0.45
1:B:375:GLN:HG3	1:B:419:THR:HG22	1.99	0.45
1:A:361:GLN:HA	1:A:364:ASN:HB2	1.99	0.45
1:A:734:TYR:CE1	1:A:784:LEU:HB3	2.51	0.45
1:A:762:LEU:HD21	1:A:784:LEU:HD11	1.98	0.45
1:B:252:ILE:O	1:B:462:GLY:HA2	2.16	0.45
1:B:725:ILE:HG21	1:B:781:LEU:HD11	1.98	0.45
2:D:98:GLU:H	2:D:100:ASN:ND2	2.14	0.45
3:F:56:VAL:HG12	3:F:108:PHE:CZ	2.51	0.45
1:A:432:LYS:HE2	1:A:432:LYS:HB3	1.74	0.45
1:A:948:THR:O	1:A:952:ARG:HG2	2.17	0.45
1:B:497:MET:HA	1:B:501:GLU:CB	2.47	0.45
1:B:669:LYS:HB2	1:B:669:LYS:HE3	1.73	0.45
1:B:690:GLU:O	1:B:691:LYS:HB3	2.16	0.45
3:E:106:ILE:HA	3:E:110:MET:HB3	1.99	0.45
1:A:490:GLN:NE2	1:A:494:ASN:HD21	2.15	0.45
1:A:614:ASN:ND2	1:A:626:LYS:HA	2.32	0.45
1:A:724:ARG:HB2	1:A:773:LYS:HD3	1.98	0.45
1:B:787:GLU:HG2	1:B:790:LEU:HD22	1.99	0.45
2:D:119:MET:HB2	2:D:124:VAL:HG12	1.98	0.45
3:F:42:ARG:HH22	3:F:124:GLU:H	1.65	0.45
1:A:823:LYS:HA	1:A:826:GLN:OE1	2.17	0.45
1:B:866:GLU:CD	1:B:869:ARG:HH21	2.25	0.45
1:A:491:GLN:HG2	1:A:522:GLN:CD	2.42	0.45
3:F:9:LYS:HA	3:F:12:LYS:N	2.31	0.45
1:A:484:TYR:HD2	1:A:663:TYR:HE2	1.65	0.45
1:B:438:LEU:HA	1:B:624:LEU:HD22	1.97	0.45
1:B:572:SER:HB3	1:B:580:GLU:O	2.17	0.45
1:A:603:ASP:HB2	1:A:659:VAL:HA	1.99	0.45
1:A:729:GLU:CD	1:A:729:GLU:H	2.25	0.45
1:B:120:PHE:CD1	1:B:497:MET:HG2	2.51	0.45
1:B:167:ASP:HB2	1:B:773:LYS:HE2	1.99	0.45
1:B:430:LEU:HD11	1:B:613:LEU:CD1	2.47	0.45
1:B:488:LYS:O	1:B:492:LEU:N	2.50	0.45
1:B:764:PRO:HA	1:B:767:TYR:CE2	2.50	0.45
1:B:839:GLN:HA	3:F:88:ARG:HB2	1.99	0.45
2:D:9:ALA:HA	2:D:12:LYS:HD2	1.99	0.45
1:B:144:LYS:HB3	1:B:149:MET:HG3	1.98	0.44
1:B:250:LYS:HD2	1:B:267:ILE:HG23	1.98	0.44
1:B:510:ILE:HG21	1:B:775:PHE:CE1	2.51	0.44
1:B:687:PRO:HB2	1:B:696:LEU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:732:GLN:HB3	2:D:94:VAL:CA	2.41	0.44
2:C:119:MET:HB3	2:C:123:GLU:HB2	1.99	0.44
1:A:506:GLN:OE1	1:A:514:PHE:HB2	2.17	0.44
1:A:607:ASP:HA	1:A:610:THR:HB	1.98	0.44
1:B:393:ILE:HD11	1:B:398:PHE:CD1	2.47	0.44
1:B:817:GLN:HG3	3:F:134:LEU:HB3	2.00	0.44
1:A:42:HIS:HB2	1:A:44:PHE:O	2.17	0.44
1:A:711:LEU:HD22	1:A:711:LEU:H	1.81	0.44
1:B:505:TYR:HB3	1:B:510:ILE:HG12	1.97	0.44
1:A:159:THR:O	1:A:163:SER:HB2	2.17	0.44
1:B:36:TRP:CD1	1:B:78:MET:HA	2.53	0.44
1:B:139:ASP:HA	1:B:142:LYS:HB2	2.00	0.44
1:B:141:TYR:CD2	1:B:149:MET:SD	3.10	0.44
1:B:199:SER:CB	1:B:221:GLU:HG2	2.48	0.44
1:B:556:VAL:O	1:B:560:ILE:HG12	2.18	0.44
3:F:54:HIS:CB	3:F:57:GLN:HB2	2.44	0.44
1:A:285:ARG:HD2	1:A:321:VAL:O	2.17	0.44
1:B:573:LYS:H	1:B:573:LYS:HD2	1.83	0.44
1:B:753:CYS:HA	1:B:756:MET:HG2	1.99	0.44
2:D:101:GLY:HA2	2:D:140:TYR:HE2	1.81	0.44
3:F:59:PHE:CD2	3:F:59:PHE:N	2.84	0.44
1:A:429:ALA:HB2	1:A:603:ASP:HA	2.00	0.44
1:B:270:TYR:O	1:B:440:ARG:NH2	2.51	0.44
3:E:158:PHE:HB3	3:E:162:GLU:HB2	2.00	0.44
3:F:12:LYS:O	3:F:15:LYS:HB2	2.17	0.44
1:A:254:ILE:O	1:A:460:PHE:HA	2.17	0.44
1:B:120:PHE:HD2	1:B:683:ARG:HG3	1.82	0.44
3:E:5:GLU:HG3	3:E:6:LYS:N	2.33	0.44
1:A:265:ALA:O	1:A:450:LEU:HB3	2.17	0.44
1:A:357:SER:O	1:A:361:GLN:HB2	2.17	0.44
1:A:477:PHE:HB3	1:A:600:LYS:HD3	1.99	0.44
1:B:158:ASP:HB2	1:B:193:TYR:OH	2.17	0.44
1:B:859:GLU:O	1:B:863:MET:N	2.51	0.44
3:E:11:LYS:HB2	3:F:77:ASN:CB	2.47	0.44
1:A:605:LEU:HD23	1:A:630:ARG:HH12	1.82	0.44
1:A:825:ILE:HG13	3:E:131:ALA:HB1	2.00	0.44
1:B:86:VAL:HG13	1:B:88:ASP:O	2.18	0.44
1:B:108:TYR:HD2	1:B:696:LEU:HD12	1.82	0.44
2:C:34:VAL:O	2:C:38:LEU:HG	2.18	0.44
1:B:15:VAL:O	1:B:17:LYS:HG3	2.18	0.43
1:B:391:MET:HB3	1:B:393:ILE:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:732:GLN:CA	2:D:94:VAL:HA	2.48	0.43
1:B:795:VAL:O	1:B:799:PHE:N	2.51	0.43
1:B:842:ARG:HB2	3:F:191:ALA:HB3	2.00	0.43
3:F:79:ILE:HG22	3:F:99:VAL:HA	1.99	0.43
1:B:497:MET:O	1:B:716:ILE:HG12	2.18	0.43
1:B:840:TRP:HA	3:F:195:GLY:HA3	2.00	0.43
1:B:115:THR:O	1:B:121:CYS:HA	2.19	0.43
3:F:130:ASN:HB3	3:F:134:LEU:HG	2.00	0.43
1:A:162:ARG:CZ	1:A:162:ARG:HA	2.49	0.43
1:A:275:SER:HA	1:A:432:LYS:HZ3	1.84	0.43
1:A:375:GLN:HA	1:A:419:THR:HA	1.99	0.43
1:B:145:LYS:NZ	1:B:789:ASP:OD2	2.52	0.43
1:B:225:LEU:O	1:B:229:PRO:HD2	2.18	0.43
2:D:35:MET:HG2	2:D:73:MET:SD	2.57	0.43
1:A:805:GLY:O	1:A:809:ARG:HG2	2.18	0.43
1:A:842:ARG:HB3	3:E:194:GLU:HB3	2.01	0.43
1:B:153:ILE:HD11	1:B:173:ILE:HG21	2.00	0.43
1:B:351:SER:O	1:B:354:ARG:HG2	2.19	0.43
1:B:776:PHE:HB2	1:B:781:LEU:HB2	1.99	0.43
1:B:860:MET:O	1:B:864:LYS:HG2	2.18	0.43
2:D:21:THR:HA	3:F:154:TRP:HZ2	1.82	0.43
2:D:103:VAL:HG12	2:D:138:ILE:HB	2.00	0.43
3:F:130:ASN:O	3:F:134:LEU:HG	2.18	0.43
1:A:311:ASN:N	1:A:311:ASN:HD22	2.15	0.43
1:A:387:VAL:HG22	1:A:434:LYS:HD2	1.99	0.43
1:A:429:ALA:O	1:A:433:ALA:HB3	2.19	0.43
1:A:470:GLU:HG2	1:A:482:ILE:HG21	2.00	0.43
1:A:526:GLU:HA	1:A:530:ARG:HB2	1.99	0.43
1:A:663:TYR:O	1:A:667:LEU:HB2	2.18	0.43
1:A:725:ILE:O	1:A:774:ILE:N	2.52	0.43
1:B:292:TYR:HB3	1:B:332:PHE:HB2	2.00	0.43
1:B:842:ARG:HD2	3:F:193:GLU:HB2	2.00	0.43
3:E:33:PRO:HA	3:E:34:PRO:HD3	1.81	0.43
3:E:141:LYS:NZ	3:E:173:ASP:O	2.51	0.43
1:A:420:LYS:HB3	1:A:421:GLU:OE2	2.18	0.43
1:A:746:PHE:HE1	1:B:303:ASN:HA	1.83	0.43
1:A:856:ARG:HH22	1:B:856:ARG:HB3	1.82	0.43
1:B:114:TYR:CD2	1:B:123:VAL:HG22	2.53	0.43
1:B:502:GLN:OE1	1:B:514:PHE:HA	2.19	0.43
2:D:101:GLY:HA2	2:D:140:TYR:CE2	2.54	0.43
2:D:102:THR:HB	2:D:137:CYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:121:GLU:H	2:D:121:GLU:CD	2.26	0.43
3:E:37:LYS:HD2	3:F:89:LEU:HD22	2.00	0.43
3:F:12:LYS:HE2	3:F:105:PRO:O	2.19	0.43
1:A:854:ALA:O	1:A:858:LYS:HG3	2.18	0.43
1:B:814:LYS:HE3	1:B:814:LYS:O	2.19	0.43
1:B:6:LEU:HB2	1:B:11:LYS:HG3	2.00	0.43
1:A:540:LEU:HD22	1:A:558:LYS:HD3	2.00	0.43
1:B:14:PHE:CD2	1:B:150:PRO:HG3	2.54	0.43
1:B:407:ILE:O	1:B:408:LYS:NZ	2.52	0.43
1:B:758:LYS:NZ	1:B:761:GLU:O	2.52	0.43
3:E:62:ALA:HB1	3:E:66:ILE:HD13	2.01	0.43
1:A:540:LEU:HD21	1:A:562:GLU:HG3	2.00	0.42
1:B:839:GLN:O	3:F:195:GLY:HA3	2.19	0.42
3:E:9:LYS:HZ2	3:F:84:ASP:CG	2.27	0.42
3:F:33:PRO:HA	3:F:34:PRO:HD2	1.87	0.42
1:A:554:SER:HA	1:A:557:GLU:HG2	2.00	0.42
1:A:908:ASN:O	1:A:911:ASP:HB2	2.19	0.42
1:B:171:GLN:O	1:B:461:LEU:HA	2.19	0.42
1:B:255:ASN:HA	1:B:460:PHE:HA	2.01	0.42
3:F:171:PRO:HB2	3:F:178:ILE:HG22	2.01	0.42
1:A:720:GLY:O	1:A:777:ARG:NH1	2.53	0.42
1:B:339:MET:SD	1:B:349:GLN:HG2	2.60	0.42
1:A:367:PHE:HE1	1:A:378:MET:SD	2.43	0.42
1:A:758:LYS:NZ	1:A:762:LEU:O	2.51	0.42
1:B:11:LYS:NZ	1:B:16:ASP:OD2	2.52	0.42
1:B:145:LYS:CB	1:B:782:ALA:HB1	2.50	0.42
1:B:163:SER:OG	1:B:724:ARG:HG3	2.20	0.42
1:B:220:LEU:O	1:B:223:GLN:HB2	2.18	0.42
1:B:381:ASN:O	1:B:385:GLN:N	2.51	0.42
1:B:578:LYS:HG2	1:B:593:ASN:ND2	2.33	0.42
3:E:2:GLY:HA2	3:F:92:GLU:HG2	2.00	0.42
1:A:361:GLN:HG3	1:A:364:ASN:HB2	2.01	0.42
1:A:547:PHE:HB3	1:A:550:ALA:CB	2.48	0.42
1:A:603:ASP:HB2	1:A:659:VAL:CA	2.50	0.42
3:F:9:LYS:O	3:F:10:LYS:NZ	2.51	0.42
3:F:12:LYS:HA	3:F:15:LYS:HG3	2.02	0.42
1:A:251:PHE:O	1:A:267:ILE:HA	2.19	0.42
1:A:437:ARG:HD2	1:A:440:ARG:HD2	2.01	0.42
1:A:844:PHE:HB2	3:E:190:GLY:O	2.20	0.42
2:D:140:TYR:HA	2:D:143:LEU:HB3	2.01	0.42
3:E:30:ALA:HA	3:E:37:LYS:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ASN:HB3	1:A:586:TYR:OH	2.19	0.42
1:B:683:ARG:NH2	1:B:708:ASN:OD1	2.52	0.42
1:B:788:ARG:O	1:B:792:ILE:HG12	2.20	0.42
2:D:95:PHE:CD2	2:D:108:ILE:HG12	2.55	0.42
2:D:120:THR:O	2:D:124:VAL:HG13	2.20	0.42
3:F:118:ARG:NH2	3:F:186:ILE:O	2.53	0.42
1:A:444:THR:HG21	1:A:620:PHE:O	2.20	0.42
1:A:923:LYS:NZ	1:A:927:GLU:OE1	2.52	0.42
1:B:387:VAL:HG12	1:B:391:MET:SD	2.60	0.42
1:B:665:GLU:O	1:B:669:LYS:NZ	2.43	0.42
3:F:17:ALA:O	3:F:20:GLU:HB2	2.20	0.42
3:F:76:LYS:HA	3:F:102:ALA:O	2.20	0.42
1:A:541:LEU:HD11	1:A:598:LEU:HA	2.01	0.42
1:B:15:VAL:HG22	1:B:87:GLU:HG2	2.02	0.42
1:B:189:LYS:HA	1:B:189:LYS:HD3	1.86	0.42
1:B:711:LEU:O	1:B:714:ILE:HB	2.19	0.42
1:A:731:ARG:HH11	1:B:385:GLN:NE2	2.18	0.42
1:B:89:MET:HB3	1:B:714:ILE:HG12	2.02	0.42
1:B:234:PHE:CE1	1:B:289:ILE:HG12	2.55	0.42
1:B:344:PHE:O	1:B:349:GLN:NE2	2.53	0.42
1:B:728:GLN:OE1	1:B:749:GLY:HA3	2.20	0.42
1:B:736:ILE:HG13	1:B:739:ALA:HB2	2.02	0.42
1:B:853:SER:HB3	3:F:54:HIS:O	2.19	0.42
2:D:48:MET:SD	2:D:54:PRO:HD2	2.60	0.42
3:E:5:GLU:HG3	3:E:6:LYS:H	1.85	0.42
3:E:41:GLN:NE2	3:F:87:GLY:O	2.52	0.42
1:A:427:ILE:HD12	1:A:427:ILE:HA	1.94	0.41
1:A:576:LYS:HD2	1:A:577:ASP:N	2.35	0.41
1:B:678:ASN:HA	1:B:679:PRO:HD2	1.86	0.41
1:B:741:ALA:O	1:B:743:PRO:HD3	2.20	0.41
1:B:834:LYS:H	1:B:834:LYS:HD2	1.84	0.41
2:D:83:GLY:HA3	2:D:88:TYR:CE2	2.44	0.41
3:E:37:LYS:HD2	3:F:89:LEU:CD2	2.50	0.41
3:E:60:LYS:HB2	3:E:60:LYS:NZ	2.35	0.41
1:A:397:ASP:HA	1:A:400:ARG:NH1	2.35	0.41
1:B:255:ASN:HD22	1:B:264:GLY:HA3	1.86	0.41
1:B:398:PHE:O	1:B:402:ILE:HB	2.20	0.41
1:B:842:ARG:HG3	3:F:193:GLU:HB2	2.01	0.41
2:D:46:GLU:O	2:D:49:LYS:HB3	2.21	0.41
1:A:273:GLU:CA	1:A:478:GLU:HG2	2.34	0.41
1:A:280:GLN:HB2	1:A:317:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:916:CYS:SG	1:B:916:CYS:SG	3.17	0.41
1:B:100:VAL:HG21	1:B:711:LEU:HD13	2.02	0.41
1:B:175:CYS:HB2	1:B:183:LYS:HG3	2.02	0.41
1:B:398:PHE:HA	1:B:609:VAL:HG23	2.02	0.41
1:B:478:GLU:CD	1:B:478:GLU:H	2.28	0.41
3:E:15:LYS:HB2	3:F:69:ASP:OD2	2.20	0.41
1:A:425:PHE:CD2	1:A:599:THR:HB	2.55	0.41
1:B:716:ILE:O	1:B:719:GLN:HG2	2.20	0.41
1:B:725:ILE:O	1:B:774:ILE:HG22	2.21	0.41
1:B:776:PHE:CD1	1:B:781:LEU:HA	2.55	0.41
1:A:199:SER:HB2	1:A:221:GLU:OE2	2.20	0.41
1:A:241:LYS:NZ	1:A:471:ILE:O	2.51	0.41
1:A:339:MET:HB3	1:A:344:PHE:HD1	1.85	0.41
1:A:428:GLU:HB2	1:A:432:LYS:CE	2.46	0.41
1:A:733:ARG:HG2	1:A:788:ARG:HD3	2.01	0.41
1:B:86:VAL:HG22	1:B:87:GLU:H	1.83	0.41
1:B:409:VAL:HB	1:B:414:VAL:HG21	2.02	0.41
1:B:727:PHE:CZ	1:B:750:LYS:HA	2.55	0.41
3:E:147:LEU:HD12	3:E:177:LEU:HD23	2.01	0.41
3:F:31:PRO:HG2	3:F:36:GLN:NE2	2.36	0.41
3:F:91:THR:OG1	3:F:93:GLN:HB3	2.20	0.41
1:A:247:ARG:HH21	1:A:273:GLU:CD	2.29	0.41
1:A:477:PHE:CZ	1:A:481:CYS:SG	3.13	0.41
1:A:602:MET:O	1:A:658:THR:HA	2.20	0.41
1:A:825:ILE:CG1	3:E:131:ALA:HB1	2.51	0.41
1:B:141:TYR:HD1	1:B:193:TYR:OH	2.04	0.41
1:B:609:VAL:O	1:B:612:LEU:HB3	2.20	0.41
1:B:733:ARG:HH12	2:D:107:GLU:CD	2.29	0.41
1:A:744:LYS:HA	1:B:303:ASN:OD1	2.20	0.41
1:B:115:THR:N	1:B:122:VAL:O	2.54	0.41
1:B:188:LYS:HA	1:B:191:ILE:HB	2.03	0.41
1:B:348:GLU:O	1:B:352:ILE:HG13	2.21	0.41
1:B:393:ILE:HD13	1:B:613:LEU:HG	2.03	0.41
1:B:442:ILE:HD13	1:B:442:ILE:HA	1.93	0.41
1:B:618:ASP:HB3	1:B:621:VAL:HG23	2.01	0.41
1:B:685:ILE:HD12	1:B:704:GLN:HB3	2.01	0.41
3:F:68:GLN:HB2	3:F:78:ASP:OD2	2.21	0.41
1:A:611:SER:O	1:A:615:GLN:NE2	2.53	0.41
1:B:49:ILE:HG23	1:B:57:VAL:CG1	2.49	0.41
3:F:74:ILE:HG23	3:F:78:ASP:HB3	2.02	0.41
1:A:173:ILE:O	1:A:463:ILE:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ILE:HG12	1:A:378:MET:HE1	2.03	0.41
1:A:491:GLN:HE22	1:A:520:ASP:HA	1.85	0.41
1:A:602:MET:HG3	1:A:604:PRO:HD3	2.02	0.41
1:A:832:TYR:HE1	1:A:836:ARG:NH1	2.18	0.41
1:B:6:LEU:HB3	1:B:10:GLU:HB3	2.02	0.41
1:B:17:LYS:HE3	1:B:87:GLU:HG3	2.01	0.41
1:B:174:LEU:HD21	1:B:674:LEU:HD22	2.03	0.41
1:B:734:TYR:CE2	1:B:788:ARG:HD3	2.56	0.41
1:B:738:ALA:HB2	1:B:759:ALA:CB	2.51	0.41
1:B:800:GLN:HE21	2:D:119:MET:HG2	1.84	0.41
3:E:129:VAL:HA	3:E:183:PHE:CD2	2.56	0.41
3:F:27:ALA:O	3:F:29:PRO:HD3	2.20	0.41
1:A:238:LYS:HD3	1:A:285:ARG:HD3	2.02	0.41
1:A:563:GLN:OE1	1:A:566:HIS:HD2	2.04	0.41
1:A:721:PHE:CB	1:A:775:PHE:HB3	2.51	0.41
1:A:769:ILE:HD13	1:A:774:ILE:HG12	2.03	0.41
1:A:804:ARG:NH2	2:C:119:MET:SD	2.94	0.41
1:B:493:PHE:HD2	1:B:494:ASN:ND2	2.19	0.41
3:E:43:SER:HA	3:F:193:GLU:O	2.20	0.41
3:F:16:LYS:N	3:F:100:ALA:O	2.53	0.41
1:A:772:SER:OG	1:A:773:LYS:HE3	2.21	0.40
1:B:361:GLN:NE2	1:B:364:ASN:ND2	2.69	0.40
1:B:399:THR:HA	1:B:402:ILE:HG22	2.02	0.40
1:B:731:ARG:NH1	1:B:749:GLY:HA2	2.36	0.40
3:E:6:LYS:O	3:E:10:LYS:NZ	2.51	0.40
1:A:52:GLU:OE1	1:A:72:LYS:NZ	2.53	0.40
1:A:603:ASP:HB2	1:A:659:VAL:HG22	2.03	0.40
1:B:251:PHE:O	1:B:267:ILE:HA	2.21	0.40
1:B:736:ILE:HG23	1:B:794:ASP:OD1	2.21	0.40
1:B:800:GLN:NE2	2:D:119:MET:HG2	2.35	0.40
2:C:53:ASN:N	2:C:54:PRO:HD3	2.35	0.40
3:F:16:LYS:H	3:F:100:ALA:HB1	1.85	0.40
1:A:58:THR:HG22	1:A:69:THR:OG1	2.21	0.40
1:A:369:LYS:HZ1	1:A:374:ASP:CG	2.30	0.40
1:A:690:GLU:HB3	1:A:692:ARG:HG3	2.03	0.40
1:B:33:LYS:O	1:B:48:SER:HA	2.21	0.40
1:B:55:ASP:O	1:B:71:SER:HA	2.22	0.40
1:B:141:TYR:HA	1:B:149:MET:SD	2.60	0.40
1:B:218:GLY:O	1:B:222:LYS:HB2	2.21	0.40
1:B:400:ARG:HH21	1:B:400:ARG:HD3	1.71	0.40
3:F:42:ARG:NH2	3:F:120:ALA:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:146:THR:O	3:F:149:ARG:NH1	2.54	0.40
3:F:195:GLY:HA2	3:F:196:ALA:O	2.21	0.40
1:B:251:PHE:CE2	1:B:674:LEU:HD21	2.57	0.40
3:F:74:ILE:CG2	3:F:106:ILE:HD12	2.51	0.40
1:A:348:GLU:O	1:A:352:ILE:HG13	2.21	0.40
1:B:176:THR:O	1:B:684:CYS:HB2	2.22	0.40
1:B:530:ARG:HH11	1:B:530:ARG:HD2	1.74	0.40
1:B:663:TYR:O	1:B:667:LEU:N	2.53	0.40
2:D:31:CYS:HB2	2:D:64:LEU:HD11	2.02	0.40
3:F:76:LYS:HG3	3:F:103:PRO:HA	2.02	0.40
3:F:142:CYS:HB3	3:F:147:LEU:HD21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	930/974 (96%)	739 (80%)	154 (17%)	37 (4%)	2	18
1	B	932/974 (96%)	764 (82%)	127 (14%)	41 (4%)	2	17
2	C	146/151 (97%)	127 (87%)	12 (8%)	7 (5%)	2	16
2	D	146/151 (97%)	122 (84%)	18 (12%)	6 (4%)	2	18
3	E	194/196 (99%)	159 (82%)	23 (12%)	12 (6%)	1	13
3	F	194/196 (99%)	118 (61%)	52 (27%)	24 (12%)	0	4
All	All	2542/2642 (96%)	2029 (80%)	386 (15%)	127 (5%)	3	16

All (127) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	ASN

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Mol	Chain	Res	Type
1	A	181	ALA
1	A	224	LEU
1	A	429	ALA
1	A	533	ASN
1	A	795	VAL
1	A	848	LYS
1	B	16	ASP
1	B	257	ASP
1	B	369	LYS
1	B	407	ILE
1	B	469	PHE
1	B	533	ASN
1	B	735	GLU
1	B	743	PRO
1	B	793	THR
1	B	794	ASP
1	B	837	ASN
1	B	848	LYS
1	B	853	SER
1	B	856	ARG
2	C	100	ASN
2	D	94	VAL
2	D	97	LYS
2	D	116	GLY
2	D	121	GLU
3	E	29	PRO
3	F	11	LYS
3	F	14	LYS
3	F	53	GLN
3	F	54	HIS
3	F	110	MET
3	F	120	ALA
3	F	123	ASP
3	F	125	GLU
3	F	188	THR
1	A	32	LYS
1	A	134	SER
1	A	288	HIS
1	A	371	ARG
1	A	508	GLU
1	A	564	GLY
1	A	605	LEU

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Mol	Chain	Res	Type
1	A	670	LEU
1	A	780	VAL
1	A	846	LYS
1	A	860	MET
1	B	77	LYS
1	B	184	THR
1	B	346	GLU
1	B	393	ILE
1	B	511	GLU
1	B	733	ARG
1	B	762	LEU
1	B	813	ALA
1	B	819	LEU
1	B	836	ARG
1	B	854	ALA
2	C	6	GLU
2	C	57	ASP
2	C	77	ALA
3	E	47	VAL
3	E	49	ALA
3	E	55	GLN
3	E	178	ILE
3	F	15	LYS
3	F	70	LYS
3	F	121	GLY
1	A	257	ASP
1	A	374	ASP
1	A	426	ALA
1	A	574	GLN
1	A	852	GLN
1	B	565	ASN
1	B	572	SER
1	B	817	GLN
1	B	839	GLN
2	D	57	ASP
3	E	188	THR
3	E	194	GLU
3	F	3	ASP
3	F	17	ALA
3	F	29	PRO
3	F	190	GLY
1	A	151	PRO

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Mol	Chain	Res	Type
1	A	603	ASP
1	A	632	VAL
1	A	717	CYS
1	A	854	ALA
1	B	151	PRO
1	B	564	GLY
1	B	567	ALA
1	B	579	THR
2	D	6	GLU
3	F	82	THR
3	F	195	GLY
1	A	92	LEU
1	A	93	THR
1	A	132	ILE
1	A	469	PHE
1	A	546	TRP
1	A	565	ASN
1	B	362	LEU
1	B	531	PRO
3	E	44	GLY
3	E	141	LYS
3	F	12	LYS
3	F	13	SER
3	F	72	GLY
3	F	95	LEU
1	B	379	PRO
1	B	629	ASP
1	B	722	PRO
1	B	725	ILE
2	C	39	GLY
2	C	94	VAL
3	E	105	PRO
1	A	743	PRO
2	C	76	ILE
3	F	44	GLY
3	F	105	PRO
1	A	393	ILE
1	A	413	VAL
3	E	87	GLY
1	B	132	ILE
3	E	140	GLY
1	B	764	PRO

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	828/859 (96%)	742 (90%)	86 (10%)	7	22
1	B	829/859 (96%)	723 (87%)	106 (13%)	4	15
2	C	127/130 (98%)	115 (91%)	12 (9%)	8	26
2	D	127/130 (98%)	106 (84%)	21 (16%)	2	10
3	E	162/162 (100%)	147 (91%)	15 (9%)	8	26
3	F	162/162 (100%)	137 (85%)	25 (15%)	2	12
All	All	2235/2302 (97%)	1970 (88%)	265 (12%)	7	18

All (265) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	26	GLN
1	A	33	LYS
1	A	42	HIS
1	A	51	GLU
1	A	55	ASP
1	A	66	LYS
1	A	79	ASN
1	A	96	ASN
1	A	103	ASN
1	A	110	SER
1	A	146	ARG
1	A	147	HIS
1	A	162	ARG
1	A	178	GLU
1	A	211	GLN
1	A	214	SER
1	A	222	LYS
1	A	228	ASN
1	A	247	ARG
1	A	259	THR
1	A	278	ILE

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Mol	Chain	Res	Type
1	A	279	ARG
1	A	280	GLN
1	A	286	THR
1	A	290	PHE
1	A	302	ARG
1	A	311	ASN
1	A	312	ASN
1	A	314	THR
1	A	342	MET
1	A	357	SER
1	A	366	VAL
1	A	375	GLN
1	A	388	CYS
1	A	396	THR
1	A	402	ILE
1	A	406	ARG
1	A	408	LYS
1	A	412	ASP
1	A	425	PHE
1	A	430	LEU
1	A	434	LYS
1	A	435	PHE
1	A	451	ASP
1	A	488	LYS
1	A	495	HIS
1	A	506	GLN
1	A	513	ASN
1	A	526	GLU
1	A	543	GLU
1	A	565	ASN
1	A	566	HIS
1	A	568	LYS
1	A	576	LYS
1	A	579	THR
1	A	586	TYR
1	A	603	ASP
1	A	605	LEU
1	A	608	ASN
1	A	615	GLN
1	A	618	ASP
1	A	623	ASP
1	A	624	LEU

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Mol	Chain	Res	Type
1	A	661	GLN
1	A	662	LEU
1	A	667	LEU
1	A	686	ILE
1	A	699	HIS
1	A	707	CYS
1	A	711	LEU
1	A	715	ARG
1	A	727	PHE
1	A	748	ASP
1	A	754	ILE
1	A	778	THR
1	A	796	ILE
1	A	833	LEU
1	A	837	ASN
1	A	843	LEU
1	A	856	ARG
1	A	865	GLU
1	A	867	PHE
1	A	869	ARG
1	A	882	LYS
1	A	932	GLU
1	B	3	GLN
1	B	14	PHE
1	B	16	ASP
1	B	21	ASN
1	B	26	GLN
1	B	33	LYS
1	B	51	GLU
1	B	66	LYS
1	B	77	LYS
1	B	103	ASN
1	B	109	PHE
1	B	124	ILE
1	B	150	PRO
1	B	162	ARG
1	B	196	VAL
1	B	200	SER
1	B	201	HIS
1	B	222	LYS
1	B	228	ASN
1	B	245	SER

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Mol	Chain	Res	Type
1	B	247	ARG
1	B	253	ARG
1	B	278	ILE
1	B	280	GLN
1	B	286	THR
1	B	303	ASN
1	B	311	ASN
1	B	314	THR
1	B	329	ASP
1	B	347	GLU
1	B	357	SER
1	B	369	LYS
1	B	370	GLU
1	B	372	ASN
1	B	382	THR
1	B	396	THR
1	B	399	THR
1	B	402	ILE
1	B	408	LYS
1	B	411	ARG
1	B	412	ASP
1	B	445	ARG
1	B	476	SER
1	B	479	GLN
1	B	480	LEU
1	B	484	TYR
1	B	494	ASN
1	B	503	GLU
1	B	504	GLU
1	B	511	GLU
1	B	513	ASN
1	B	515	ILE
1	B	532	THR
1	B	538	LEU
1	B	543	GLU
1	B	553	THR
1	B	565	ASN
1	B	568	LYS
1	B	570	GLN
1	B	573	LYS
1	B	576	LYS
1	B	579	THR

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Mol	Chain	Res	Type
1	B	613	LEU
1	B	665	GLU
1	B	675	ARG
1	B	682	VAL
1	B	686	ILE
1	B	691	LYS
1	B	711	LEU
1	B	716	ILE
1	B	718	ARG
1	B	719	GLN
1	B	724	ARG
1	B	728	GLN
1	B	729	GLU
1	B	730	PHE
1	B	731	ARG
1	B	733	ARG
1	B	744	LYS
1	B	757	ILE
1	B	760	LEU
1	B	761	GLU
1	B	772	SER
1	B	778	THR
1	B	781	LEU
1	B	791	LYS
1	B	812	PHE
1	B	814	LYS
1	B	833	LEU
1	B	834	LYS
1	B	839	GLN
1	B	843	LEU
1	B	846	LYS
1	B	849	PRO
1	B	852	GLN
1	B	853	SER
1	B	856	ARG
1	B	862	SER
1	B	886	GLU
1	B	891	LEU
1	B	907	ASP
1	B	911	ASP
1	B	932	GLU
1	B	939	ASP

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Mol	Chain	Res	Type
1	B	960	GLU
1	B	974	LYS
2	C	25	LYS
2	C	50	VAL
2	C	55	LYS
2	C	60	ASN
2	C	67	GLU
2	C	73	MET
2	C	78	LYS
2	C	80	LYS
2	C	82	GLN
2	C	121	GLU
2	C	132	GLU
2	C	134	SER
2	D	21	THR
2	D	25	LYS
2	D	50	VAL
2	D	55	LYS
2	D	60	ASN
2	D	73	MET
2	D	78	LYS
2	D	80	LYS
2	D	82	GLN
2	D	90	GLU
2	D	96	ASP
2	D	102	THR
2	D	103	VAL
2	D	108	ILE
2	D	110	HIS
2	D	111	VAL
2	D	121	GLU
2	D	122	GLU
2	D	124	VAL
2	D	132	GLU
2	D	148	LEU
3	E	15	LYS
3	E	16	LYS
3	E	29	PRO
3	E	37	LYS
3	E	41	GLN
3	E	71	ASP
3	E	115	PHE

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Mol	Chain	Res	Type
3	E	123	ASP
3	E	126	ASP
3	E	145	GLU
3	E	147	LEU
3	E	173	ASP
3	E	187	LEU
3	E	189	LYS
3	E	193	GLU
3	F	10	LYS
3	F	14	LYS
3	F	29	PRO
3	F	33	PRO
3	F	42	ARG
3	F	48	PHE
3	F	50	MET
3	F	61	GLU
3	F	67	ASP
3	F	70	LYS
3	F	80	ARG
3	F	84	ASP
3	F	85	SER
3	F	86	LEU
3	F	88	ARG
3	F	89	LEU
3	F	90	CYS
3	F	95	LEU
3	F	110	MET
3	F	118	ARG
3	F	124	GLU
3	F	145	GLU
3	F	165	GLN
3	F	187	LEU
3	F	193	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	62	GLN
1	A	171	GLN
1	A	223	GLN
1	A	312	ASN

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Mol	Chain	Res	Type
1	A	333	GLN
1	A	364	ASN
1	A	375	GLN
1	A	486	ASN
1	A	494	ASN
1	A	565	ASN
1	A	566	HIS
1	A	593	ASN
1	A	608	ASN
1	A	614	ASN
1	A	615	GLN
1	A	678	ASN
1	A	680	ASN
1	A	728	GLN
1	A	802	GLN
1	A	828	ASN
1	A	839	GLN
1	A	852	GLN
1	A	893	GLN
1	A	906	GLN
1	A	908	ASN
1	B	171	GLN
1	B	186	ASN
1	B	266	ASN
1	B	311	ASN
1	B	326	GLN
1	B	361	GLN
1	B	364	ASN
1	B	372	ASN
1	B	385	GLN
1	B	389	HIS
1	B	415	GLN
1	B	479	GLN
1	B	494	ASN
1	B	495	HIS
1	B	593	ASN
1	B	608	ASN
1	B	680	ASN
1	B	751	GLN
1	B	800	GLN
1	B	817	GLN
1	B	818	GLN

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Mol	Chain	Res	Type
1	B	828	ASN
1	B	852	GLN
1	B	899	GLN
2	C	30	GLN
2	C	60	ASN
2	C	74	GLN
2	C	110	HIS
2	D	7	GLN
2	D	16	GLN
2	D	30	GLN
2	D	60	ASN
2	D	74	GLN
2	D	100	ASN
2	D	135	ASN
3	E	41	GLN
3	E	57	GLN
3	E	130	ASN
3	E	133	ASN
3	E	165	GLN
3	F	46	ASN
3	F	55	GLN
3	F	130	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6370. These allow visual inspection of the internal detail of the map and identification of artifacts.

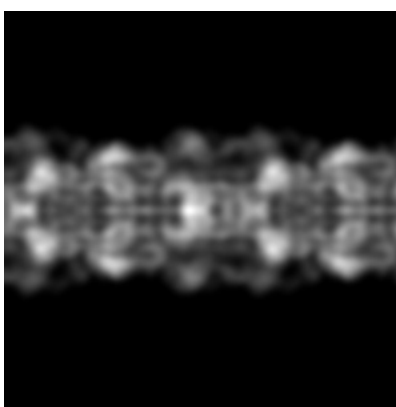
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

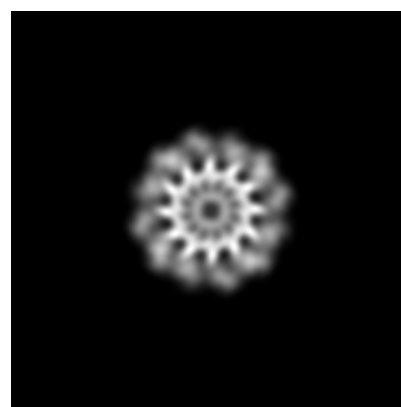
6.1.1 Primary map



X



Y

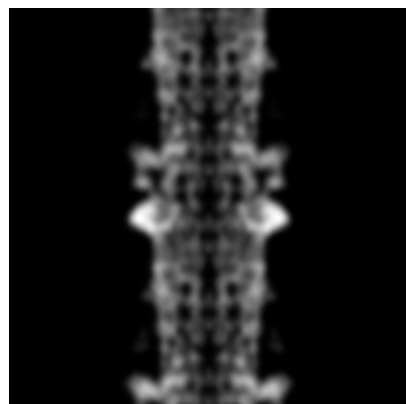


Z

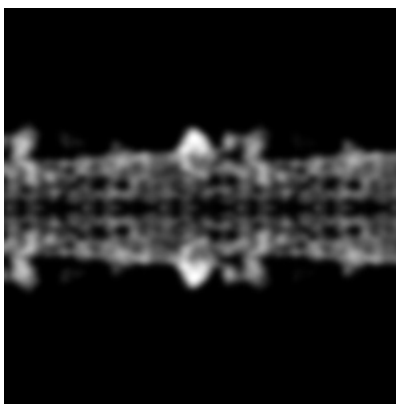
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 65



Y Index: 65

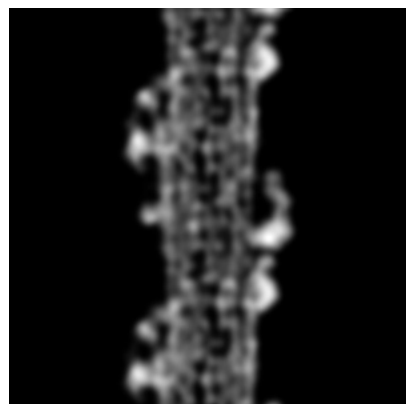


Z Index: 65

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

6.3 Largest variance slices [i](#)

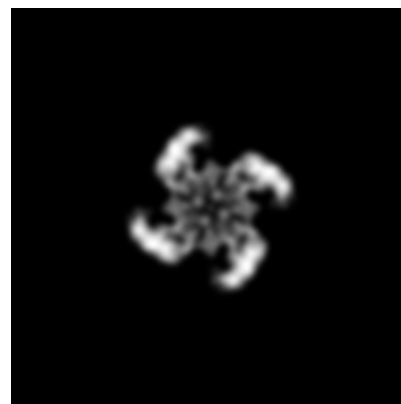
6.3.1 Primary map



X Index: 73



Y Index: 73

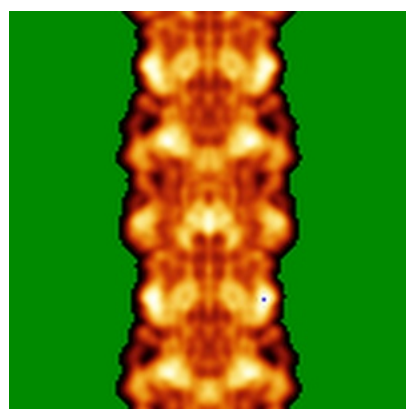


Z Index: 11

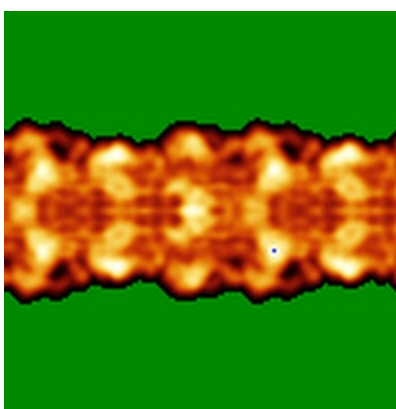
The images above show the largest variance slices of the map in three orthogonal directions.

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

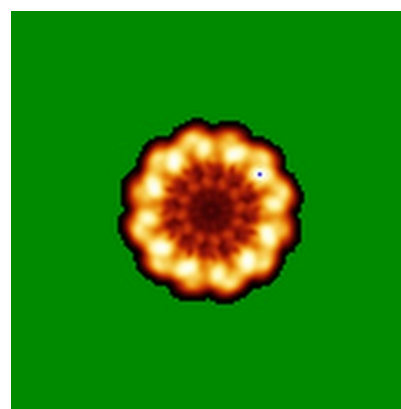
6.4.1 Primary map



X



Y



Z

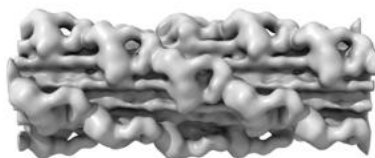
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

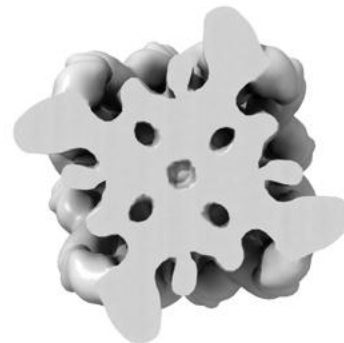
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

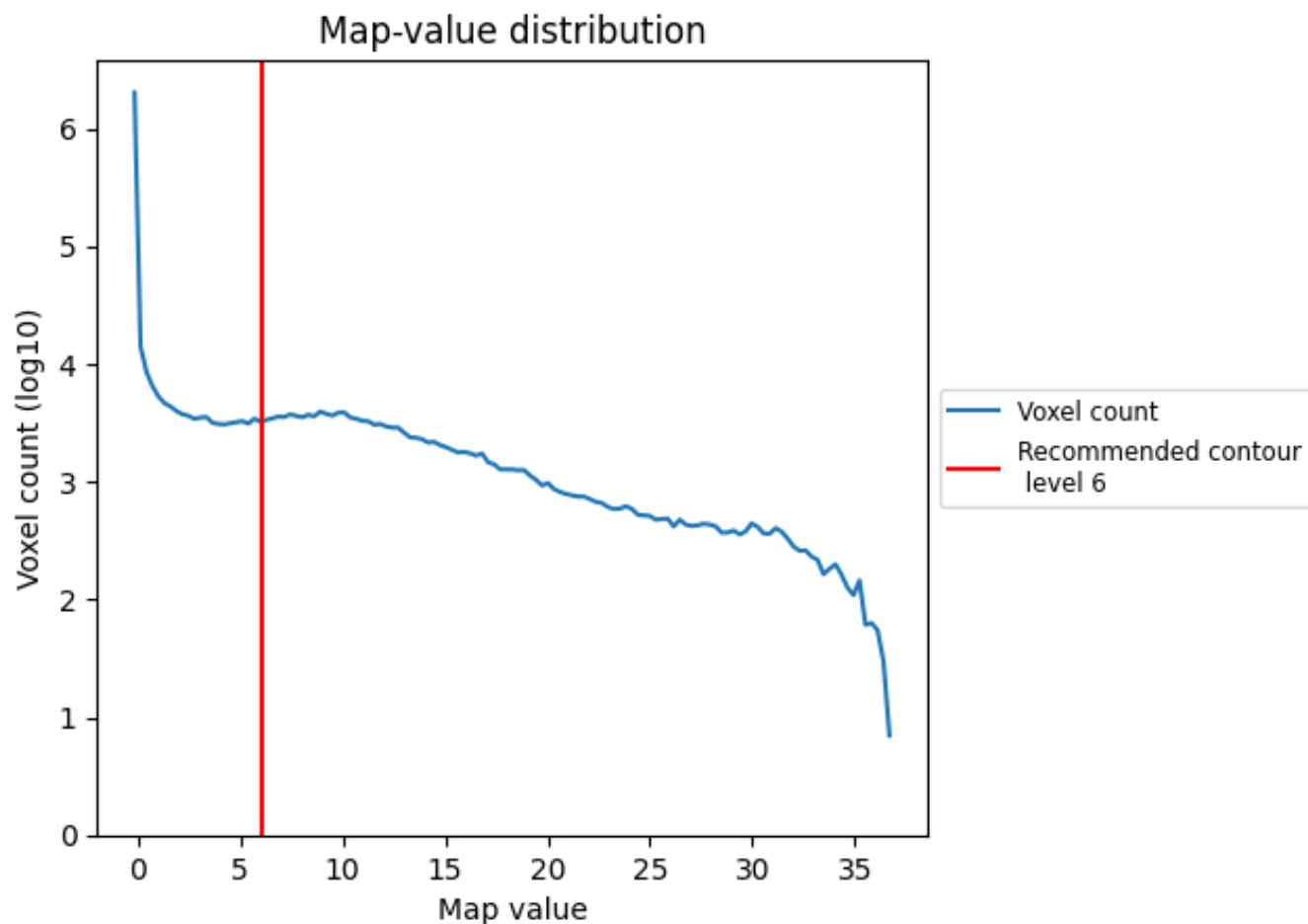
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

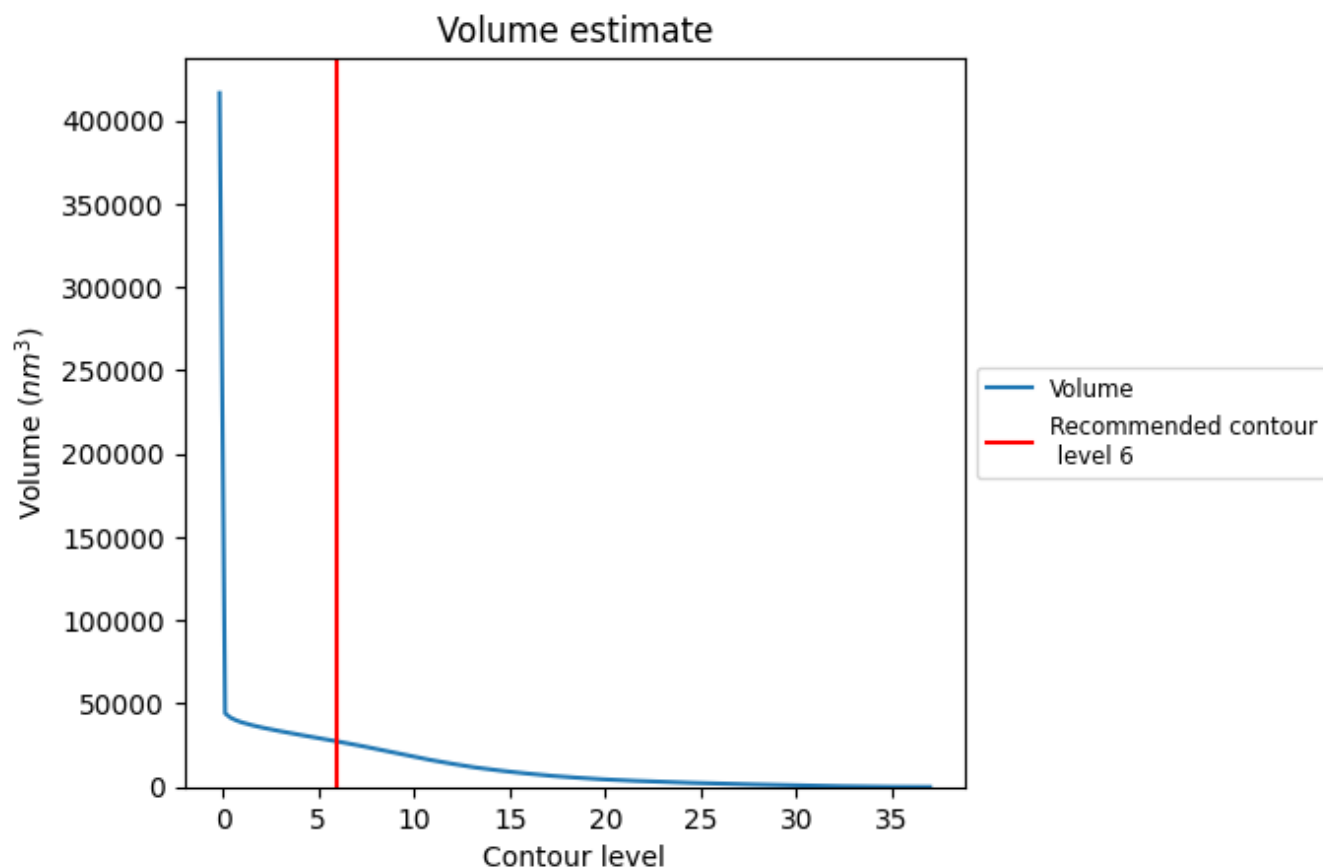
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

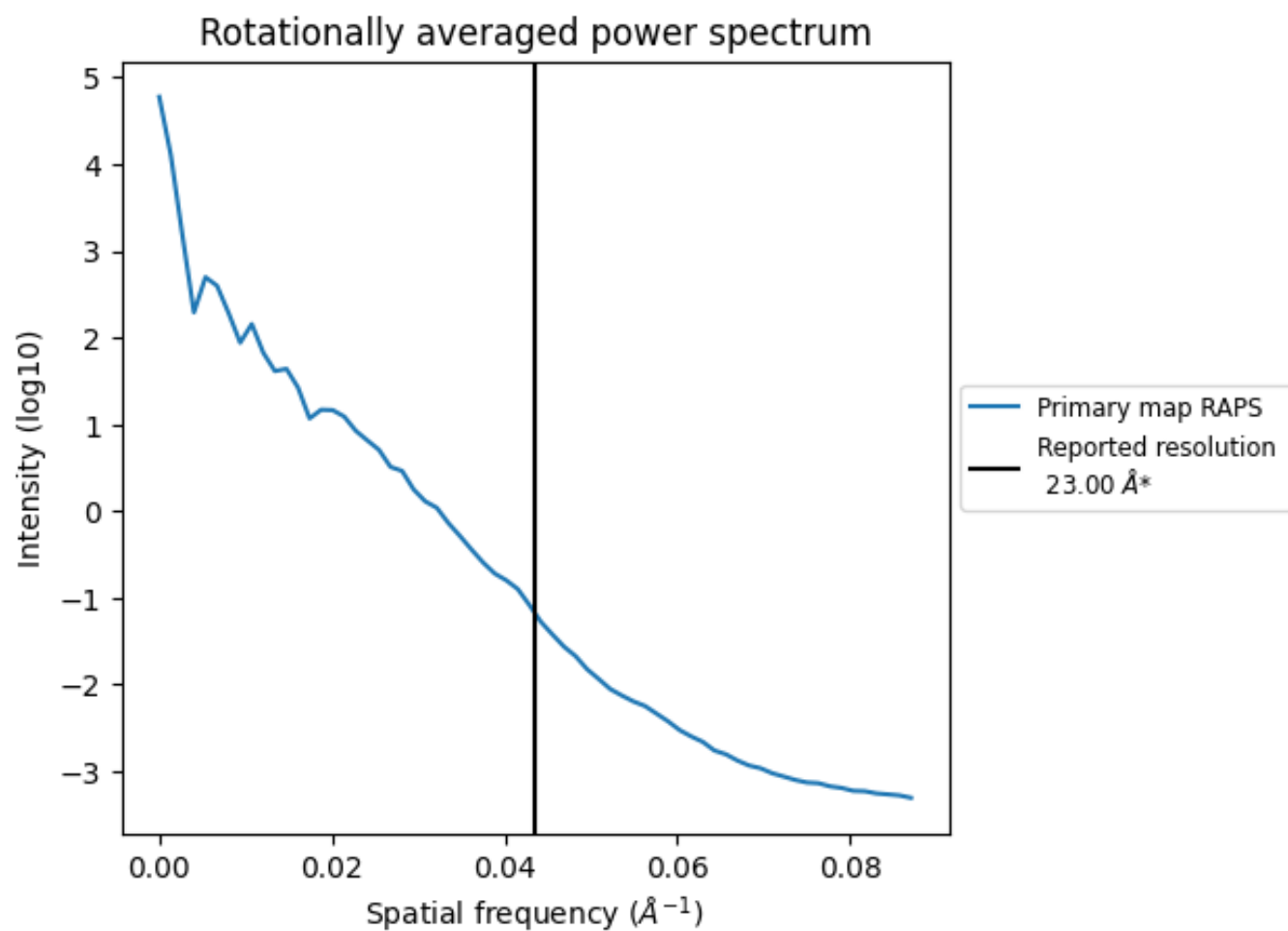
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 27308 nm^3 ; this corresponds to an approximate mass of 24668 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 ⓘ

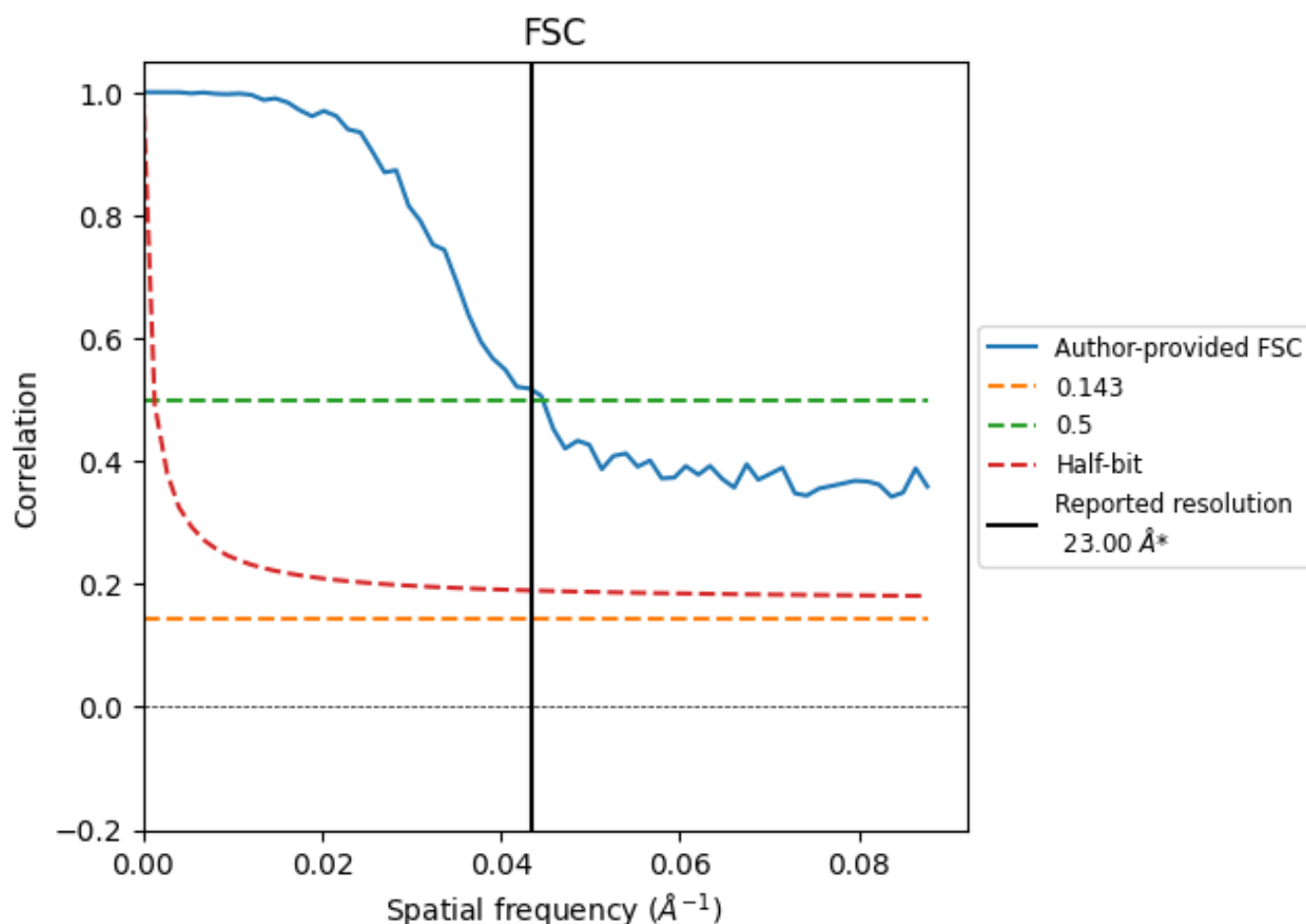


*Reported resolution corresponds to spatial frequency of 0.043 Å⁻¹

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 0.043 Å⁻¹

8.2 Resolution estimates [i](#)

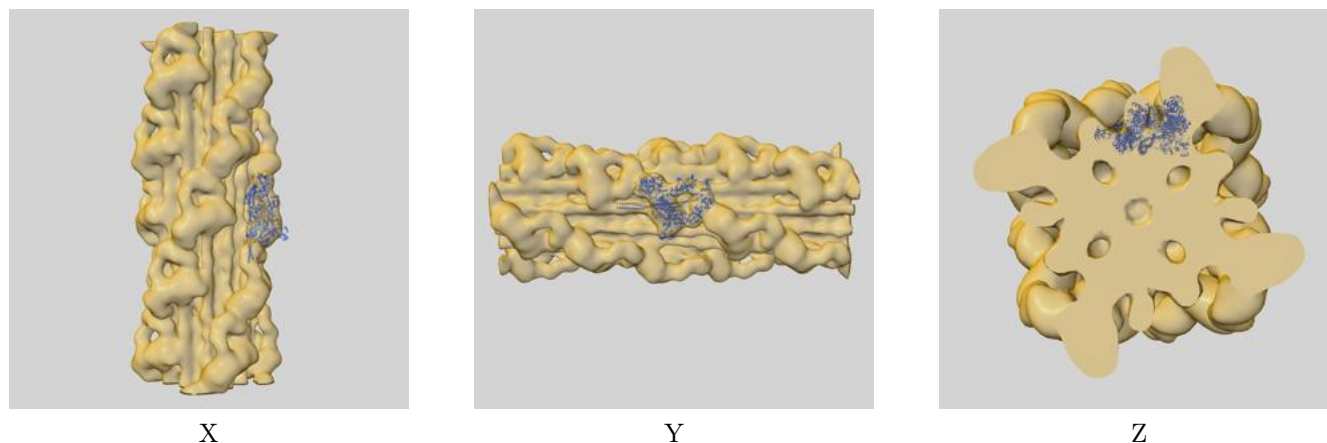
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	23.00	-
Author-provided FSC curve	-	22.37	-
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

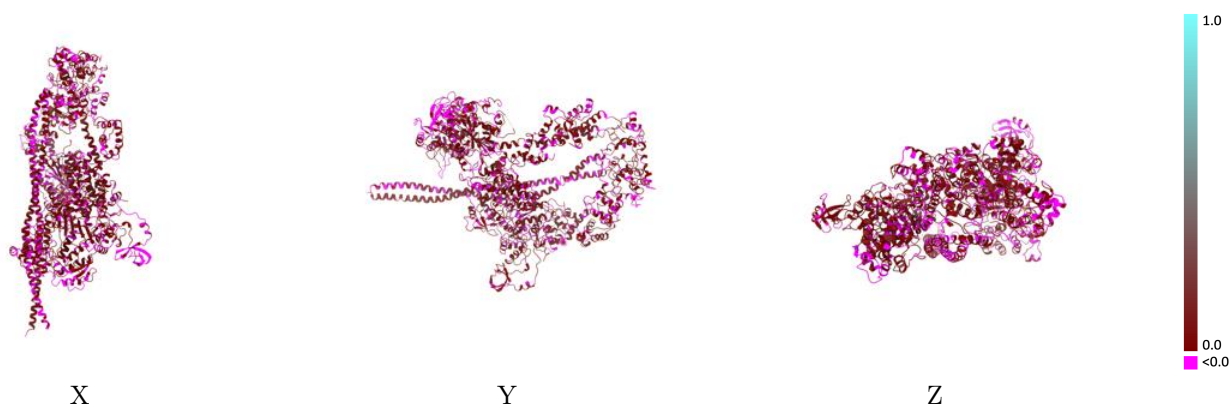
This section contains information regarding the fit between EMDB map EMD-6370 and PDB model 3JAX. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



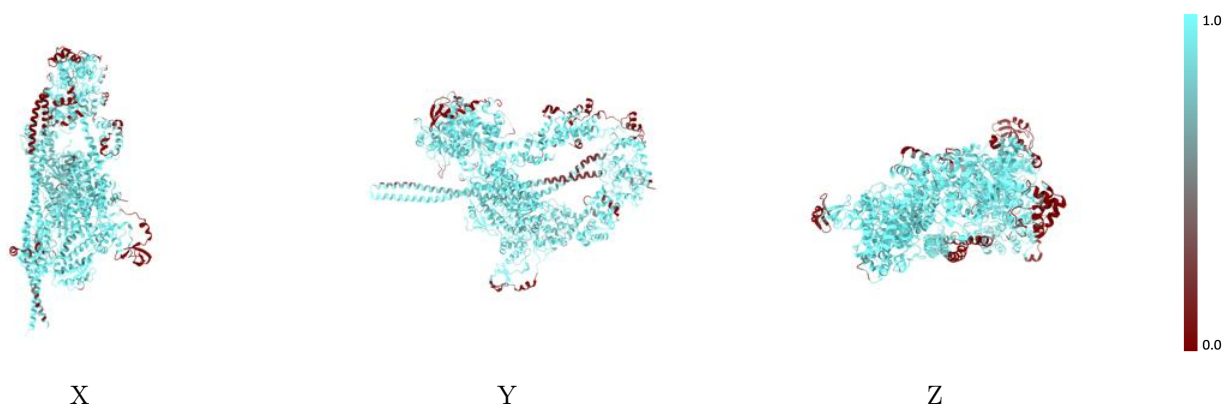
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



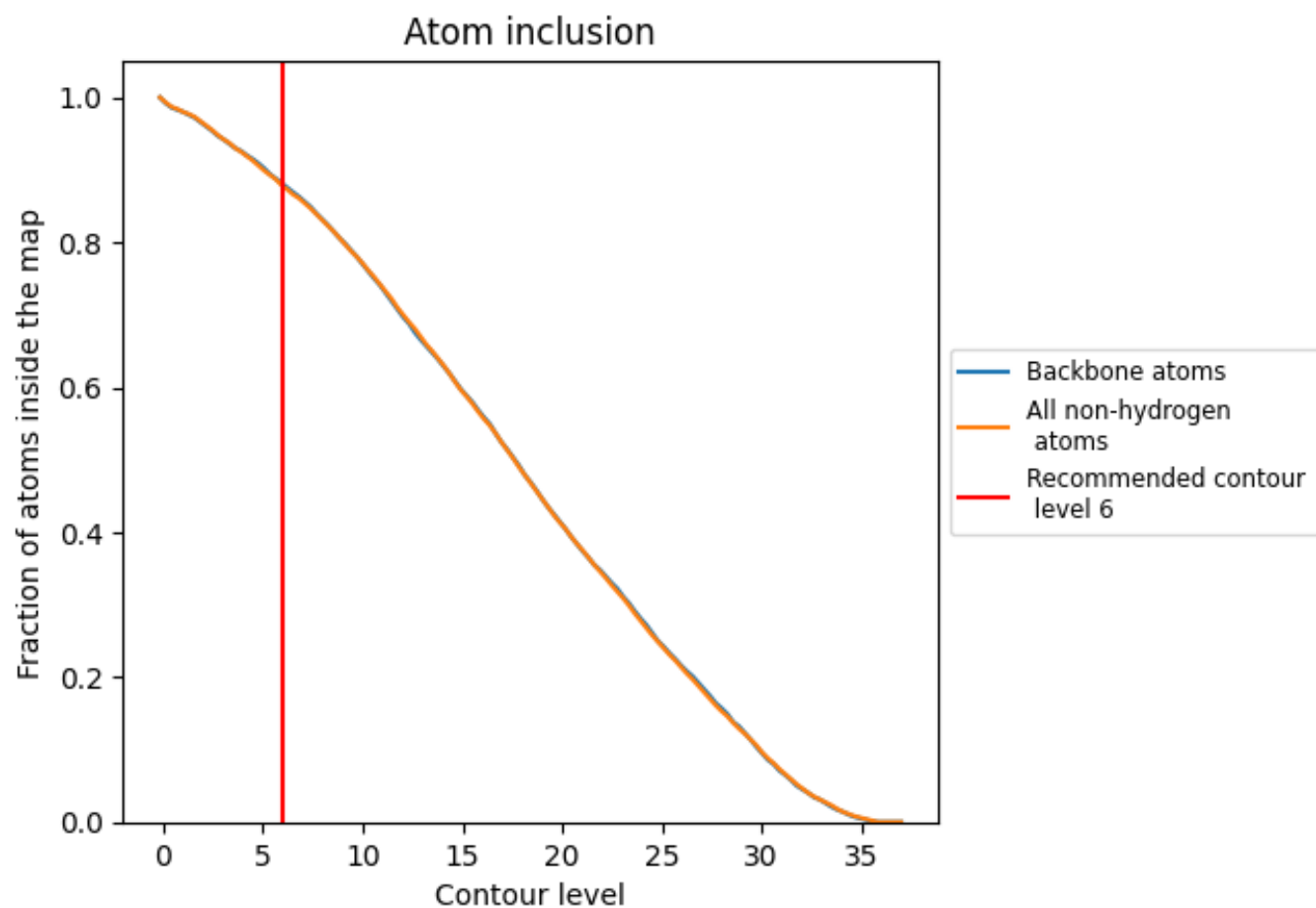
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 88% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8770	0.0400
A	0.8620	0.0310
B	0.9320	0.0460
C	0.7840	0.0380
D	0.9900	0.0750
E	0.6320	0.0330
F	0.9340	0.0430

1.0

0.0

<0.0