



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:01 AM UTC

PDB ID : 2DFS / pdb_00002dfs
EMDB ID : EMD-1201
Title : 3-D structure of Myosin-V inhibited state
Authors : Liu, J.; Taylor, D.W.; Krementsova, E.B.; Trybus, K.M.; Taylor, K.A.
Deposited on : 2006-03-03
Resolution : 24.00 Å (reported)
Based on initial models : 1N2D, 1W7I

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:

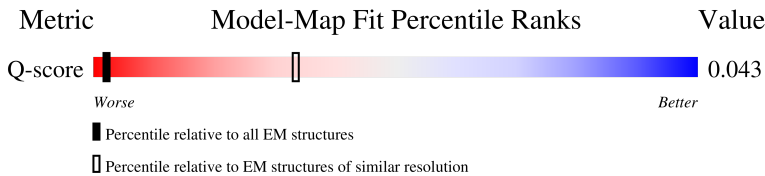
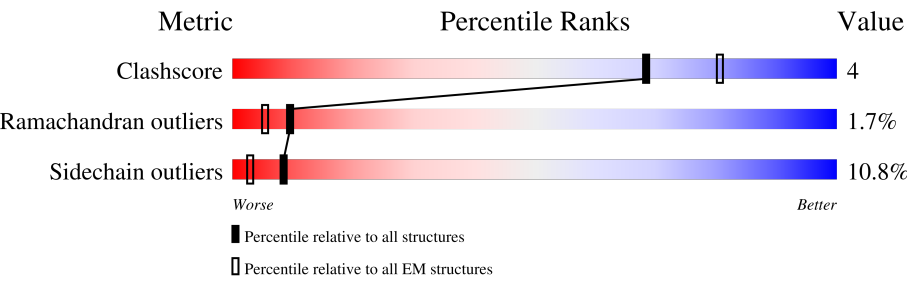
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 CRYSTALLOGRAPHY

The reported resolution of this entry is 24.00 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.



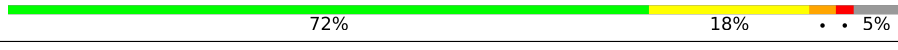
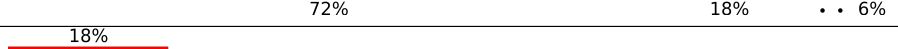
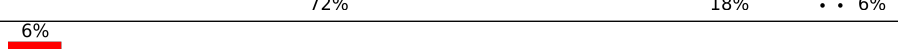
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9 (23.50 - 24.00)

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	1080	6% 73%16%8%
1	M	1080	10% 74%15%8%
2	B	148	53%29%9%6%
2	C	148	65%25%5%5%

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Mol	Chain	Length	Quality of chain
2	D	148	 74%16%••6%
2	E	148	 72%18%••5%
2	F	148	 72%18%••6%
2	G	148	 18%54%30%7%•5%
2	N	148	 57%26%7%•6%
2	O	148	 66%23%6%5%
2	P	148	 7%73%18%••6%
2	Q	148	 71%20%••5%
2	R	148	 72%18%••6%
2	S	148	 6%60%24%7%•5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29614 atoms, of which 0 are hydrogens and 0 are deuteriums.

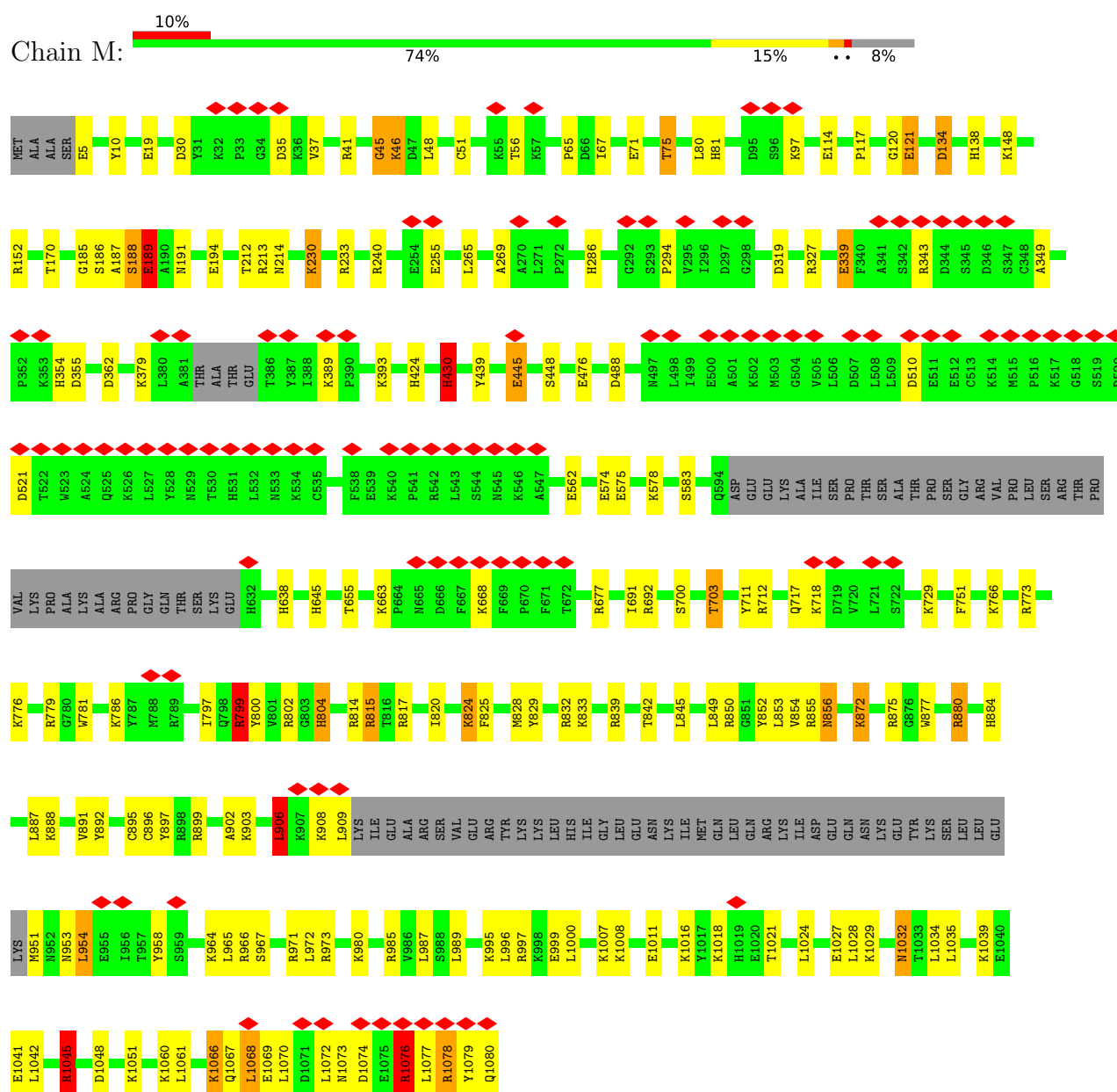
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Myosin-5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	994	Total	C	N	O	S	0	0
			8198	5219	1445	1486	48		
1	M	994	Total	C	N	O	S	0	0
			8198	5219	1445	1486	48		

- Molecule 2 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	139	Total	C	N	O	S	0	0
			1093	671	177	236	9		
2	C	141	Total	C	N	O	S	0	0
			1110	682	180	239	9		
2	D	139	Total	C	N	O	S	0	0
			1093	671	177	236	9		
2	E	141	Total	C	N	O	S	0	0
			1110	682	180	239	9		
2	F	139	Total	C	N	O	S	0	0
			1093	671	177	236	9		
2	G	141	Total	C	N	O	S	0	0
			1110	682	180	239	9		
2	N	139	Total	C	N	O	S	0	0
			1093	671	177	236	9		
2	O	141	Total	C	N	O	S	0	0
			1110	682	180	239	9		
2	P	139	Total	C	N	O	S	0	0
			1093	671	177	236	9		
2	Q	141	Total	C	N	O	S	0	0
			1110	682	180	239	9		
2	R	139	Total	C	N	O	S	0	0
			1093	671	177	236	9		
2	S	141	Total	C	N	O	S	0	0
			1110	682	180	239	9		

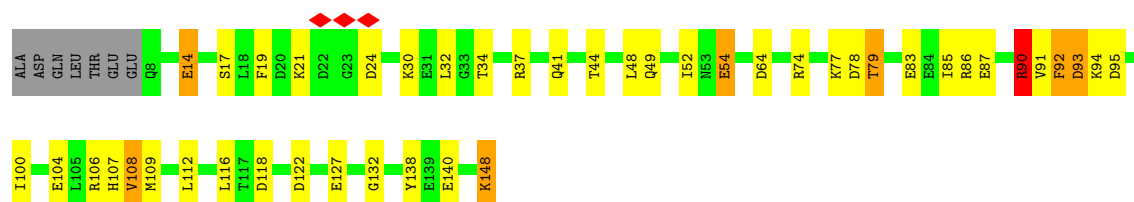


• Molecule 2: Calmodulin

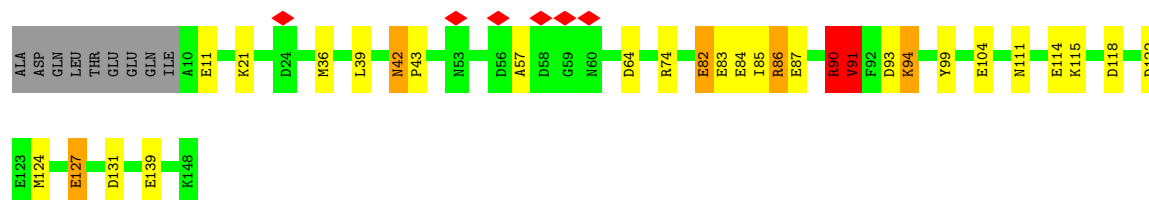


• Molecule 2: Calmodulin

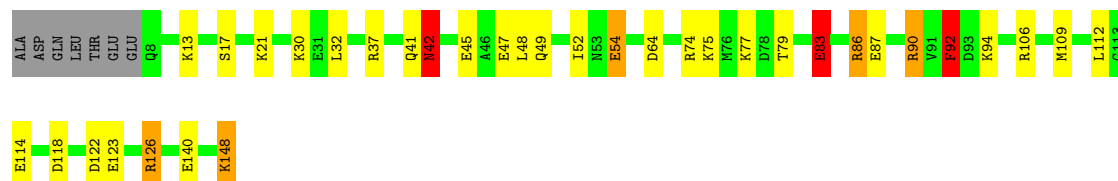




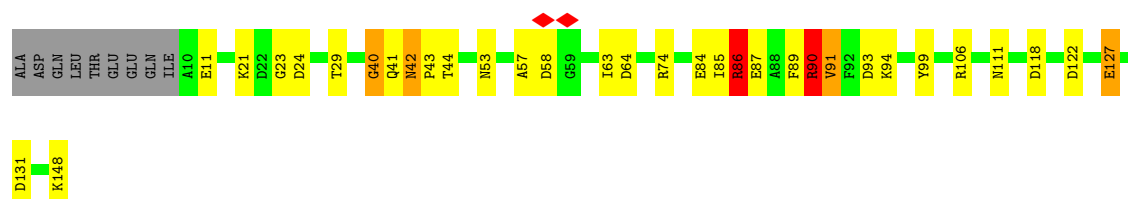
• Molecule 2: Calmodulin



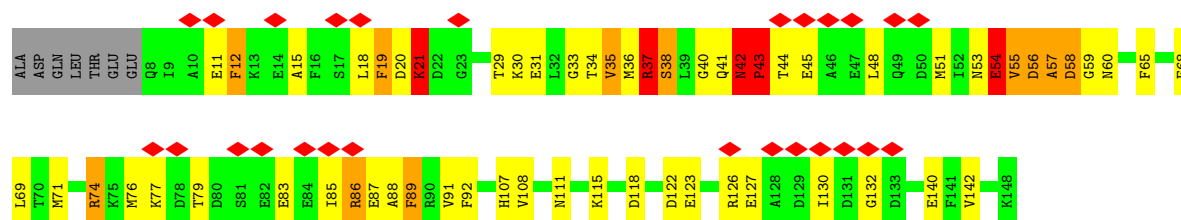
• Molecule 2: Calmodulin



• Molecule 2: Calmodulin

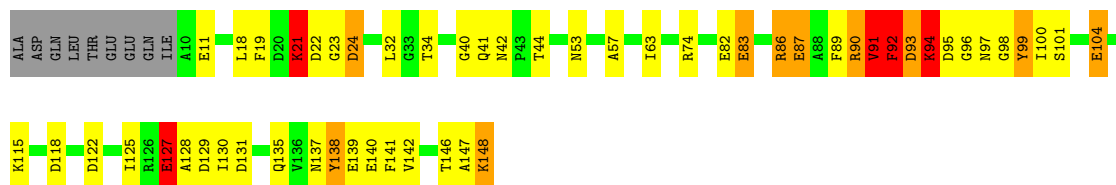


• Molecule 2: Calmodulin



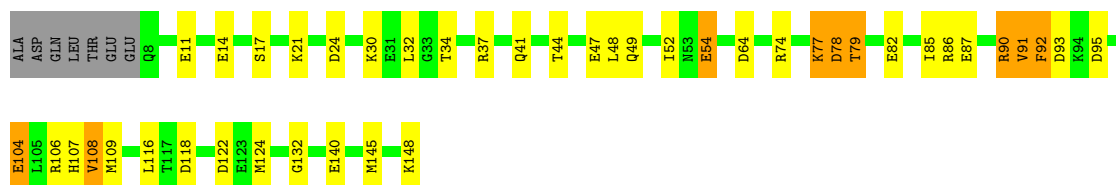
• Molecule 2: Calmodulin

Chain N:  57% 26% 7% 6%



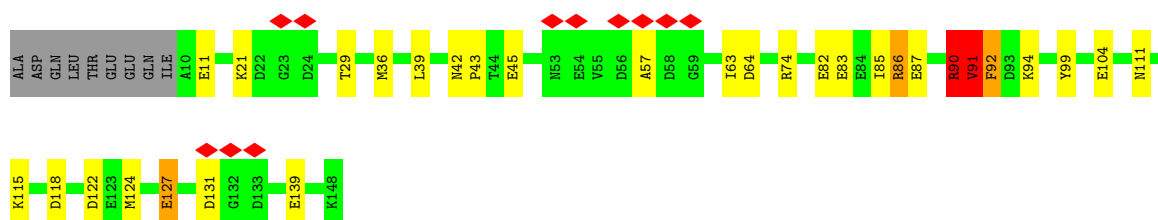
• Molecule 2: Calmodulin

Chain O:  66% 23% 6% 5%



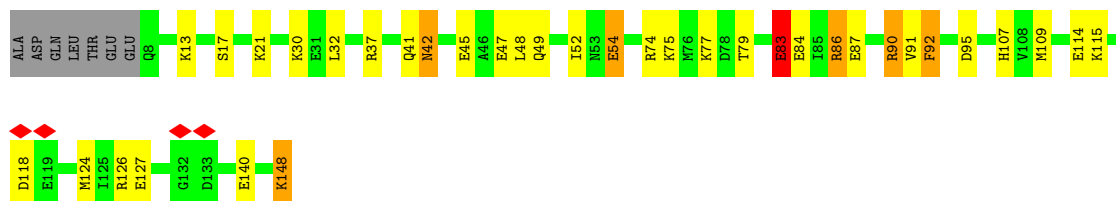
• Molecule 2: Calmodulin

Chain P:  73% 18% 7% 6%



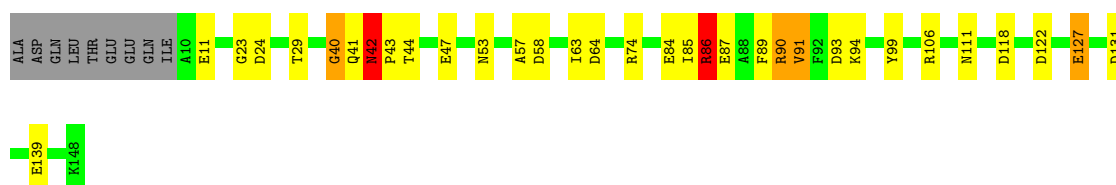
• Molecule 2: Calmodulin

Chain Q:  71% 20% 5% 6%

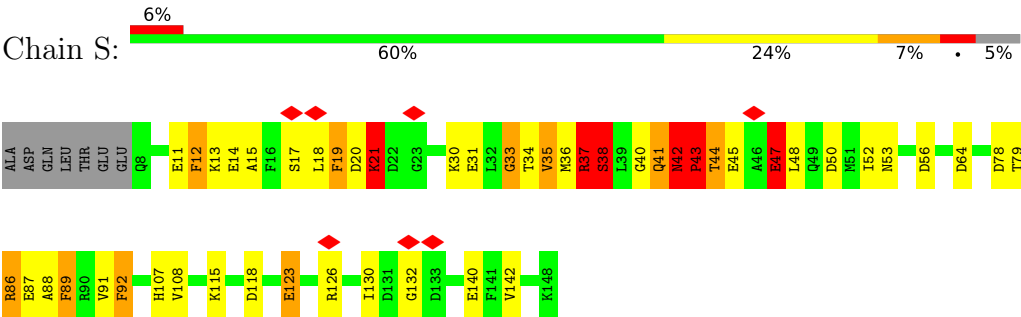


• Molecule 2: Calmodulin

Chain R:  72% 18% 5% 6%



● Molecule 2: Calmodulin



4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	2D CRYSTAL, a =Not provided Å, b =Not provided Å, c =Not provided Å, γ =Not provided°, space group=Not provided	Depositor
Number of tilted images used	4029	Depositor
Resolution determination method	Not provided	
CTF correction method	CTF gradient correction	Depositor
Microscope	FEI/PHILIPS CM300FEG/ST	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	12000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	24000	Depositor
Image detector	TVIPS TEMCAM-F224 (2k x 2k)	Depositor
Maximum voxel value	13.857	Depositor
Minimum voxel value	-0.411	Depositor
Average voxel value	0.042	Depositor
Voxel value standard deviation	0.651	Depositor
Recommended contour level	0.65	Depositor
Tomogram size (Å)	1000.8, 1000.8, 333.6	wwPDB
Tomogram dimensions	180, 180, 60	wwPDB
Tomogram angles (°)	90, 90, 90	wwPDB
Grid spacing (Å)	5.56, 5.56, 5.56	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	0.92	0/8359	1.63	63/11241 (0.6%)
1	M	0.92	0/8359	1.63	63/11241 (0.6%)
2	B	0.94	0/1105	1.85	22/1482 (1.5%)
2	C	0.89	0/1122	1.78	18/1505 (1.2%)
2	D	0.93	0/1105	1.83	25/1482 (1.7%)
2	E	0.88	0/1122	1.72	15/1505 (1.0%)
2	F	0.92	0/1105	1.79	21/1482 (1.4%)
2	G	1.11	3/1122 (0.3%)	2.02	37/1505 (2.5%)
2	N	0.93	0/1105	1.83	19/1482 (1.3%)
2	O	0.90	0/1122	1.79	18/1505 (1.2%)
2	P	0.95	1/1105 (0.1%)	1.80	20/1482 (1.3%)
2	Q	0.88	0/1122	1.70	10/1505 (0.7%)
2	R	0.92	0/1105	1.79	22/1482 (1.5%)
2	S	0.97	1/1122 (0.1%)	1.89	26/1505 (1.7%)
All	All	0.93	5/30080 (0.0%)	1.71	379/40404 (0.9%)

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	M	0	30
2	B	0	8
2	C	0	7
2	D	0	4
2	E	0	8
2	F	0	5
2	G	0	7
2	N	0	8
2	O	0	6
2	P	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	Q	0	7
2	R	0	4
2	S	0	9
All	All	0	140

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	57	ALA	CA-C	10.51	1.65	1.52
2	G	56	ASP	CA-C	8.96	1.64	1.52
2	G	57	ALA	N-CA	6.64	1.54	1.45
2	P	42	ASN	N-CA	-5.05	1.41	1.46
2	S	33	GLY	CA-C	-5.01	1.46	1.52

All (379) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	57	ALA	N-CA-C	12.70	130.22	113.97
1	A	430	HIS	CA-CB-CG	12.51	126.31	113.80
1	M	430	HIS	CA-CB-CG	12.50	126.30	113.80
1	A	825	PHE	CA-CB-CG	11.79	125.59	113.80
1	M	825	PHE	CA-CB-CG	10.50	124.30	113.80
1	M	804	HIS	CA-CB-CG	10.12	123.92	113.80
2	G	57	ALA	CA-C-N	9.29	137.87	122.54
2	G	57	ALA	C-N-CA	9.29	137.87	122.54
2	D	42	ASN	O-C-N	-9.23	112.58	121.17
2	P	42	ASN	O-C-N	-9.06	112.75	121.17
2	O	21	LYS	CA-C-N	8.90	132.21	120.28
2	O	21	LYS	C-N-CA	8.90	132.21	120.28
2	B	23	GLY	CA-C-N	8.82	132.10	120.28
2	B	23	GLY	C-N-CA	8.82	132.10	120.28
2	B	83	GLU	CA-CB-CG	8.81	131.73	114.10
2	F	89	PHE	N-CA-C	8.79	122.31	110.35
2	R	89	PHE	N-CA-C	8.78	122.30	110.35
2	N	57	ALA	CA-C-N	8.72	132.31	120.54
2	N	57	ALA	C-N-CA	8.72	132.31	120.54
2	N	23	GLY	CA-C-N	8.64	133.44	120.31
2	N	23	GLY	C-N-CA	8.64	133.44	120.31
1	A	355	ASP	CA-CB-CG	-8.57	104.03	112.60
2	C	21	LYS	CA-C-N	8.51	131.69	120.28
2	C	21	LYS	C-N-CA	8.51	131.69	120.28
2	F	90	ARG	CA-C-N	8.46	136.92	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	90	ARG	C-N-CA	8.46	136.92	121.70
1	A	951	MET	CA-CB-CG	8.42	130.94	114.10
2	B	94	LYS	CA-C-N	8.36	131.48	120.28
2	B	94	LYS	C-N-CA	8.36	131.48	120.28
2	F	94	LYS	CA-C-N	8.34	131.46	120.28
2	F	94	LYS	C-N-CA	8.34	131.46	120.28
2	R	90	ARG	CA-C-N	8.34	136.72	121.70
2	R	90	ARG	C-N-CA	8.34	136.72	121.70
2	D	94	LYS	CA-C-N	8.34	131.46	120.28
2	D	94	LYS	C-N-CA	8.34	131.46	120.28
2	S	41	GLN	N-CA-C	8.30	122.26	110.23
2	B	21	LYS	N-CA-C	-8.23	101.73	112.68
2	R	42	ASN	O-C-N	-8.21	111.88	121.32
1	A	48	LEU	N-CA-C	8.19	122.40	110.28
2	N	94	LYS	CA-C-N	8.14	131.85	120.29
2	N	94	LYS	C-N-CA	8.14	131.85	120.29
1	A	951	MET	N-CA-CB	8.10	124.26	110.50
1	M	1048	ASP	CA-CB-CG	7.99	120.59	112.60
2	G	41	GLN	N-CA-C	7.91	121.69	110.23
2	D	90	ARG	CA-C-N	7.88	135.88	121.70
2	D	90	ARG	C-N-CA	7.88	135.88	121.70
1	A	1073	ASN	CA-CB-CG	7.87	120.47	112.60
1	A	35	ASP	CA-CB-CG	7.78	120.38	112.60
1	A	1032	ASN	CA-CB-CG	7.78	120.38	112.60
2	S	21	LYS	CA-C-N	7.69	131.21	120.29
2	S	21	LYS	C-N-CA	7.69	131.21	120.29
2	F	93	ASP	N-CA-C	-7.69	95.61	108.75
1	A	884	HIS	CA-CB-CG	7.67	121.47	113.80
1	A	1015	ASP	CA-CB-CG	7.63	120.23	112.60
1	M	35	ASP	CA-CB-CG	7.60	120.20	112.60
2	R	94	LYS	CA-C-N	7.58	130.44	120.28
2	R	94	LYS	C-N-CA	7.58	130.44	120.28
1	M	1032	ASN	CA-CB-CG	7.55	120.15	112.60
1	M	355	ASP	CA-CB-CG	-7.54	105.06	112.60
2	P	90	ARG	CA-C-N	7.51	135.22	121.70
2	P	90	ARG	C-N-CA	7.51	135.22	121.70
2	G	56	ASP	O-C-N	-7.50	114.05	122.23
2	P	21	LYS	N-CA-C	-7.48	104.00	113.43
2	B	22	ASP	CA-CB-CG	7.47	120.07	112.60
2	G	91	VAL	N-CA-C	-7.41	96.60	108.90
2	G	43	PRO	N-CA-C	7.39	127.70	112.47
2	D	93	ASP	N-CA-C	-7.36	96.16	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	21	LYS	CA-C-N	7.35	130.86	120.28
2	B	21	LYS	C-N-CA	7.35	130.86	120.28
1	A	430	HIS	CB-CG-CD2	-7.34	121.65	131.20
1	M	430	HIS	CB-CG-CD2	-7.32	121.68	131.20
1	A	968	ASP	CA-CB-CG	-7.32	105.28	112.60
2	G	21	LYS	CA-C-N	7.30	130.66	120.29
2	G	21	LYS	C-N-CA	7.30	130.66	120.29
2	P	94	LYS	CA-C-N	7.30	130.06	120.28
2	P	94	LYS	C-N-CA	7.30	130.06	120.28
2	N	21	LYS	N-CA-C	-7.29	103.48	112.88
2	C	108	VAL	CB-CA-C	-7.26	102.33	112.14
1	A	856	ASN	CA-CB-CG	7.22	119.82	112.60
2	S	91	VAL	N-CA-C	-7.20	96.94	108.90
2	R	93	ASP	N-CA-C	-7.17	95.57	108.48
2	D	21	LYS	N-CA-C	-7.12	104.58	113.55
2	D	83	GLU	CA-CB-CG	7.11	128.32	114.10
2	S	43	PRO	N-CA-C	7.11	127.11	112.47
2	R	43	PRO	N-CA-C	7.07	122.78	111.26
2	B	57	ALA	CA-C-N	7.03	132.37	121.19
2	B	57	ALA	C-N-CA	7.03	132.37	121.19
2	B	44	THR	N-CA-CB	7.01	119.99	110.38
2	D	21	LYS	CA-C-N	6.99	129.65	120.28
2	D	21	LYS	C-N-CA	6.99	129.65	120.28
1	M	906	LEU	CB-CA-C	6.99	119.81	111.22
2	O	93	ASP	N-CA-CB	-6.92	99.85	110.65
1	M	884	HIS	CA-CB-CG	6.92	120.72	113.80
1	A	319	ASP	CA-CB-CG	-6.92	105.68	112.60
2	P	83	GLU	CA-CB-CG	6.89	127.87	114.10
1	M	319	ASP	CA-CB-CG	-6.86	105.74	112.60
1	A	703	THR	N-CA-CB	6.85	120.16	110.36
1	M	703	THR	N-CA-CB	6.82	120.11	110.36
2	P	21	LYS	CA-C-N	6.77	129.36	120.28
2	P	21	LYS	C-N-CA	6.77	129.36	120.28
2	G	54	GLU	CA-CB-CG	6.77	127.64	114.10
1	M	65	PRO	CA-C-N	6.74	129.99	120.28
1	M	65	PRO	C-N-CA	6.74	129.99	120.28
1	M	1076	ARG	N-CA-C	6.74	118.42	111.14
2	S	64	ASP	CA-CB-CG	6.74	119.33	112.60
2	O	108	VAL	CB-CA-C	-6.72	103.06	112.14
2	N	40	GLY	CA-C-N	6.67	134.28	121.54
2	N	40	GLY	C-N-CA	6.67	134.28	121.54
2	F	42	ASN	O-C-N	-6.66	113.66	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	877	TRP	CB-CG-CD2	-6.60	117.56	126.80
2	S	83	GLU	CA-CB-CG	6.59	127.29	114.10
2	C	132	GLY	CA-C-N	6.57	129.08	120.28
2	C	132	GLY	C-N-CA	6.57	129.08	120.28
2	G	37	ARG	CB-CG-CD	6.54	126.34	111.30
2	G	35	VAL	N-CA-C	6.52	117.27	110.62
2	P	118	ASP	CA-CB-CG	-6.47	106.13	112.60
2	O	132	GLY	CA-C-N	6.42	128.89	120.28
2	O	132	GLY	C-N-CA	6.42	128.89	120.28
2	N	118	ASP	CA-CB-CG	-6.41	106.19	112.60
2	S	35	VAL	N-CA-C	6.39	117.18	110.72
2	N	44	THR	N-CA-CB	6.39	119.40	110.26
2	S	37	ARG	CB-CG-CD	6.36	125.93	111.30
1	M	820	ILE	N-CA-CB	6.36	117.99	110.55
1	A	1041	GLU	N-CA-C	6.33	117.84	111.07
1	A	1076	ARG	N-CA-C	6.32	117.84	111.07
2	G	57	ALA	O-C-N	-6.31	114.84	122.48
1	M	48	LEU	N-CA-C	6.31	120.35	110.32
2	D	118	ASP	CA-CB-CG	-6.30	106.30	112.60
2	B	92	PHE	CA-CB-CG	-6.29	107.51	113.80
1	A	877	TRP	CB-CG-CD2	-6.28	118.00	126.80
1	M	825	PHE	CB-CA-C	-6.28	100.36	110.79
2	E	21	LYS	CA-C-N	6.28	128.69	120.28
2	E	21	LYS	C-N-CA	6.28	128.69	120.28
2	Q	45	GLU	CA-CB-CG	-6.27	101.57	114.10
2	E	45	GLU	CA-CB-CG	-6.26	101.58	114.10
1	M	1074	ASP	CA-CB-CG	-6.25	106.35	112.60
2	O	95	ASP	CA-CB-CG	-6.25	106.36	112.60
2	R	42	ASN	CA-C-O	-6.23	111.62	120.16
2	G	79	THR	CA-C-N	6.21	128.61	120.28
2	G	79	THR	C-N-CA	6.21	128.61	120.28
1	M	354	HIS	CA-C-N	6.21	128.59	120.26
1	M	354	HIS	C-N-CA	6.21	128.59	120.26
2	N	92	PHE	CA-CB-CG	-6.21	107.59	113.80
1	M	856	ASN	CA-CB-CG	6.21	118.81	112.60
2	G	54	GLU	O-C-N	-6.19	114.53	122.20
2	G	55	VAL	N-CA-CB	6.19	121.44	111.23
2	D	90	ARG	O-C-N	-6.17	116.00	123.10
2	G	42	ASN	CA-CB-CG	6.14	118.74	112.60
2	E	45	GLU	CB-CG-CD	6.13	123.02	112.60
2	F	90	ARG	O-C-N	-6.06	115.27	123.15
2	B	118	ASP	CA-CB-CG	-6.03	106.57	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	123	GLU	CB-CG-CD	6.03	122.85	112.60
1	A	188	SER	N-CA-C	6.03	117.65	111.14
2	Q	21	LYS	CA-C-N	6.02	128.34	120.28
2	Q	21	LYS	C-N-CA	6.02	128.34	120.28
2	C	21	LYS	N-CA-C	-6.00	105.87	113.43
2	S	42	ASN	CA-CB-CG	6.00	118.60	112.60
1	A	825	PHE	CB-CA-C	-5.99	100.84	110.79
1	M	188	SER	N-CA-C	5.98	117.60	111.14
2	C	95	ASP	CA-CB-CG	-5.98	106.62	112.60
2	E	83	GLU	CA-C-N	5.97	128.21	120.44
2	E	83	GLU	C-N-CA	5.97	128.21	120.44
2	R	23	GLY	CA-C-N	5.95	128.25	120.28
2	R	23	GLY	C-N-CA	5.95	128.25	120.28
2	G	58	ASP	CA-C-O	5.95	126.31	119.35
2	G	83	GLU	CA-CB-CG	5.94	125.98	114.10
1	A	362	ASP	CA-CB-CG	5.93	118.53	112.60
1	M	877	TRP	CB-CG-CD1	5.93	135.80	126.90
1	M	953	ASN	CA-CB-CG	5.92	118.53	112.60
1	A	286	HIS	CA-CB-CG	5.88	119.68	113.80
2	F	42	ASN	CA-C-O	-5.88	112.10	120.16
2	G	56	ASP	N-CA-C	5.87	123.17	113.89
2	P	90	ARG	O-C-N	-5.86	116.36	123.10
2	G	36	MET	CG-SD-CE	-5.86	88.01	100.90
2	R	90	ARG	O-C-N	-5.86	115.53	123.15
2	F	43	PRO	N-CA-C	5.85	120.43	110.95
2	D	57	ALA	CA-C-N	5.84	132.69	121.54
2	D	57	ALA	C-N-CA	5.84	132.69	121.54
2	P	57	ALA	CA-C-N	5.84	132.69	121.54
2	P	57	ALA	C-N-CA	5.84	132.69	121.54
2	G	85	ILE	N-CA-C	5.82	117.08	109.58
1	A	134	ASP	CA-CB-CG	5.81	118.41	112.60
2	Q	83	GLU	CA-C-N	5.80	127.98	120.44
2	Q	83	GLU	C-N-CA	5.80	127.98	120.44
2	O	11	GLU	CB-CG-CD	5.80	122.46	112.60
1	M	286	HIS	CA-CB-CG	5.80	119.60	113.80
1	A	48	LEU	N-CA-CB	-5.79	101.45	109.97
2	F	57	ALA	CA-C-N	5.79	132.60	121.54
2	F	57	ALA	C-N-CA	5.79	132.60	121.54
2	R	57	ALA	CA-C-N	5.79	132.59	121.54
2	R	57	ALA	C-N-CA	5.79	132.59	121.54
1	A	951	MET	N-CA-C	5.79	127.20	111.00
1	A	354	HIS	CA-C-N	5.78	128.00	120.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	HIS	C-N-CA	5.78	128.00	120.26
1	M	362	ASP	CA-CB-CG	5.77	118.37	112.60
2	C	94	LYS	N-CA-C	-5.74	106.62	113.97
2	P	42	ASN	CB-CA-C	5.74	118.73	111.21
2	C	118	ASP	CA-CB-CG	-5.73	106.87	112.60
2	C	79	THR	CA-C-N	5.72	127.94	120.28
2	C	79	THR	C-N-CA	5.72	127.94	120.28
2	D	42	ASN	CB-CA-C	5.71	118.69	111.21
2	S	47	GLU	CA-C-N	5.71	127.93	120.28
2	S	47	GLU	C-N-CA	5.71	127.93	120.28
2	S	132	GLY	CA-C-N	5.71	128.40	120.29
2	S	132	GLY	C-N-CA	5.71	128.40	120.29
1	M	269	ALA	N-CA-C	5.70	118.27	111.71
2	O	79	THR	CA-C-N	5.70	127.92	120.28
2	O	79	THR	C-N-CA	5.70	127.92	120.28
1	A	269	ALA	N-CA-C	5.70	118.26	111.71
1	M	120	GLY	CA-C-N	5.70	127.91	120.28
1	M	120	GLY	C-N-CA	5.70	127.91	120.28
2	B	92	PHE	CB-CA-C	5.68	121.73	110.42
2	C	90	ARG	CA-C-N	5.68	132.20	121.97
2	C	90	ARG	C-N-CA	5.68	132.20	121.97
2	S	85	ILE	N-CA-C	5.68	116.91	109.58
1	M	134	ASP	CA-CB-CG	5.67	118.28	112.60
2	N	104	GLU	CB-CG-CD	-5.66	102.97	112.60
2	S	21	LYS	N-CA-C	-5.66	105.47	112.72
1	A	877	TRP	CB-CG-CD1	5.66	135.39	126.90
2	G	132	GLY	CA-C-N	5.64	128.30	120.29
2	G	132	GLY	C-N-CA	5.64	128.30	120.29
2	N	92	PHE	CB-CA-C	5.64	121.64	110.42
1	A	120	GLY	CA-C-N	5.63	127.82	120.28
1	A	120	GLY	C-N-CA	5.63	127.82	120.28
1	A	189	GLU	N-CA-C	-5.63	106.96	113.88
1	A	645	HIS	CA-CB-CG	-5.63	108.17	113.80
2	C	93	ASP	N-CA-C	-5.63	98.81	110.80
2	G	65	PHE	CA-C-N	5.63	125.73	119.32
2	G	65	PHE	C-N-CA	5.63	125.73	119.32
1	A	583	SER	N-CA-C	5.62	117.79	110.43
2	B	88	ALA	CB-CA-C	-5.61	104.47	111.43
1	A	804	HIS	CA-CB-CG	-5.61	108.19	113.80
2	O	118	ASP	CA-CB-CG	-5.60	107.00	112.60
1	A	908	LYS	CA-CB-CG	5.60	125.29	114.10
1	M	853	LEU	CB-CA-C	-5.59	102.10	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	122	ASP	CA-CB-CG	-5.58	107.02	112.60
1	M	189	GLU	N-CA-C	-5.58	107.02	113.88
2	Q	45	GLU	CB-CG-CD	5.58	122.08	112.60
2	S	36	MET	CA-C-N	5.56	128.00	120.38
2	S	36	MET	C-N-CA	5.56	128.00	120.38
1	M	45	GLY	N-CA-C	5.56	126.36	113.18
2	O	104	GLU	CB-CA-C	-5.55	102.17	110.88
2	S	42	ASN	N-CA-C	5.54	122.06	109.81
1	A	909	LEU	N-CA-C	-5.53	95.51	111.00
2	G	53	ASN	CA-C-N	5.53	132.47	122.02
2	G	53	ASN	C-N-CA	5.53	132.47	122.02
2	B	104	GLU	CB-CG-CD	-5.52	103.21	112.60
2	B	21	LYS	CB-CA-C	5.52	119.45	110.24
2	F	23	GLY	CA-C-N	5.51	127.66	120.28
2	F	23	GLY	C-N-CA	5.51	127.66	120.28
1	A	1074	ASP	CA-CB-CG	-5.50	107.10	112.60
2	R	43	PRO	CB-CA-C	-5.50	104.65	111.64
2	S	53	ASN	CA-CB-CG	5.50	118.10	112.60
1	A	820	ILE	N-CA-CB	5.50	116.98	110.55
1	M	583	SER	N-CA-C	5.49	117.63	110.43
1	A	47	ASP	CA-C-N	5.49	128.67	120.87
1	A	47	ASP	C-N-CA	5.49	128.67	120.87
2	P	122	ASP	CA-CB-CG	-5.49	107.11	112.60
2	G	42	ASN	N-CA-C	5.48	121.93	109.81
2	D	43	PRO	CA-C-O	-5.47	114.92	121.48
2	D	36	MET	CG-SD-CE	-5.46	88.89	100.90
1	M	185	GLY	CA-C-N	5.46	131.96	121.54
1	M	185	GLY	C-N-CA	5.46	131.96	121.54
2	P	127	GLU	CA-CB-CG	5.46	125.02	114.10
2	B	84	GLU	N-CA-C	5.45	117.03	111.14
2	G	21	LYS	N-CA-C	-5.45	105.75	112.72
2	S	118	ASP	CA-CB-CG	-5.43	107.17	112.60
1	A	45	GLY	N-CA-C	5.43	126.04	113.18
1	A	185	GLY	CA-C-N	5.43	131.90	121.54
1	A	185	GLY	C-N-CA	5.43	131.90	121.54
1	A	843	ILE	N-CA-CB	5.42	117.91	110.54
1	M	645	HIS	CA-CB-CG	-5.42	108.39	113.80
1	M	877	TRP	CA-CB-CG	5.41	123.89	113.60
2	R	122	ASP	CA-CB-CG	-5.41	107.19	112.60
1	M	779	ARG	CA-CB-CG	5.41	124.91	114.10
1	M	908	LYS	CA-CB-CG	5.40	124.89	114.10
2	O	91	VAL	CB-CA-C	5.39	120.14	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	127	GLU	CA-CB-CG	5.38	124.85	114.10
2	F	64	ASP	CA-CB-CG	5.35	117.95	112.60
2	E	114	GLU	N-CA-CB	5.34	118.58	109.87
2	R	127	GLU	CA-CB-CG	5.34	124.78	114.10
2	P	36	MET	CG-SD-CE	-5.33	89.16	100.90
2	E	92	PHE	CA-CB-CG	-5.33	108.47	113.80
2	F	85	ILE	N-CA-C	5.32	115.87	108.84
2	E	118	ASP	CA-CB-CG	-5.32	107.28	112.60
1	M	48	LEU	N-CA-CB	-5.32	101.75	110.41
2	S	20	ASP	CB-CA-C	5.30	117.80	109.84
1	A	81	HIS	CA-CB-CG	5.30	119.10	113.80
1	M	1041	GLU	N-CA-C	5.30	116.74	111.07
2	R	64	ASP	CA-CB-CG	5.29	117.89	112.60
2	R	90	ARG	N-CA-C	-5.29	101.31	109.52
1	M	909	LEU	N-CA-C	-5.29	96.19	111.00
1	M	448	SER	CA-C-N	5.29	127.36	120.28
1	M	448	SER	C-N-CA	5.29	127.36	120.28
1	A	448	SER	CA-C-N	5.28	127.36	120.28
1	A	448	SER	C-N-CA	5.28	127.36	120.28
2	F	122	ASP	CA-CB-CG	-5.27	107.33	112.60
2	Q	118	ASP	CA-CB-CG	-5.26	107.34	112.60
1	M	638	HIS	CA-CB-CG	5.25	119.05	113.80
2	P	43	PRO	CA-C-O	-5.24	115.19	121.48
2	Q	95	ASP	N-CA-C	-5.24	107.05	113.50
2	O	21	LYS	N-CA-C	-5.24	105.97	112.93
2	N	24	ASP	CA-CB-CG	5.23	117.83	112.60
2	D	64	ASP	CA-CB-CG	5.23	117.83	112.60
2	D	84	GLU	CA-C-N	5.22	127.49	120.50
2	D	84	GLU	C-N-CA	5.22	127.49	120.50
2	C	64	ASP	CA-C-N	5.21	126.61	120.09
2	C	64	ASP	C-N-CA	5.21	126.61	120.09
2	D	114	GLU	CA-C-N	5.21	131.50	121.54
2	D	114	GLU	C-N-CA	5.21	131.50	121.54
2	G	36	MET	CA-C-N	5.19	127.50	120.38
2	G	36	MET	C-N-CA	5.19	127.50	120.38
2	E	42	ASN	CA-C-N	5.19	126.33	119.84
2	E	42	ASN	C-N-CA	5.19	126.33	119.84
2	P	90	ARG	N-CA-C	-5.19	101.22	108.96
2	N	142	VAL	N-CA-CB	5.18	118.36	110.58
2	P	64	ASP	CA-CB-CG	5.18	117.78	112.60
1	M	1045	ARG	N-CA-C	5.18	116.93	111.28
1	A	148	LYS	N-CA-C	5.18	116.73	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	901	MET	CG-SD-CE	-5.17	89.52	100.90
2	R	85	ILE	N-CA-C	5.16	115.75	109.30
2	O	78	ASP	CA-C-N	5.16	127.61	120.29
2	O	78	ASP	C-N-CA	5.16	127.61	120.29
2	G	55	VAL	CB-CA-C	5.15	119.74	111.29
2	Q	42	ASN	CA-C-N	5.14	126.27	119.84
2	Q	42	ASN	C-N-CA	5.14	126.27	119.84
1	M	148	LYS	N-CA-C	5.14	116.69	111.14
2	O	64	ASP	CA-C-N	5.14	126.52	120.09
2	O	64	ASP	C-N-CA	5.14	126.52	120.09
2	S	92	PHE	CA-CB-CG	-5.14	108.66	113.80
1	A	853	LEU	CB-CA-C	-5.14	102.82	110.88
1	M	75	THR	CA-C-N	5.14	127.16	120.28
1	M	75	THR	C-N-CA	5.14	127.16	120.28
1	A	187	ALA	CA-C-N	5.13	127.42	120.44
1	A	187	ALA	C-N-CA	5.13	127.42	120.44
1	M	81	HIS	CA-CB-CG	5.13	118.93	113.80
1	A	121	GLU	CA-C-N	5.12	127.09	120.44
1	A	121	GLU	C-N-CA	5.12	127.09	120.44
2	N	122	ASP	CA-CB-CG	-5.12	107.48	112.60
1	A	638	HIS	CA-CB-CG	5.11	118.91	113.80
2	S	78	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	65	PRO	CA-C-N	5.10	129.24	120.72
1	A	65	PRO	C-N-CA	5.10	129.24	120.72
2	G	122	ASP	CA-CB-CG	-5.10	107.50	112.60
1	M	833	LYS	CB-CA-C	-5.10	102.88	110.88
1	A	1047	HIS	CA-C-N	5.09	127.06	120.44
1	A	1047	HIS	C-N-CA	5.09	127.06	120.44
1	M	786	LYS	CA-C-N	5.09	127.06	120.44
1	M	786	LYS	C-N-CA	5.09	127.06	120.44
2	S	38	SER	N-CA-C	5.08	119.57	113.17
2	E	94	LYS	N-CA-C	-5.08	107.47	113.97
2	C	78	ASP	CA-C-N	5.08	127.50	120.29
2	C	78	ASP	C-N-CA	5.08	127.50	120.29
1	M	121	GLU	CA-C-N	5.07	127.04	120.44
1	M	121	GLU	C-N-CA	5.07	127.04	120.44
2	N	83	GLU	CA-CB-CG	5.07	124.24	114.10
2	N	127	GLU	CB-CG-CD	5.07	121.22	112.60
1	M	265	LEU	N-CA-C	5.07	116.61	111.14
2	R	40	GLY	CA-C-N	5.07	131.22	121.54
2	R	40	GLY	C-N-CA	5.07	131.22	121.54
1	A	954	LEU	N-CA-CB	5.06	117.74	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	187	ALA	CA-C-N	5.06	127.32	120.44
1	M	187	ALA	C-N-CA	5.06	127.32	120.44
2	F	40	GLY	CA-C-N	5.05	131.19	121.54
2	F	40	GLY	C-N-CA	5.05	131.19	121.54
2	G	20	ASP	CB-CA-C	5.05	117.42	109.84
1	M	799	ARG	N-CA-C	5.05	116.47	111.07
2	D	90	ARG	N-CA-C	-5.05	101.44	108.96
1	A	997	ARG	CB-CG-CD	5.04	122.90	111.30
2	F	90	ARG	N-CA-C	-5.04	101.71	109.52
1	M	1011	GLU	CB-CG-CD	5.04	121.17	112.60
2	F	127	GLU	CA-CB-CG	5.04	124.17	114.10
2	G	118	ASP	CA-CB-CG	-5.04	107.56	112.60
2	E	112	LEU	N-CA-C	5.03	116.59	108.34
2	B	40	GLY	CA-C-N	5.01	131.11	121.54
2	B	40	GLY	C-N-CA	5.01	131.11	121.54
2	B	142	VAL	N-CA-CB	5.01	118.09	110.58
2	E	64	ASP	CA-C-N	5.00	126.34	120.09
2	E	64	ASP	C-N-CA	5.00	126.34	120.09

There are no chirality outliers.

All (140) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1076	ARG	Sidechain
1	A	1078	ARG	Sidechain
1	A	1079	TYR	Sidechain
1	A	152	ARG	Sidechain
1	A	191	ASN	Peptide
1	A	213	ARG	Sidechain
1	A	233	ARG	Sidechain
1	A	240	ARG	Sidechain
1	A	327	ARG	Sidechain
1	A	41	ARG	Sidechain
1	A	430	HIS	Sidechain
1	A	677	ARG	Sidechain
1	A	692	ARG	Sidechain
1	A	711	TYR	Sidechain
1	A	773	ARG	Sidechain
1	A	799	ARG	Sidechain
1	A	800	TYR	Sidechain
1	A	807	ARG	Sidechain
1	A	815	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	829	TYR	Sidechain
1	A	832	ARG	Sidechain
1	A	839	ARG	Sidechain
1	A	852	TYR	Sidechain
1	A	855	ARG	Sidechain
1	A	875	ARG	Sidechain
1	A	880	ARG	Sidechain
1	A	884	HIS	Sidechain
1	A	892	TYR	Sidechain
1	A	904	ARG	Sidechain
1	A	951	MET	Peptide
1	A	971	ARG	Sidechain
1	A	973	ARG	Sidechain
2	B	138	TYR	Sidechain
2	B	19	PHE	Peptide
2	B	74	ARG	Sidechain
2	B	82	GLU	Peptide
2	B	86	ARG	Sidechain
2	B	90	ARG	Peptide,Sidechain
2	B	99	TYR	Sidechain
2	C	19	PHE	Peptide
2	C	37	ARG	Sidechain
2	C	54	GLU	Peptide
2	C	74	ARG	Sidechain
2	C	86	ARG	Sidechain
2	C	90	ARG	Sidechain
2	C	92	PHE	Sidechain
2	D	74	ARG	Sidechain
2	D	86	ARG	Sidechain
2	D	90	ARG	Sidechain
2	D	99	TYR	Sidechain
2	E	126	ARG	Sidechain
2	E	42	ASN	Peptide
2	E	54	GLU	Peptide
2	E	74	ARG	Sidechain
2	E	86	ARG	Sidechain
2	E	90	ARG	Sidechain
2	E	92	PHE	Peptide,Sidechain
2	F	106	ARG	Sidechain
2	F	74	ARG	Sidechain
2	F	86	ARG	Sidechain
2	F	90	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	F	99	TYR	Sidechain
2	G	12	PHE	Sidechain
2	G	126	ARG	Sidechain
2	G	19	PHE	Sidechain
2	G	37	ARG	Sidechain
2	G	38	SER	Peptide
2	G	86	ARG	Sidechain
2	G	89	PHE	Sidechain
1	M	10	TYR	Sidechain
1	M	1045	ARG	Sidechain
1	M	1076	ARG	Sidechain
1	M	1078	ARG	Sidechain
1	M	1079	TYR	Sidechain
1	M	152	ARG	Sidechain
1	M	191	ASN	Peptide
1	M	213	ARG	Sidechain
1	M	233	ARG	Sidechain
1	M	240	ARG	Sidechain
1	M	327	ARG	Sidechain
1	M	41	ARG	Sidechain
1	M	430	HIS	Sidechain
1	M	677	ARG	Sidechain
1	M	692	ARG	Sidechain
1	M	711	TYR	Sidechain
1	M	773	ARG	Sidechain
1	M	799	ARG	Sidechain
1	M	800	TYR	Sidechain
1	M	815	ARG	Sidechain
1	M	817	ARG	Sidechain
1	M	829	TYR	Sidechain
1	M	832	ARG	Sidechain
1	M	839	ARG	Sidechain
1	M	852	TYR	Sidechain
1	M	855	ARG	Sidechain
1	M	875	ARG	Sidechain
1	M	880	ARG	Sidechain
1	M	892	TYR	Sidechain
1	M	973	ARG	Sidechain
2	N	138	TYR	Sidechain
2	N	19	PHE	Peptide
2	N	74	ARG	Sidechain
2	N	86	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	N	90	ARG	Peptide,Sidechain
2	N	91	VAL	Peptide
2	N	99	TYR	Sidechain
2	O	37	ARG	Sidechain
2	O	54	GLU	Peptide
2	O	74	ARG	Sidechain
2	O	86	ARG	Sidechain
2	O	90	ARG	Sidechain
2	O	92	PHE	Sidechain
2	P	74	ARG	Sidechain
2	P	86	ARG	Sidechain
2	P	90	ARG	Sidechain
2	P	92	PHE	Peptide
2	P	99	TYR	Sidechain
2	Q	126	ARG	Sidechain
2	Q	54	GLU	Peptide
2	Q	74	ARG	Sidechain
2	Q	86	ARG	Sidechain
2	Q	90	ARG	Sidechain
2	Q	91	VAL	Peptide
2	Q	92	PHE	Peptide
2	R	106	ARG	Sidechain
2	R	74	ARG	Sidechain
2	R	86	ARG	Sidechain
2	R	99	TYR	Sidechain
2	S	107	HIS	Sidechain
2	S	12	PHE	Sidechain
2	S	126	ARG	Sidechain
2	S	14	GLU	Peptide
2	S	19	PHE	Sidechain
2	S	37	ARG	Sidechain
2	S	38	SER	Peptide
2	S	86	ARG	Sidechain
2	S	89	PHE	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	8198	0	8280	67	72
1	M	8198	0	8280	64	56
2	B	1093	0	1027	12	371
2	C	1110	0	1046	18	0
2	D	1093	0	1027	2	0
2	E	1110	0	1046	12	0
2	F	1093	0	1027	4	0
2	G	1110	0	1046	55	0
2	N	1093	0	1027	9	387
2	O	1110	0	1046	17	0
2	P	1093	0	1027	3	0
2	Q	1110	0	1046	14	0
2	R	1093	0	1027	4	0
2	S	1110	0	1046	32	0
All	All	29614	0	28998	216	443

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 4.

All (216) 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:A:906:LEU:HD21	2:G:15:ALA:HB1	1.58	0.84
2:C:92:PHE:CE2	2:C:108:VAL:HG22	2.14	0.83
1:M:906:LEU:HD21	2:S:15:ALA:HB1	1.61	0.81
1:A:951:MET:HG3	2:G:59:GLY:H	1.46	0.81
1:A:906:LEU:CD2	2:G:15:ALA:HB1	2.17	0.74
1:M:899:ARG:HD3	2:S:37:ARG:HG2	1.74	0.69
1:A:899:ARG:HD3	2:G:37:ARG:HG2	1.74	0.68
1:M:902:ALA:HB3	2:S:37:ARG:CD	2.24	0.68
1:A:951:MET:N	2:G:58:ASP:H	1.92	0.67
2:G:54:GLU:HG3	2:G:56:ASP:H	1.59	0.67
1:M:872:LYS:HD3	2:R:44:THR:HA	1.78	0.66
2:O:92:PHE:CE2	2:O:108:VAL:HG22	2.32	0.65
1:A:951:MET:CA	2:G:58:ASP:H	2.11	0.64
2:S:89:PHE:CZ	2:S:108:VAL:HG21	2.34	0.63
1:A:902:ALA:HB3	2:G:37:ARG:CD	2.30	0.62
2:O:104:GLU:O	2:O:108:VAL:HG23	2.00	0.61
2:O:92:PHE:CZ	2:O:108:VAL:HG22	2.36	0.61
2:Q:109:MET:HE2	2:Q:109:MET:HA	1.83	0.60
1:A:814:ARG:HG2	1:A:814:ARG:HH11	1.67	0.60
1:A:906:LEU:HB3	2:G:38:SER:CB	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:37:ARG:HH22	2:S:45:GLU:CD	2.09	0.59
1:A:768:ARG:HA	2:B:112:LEU:HB3	1.83	0.59
1:M:906:LEU:HB3	2:S:38:SER:HB3	1.83	0.59
1:M:903:LYS:HA	2:S:38:SER:HA	1.85	0.59
2:C:104:GLU:O	2:C:108:VAL:HG23	2.03	0.58
1:M:906:LEU:HD22	2:S:38:SER:HB3	1.85	0.58
1:M:899:ARG:NE	2:S:37:ARG:HE	2.02	0.58
1:M:954:LEU:HD22	1:M:954:LEU:H	1.68	0.58
1:A:906:LEU:HD13	2:G:35:VAL:HG23	1.86	0.58
2:G:12:PHE:O	2:G:15:ALA:HB3	2.03	0.58
1:A:189:GLU:H	1:A:189:GLU:CD	2.12	0.57
1:A:951:MET:HB3	2:G:56:ASP:HA	1.86	0.57
2:C:49:GLN:HA	2:C:52:ILE:HG22	1.87	0.57
1:M:189:GLU:H	1:M:189:GLU:CD	2.12	0.57
2:O:49:GLN:HA	2:O:52:ILE:HG22	1.87	0.57
1:M:906:LEU:HB3	2:S:38:SER:CB	2.34	0.57
1:A:903:LYS:HA	2:G:38:SER:HA	1.87	0.56
1:M:824:LYS:HB3	1:M:824:LYS:HZ2	1.69	0.56
1:A:951:MET:HB3	2:G:56:ASP:CA	2.36	0.56
1:M:230:LYS:HA	1:M:430:HIS:CD2	2.41	0.56
2:B:21:LYS:HA	2:C:92:PHE:CE2	2.41	0.56
1:M:906:LEU:HD13	2:S:35:VAL:HG23	1.88	0.56
1:A:445:GLU:CD	1:A:445:GLU:H	2.14	0.56
2:E:109:MET:HE2	2:E:109:MET:HA	1.87	0.56
2:G:89:PHE:CZ	2:G:108:VAL:HG21	2.41	0.56
2:Q:49:GLN:HA	2:Q:52:ILE:HG22	1.88	0.56
1:A:230:LYS:HA	1:A:430:HIS:CD2	2.41	0.56
1:M:445:GLU:CD	1:M:445:GLU:H	2.13	0.56
2:E:49:GLN:HA	2:E:52:ILE:HG22	1.88	0.55
1:A:906:LEU:HB3	2:G:38:SER:HB3	1.88	0.55
1:M:906:LEU:CD2	2:S:15:ALA:HB1	2.34	0.55
2:N:21:LYS:HA	2:O:92:PHE:CE2	2.43	0.54
2:S:41:GLN:HG2	2:S:79:THR:HG22	1.89	0.54
1:M:776:LYS:HZ1	2:N:82:GLU:CD	2.15	0.54
2:C:32:LEU:HD22	2:C:52:ILE:HD13	1.90	0.54
1:A:842:THR:CG2	2:E:90:ARG:HE	2.21	0.53
2:F:84:GLU:CD	2:F:86:ARG:HH12	2.17	0.53
2:N:21:LYS:O	2:O:92:PHE:HA	2.09	0.53
1:A:899:ARG:NE	2:G:37:ARG:HE	2.06	0.53
2:O:32:LEU:HD22	2:O:52:ILE:HD13	1.90	0.53
2:S:12:PHE:O	2:S:15:ALA:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:90:ARG:HH22	2:C:109:MET:HE3	1.74	0.52
2:S:33:GLY:O	2:S:37:ARG:HG3	2.10	0.52
2:G:33:GLY:O	2:G:37:ARG:HG3	2.09	0.52
1:M:814:ARG:HG2	1:M:814:ARG:HH11	1.73	0.52
1:M:845:LEU:HD23	2:Q:109:MET:HE3	1.92	0.52
2:Q:83:GLU:CD	2:Q:148:LYS:HZ3	2.18	0.52
1:A:906:LEU:HD22	2:G:38:SER:HB3	1.91	0.52
1:M:824:LYS:HZ2	1:M:824:LYS:CB	2.23	0.52
2:E:32:LEU:HD22	2:E:52:ILE:HD13	1.93	0.51
2:O:41:GLN:HG2	2:O:79:THR:HG22	1.92	0.51
2:R:84:GLU:CD	2:R:86:ARG:HH12	2.19	0.51
1:A:903:LYS:HA	2:G:38:SER:CA	2.40	0.51
1:A:902:ALA:HB1	2:G:34:THR:HA	1.93	0.51
1:M:343:ARG:CZ	1:M:349:ALA:HB3	2.41	0.51
2:Q:32:LEU:HD22	2:Q:52:ILE:HD13	1.93	0.51
2:G:55:VAL:O	2:G:55:VAL:HG22	2.11	0.51
1:A:339:GLU:CD	1:A:393:LYS:HZ1	2.19	0.50
1:M:856:ASN:HD22	2:Q:127:GLU:CD	2.19	0.50
1:A:343:ARG:CZ	1:A:349:ALA:HB3	2.41	0.50
2:C:41:GLN:HG2	2:C:79:THR:HG22	1.93	0.50
1:M:899:ARG:CD	2:S:37:ARG:HG2	2.40	0.50
2:O:90:ARG:HH22	2:O:109:MET:HE3	1.76	0.50
1:M:903:LYS:HA	2:S:38:SER:CA	2.42	0.50
1:M:906:LEU:CD2	2:S:38:SER:HB3	2.42	0.50
1:A:958:TYR:CZ	1:M:958:TYR:HB2	2.47	0.50
1:A:902:ALA:CB	2:G:34:THR:HA	2.42	0.49
2:B:17:SER:O	2:C:112:LEU:HD21	2.12	0.49
2:B:94:LYS:NZ	2:B:94:LYS:HA	2.27	0.49
1:A:899:ARG:CD	2:G:37:ARG:HG2	2.40	0.49
2:C:83:GLU:CD	2:C:148:LYS:HZ3	2.20	0.49
2:G:51:MET:HE2	1:M:951:MET:SD	2.52	0.49
1:M:339:GLU:CD	1:M:393:LYS:HZ1	2.20	0.49
1:M:902:ALA:CB	2:S:34:THR:HA	2.43	0.49
1:M:872:LYS:HG3	2:R:42:ASN:O	2.13	0.49
1:M:37:VAL:HG12	1:M:51:CYS:HA	1.95	0.48
2:P:90:ARG:HA	2:P:91:VAL:HG12	1.95	0.48
1:M:899:ARG:CB	2:S:42:ASN:HA	2.43	0.48
1:A:37:VAL:HG12	1:A:51:CYS:HA	1.96	0.48
2:B:90:ARG:HB3	2:B:92:PHE:H	1.78	0.48
2:N:90:ARG:HB3	2:N:92:PHE:H	1.79	0.48
2:E:41:GLN:HG2	2:E:79:THR:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:47:GLU:CD	2:Q:75:LYS:HZ1	2.21	0.48
1:A:955:GLU:CD	2:G:55:VAL:HG21	2.39	0.47
1:M:902:ALA:HB1	2:S:34:THR:HA	1.96	0.47
1:A:814:ARG:HH12	2:C:14:GLU:CD	2.23	0.47
1:M:815:ARG:HH21	2:P:92:PHE:HA	1.78	0.47
2:S:19:PHE:CZ	2:S:31:GLU:HB3	2.49	0.47
1:A:872:LYS:HD2	1:A:872:LYS:HA	1.77	0.47
1:A:951:MET:HA	2:G:54:GLU:O	2.14	0.47
2:B:144:MET:O	2:B:148:LYS:HD2	2.14	0.47
1:A:903:LYS:HA	2:G:38:SER:CB	2.45	0.47
2:Q:41:GLN:HG2	2:Q:79:THR:HG22	1.96	0.46
2:C:109:MET:HE2	2:C:109:MET:HA	1.97	0.46
2:G:19:PHE:CZ	2:G:31:GLU:HB3	2.51	0.46
2:N:94:LYS:NZ	2:N:94:LYS:HA	2.29	0.46
1:A:899:ARG:CZ	2:G:43:PRO:HB2	2.46	0.46
1:A:951:MET:HB3	2:G:56:ASP:N	2.30	0.46
1:A:951:MET:HG2	2:G:56:ASP:C	2.41	0.46
1:A:877:TRP:NE1	1:A:880:ARG:HH21	2.14	0.46
1:M:902:ALA:HB3	2:S:37:ARG:HD3	1.98	0.46
1:A:854:VAL:HG21	2:E:37:ARG:CB	2.46	0.46
1:A:899:ARG:CB	2:G:42:ASN:HA	2.45	0.46
1:M:842:THR:CG2	2:Q:90:ARG:HE	2.28	0.46
2:D:42:ASN:HB2	2:D:82:GLU:HB3	1.99	0.45
1:A:900:MET:HG3	1:A:904:ARG:HH21	1.81	0.45
2:G:107:HIS:CE1	2:G:111:ASN:HD22	2.34	0.45
1:A:866:LYS:HZ2	1:A:869:ILE:HG13	1.81	0.45
2:G:51:MET:O	1:M:951:MET:HB3	2.17	0.45
2:N:22:ASP:HA	2:O:104:GLU:HG2	1.97	0.45
1:M:895:CYS:SG	2:S:44:THR:HG22	2.57	0.45
2:G:71:MET:HE1	2:G:74:ARG:HH22	1.82	0.45
1:M:880:ARG:HG3	1:M:880:ARG:HH11	1.82	0.45
1:M:849:LEU:HD21	2:Q:124:MET:HB2	1.99	0.45
2:Q:107:HIS:C	2:Q:107:HIS:CD2	2.94	0.45
2:B:17:SER:C	2:C:112:LEU:HD21	2.42	0.45
2:G:71:MET:HB3	1:M:951:MET:SD	2.57	0.45
1:A:880:ARG:HH12	2:F:148:LYS:C	2.24	0.45
2:C:92:PHE:CZ	2:C:108:VAL:HG22	2.51	0.44
1:A:952:ASN:H	2:G:59:GLY:N	2.15	0.44
2:C:92:PHE:O	2:C:100:ILE:HG22	2.17	0.44
2:D:90:ARG:HA	2:D:91:VAL:HG12	2.00	0.44
2:G:107:HIS:CD2	2:G:107:HIS:C	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:781:TRP:HE1	2:N:148:LYS:CB	2.30	0.44
1:M:854:VAL:HG21	2:Q:37:ARG:CB	2.47	0.44
1:A:899:ARG:HD3	2:G:37:ARG:CG	2.47	0.44
1:A:854:VAL:HG21	2:E:37:ARG:HB3	2.00	0.44
2:G:35:VAL:HG13	2:G:68:PHE:CE1	2.53	0.44
1:M:824:LYS:HD2	1:M:824:LYS:HA	1.75	0.44
1:M:854:VAL:HG21	2:Q:37:ARG:HB3	2.00	0.44
1:A:906:LEU:CG	2:G:15:ALA:HB1	2.47	0.44
1:M:888:LYS:HA	1:M:891:VAL:HG22	1.99	0.43
1:M:80:LEU:HG	1:M:691:ILE:HG23	2.01	0.43
1:A:824:LYS:HD2	1:A:824:LYS:HA	1.75	0.43
2:G:37:ARG:HH22	2:G:45:GLU:CD	2.26	0.43
2:N:32:LEU:HD13	2:N:63:ILE:CD1	2.49	0.43
2:N:94:LYS:HA	2:N:94:LYS:HZ3	1.84	0.43
1:A:849:LEU:HD23	1:A:853:LEU:HG	2.01	0.43
2:E:47:GLU:CD	2:E:75:LYS:HZ1	2.26	0.43
1:A:97:LYS:HZ1	1:A:114:GLU:CD	2.26	0.42
1:M:802:ARG:HH11	2:O:116:LEU:HD22	1.84	0.42
1:A:824:LYS:HZ2	1:A:824:LYS:HB3	1.84	0.42
1:M:896:CYS:HA	2:S:42:ASN:HB3	2.02	0.42
2:G:21:LYS:HA	2:G:21:LYS:HZ2	1.84	0.42
1:A:781:TRP:CD2	2:B:145:MET:O	2.73	0.42
1:A:904:ARG:HH22	2:G:127:GLU:CD	2.27	0.42
2:S:43:PRO:HB3	2:S:47:GLU:HG3	2.00	0.42
1:A:824:LYS:HB3	1:A:824:LYS:NZ	2.35	0.42
1:A:954:LEU:C	1:A:954:LEU:HD22	2.45	0.42
2:F:21:LYS:HA	2:G:107:HIS:CE1	2.55	0.42
2:S:88:ALA:HB3	2:S:142:VAL:HG11	2.02	0.42
1:A:776:LYS:HZ3	2:B:82:GLU:CD	2.28	0.42
1:A:845:LEU:HD23	2:E:109:MET:HE3	2.01	0.42
1:A:802:ARG:HH11	2:C:116:LEU:HD22	1.85	0.41
2:F:29:THR:HG22	2:F:63:ILE:HG23	2.02	0.41
1:M:379:LYS:NZ	1:M:574:GLU:OE1	2.46	0.41
1:M:1066:LYS:HZ2	1:M:1069:GLU:CD	2.27	0.41
2:C:100:ILE:HG23	2:C:138:TYR:CD2	2.55	0.41
2:O:77:LYS:NZ	2:O:78:ASP:OD1	2.48	0.41
2:E:123:GLU:HG3	2:E:126:ARG:HE	1.86	0.41
1:M:799:ARG:HH21	2:O:82:GLU:CD	2.29	0.41
2:S:43:PRO:HG3	2:S:82:GLU:HG3	2.03	0.41
1:A:954:LEU:CD1	2:G:54:GLU:O	2.68	0.41
1:M:700:SER:HB2	1:M:751:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:804:HIS:CD2	2:O:145:MET:HA	2.55	0.41
1:M:1068:LEU:HD13	1:M:1068:LEU:H	1.86	0.41
2:R:29:THR:HG22	2:R:63:ILE:HG23	2.02	0.41
2:G:107:HIS:HE1	2:G:111:ASN:HD22	1.67	0.41
2:B:32:LEU:HD13	2:B:63:ILE:CD1	2.51	0.41
1:M:804:HIS:CD2	2:O:124:MET:SD	3.14	0.41
1:A:393:LYS:HE3	1:A:397:ILE:HD11	2.03	0.41
1:M:899:ARG:HB3	2:S:42:ASN:HA	2.03	0.41
2:P:29:THR:HG22	2:P:63:ILE:HG23	2.03	0.41
2:S:21:LYS:HZ1	2:S:21:LYS:HA	1.85	0.41
1:A:895:CYS:SG	2:G:44:THR:HG22	2.61	0.41
1:A:906:LEU:CD1	2:G:35:VAL:HG23	2.51	0.41
2:C:106:ARG:HH22	2:C:122:ASP:CG	2.29	0.41
2:E:106:ARG:HH22	2:E:122:ASP:CG	2.29	0.41
2:G:71:MET:CE	2:G:74:ARG:HH22	2.34	0.41
1:M:903:LYS:HA	2:S:38:SER:CB	2.50	0.41
2:O:106:ARG:HH22	2:O:122:ASP:CG	2.28	0.41
2:B:94:LYS:HA	2:B:94:LYS:HZ3	1.86	0.41
2:B:105:LEU:HD21	2:B:141:PHE:CE2	2.56	0.41
2:G:88:ALA:HB3	2:G:142:VAL:HG11	2.03	0.41
1:A:797:ILE:HG21	2:C:90:ARG:HH21	1.85	0.40
1:M:97:LYS:HZ1	1:M:114:GLU:CD	2.29	0.40
1:A:700:SER:HB2	1:A:751:PHE:HB2	2.03	0.40
1:A:902:ALA:HB3	2:G:37:ARG:CB	2.51	0.40
1:M:850:ARG:HH22	2:Q:114:GLU:CD	2.29	0.40
1:M:899:ARG:HD3	2:S:37:ARG:CG	2.47	0.40
1:A:888:LYS:HA	1:A:891:VAL:HG22	2.03	0.40
2:E:83:GLU:CD	2:E:148:LYS:HZ3	2.29	0.40
2:G:54:GLU:HB2	1:M:954:LEU:HD11	2.04	0.40
1:A:951:MET:N	2:G:57:ALA:H	2.20	0.40
1:M:339:GLU:OE2	1:M:393:LYS:NZ	2.55	0.40
1:M:797:ILE:HG21	2:O:90:ARG:HH21	1.86	0.40

All (443) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:TYR:CA	2:N:94:LYS:N[5_555]	0.37	1.83
2:B:99:TYR:CD1	2:N:94:LYS:CG[5_555]	0.39	1.81
2:B:92:PHE:CB	2:N:97:ASN:O[5_555]	0.41	1.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:ASP:CG	1:M:712:ARG:CB[5_555]	0.48	1.72
2:B:91:VAL:O	2:N:99:TYR:CE2[5_555]	0.50	1.70
2:B:139:GLU:CB	2:N:90:ARG:CA[5_555]	0.50	1.70
1:A:718:LYS:CB	2:N:127:GLU:CB[5_555]	0.54	1.66
2:B:86:ARG:CA	2:N:86:ARG:O[5_555]	0.54	1.66
2:B:129:ASP:OD2	1:M:712:ARG:CA[5_555]	0.57	1.63
2:B:89:PHE:CZ	2:N:140:GLU:CA[5_555]	0.58	1.62
2:B:138:TYR:CD1	2:N:138:TYR:OH[5_555]	0.59	1.61
2:B:96:GLY:O	2:N:104:GLU:CD[5_555]	0.63	1.57
2:B:98:GLY:CA	2:N:93:ASP:N[5_555]	0.63	1.57
1:A:717:GLN:CB	2:N:128:ALA:CA[5_555]	0.64	1.56
2:B:96:GLY:O	2:N:104:GLU:OE2[5_555]	0.66	1.54
1:A:718:LYS:N	2:N:127:GLU:C[5_555]	0.68	1.52
1:A:712:ARG:CG	2:N:130:ILE:O[5_555]	0.70	1.50
1:A:718:LYS:CA	2:N:127:GLU:CA[5_555]	0.74	1.46
2:B:91:VAL:C	2:N:99:TYR:CE2[5_555]	0.76	1.44
2:B:143:GLN:CB	2:N:89:PHE:CE1[5_555]	0.76	1.44
2:B:100:ILE:CB	2:N:96:GLY:N[5_555]	0.77	1.43
1:A:717:GLN:C	2:N:127:GLU:C[5_555]	0.78	1.42
2:B:138:TYR:CE1	2:N:138:TYR:CZ[5_555]	0.79	1.41
2:B:129:ASP:CA	1:M:712:ARG:CG[5_555]	0.80	1.40
2:B:143:GLN:CB	2:N:89:PHE:CD1[5_555]	0.80	1.40
2:B:100:ILE:CB	2:N:96:GLY:CA[5_555]	0.81	1.39
2:B:137:ASN:CA	2:N:94:LYS:NZ[5_555]	0.82	1.38
2:B:89:PHE:CB	2:N:139:GLU:N[5_555]	0.83	1.37
2:B:100:ILE:CA	2:N:96:GLY:N[5_555]	0.83	1.37
2:B:138:TYR:CE1	2:N:138:TYR:OH[5_555]	0.86	1.34
2:B:94:LYS:CA	2:N:135:GLN:CD[5_555]	0.87	1.33
2:B:100:ILE:CA	2:N:95:ASP:C[5_555]	0.89	1.31
1:A:712:ARG:NE	2:N:130:ILE:CG2[5_555]	0.90	1.30
2:B:89:PHE:CB	2:N:138:TYR:C[5_555]	0.90	1.30
2:B:89:PHE:CA	2:N:139:GLU:N[5_555]	0.90	1.30
1:A:717:GLN:CG	2:N:128:ALA:CB[5_555]	0.92	1.28
2:B:94:LYS:C	2:N:135:GLN:CD[5_555]	0.92	1.28
2:B:128:ALA:N	1:M:712:ARG:NH2[5_555]	0.93	1.27
2:B:91:VAL:CG2	2:N:99:TYR:OH[5_555]	0.94	1.26
2:B:98:GLY:C	2:N:93:ASP:N[5_555]	0.95	1.25
2:B:129:ASP:CB	1:M:712:ARG:CG[5_555]	0.96	1.24
2:B:100:ILE:C	2:N:95:ASP:C[5_555]	0.97	1.23
2:B:92:PHE:CB	2:N:97:ASN:C[5_555]	1.00	1.20
2:B:129:ASP:OD2	1:M:712:ARG:N[5_555]	1.03	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:ILE:CG1	2:N:96:GLY:CA[5_555]	1.04	1.16
2:B:89:PHE:N	2:N:139:GLU:CA[5_555]	1.05	1.15
1:A:715:MET:N	2:N:129:ASP:OD2[5_555]	1.06	1.14
1:A:718:LYS:CA	2:N:127:GLU:CB[5_555]	1.07	1.13
2:B:126:ARG:O	1:M:717:GLN:NE2[5_555]	1.08	1.12
2:B:139:GLU:OE1	2:N:90:ARG:CD[5_555]	1.08	1.12
2:B:94:LYS:C	2:N:135:GLN:CG[5_555]	1.09	1.11
2:B:139:GLU:O	2:N:89:PHE:CB[5_555]	1.09	1.11
2:B:138:TYR:CE2	2:N:93:ASP:CB[5_555]	1.10	1.10
1:A:717:GLN:CA	2:N:128:ALA:CA[5_555]	1.11	1.09
1:A:717:GLN:C	2:N:128:ALA:N[5_555]	1.11	1.09
1:A:717:GLN:OE1	2:N:128:ALA:O[5_555]	1.11	1.09
2:B:135:GLN:OE1	2:N:95:ASP:CG[5_555]	1.11	1.09
2:B:94:LYS:O	2:N:135:GLN:CG[5_555]	1.12	1.08
2:B:127:GLU:OE1	1:M:717:GLN:CB[5_555]	1.12	1.08
2:B:89:PHE:CD2	2:N:140:GLU:N[5_555]	1.13	1.07
2:B:139:GLU:CB	2:N:90:ARG:N[5_555]	1.13	1.07
1:A:712:ARG:NH1	2:N:130:ILE:N[5_555]	1.14	1.06
1:A:717:GLN:CB	2:N:128:ALA:CB[5_555]	1.15	1.05
2:B:99:TYR:CE1	2:N:94:LYS:CG[5_555]	1.15	1.05
2:B:89:PHE:CE1	2:N:140:GLU:CA[5_555]	1.16	1.04
1:A:718:LYS:N	2:N:127:GLU:O[5_555]	1.17	1.03
2:B:96:GLY:C	2:N:104:GLU:OE1[5_555]	1.18	1.02
2:B:100:ILE:CG2	2:N:97:ASN:N[5_555]	1.18	1.02
2:B:143:GLN:CG	2:N:89:PHE:CD1[5_555]	1.18	1.02
2:B:92:PHE:CA	2:N:97:ASN:O[5_555]	1.19	1.01
2:B:127:GLU:OE1	1:M:717:GLN:CA[5_555]	1.19	1.01
2:B:88:ALA:C	2:N:139:GLU:OE2[5_555]	1.20	1.00
2:B:89:PHE:CG	2:N:140:GLU:N[5_555]	1.20	1.00
2:B:98:GLY:O	2:N:92:PHE:O[5_555]	1.20	1.00
2:B:99:TYR:CD1	2:N:94:LYS:CB[5_555]	1.21	0.99
2:B:135:GLN:NE2	2:N:95:ASP:OD1[5_555]	1.21	0.99
2:B:89:PHE:CA	2:N:139:GLU:CA[5_555]	1.22	0.98
2:B:98:GLY:C	2:N:93:ASP:CA[5_555]	1.22	0.98
2:B:101:SER:N	2:N:95:ASP:O[5_555]	1.22	0.98
2:B:129:ASP:CG	1:M:712:ARG:CA[5_555]	1.22	0.98
2:B:89:PHE:CE2	2:N:140:GLU:CB[5_555]	1.23	0.97
2:B:138:TYR:CE2	2:N:93:ASP:CG[5_555]	1.23	0.97
1:A:718:LYS:CB	2:N:127:GLU:CG[5_555]	1.24	0.96
2:B:86:ARG:O	2:N:87:GLU:CA[5_555]	1.24	0.96
2:B:139:GLU:CG	2:N:89:PHE:O[5_555]	1.24	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:LYS:N	2:N:135:GLN:OE1[5_555]	1.25	0.95
2:B:128:ALA:CA	1:M:712:ARG:NH2[5_555]	1.25	0.95
2:B:96:GLY:CA	2:N:104:GLU:OE1[5_555]	1.26	0.94
2:B:99:TYR:N	2:N:93:ASP:CA[5_555]	1.27	0.93
2:B:135:GLN:CD	2:N:95:ASP:OD1[5_555]	1.27	0.93
1:A:715:MET:CA	2:N:129:ASP:OD2[5_555]	1.28	0.92
1:A:717:GLN:CA	2:N:128:ALA:C[5_555]	1.28	0.92
2:B:99:TYR:CE1	2:N:94:LYS:CD[5_555]	1.28	0.92
2:B:127:GLU:CD	1:M:717:GLN:C[5_555]	1.29	0.91
1:A:717:GLN:C	2:N:127:GLU:O[5_555]	1.30	0.90
2:B:139:GLU:CA	2:N:90:ARG:N[5_555]	1.30	0.90
2:B:89:PHE:CE1	2:N:140:GLU:C[5_555]	1.31	0.89
2:B:129:ASP:OD1	1:M:712:ARG:CB[5_555]	1.32	0.88
2:B:137:ASN:CA	2:N:94:LYS:CE[5_555]	1.32	0.88
2:B:137:ASN:N	2:N:94:LYS:NZ[5_555]	1.32	0.88
2:B:89:PHE:O	2:N:139:GLU:CB[5_555]	1.33	0.87
2:B:139:GLU:CG	2:N:89:PHE:C[5_555]	1.33	0.87
2:B:92:PHE:O	2:N:99:TYR:CD2[5_555]	1.34	0.86
2:B:129:ASP:CB	1:M:712:ARG:CB[5_555]	1.34	0.86
2:B:88:ALA:O	2:N:139:GLU:OE2[5_555]	1.35	0.85
2:B:89:PHE:CE2	2:N:140:GLU:CA[5_555]	1.35	0.85
2:B:96:GLY:C	2:N:104:GLU:CD[5_555]	1.35	0.85
2:B:91:VAL:O	2:N:99:TYR:CZ[5_555]	1.36	0.84
2:B:99:TYR:CA	2:N:93:ASP:C[5_555]	1.36	0.84
2:B:100:ILE:C	2:N:95:ASP:O[5_555]	1.36	0.84
2:B:89:PHE:CD1	2:N:139:GLU:C[5_555]	1.37	0.83
2:B:93:ASP:O	2:N:99:TYR:CB[5_555]	1.37	0.83
2:B:98:GLY:CA	2:N:92:PHE:C[5_555]	1.37	0.83
2:B:128:ALA:C	1:M:712:ARG:CZ[5_555]	1.37	0.83
2:B:138:TYR:OH	2:N:138:TYR:CE2[5_555]	1.37	0.83
1:A:712:ARG:CZ	2:N:130:ILE:CG2[5_555]	1.38	0.82
2:B:88:ALA:CA	2:N:139:GLU:OE2[5_555]	1.38	0.82
2:B:88:ALA:CB	2:N:139:GLU:OE2[5_555]	1.39	0.81
2:B:89:PHE:CG	2:N:139:GLU:C[5_555]	1.39	0.81
2:B:92:PHE:O	2:N:99:TYR:CG[5_555]	1.39	0.81
2:B:139:GLU:CG	2:N:90:ARG:N[5_555]	1.39	0.81
2:B:98:GLY:C	2:N:92:PHE:C[5_555]	1.40	0.80
2:B:104:GLU:OE2	2:N:97:ASN:OD1[5_555]	1.40	0.80
2:B:135:GLN:OE1	2:N:95:ASP:OD1[5_555]	1.40	0.80
2:B:94:LYS:CA	2:N:135:GLN:OE1[5_555]	1.41	0.79
2:B:139:GLU:CB	2:N:90:ARG:C[5_555]	1.42	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:ARG:CG	2:N:130:ILE:C[5_555]	1.43	0.77
1:A:717:GLN:CD	2:N:128:ALA:O[5_555]	1.44	0.76
2:B:100:ILE:N	2:N:95:ASP:N[5_555]	1.44	0.76
2:B:100:ILE:CG2	2:N:96:GLY:C[5_555]	1.44	0.76
2:B:90:ARG:O	2:N:137:ASN:CG[5_555]	1.45	0.75
2:B:89:PHE:CD1	2:N:139:GLU:O[5_555]	1.46	0.74
2:B:138:TYR:CE2	2:N:93:ASP:OD2[5_555]	1.46	0.74
2:B:91:VAL:C	2:N:99:TYR:CZ[5_555]	1.47	0.73
2:B:95:ASP:N	2:N:135:GLN:CD[5_555]	1.48	0.72
2:B:89:PHE:CE2	2:N:140:GLU:N[5_555]	1.49	0.71
2:B:137:ASN:ND2	2:N:91:VAL:CA[5_555]	1.49	0.71
2:B:91:VAL:C	2:N:99:TYR:CD2[5_555]	1.50	0.70
2:B:94:LYS:CA	2:N:135:GLN:CG[5_555]	1.50	0.70
2:B:99:TYR:N	2:N:93:ASP:C[5_555]	1.50	0.70
2:B:89:PHE:CZ	2:N:140:GLU:CB[5_555]	1.51	0.69
2:B:93:ASP:CG	2:N:99:TYR:O[5_555]	1.51	0.69
2:B:137:ASN:CB	2:N:94:LYS:CE[5_555]	1.51	0.69
2:B:140:GLU:N	2:N:90:ARG:O[5_555]	1.52	0.68
2:B:100:ILE:C	2:N:95:ASP:CA[5_555]	1.53	0.67
2:B:127:GLU:CG	1:M:717:GLN:O[5_555]	1.53	0.67
2:B:143:GLN:NE2	2:N:89:PHE:CE2[5_555]	1.53	0.67
1:A:712:ARG:CZ	2:N:130:ILE:CB[5_555]	1.54	0.66
2:B:87:GLU:OE1	2:N:146:THR:OG1[5_555]	1.54	0.66
2:B:90:ARG:CB	2:N:98:GLY:O[5_555]	1.54	0.66
2:B:93:ASP:CB	2:N:99:TYR:O[5_555]	1.55	0.65
2:B:95:ASP:N	2:N:135:GLN:NE2[5_555]	1.55	0.65
2:B:138:TYR:CZ	2:N:138:TYR:CE2[5_555]	1.55	0.65
2:B:139:GLU:CG	2:N:90:ARG:CA[5_555]	1.55	0.65
2:B:139:GLU:OE1	2:N:90:ARG:NE[5_555]	1.55	0.65
1:A:712:ARG:CD	2:N:130:ILE:O[5_555]	1.56	0.64
2:B:89:PHE:CD1	2:N:140:GLU:N[5_555]	1.56	0.64
2:B:91:VAL:CA	2:N:99:TYR:CZ[5_555]	1.56	0.64
2:B:99:TYR:CG	2:N:94:LYS:CG[5_555]	1.56	0.64
2:B:137:ASN:OD1	2:N:91:VAL:N[5_555]	1.56	0.64
2:B:138:TYR:CD2	2:N:93:ASP:OD2[5_555]	1.56	0.64
1:A:717:GLN:O	2:N:127:GLU:C[5_555]	1.57	0.63
2:B:92:PHE:CG	2:N:97:ASN:O[5_555]	1.57	0.63
2:B:94:LYS:N	2:N:135:GLN:CD[5_555]	1.57	0.63
2:B:96:GLY:C	2:N:104:GLU:OE2[5_555]	1.57	0.63
2:B:99:TYR:C	2:N:94:LYS:N[5_555]	1.57	0.63
2:B:143:GLN:CA	2:N:89:PHE:CD1[5_555]	1.57	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:PHE:O	2:N:99:TYR:CB[5_555]	1.58	0.62
2:B:127:GLU:O	1:M:712:ARG:NH1[5_555]	1.58	0.62
2:B:129:ASP:OD2	1:M:712:ARG:CB[5_555]	1.58	0.62
2:B:139:GLU:O	2:N:89:PHE:CG[5_555]	1.58	0.62
2:B:93:ASP:O	2:N:99:TYR:C[5_555]	1.59	0.61
2:B:137:ASN:OD1	2:N:91:VAL:CA[5_555]	1.59	0.61
1:A:718:LYS:N	2:N:127:GLU:CA[5_555]	1.60	0.60
2:B:99:TYR:CB	2:N:94:LYS:N[5_555]	1.60	0.60
2:B:86:ARG:C	2:N:86:ARG:O[5_555]	1.61	0.59
2:B:101:SER:N	2:N:95:ASP:C[5_555]	1.61	0.59
1:A:718:LYS:CG	2:N:127:GLU:CG[5_555]	1.62	0.58
2:B:98:GLY:O	2:N:92:PHE:C[5_555]	1.62	0.58
2:B:100:ILE:CG2	2:N:96:GLY:CA[5_555]	1.62	0.58
2:B:100:ILE:CA	2:N:95:ASP:CA[5_555]	1.62	0.58
2:B:143:GLN:CG	2:N:89:PHE:CE1[5_555]	1.62	0.58
2:B:96:GLY:O	2:N:104:GLU:OE1[5_555]	1.63	0.57
2:B:127:GLU:CD	1:M:717:GLN:CA[5_555]	1.63	0.57
1:A:715:MET:O	2:N:129:ASP:CB[5_555]	1.64	0.56
2:B:90:ARG:O	2:N:137:ASN:CA[5_555]	1.64	0.56
2:B:90:ARG:CB	2:N:98:GLY:CA[5_555]	1.64	0.56
2:B:93:ASP:O	2:N:99:TYR:CA[5_555]	1.64	0.56
2:B:93:ASP:N	2:N:97:ASN:CB[5_555]	1.64	0.56
2:B:88:ALA:CB	2:N:139:GLU:CD[5_555]	1.65	0.55
1:A:712:ARG:CB	2:N:130:ILE:O[5_555]	1.66	0.54
2:B:137:ASN:CG	2:N:91:VAL:CA[5_555]	1.66	0.54
2:B:138:TYR:CE1	2:N:138:TYR:CE2[5_555]	1.66	0.54
2:B:138:TYR:CD2	2:N:93:ASP:CG[5_555]	1.66	0.54
1:A:717:GLN:CG	2:N:128:ALA:CA[5_555]	1.67	0.53
2:B:86:ARG:O	2:N:87:GLU:N[5_555]	1.67	0.53
2:B:94:LYS:CE	2:N:99:TYR:CD1[5_555]	1.67	0.53
2:B:127:GLU:CD	1:M:717:GLN:O[5_555]	1.67	0.53
2:B:128:ALA:C	1:M:712:ARG:NH2[5_555]	1.67	0.53
2:B:129:ASP:N	1:M:712:ARG:NE[5_555]	1.67	0.53
2:B:99:TYR:CG	2:N:94:LYS:CB[5_555]	1.68	0.52
2:B:100:ILE:O	2:N:94:LYS:O[5_555]	1.68	0.52
1:A:718:LYS:CA	2:N:127:GLU:C[5_555]	1.69	0.51
2:B:89:PHE:CB	2:N:138:TYR:O[5_555]	1.69	0.51
2:B:91:VAL:CA	2:N:99:TYR:CE1[5_555]	1.69	0.51
2:B:91:VAL:CB	2:N:99:TYR:OH[5_555]	1.69	0.51
2:B:92:PHE:N	2:N:99:TYR:CD2[5_555]	1.69	0.51
2:B:98:GLY:C	2:N:92:PHE:O[5_555]	1.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:ASN:N	2:N:94:LYS:CE[5_555]	1.69	0.51
2:B:90:ARG:CB	2:N:98:GLY:C[5_555]	1.70	0.50
2:B:100:ILE:CB	2:N:96:GLY:C[5_555]	1.70	0.50
2:B:127:GLU:C	1:M:712:ARG:NH2[5_555]	1.70	0.50
2:B:127:GLU:OE1	1:M:717:GLN:C[5_555]	1.70	0.50
1:A:717:GLN:CB	2:N:128:ALA:C[5_555]	1.71	0.49
2:B:128:ALA:CA	1:M:712:ARG:CZ[5_555]	1.71	0.49
2:B:129:ASP:CA	1:M:712:ARG:CD[5_555]	1.71	0.49
2:B:86:ARG:CA	2:N:86:ARG:C[5_555]	1.72	0.48
2:B:91:VAL:O	2:N:99:TYR:CD2[5_555]	1.72	0.48
2:B:128:ALA:C	1:M:712:ARG:NE[5_555]	1.72	0.48
2:B:129:ASP:N	1:M:712:ARG:CZ[5_555]	1.72	0.48
2:B:139:GLU:OE1	2:N:90:ARG:CG[5_555]	1.72	0.48
2:B:146:THR:OG1	2:N:87:GLU:CG[5_555]	1.72	0.48
1:A:715:MET:CB	2:N:129:ASP:OD1[5_555]	1.73	0.47
2:B:86:ARG:NE	2:N:146:THR:CB[5_555]	1.73	0.47
2:B:127:GLU:CD	1:M:717:GLN:CB[5_555]	1.73	0.47
2:B:136:VAL:N	2:N:94:LYS:O[5_555]	1.73	0.47
1:A:717:GLN:CA	2:N:129:ASP:N[5_555]	1.74	0.46
2:B:86:ARG:NE	2:N:146:THR:OG1[5_555]	1.74	0.46
2:B:86:ARG:CB	2:N:86:ARG:O[5_555]	1.74	0.46
2:B:90:ARG:O	2:N:137:ASN:CB[5_555]	1.74	0.46
2:B:99:TYR:N	2:N:94:LYS:N[5_555]	1.74	0.46
2:B:138:TYR:CG	2:N:138:TYR:OH[5_555]	1.74	0.46
1:A:717:GLN:O	2:N:128:ALA:N[5_555]	1.75	0.45
2:B:84:GLU:OE2	2:N:147:ALA:CB[5_555]	1.75	0.45
2:B:89:PHE:C	2:N:139:GLU:N[5_555]	1.75	0.45
2:B:91:VAL:N	2:N:98:GLY:O[5_555]	1.75	0.45
2:B:100:ILE:CB	2:N:95:ASP:C[5_555]	1.75	0.45
2:B:98:GLY:N	2:N:93:ASP:N[5_555]	1.76	0.44
2:B:89:PHE:CB	2:N:139:GLU:CA[5_555]	1.77	0.43
2:B:94:LYS:C	2:N:135:GLN:OE1[5_555]	1.77	0.43
2:B:127:GLU:CB	1:M:717:GLN:O[5_555]	1.77	0.43
2:B:129:ASP:CG	1:M:712:ARG:CG[5_555]	1.77	0.43
2:B:143:GLN:CG	2:N:89:PHE:CG[5_555]	1.77	0.43
1:A:717:GLN:CA	2:N:128:ALA:N[5_555]	1.78	0.42
2:B:90:ARG:CA	2:N:98:GLY:O[5_555]	1.78	0.42
2:B:93:ASP:OD2	2:N:99:TYR:O[5_555]	1.78	0.42
2:B:99:TYR:CD1	2:N:94:LYS:CD[5_555]	1.78	0.42
2:B:127:GLU:O	1:M:712:ARG:CZ[5_555]	1.78	0.42
2:B:92:PHE:N	2:N:99:TYR:CE2[5_555]	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:ILE:CD1	2:N:96:GLY:CA[5_555]	1.79	0.41
2:B:100:ILE:N	2:N:96:GLY:N[5_555]	1.79	0.41
1:A:718:LYS:N	2:N:128:ALA:N[5_555]	1.80	0.40
2:B:89:PHE:CZ	2:N:140:GLU:N[5_555]	1.80	0.40
2:B:89:PHE:C	2:N:139:GLU:CB[5_555]	1.80	0.40
2:B:93:ASP:C	2:N:135:GLN:OE1[5_555]	1.80	0.40
2:B:98:GLY:C	2:N:93:ASP:C[5_555]	1.80	0.40
2:B:99:TYR:CA	2:N:94:LYS:CA[5_555]	1.80	0.40
1:A:715:MET:CB	2:N:129:ASP:CG[5_555]	1.81	0.39
2:B:86:ARG:NH2	2:N:146:THR:OG1[5_555]	1.81	0.39
2:B:90:ARG:C	2:N:98:GLY:O[5_555]	1.81	0.39
2:B:89:PHE:CE1	2:N:140:GLU:O[5_555]	1.82	0.38
2:B:98:GLY:O	2:N:93:ASP:O[5_555]	1.82	0.38
2:B:100:ILE:N	2:N:94:LYS:C[5_555]	1.82	0.38
2:B:89:PHE:N	2:N:139:GLU:CB[5_555]	1.83	0.37
2:B:89:PHE:CE1	2:N:140:GLU:N[5_555]	1.83	0.37
2:B:93:ASP:C	2:N:99:TYR:CB[5_555]	1.83	0.37
2:B:98:GLY:O	2:N:93:ASP:C[5_555]	1.83	0.37
2:B:99:TYR:O	2:N:93:ASP:OD1[5_555]	1.83	0.37
2:B:100:ILE:CG2	2:N:96:GLY:N[5_555]	1.83	0.37
2:B:127:GLU:CD	1:M:717:GLN:CG[5_555]	1.83	0.37
2:B:91:VAL:CB	2:N:137:ASN:ND2[5_555]	1.84	0.36
2:B:127:GLU:CG	1:M:717:GLN:CD[5_555]	1.84	0.36
2:B:135:GLN:OE1	2:N:95:ASP:CB[5_555]	1.84	0.36
2:B:139:GLU:OE1	2:N:90:ARG:CZ[5_555]	1.84	0.36
2:B:89:PHE:CA	2:N:138:TYR:C[5_555]	1.85	0.35
2:B:143:GLN:NE2	2:N:89:PHE:CD2[5_555]	1.85	0.35
2:B:86:ARG:O	2:N:87:GLU:C[5_555]	1.86	0.34
2:B:91:VAL:CG2	2:N:99:TYR:CZ[5_555]	1.86	0.34
2:B:94:LYS:C	2:N:135:GLN:NE2[5_555]	1.86	0.34
2:B:135:GLN:OE1	2:N:95:ASP:OD2[5_555]	1.86	0.34
1:A:712:ARG:NH1	2:N:130:ILE:CA[5_555]	1.87	0.33
1:A:712:ARG:NH2	2:N:130:ILE:CB[5_555]	1.87	0.33
2:B:86:ARG:N	2:N:86:ARG:O[5_555]	1.87	0.33
2:B:137:ASN:C	2:N:94:LYS:NZ[5_555]	1.87	0.33
1:A:718:LYS:C	2:N:127:GLU:CA[5_555]	1.88	0.32
2:B:101:SER:N	2:N:95:ASP:CA[5_555]	1.88	0.32
2:B:127:GLU:CG	1:M:717:GLN:C[5_555]	1.88	0.32
1:A:712:ARG:NH1	2:N:129:ASP:C[5_555]	1.89	0.31
2:B:89:PHE:CD1	2:N:140:GLU:C[5_555]	1.89	0.31
2:B:92:PHE:C	2:N:99:TYR:CD2[5_555]	1.89	0.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:TYR:N	2:N:93:ASP:N[5_555]	1.90	0.30
2:B:138:TYR:CZ	2:N:138:TYR:CZ[5_555]	1.90	0.30
2:B:88:ALA:C	2:N:139:GLU:CD[5_555]	1.91	0.29
2:B:90:ARG:O	2:N:137:ASN:OD1[5_555]	1.91	0.29
1:A:712:ARG:NH2	2:N:130:ILE:CG2[5_555]	1.92	0.28
1:A:715:MET:C	2:N:129:ASP:OD2[5_555]	1.92	0.28
1:A:717:GLN:C	2:N:128:ALA:CA[5_555]	1.92	0.28
2:B:89:PHE:CZ	2:N:140:GLU:C[5_555]	1.92	0.28
2:B:89:PHE:CG	2:N:139:GLU:N[5_555]	1.92	0.28
2:B:94:LYS:CB	2:N:135:GLN:CG[5_555]	1.92	0.28
2:B:100:ILE:CG1	2:N:96:GLY:N[5_555]	1.92	0.28
2:B:138:TYR:CD1	2:N:138:TYR:CZ[5_555]	1.92	0.28
1:A:716:LYS:O	2:N:127:GLU:O[5_555]	1.93	0.27
2:B:90:ARG:CG	2:N:98:GLY:CA[5_555]	1.93	0.27
2:B:98:GLY:O	2:N:93:ASP:N[5_555]	1.93	0.27
2:B:126:ARG:C	1:M:717:GLN:NE2[5_555]	1.93	0.27
2:B:127:GLU:CG	1:M:717:GLN:CA[5_555]	1.93	0.27
1:A:718:LYS:CG	2:N:127:GLU:CB[5_555]	1.94	0.26
2:B:91:VAL:CB	2:N:99:TYR:CZ[5_555]	1.94	0.26
2:B:94:LYS:CA	2:N:135:GLN:NE2[5_555]	1.94	0.26
2:B:136:VAL:C	2:N:94:LYS:NZ[5_555]	1.94	0.26
2:B:138:TYR:CZ	2:N:138:TYR:OH[5_555]	1.94	0.26
1:A:715:MET:CA	2:N:129:ASP:CG[5_555]	1.95	0.25
1:A:717:GLN:N	2:N:129:ASP:N[5_555]	1.95	0.25
2:B:137:ASN:ND2	2:N:91:VAL:C[5_555]	1.95	0.25
2:B:138:TYR:CD2	2:N:93:ASP:CB[5_555]	1.95	0.25
2:B:139:GLU:OE1	2:N:90:ARG:NH1[5_555]	1.95	0.25
2:B:86:ARG:CZ	2:N:146:THR:OG1[5_555]	1.96	0.24
2:B:89:PHE:CD1	2:N:140:GLU:CA[5_555]	1.96	0.24
2:B:96:GLY:O	2:N:104:GLU:CG[5_555]	1.96	0.24
2:B:139:GLU:C	2:N:90:ARG:O[5_555]	1.96	0.24
2:B:143:GLN:CB	2:N:89:PHE:CZ[5_555]	1.96	0.24
2:B:143:GLN:CD	2:N:89:PHE:CZ[5_555]	1.96	0.24
2:B:89:PHE:CG	2:N:139:GLU:CA[5_555]	1.97	0.23
2:B:91:VAL:CG1	2:N:137:ASN:ND2[5_555]	1.97	0.23
2:B:94:LYS:CA	2:N:135:GLN:CB[5_555]	1.97	0.23
2:B:99:TYR:C	2:N:95:ASP:N[5_555]	1.97	0.23
2:B:99:TYR:CB	2:N:94:LYS:CB[5_555]	1.97	0.23
2:B:99:TYR:CB	2:N:94:LYS:CA[5_555]	1.97	0.23
2:B:129:ASP:OD2	1:M:712:ARG:C[5_555]	1.97	0.23
2:B:135:GLN:OE1	2:N:95:ASP:N[5_555]	1.97	0.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:ASN:OD1	2:N:90:ARG:O[5_555]	1.97	0.23
2:B:139:GLU:CB	2:N:90:ARG:CB[5_555]	1.97	0.23
2:B:92:PHE:CA	2:N:97:ASN:C[5_555]	1.98	0.22
2:B:95:ASP:O	2:N:101:SER:OG[5_555]	1.98	0.22
2:B:135:GLN:CD	2:N:95:ASP:CG[5_555]	1.98	0.22
2:B:139:GLU:CD	2:N:89:PHE:C[5_555]	1.98	0.22
2:B:100:ILE:CA	2:N:95:ASP:N[5_555]	1.99	0.21
2:B:129:ASP:C	1:M:712:ARG:CG[5_555]	1.99	0.21
2:B:139:GLU:O	2:N:89:PHE:CD2[5_555]	1.99	0.21
2:B:139:GLU:CA	2:N:90:ARG:CA[5_555]	1.99	0.21
2:B:89:PHE:CE1	2:N:139:GLU:O[5_555]	2.00	0.20
2:B:90:ARG:NH1	2:N:139:GLU:OE1[5_555]	2.00	0.20
2:B:94:LYS:N	2:N:135:GLN:NE2[5_555]	2.00	0.20
2:B:98:GLY:O	2:N:93:ASP:CA[5_555]	2.00	0.20
2:B:128:ALA:N	1:M:712:ARG:CZ[5_555]	2.00	0.20
2:B:143:GLN:CB	2:N:89:PHE:CG[5_555]	2.00	0.20
1:A:717:GLN:OE1	2:N:128:ALA:C[5_555]	2.01	0.19
1:A:717:GLN:CB	2:N:128:ALA:N[5_555]	2.01	0.19
2:B:139:GLU:CD	2:N:90:ARG:N[5_555]	2.01	0.19
2:B:139:GLU:CD	2:N:90:ARG:CG[5_555]	2.01	0.19
1:A:715:MET:CB	2:N:129:ASP:OD2[5_555]	2.02	0.18
1:A:717:GLN:CA	2:N:127:GLU:O[5_555]	2.02	0.18
2:B:92:PHE:CA	2:N:99:TYR:CD2[5_555]	2.02	0.18
2:B:100:ILE:CG2	2:N:93:ASP:OD1[5_555]	2.02	0.18
2:B:127:GLU:OE2	1:M:717:GLN:C[5_555]	2.02	0.18
2:B:128:ALA:O	1:M:712:ARG:NE[5_555]	2.02	0.18
2:B:137:ASN:OD1	2:N:90:ARG:C[5_555]	2.02	0.18
2:B:138:TYR:OH	2:N:138:TYR:CD2[5_555]	2.02	0.18
2:B:89:PHE:CD2	2:N:137:ASN:OD1[5_555]	2.03	0.17
2:B:94:LYS:CB	2:N:135:GLN:CD[5_555]	2.03	0.17
2:B:127:GLU:OE2	1:M:717:GLN:O[5_555]	2.03	0.17
2:B:129:ASP:CB	1:M:712:ARG:CA[5_555]	2.03	0.17
2:B:135:GLN:OE1	2:N:95:ASP:CA[5_555]	2.03	0.17
2:B:100:ILE:C	2:N:96:GLY:N[5_555]	2.04	0.16
2:B:129:ASP:N	1:M:712:ARG:CG[5_555]	2.04	0.16
2:B:137:ASN:ND2	2:N:91:VAL:O[5_555]	2.04	0.16
2:B:89:PHE:CA	2:N:139:GLU:CB[5_555]	2.05	0.15
2:B:95:ASP:N	2:N:135:GLN:OE1[5_555]	2.05	0.15
2:B:129:ASP:N	1:M:712:ARG:NH1[5_555]	2.05	0.15
2:B:139:GLU:CD	2:N:89:PHE:O[5_555]	2.05	0.15
2:B:95:ASP:OD2	2:N:135:GLN:NE2[5_555]	2.06	0.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:ASP:O	2:N:101:SER:CB[5_555]	2.06	0.14
2:B:98:GLY:CA	2:N:93:ASP:CA[5_555]	2.06	0.14
2:B:127:GLU:OE1	1:M:717:GLN:N[5_555]	2.06	0.14
2:B:129:ASP:CA	1:M:712:ARG:NE[5_555]	2.06	0.14
2:B:139:GLU:CA	2:N:90:ARG:C[5_555]	2.06	0.14
1:A:718:LYS:C	2:N:127:GLU:CB[5_555]	2.07	0.13
2:B:88:ALA:CA	2:N:139:GLU:CD[5_555]	2.07	0.13
2:B:92:PHE:N	2:N:97:ASN:O[5_555]	2.07	0.13
2:B:99:TYR:C	2:N:93:ASP:C[5_555]	2.07	0.13
2:B:127:GLU:C	1:M:712:ARG:CZ[5_555]	2.07	0.13
2:B:136:VAL:O	2:N:94:LYS:NZ[5_555]	2.07	0.13
2:B:138:TYR:CE1	2:N:138:TYR:CE1[5_555]	2.07	0.13
2:B:87:GLU:OE1	2:N:146:THR:CG2[5_555]	2.08	0.12
2:B:89:PHE:CD2	2:N:140:GLU:CA[5_555]	2.08	0.12
2:B:92:PHE:CB	2:N:98:GLY:N[5_555]	2.08	0.12
2:B:100:ILE:CA	2:N:95:ASP:O[5_555]	2.08	0.12
1:A:718:LYS:CB	2:N:127:GLU:CA[5_555]	2.09	0.11
2:B:94:LYS:O	2:N:135:GLN:CD[5_555]	2.09	0.11
2:B:104:GLU:CD	2:N:97:ASN:OD1[5_555]	2.09	0.11
2:B:129:ASP:OD1	1:M:712:ARG:CG[5_555]	2.09	0.11
2:B:143:GLN:N	2:N:89:PHE:CD1[5_555]	2.09	0.11
1:A:712:ARG:NE	2:N:130:ILE:CB[5_555]	2.10	0.10
1:A:715:MET:O	2:N:129:ASP:OD2[5_555]	2.10	0.10
1:A:717:GLN:NE2	2:N:125:ILE:O[5_555]	2.10	0.10
2:B:89:PHE:N	2:N:139:GLU:N[5_555]	2.10	0.10
2:B:89:PHE:C	2:N:139:GLU:CA[5_555]	2.10	0.10
2:B:91:VAL:CA	2:N:99:TYR:CE2[5_555]	2.10	0.10
2:B:94:LYS:NZ	2:N:99:TYR:CD1[5_555]	2.10	0.10
2:B:128:ALA:CA	1:M:712:ARG:NH1[5_555]	2.10	0.10
2:B:139:GLU:CB	2:N:90:ARG:O[5_555]	2.10	0.10
2:B:93:ASP:O	2:N:100:ILE:N[5_555]	2.11	0.09
2:B:96:GLY:N	2:N:104:GLU:OE1[5_555]	2.11	0.09
2:B:128:ALA:N	1:M:717:GLN:OE1[5_555]	2.11	0.09
1:A:712:ARG:NH1	2:N:130:ILE:CB[5_555]	2.12	0.08
1:A:712:ARG:O	2:N:129:ASP:OD1[5_555]	2.12	0.08
1:A:718:LYS:CG	2:N:127:GLU:CD[5_555]	2.12	0.08
1:A:718:LYS:CA	2:N:127:GLU:N[5_555]	2.12	0.08
2:B:86:ARG:CB	2:N:86:ARG:C[5_555]	2.12	0.08
2:B:88:ALA:O	2:N:139:GLU:CD[5_555]	2.12	0.08
2:B:100:ILE:O	2:N:95:ASP:C[5_555]	2.12	0.08
2:B:139:GLU:CA	2:N:90:ARG:O[5_555]	2.12	0.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:PHE:CD1	2:N:141:PHE:N[5_555]	2.13	0.07
2:B:128:ALA:O	1:M:712:ARG:NH2[5_555]	2.13	0.07
2:B:129:ASP:CB	1:M:712:ARG:C[5_555]	2.13	0.07
2:B:139:GLU:CD	2:N:90:ARG:NH1[5_555]	2.13	0.07
2:B:89:PHE:CB	2:N:138:TYR:CA[5_555]	2.15	0.05
2:B:129:ASP:CB	1:M:712:ARG:CD[5_555]	2.15	0.05
2:B:143:GLN:CD	2:N:89:PHE:CE2[5_555]	2.15	0.05
2:B:143:GLN:CD	2:N:89:PHE:CE1[5_555]	2.15	0.05
1:A:715:MET:C	2:N:129:ASP:CB[5_555]	2.16	0.04
2:B:92:PHE:CB	2:N:97:ASN:CA[5_555]	2.16	0.04
2:B:129:ASP:N	1:M:712:ARG:CD[5_555]	2.16	0.04
2:B:138:TYR:CZ	2:N:93:ASP:OD2[5_555]	2.16	0.04
1:A:715:MET:C	2:N:129:ASP:CG[5_555]	2.17	0.03
1:A:717:GLN:CD	2:N:128:ALA:C[5_555]	2.17	0.03
1:A:717:GLN:CA	2:N:127:GLU:C[5_555]	2.17	0.03
2:B:99:TYR:CZ	2:N:94:LYS:CG[5_555]	2.17	0.03
2:B:139:GLU:OE2	2:N:89:PHE:C[5_555]	2.17	0.03
1:A:714:LEU:C	2:N:129:ASP:OD2[5_555]	2.18	0.02
1:A:717:GLN:N	2:N:127:GLU:O[5_555]	2.18	0.02
1:A:718:LYS:N	2:N:127:GLU:CB[5_555]	2.18	0.02
2:B:86:ARG:O	2:N:86:ARG:C[5_555]	2.18	0.02
2:B:94:LYS:CB	2:N:135:GLN:CB[5_555]	2.18	0.02
2:B:139:GLU:CB	2:N:89:PHE:C[5_555]	2.18	0.02
2:B:139:GLU:CD	2:N:90:ARG:CD[5_555]	2.18	0.02
1:A:715:MET:O	2:N:129:ASP:CG[5_555]	2.19	0.01
1:A:717:GLN:C	2:N:127:GLU:CA[5_555]	2.19	0.01
2:B:89:PHE:CE1	2:N:139:GLU:C[5_555]	2.19	0.01
2:B:138:TYR:CZ	2:N:93:ASP:CB[5_555]	2.19	0.01
2:B:139:GLU:C	2:N:89:PHE:CB[5_555]	2.19	0.01
2:B:139:GLU:OE2	2:N:90:ARG:N[5_555]	2.19	0.01

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	986/1080 (91%)	939 (95%)	39 (4%)	8 (1%)	16	54
1	M	986/1080 (91%)	942 (96%)	37 (4%)	7 (1%)	18	56
2	B	137/148 (93%)	123 (90%)	7 (5%)	7 (5%)	1	15
2	C	139/148 (94%)	129 (93%)	8 (6%)	2 (1%)	9	40
2	D	137/148 (93%)	124 (90%)	11 (8%)	2 (2%)	8	40
2	E	139/148 (94%)	129 (93%)	8 (6%)	2 (1%)	9	40
2	F	137/148 (93%)	124 (90%)	7 (5%)	6 (4%)	2	17
2	G	139/148 (94%)	128 (92%)	5 (4%)	6 (4%)	2	17
2	N	137/148 (93%)	123 (90%)	8 (6%)	6 (4%)	2	17
2	O	139/148 (94%)	128 (92%)	10 (7%)	1 (1%)	18	56
2	P	137/148 (93%)	127 (93%)	8 (6%)	2 (2%)	8	40
2	Q	139/148 (94%)	128 (92%)	8 (6%)	3 (2%)	5	29
2	R	137/148 (93%)	123 (90%)	9 (7%)	5 (4%)	2	20
2	S	139/148 (94%)	129 (93%)	4 (3%)	6 (4%)	2	17
All	All	3628/3936 (92%)	3396 (94%)	169 (5%)	63 (2%)	9	36

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	SER
2	B	41	GLN
2	B	91	VAL
2	B	93	ASP
2	B	115	LYS
2	C	91	VAL
2	C	93	ASP
2	D	91	VAL
2	D	115	LYS
2	F	41	GLN
2	G	76	MET
2	G	92	PHE
1	M	186	SER
2	N	41	GLN
2	N	91	VAL
2	N	93	ASP
2	O	91	VAL
2	R	41	GLN
2	S	92	PHE

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Mol	Chain	Res	Type
2	S	115	LYS
1	A	46	LYS
2	E	92	PHE
2	G	115	LYS
1	M	46	LYS
1	M	71	GLU
2	N	115	LYS
2	P	91	VAL
2	P	115	LYS
2	Q	92	PHE
1	A	71	GLU
1	A	439	TYR
2	B	92	PHE
2	F	44	THR
2	F	58	ASP
2	G	43	PRO
2	R	58	ASP
2	S	43	PRO
2	S	44	THR
1	A	45	GLY
1	A	294	PRO
2	F	42	ASN
1	M	294	PRO
2	Q	115	LYS
2	B	42	ASN
2	F	91	VAL
2	G	42	ASN
1	M	45	GLY
1	M	439	TYR
2	N	92	PHE
2	R	42	ASN
2	S	42	ASN
1	A	633	LYS
2	N	42	ASN
2	F	40	GLY
2	R	40	GLY
2	R	91	VAL
2	B	40	GLY
2	G	40	GLY
1	M	117	PRO
2	S	40	GLY
2	E	42	ASN

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Mol	Chain	Res	Type
2	Q	42	ASN
1	A	117	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	886/961 (92%)	789 (89%)	97 (11%)	6	21
1	M	886/961 (92%)	800 (90%)	86 (10%)	8	24
2	B	118/126 (94%)	106 (90%)	12 (10%)	7	23
2	C	120/126 (95%)	105 (88%)	15 (12%)	4	16
2	D	118/126 (94%)	104 (88%)	14 (12%)	5	18
2	E	120/126 (95%)	109 (91%)	11 (9%)	8	27
2	F	118/126 (94%)	107 (91%)	11 (9%)	8	26
2	G	120/126 (95%)	104 (87%)	16 (13%)	4	14
2	N	118/126 (94%)	106 (90%)	12 (10%)	7	23
2	O	120/126 (95%)	105 (88%)	15 (12%)	4	16
2	P	118/126 (94%)	104 (88%)	14 (12%)	5	18
2	Q	120/126 (95%)	108 (90%)	12 (10%)	7	24
2	R	118/126 (94%)	105 (89%)	13 (11%)	6	20
2	S	120/126 (95%)	103 (86%)	17 (14%)	3	13
All	All	3200/3434 (93%)	2855 (89%)	345 (11%)	8	21

All (345) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	6	LEU
1	A	19	GLU
1	A	30	ASP
1	A	46	LYS

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Mol	Chain	Res	Type
1	A	56	THR
1	A	67	ILE
1	A	121	GLU
1	A	134	ASP
1	A	138	HIS
1	A	170	THR
1	A	188	SER
1	A	189	GLU
1	A	194	GLU
1	A	212	THR
1	A	214	ASN
1	A	230	LYS
1	A	255	GLU
1	A	339	GLU
1	A	389	LYS
1	A	445	GLU
1	A	476	GLU
1	A	488	ASP
1	A	510	ASP
1	A	521	ASP
1	A	562	GLU
1	A	575	GLU
1	A	578	LYS
1	A	655	THR
1	A	663	LYS
1	A	668	LYS
1	A	703	THR
1	A	713	VAL
1	A	718	LYS
1	A	719	ASP
1	A	729	LYS
1	A	771	CYS
1	A	808	CYS
1	A	824	LYS
1	A	828	MET
1	A	846	GLN
1	A	862	LEU
1	A	872	LYS
1	A	887	LEU
1	A	897	TYR
1	A	903	LYS
1	A	906	LEU

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Mol	Chain	Res	Type
1	A	954	LEU
1	A	963	GLU
1	A	964	LYS
1	A	965	LEU
1	A	966	ARG
1	A	970	GLU
1	A	971	ARG
1	A	972	LEU
1	A	980	LYS
1	A	985	ARG
1	A	986	VAL
1	A	987	LEU
1	A	989	LEU
1	A	995	LYS
1	A	996	LEU
1	A	997	ARG
1	A	1000	LEU
1	A	1007	LYS
1	A	1008	LYS
1	A	1010	ILE
1	A	1015	ASP
1	A	1016	LYS
1	A	1018	LYS
1	A	1024	LEU
1	A	1027	GLU
1	A	1028	LEU
1	A	1029	LYS
1	A	1032	ASN
1	A	1033	THR
1	A	1034	LEU
1	A	1035	LEU
1	A	1039	LYS
1	A	1041	GLU
1	A	1042	LEU
1	A	1045	ARG
1	A	1051	LYS
1	A	1055	GLU
1	A	1056	THR
1	A	1060	LYS
1	A	1061	LEU
1	A	1064	GLU
1	A	1065	THR

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Mol	Chain	Res	Type
1	A	1068	LEU
1	A	1070	LEU
1	A	1072	LEU
1	A	1073	ASN
1	A	1076	ARG
1	A	1077	LEU
1	A	1078	ARG
1	A	1080	GLN
2	B	11	GLU
2	B	18	LEU
2	B	22	ASP
2	B	34	THR
2	B	53	ASN
2	B	85	ILE
2	B	86	ARG
2	B	87	GLU
2	B	94	LYS
2	B	120	GLU
2	B	127	GLU
2	B	131	ASP
2	C	14	GLU
2	C	17	SER
2	C	24	ASP
2	C	30	LYS
2	C	34	THR
2	C	44	THR
2	C	48	LEU
2	C	54	GLU
2	C	77	LYS
2	C	85	ILE
2	C	87	GLU
2	C	107	HIS
2	C	127	GLU
2	C	140	GLU
2	C	148	LYS
2	D	11	GLU
2	D	39	LEU
2	D	82	GLU
2	D	85	ILE
2	D	86	ARG
2	D	87	GLU
2	D	91	VAL

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Mol	Chain	Res	Type
2	D	94	LYS
2	D	104	GLU
2	D	111	ASN
2	D	124	MET
2	D	127	GLU
2	D	131	ASP
2	D	139	GLU
2	E	13	LYS
2	E	17	SER
2	E	30	LYS
2	E	48	LEU
2	E	54	GLU
2	E	77	LYS
2	E	83	GLU
2	E	86	ARG
2	E	87	GLU
2	E	140	GLU
2	E	148	LYS
2	F	11	GLU
2	F	24	ASP
2	F	53	ASN
2	F	86	ARG
2	F	87	GLU
2	F	90	ARG
2	F	91	VAL
2	F	111	ASN
2	F	118	ASP
2	F	127	GLU
2	F	131	ASP
2	G	11	GLU
2	G	18	LEU
2	G	21	LYS
2	G	29	THR
2	G	30	LYS
2	G	48	LEU
2	G	54	GLU
2	G	60	ASN
2	G	69	LEU
2	G	74	ARG
2	G	77	LYS
2	G	86	ARG
2	G	87	GLU

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Mol	Chain	Res	Type
2	G	123	GLU
2	G	130	ILE
2	G	140	GLU
1	M	5	GLU
1	M	19	GLU
1	M	30	ASP
1	M	46	LYS
1	M	56	THR
1	M	67	ILE
1	M	75	THR
1	M	121	GLU
1	M	134	ASP
1	M	138	HIS
1	M	170	THR
1	M	188	SER
1	M	189	GLU
1	M	194	GLU
1	M	212	THR
1	M	214	ASN
1	M	230	LYS
1	M	255	GLU
1	M	339	GLU
1	M	389	LYS
1	M	424	HIS
1	M	445	GLU
1	M	476	GLU
1	M	488	ASP
1	M	510	ASP
1	M	521	ASP
1	M	562	GLU
1	M	575	GLU
1	M	578	LYS
1	M	655	THR
1	M	663	LYS
1	M	668	LYS
1	M	703	THR
1	M	718	LYS
1	M	729	LYS
1	M	766	LYS
1	M	824	LYS
1	M	828	MET
1	M	872	LYS

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Mol	Chain	Res	Type
1	M	887	LEU
1	M	897	TYR
1	M	906	LEU
1	M	954	LEU
1	M	964	LYS
1	M	965	LEU
1	M	966	ARG
1	M	967	SER
1	M	971	ARG
1	M	972	LEU
1	M	980	LYS
1	M	985	ARG
1	M	987	LEU
1	M	989	LEU
1	M	995	LYS
1	M	996	LEU
1	M	997	ARG
1	M	999	GLU
1	M	1000	LEU
1	M	1007	LYS
1	M	1008	LYS
1	M	1016	LYS
1	M	1018	LYS
1	M	1021	THR
1	M	1024	LEU
1	M	1027	GLU
1	M	1028	LEU
1	M	1029	LYS
1	M	1032	ASN
1	M	1034	LEU
1	M	1035	LEU
1	M	1039	LYS
1	M	1042	LEU
1	M	1045	ARG
1	M	1051	LYS
1	M	1060	LYS
1	M	1061	LEU
1	M	1066	LYS
1	M	1067	GLN
1	M	1068	LEU
1	M	1070	LEU
1	M	1072	LEU

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Mol	Chain	Res	Type
1	M	1073	ASN
1	M	1076	ARG
1	M	1077	LEU
1	M	1078	ARG
1	M	1080	GLN
2	N	11	GLU
2	N	18	LEU
2	N	21	LYS
2	N	24	ASP
2	N	34	THR
2	N	53	ASN
2	N	83	GLU
2	N	87	GLU
2	N	94	LYS
2	N	127	GLU
2	N	131	ASP
2	N	148	LYS
2	O	14	GLU
2	O	17	SER
2	O	24	ASP
2	O	30	LYS
2	O	34	THR
2	O	44	THR
2	O	47	GLU
2	O	48	LEU
2	O	54	GLU
2	O	77	LYS
2	O	85	ILE
2	O	87	GLU
2	O	107	HIS
2	O	140	GLU
2	O	148	LYS
2	P	11	GLU
2	P	39	LEU
2	P	45	GLU
2	P	82	GLU
2	P	85	ILE
2	P	86	ARG
2	P	87	GLU
2	P	91	VAL
2	P	104	GLU
2	P	111	ASN

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Mol	Chain	Res	Type
2	P	124	MET
2	P	127	GLU
2	P	131	ASP
2	P	139	GLU
2	Q	13	LYS
2	Q	17	SER
2	Q	30	LYS
2	Q	48	LEU
2	Q	54	GLU
2	Q	77	LYS
2	Q	83	GLU
2	Q	84	GLU
2	Q	86	ARG
2	Q	87	GLU
2	Q	140	GLU
2	Q	148	LYS
2	R	11	GLU
2	R	24	ASP
2	R	47	GLU
2	R	53	ASN
2	R	86	ARG
2	R	87	GLU
2	R	90	ARG
2	R	91	VAL
2	R	111	ASN
2	R	118	ASP
2	R	127	GLU
2	R	131	ASP
2	R	139	GLU
2	S	11	GLU
2	S	13	LYS
2	S	17	SER
2	S	18	LEU
2	S	21	LYS
2	S	30	LYS
2	S	42	ASN
2	S	47	GLU
2	S	48	LEU
2	S	50	ASP
2	S	52	ILE
2	S	56	ASP
2	S	86	ARG

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Mol	Chain	Res	Type
2	S	87	GLU
2	S	123	GLU
2	S	130	ILE
2	S	140	GLU

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

Mol	Chain	Res	Type
1	A	81	HIS
1	A	214	ASN
1	A	322	GLN
1	A	334	HIS
1	A	395	HIS
1	A	430	HIS
1	A	464	GLN
1	A	493	GLN
1	A	497	ASN
1	A	525	GLN
1	A	652	ASN
1	A	873	HIS
2	B	107	HIS
2	B	111	ASN
2	B	135	GLN
2	D	107	HIS
2	E	107	HIS
2	F	107	HIS
2	F	111	ASN
2	G	107	HIS
1	M	81	HIS
1	M	322	GLN
1	M	334	HIS
1	M	395	HIS
1	M	430	HIS
1	M	464	GLN
1	M	493	GLN
1	M	497	ASN
1	M	525	GLN
1	M	652	ASN
1	M	804	HIS
1	M	805	GLN
1	M	1067	GLN
1	M	1080	GLN

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Mol	Chain	Res	Type
2	N	111	ASN
2	N	135	GLN
2	P	107	HIS
2	Q	107	HIS
2	R	107	HIS
2	R	111	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.

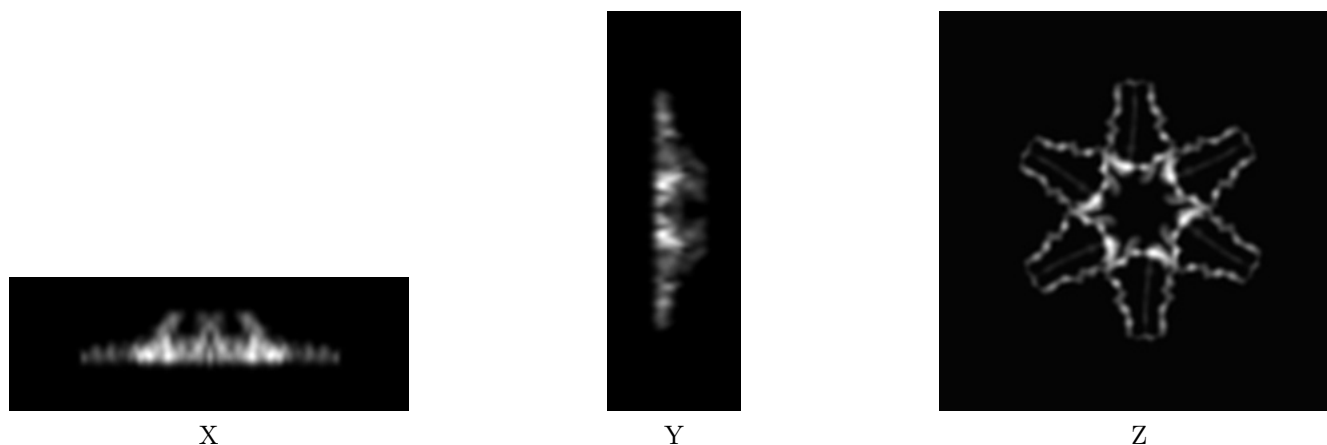
5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Tomogram visualisation [i](#)

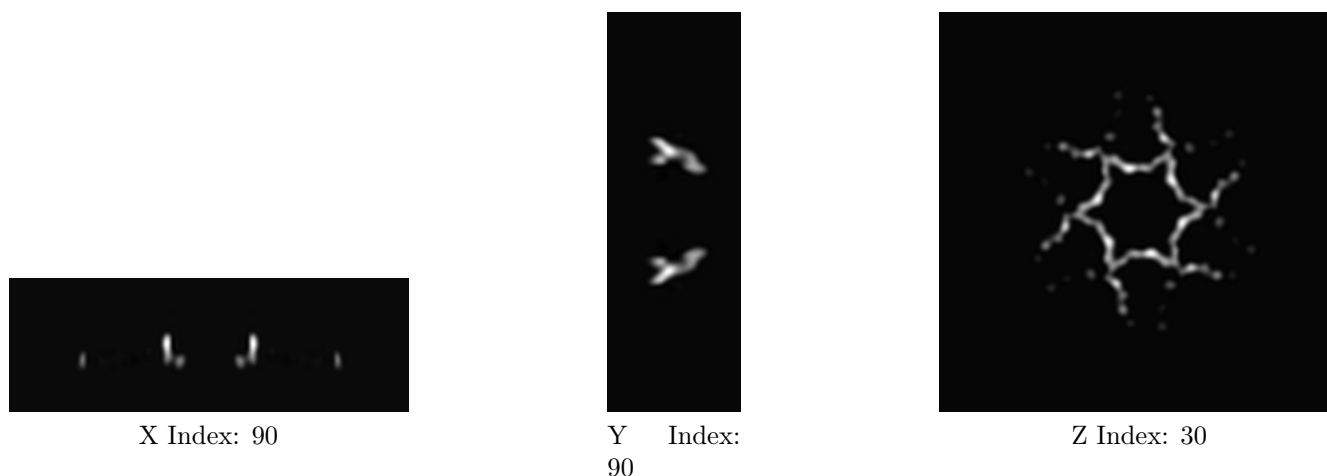
This section contains visualisations of the EMDB entry EMD-1201. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



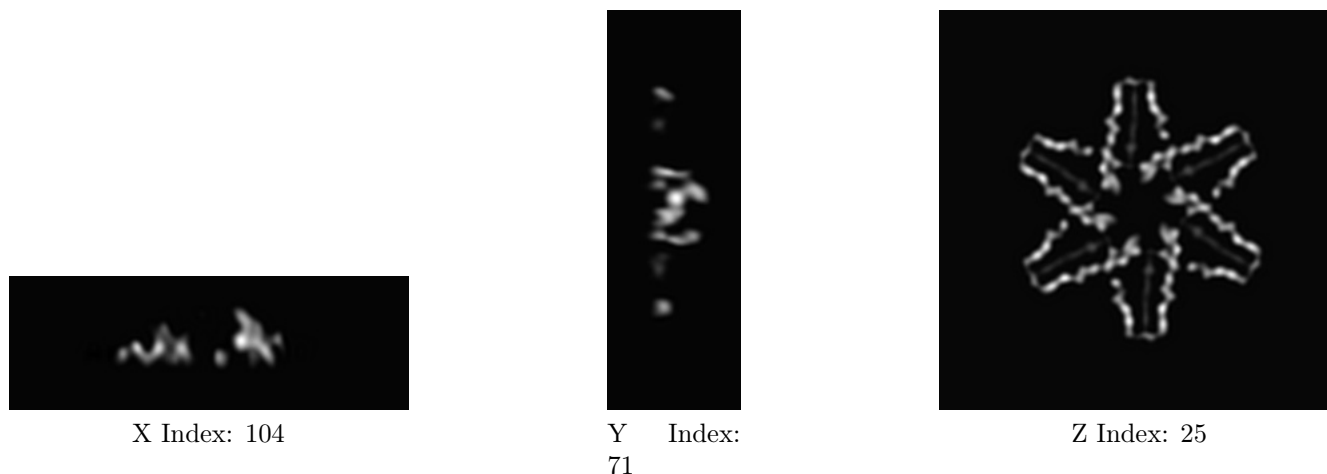
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)



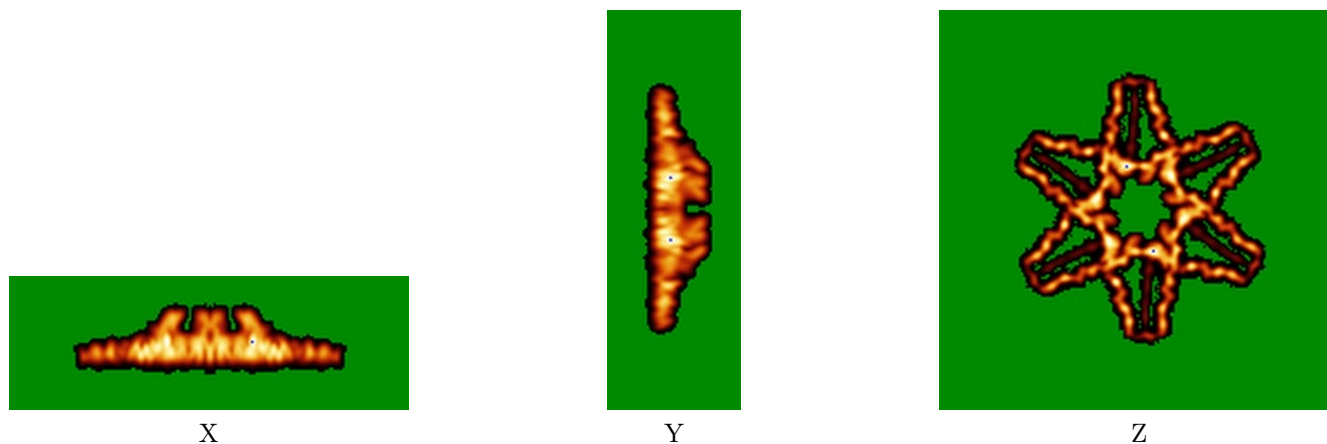
The images above show central slices of the tomogram in three orthogonal directions.

6.3 Largest variance slices [i](#)



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

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



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

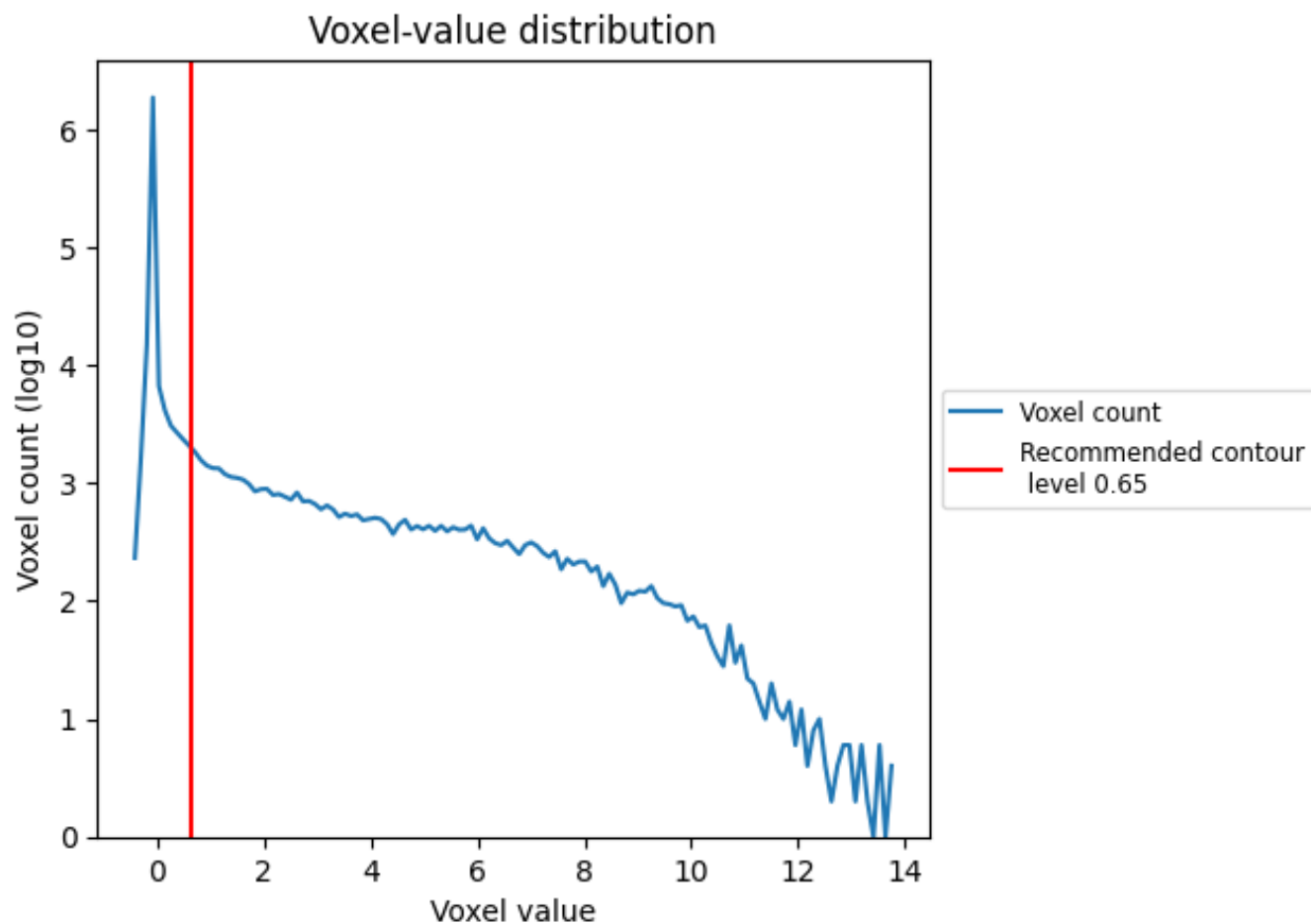
6.5 Mask visualisation [i](#)

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

7 Tomogram analysis [i](#)

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

7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

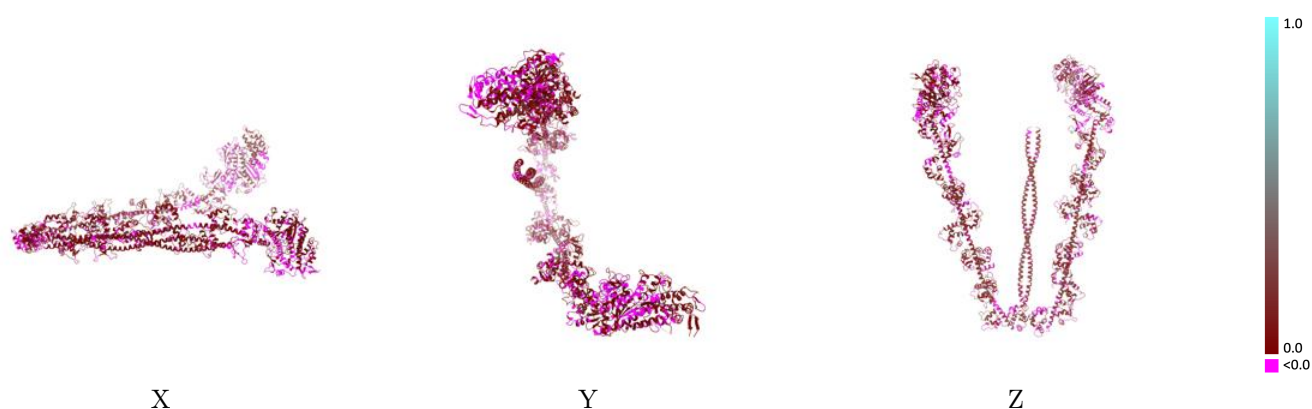
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1201 and PDB model 2DFS. Per-residue inclusion information can be found in section 3 on page 5.

8.1 Map-model overlay [i](#)

This section was not generated.

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

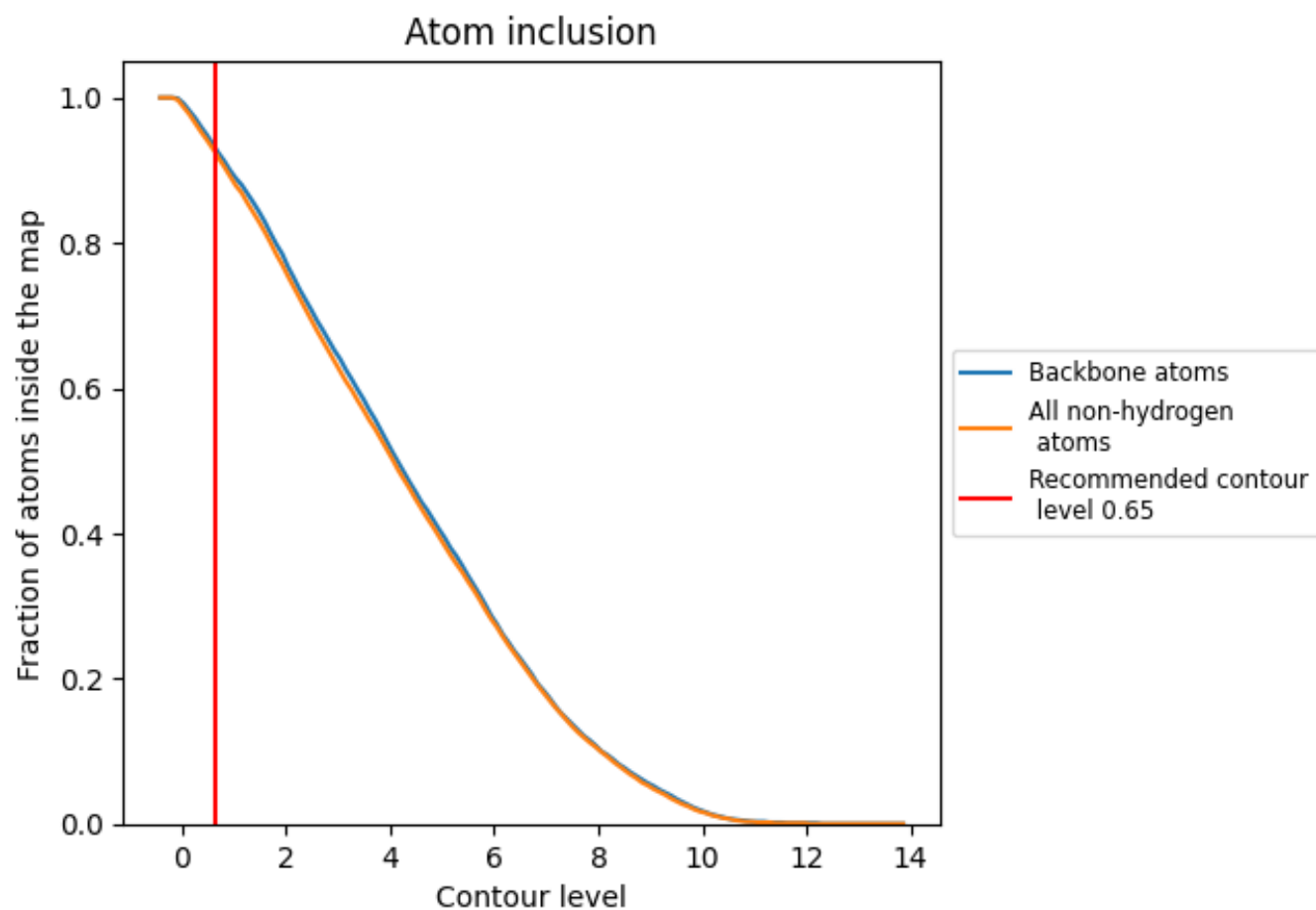


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

8.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9240	0.0430
A	0.9260	0.0400
B	0.9510	0.0460
C	0.9790	0.0490
D	0.9540	0.0620
E	0.9940	0.0550
F	0.9900	0.0600
G	0.7940	0.0350
M	0.8740	0.0300
N	0.9980	0.0700
O	0.9940	0.0610
P	0.9140	0.0460
Q	0.9660	0.0520
R	0.9870	0.0560
S	0.9120	0.0400

1.0

0.0

<0.0