



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:31 PM UTC

PDB ID : 9EKA / pdb\_00009eka  
EMDB ID : EMD-48116  
Title : CRISPR-associated deaminase Cad1 in Apo form  
Authors : Zhao, Y.; Whyms, C.T.; Li, H.  
Deposited on : 2024-12-02  
Resolution : 3.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

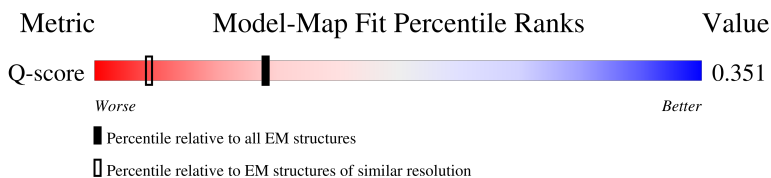
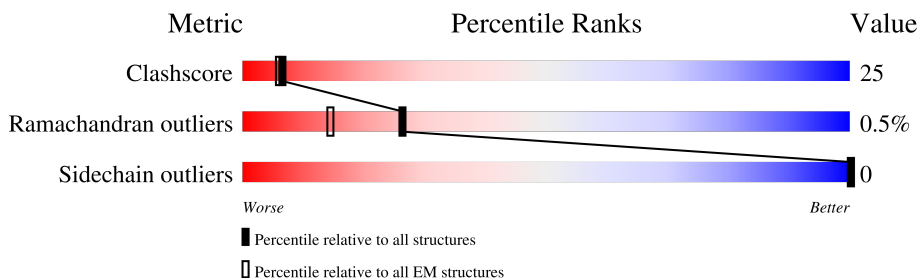
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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	14724 ( 2.60 - 3.60 )

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  $\geq 3$ , 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	625	<div> <div>31%</div> <div>63%</div> <div>29%</div> <div>5%</div> <div>.</div> </div>
1	B	625	<div> <div>32%</div> <div>58%</div> <div>34%</div> <div>5%</div> <div>..</div> </div>
1	E	625	<div> <div>30%</div> <div>61%</div> <div>29%</div> <div>6%</div> <div>..</div> </div>
1	F	625	<div> <div>32%</div> <div>59%</div> <div>34%</div> <div>.</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	625	<div><div></div><div>30%</div><div>63%</div><div>29%</div><div>5%</div><div></div></div>
1	H	625	<div><div></div><div>33%</div><div>60%</div><div>31%</div><div>6%</div><div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 28590 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 CRISPR-associated ring nuclease and adenosine deaminase, subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	608	Total	C	N	O	S	0	0
			4760	3014	869	856	21		
1	A	609	Total	C	N	O	S	0	0
			4768	3018	870	859	21		
1	F	608	Total	C	N	O	S	0	0
			4760	3014	869	856	21		
1	E	609	Total	C	N	O	S	0	0
			4768	3018	870	859	21		
1	H	608	Total	C	N	O	S	0	0
			4760	3014	869	856	21		
1	G	609	Total	C	N	O	S	0	0
			4768	3018	870	859	21		

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	B	1	Total	Zn	0
			1	1	
2	A	1	Total	Zn	0
			1	1	
2	F	1	Total	Zn	0
			1	1	
2	E	1	Total	Zn	0
			1	1	
2	H	1	Total	Zn	0
			1	1	
2	G	1	Total	Zn	0
			1	1	

### 3 Residue-property plots

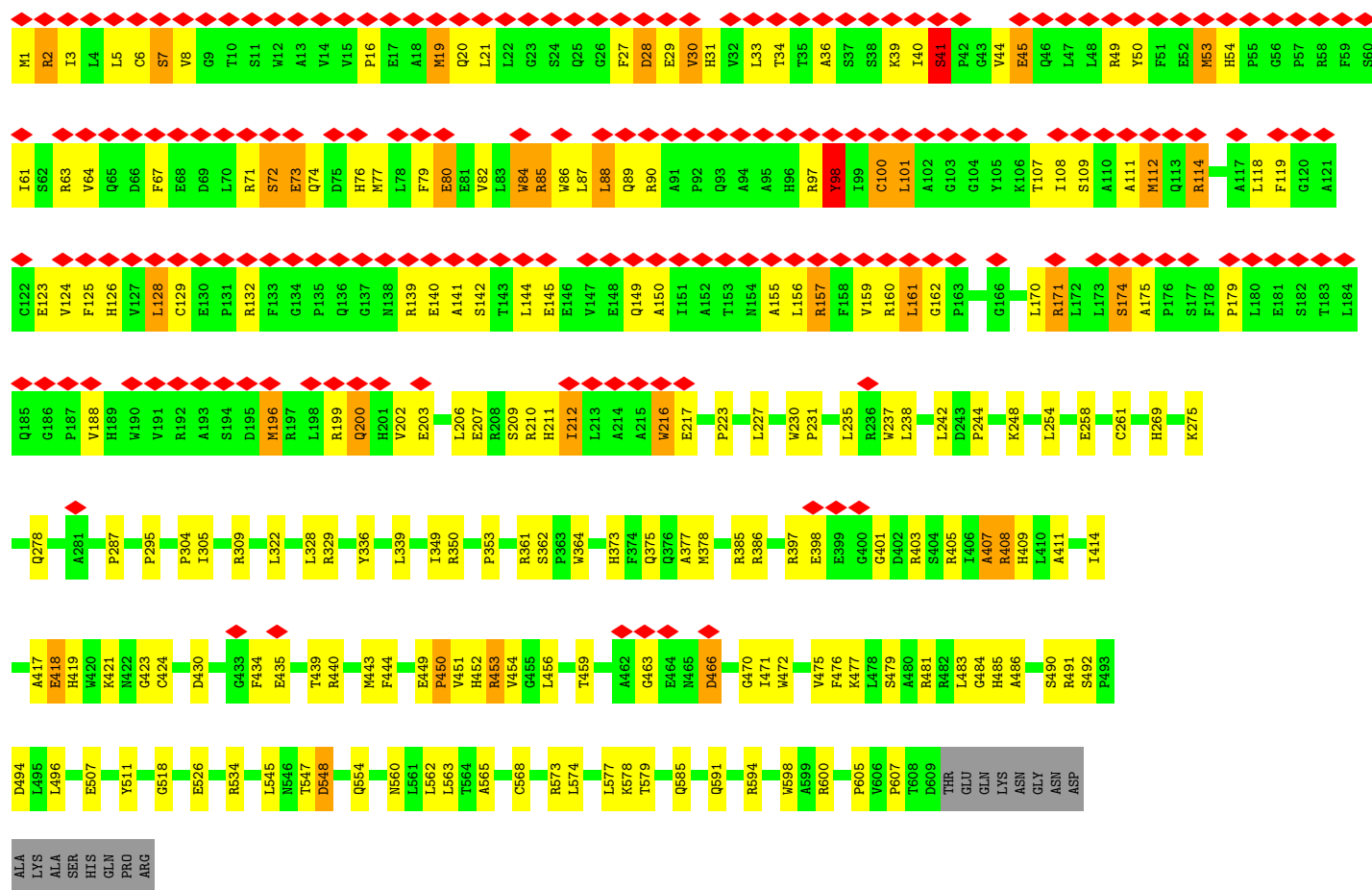
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

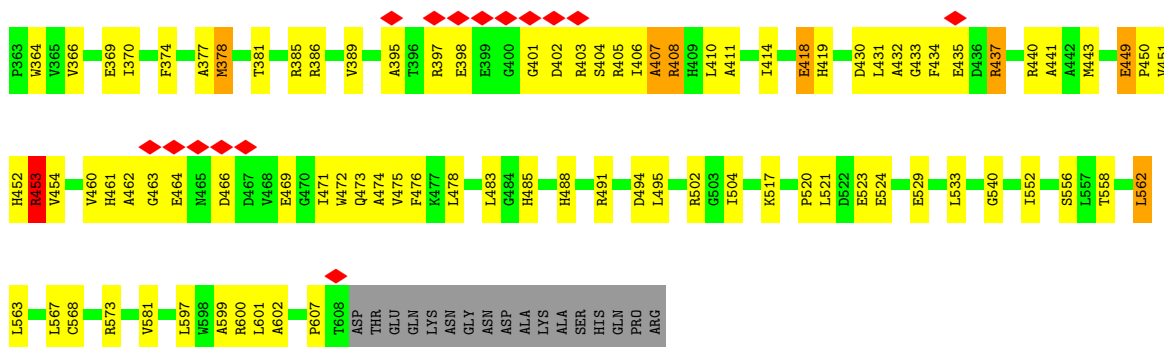
- Molecule 1: CRISPR-associated ring nuclease and adenosine deaminase, subunit A



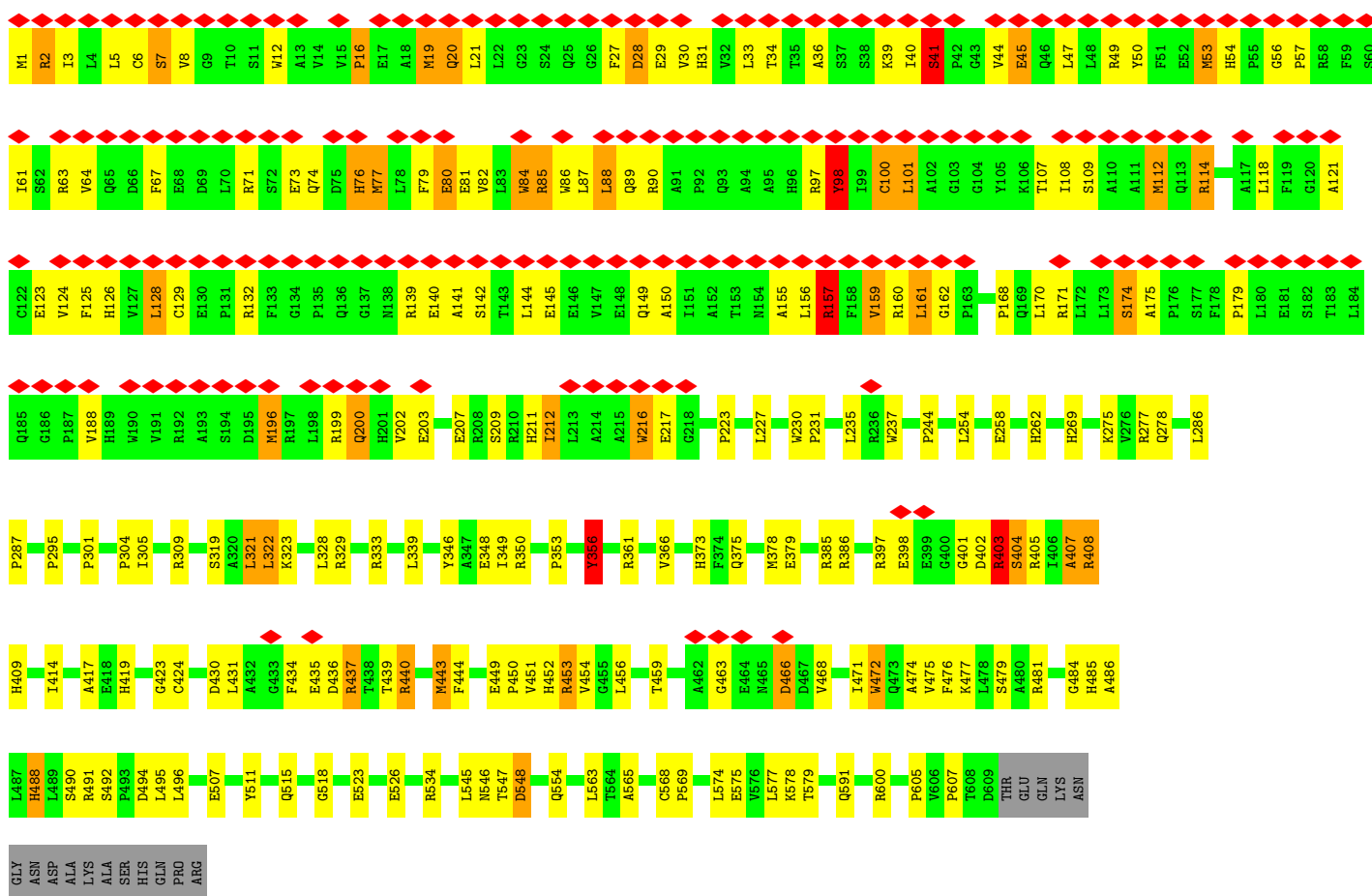
- Molecule 1: CRISPR-associated ring nuclease and adenosine deaminase, subunit A





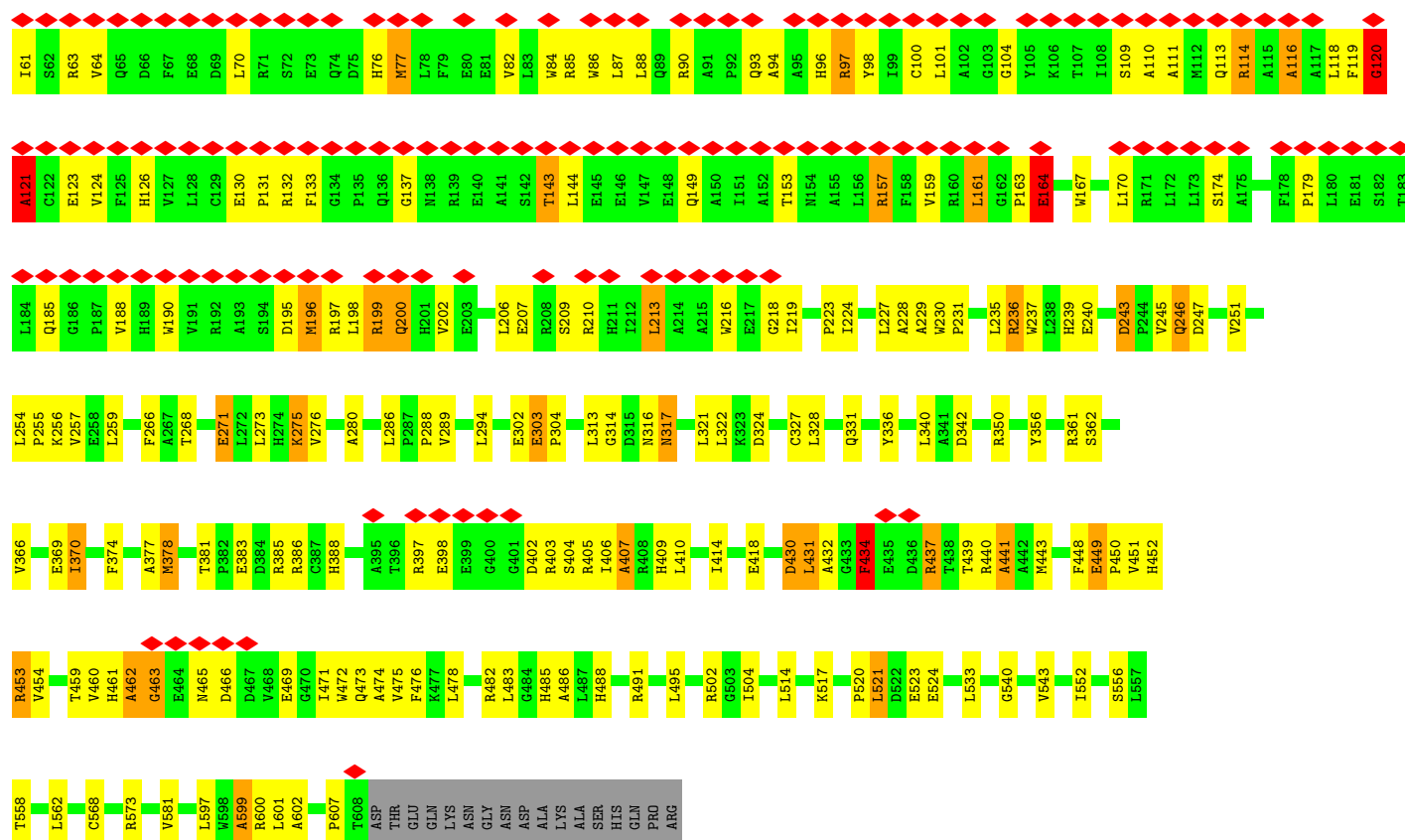


• Molecule 1: CRISPR-associated ring nuclease and adenosine deaminase, subunit A

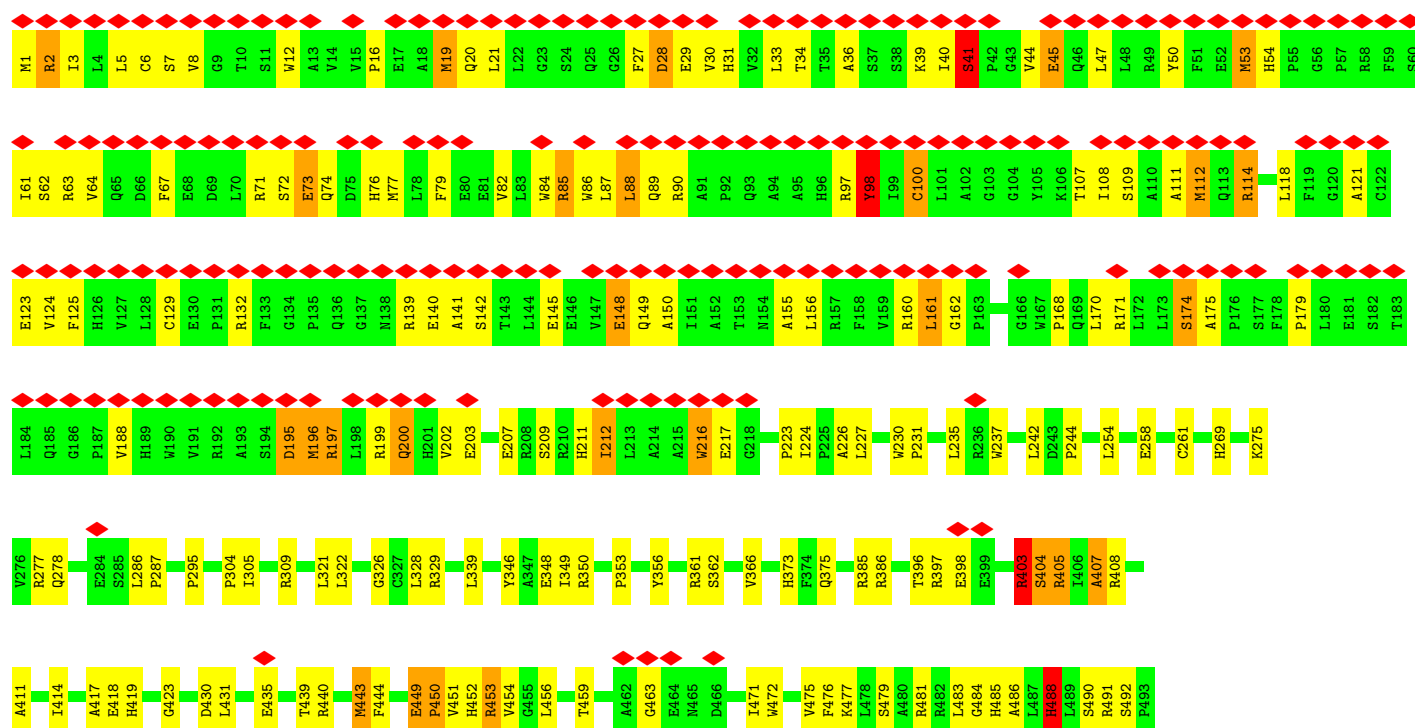


• Molecule 1: CRISPR-associated ring nuclease and adenosine deaminase, subunit A





• Molecule 1: CRISPR-associated ring nuclease and adenosine deaminase, subunit A







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15816	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.734	Depositor
Minimum map value	-2.491	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.114	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	1.30	63/4888 (1.3%)	1.03	42/6659 (0.6%)
1	B	1.30	56/4880 (1.1%)	0.97	48/6648 (0.7%)
1	E	1.41	75/4888 (1.5%)	1.07	47/6659 (0.7%)
1	F	1.22	45/4880 (0.9%)	0.93	38/6648 (0.6%)
1	G	1.29	58/4888 (1.2%)	1.02	46/6659 (0.7%)
1	H	1.46	65/4880 (1.3%)	1.03	54/6648 (0.8%)
All	All	1.33	362/29304 (1.2%)	1.01	275/39921 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
1	E	0	6
1	F	0	4
1	G	0	5
1	H	0	3
All	All	0	25

All (362) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	196	MET	SD-CE	-36.06	0.89	1.79
1	G	403	ARG	CB-CG	-24.75	0.78	1.52
1	E	157	ARG	CG-CD	-20.62	0.90	1.52
1	H	164	GLU	CD-OE2	-20.61	0.86	1.25
1	B	164	GLU	CD-OE2	-20.58	0.86	1.25
1	G	231	PRO	CA-C	20.45	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	164	GLU	CD-OE2	-20.34	0.86	1.25
1	A	295	PRO	CA-C	20.22	1.63	1.51
1	G	216	TRP	CZ3-CH2	-20.14	0.90	1.40
1	F	116	ALA	C-O	-19.84	0.97	1.24
1	H	116	ALA	C-O	-19.79	0.97	1.24
1	H	114	ARG	CZ-NH1	-19.76	1.05	1.32
1	B	378	MET	SD-CE	-19.66	1.30	1.79
1	A	287	PRO	CA-C	19.66	1.62	1.51
1	H	199	ARG	CD-NE	-19.54	1.18	1.46
1	G	403	ARG	CG-CD	19.34	2.10	1.52
1	B	116	ALA	C-O	-19.27	0.98	1.24
1	B	49	ARG	CG-CD	-19.19	0.94	1.52
1	F	49	ARG	CG-CD	-19.19	0.94	1.52
1	H	49	ARG	CG-CD	-19.16	0.94	1.52
1	A	216	TRP	CZ3-CH2	-18.91	0.93	1.40
1	E	216	TRP	CZ3-CH2	-18.87	0.93	1.40
1	E	295	PRO	CA-C	18.79	1.62	1.51
1	B	114	ARG	CZ-NH1	-18.53	1.06	1.32
1	A	231	PRO	CA-C	18.44	1.62	1.51
1	F	231	PRO	CA-C	17.93	1.61	1.51
1	H	434	PHE	CG-CD2	-17.88	1.01	1.38
1	E	322	LEU	CA-CB	-17.80	1.27	1.53
1	G	287	PRO	CA-C	17.65	1.61	1.51
1	H	378	MET	SD-CE	-17.60	1.35	1.79
1	H	199	ARG	CA-CB	-17.53	1.22	1.53
1	E	231	PRO	CA-C	17.51	1.61	1.51
1	E	128	LEU	CG-CD1	-17.00	0.96	1.52
1	G	216	TRP	CZ2-CH2	-16.93	1.05	1.37
1	B	449	GLU	CD-OE1	-16.58	0.93	1.25
1	F	378	MET	SD-CE	-16.48	1.38	1.79
1	E	112	MET	SD-CE	-16.40	1.38	1.79
1	A	112	MET	SD-CE	-16.33	1.38	1.79
1	A	216	TRP	CD2-CE3	-16.23	1.14	1.40
1	E	216	TRP	CD2-CE3	-16.17	1.14	1.40
1	G	295	PRO	CA-C	15.98	1.60	1.51
1	G	216	TRP	CD2-CE3	-15.77	1.15	1.40
1	G	216	TRP	CE3-CZ3	15.42	1.84	1.38
1	F	453	ARG	CZ-NH2	-15.17	1.13	1.33
1	G	112	MET	SD-CE	-15.05	1.42	1.79
1	E	356	TYR	CG-CD1	-15.01	1.07	1.39
1	E	287	PRO	CA-C	14.96	1.60	1.51
1	B	246	GLN	CD-OE1	-14.92	0.95	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	246	GLN	CD-OE1	-14.91	0.95	1.23
1	A	216	TRP	CE3-CZ3	14.87	1.83	1.38
1	E	216	TRP	CE3-CZ3	14.86	1.83	1.38
1	H	434	PHE	CE1-CZ	-14.69	0.94	1.38
1	A	216	TRP	CZ2-CH2	-14.45	1.09	1.37
1	E	216	TRP	CZ2-CH2	-14.36	1.09	1.37
1	H	231	PRO	CA-C	14.22	1.59	1.51
1	B	323	LYS	CE-NZ	-14.13	1.06	1.49
1	B	403	ARG	CZ-NH1	-14.06	1.13	1.32
1	A	157	ARG	CG-CD	-13.89	1.10	1.52
1	H	370	ILE	CG1-CD1	-13.32	0.99	1.51
1	B	231	PRO	CA-C	13.28	1.59	1.51
1	E	466	ASP	CG-OD1	-13.26	1.00	1.25
1	E	84	TRP	CZ2-CH2	-12.99	1.12	1.37
1	A	114	ARG	NE-CZ	-12.97	1.18	1.33
1	F	114	ARG	NE-CZ	-12.88	1.18	1.33
1	F	418	GLU	CD-OE1	-12.87	1.00	1.25
1	B	72	SER	CA-CB	-12.73	1.28	1.53
1	E	7	SER	CB-OG	-12.60	1.17	1.42
1	A	7	SER	CB-OG	-12.58	1.17	1.42
1	F	407	ALA	CA-CB	-12.08	1.34	1.53
1	A	128	LEU	CG-CD1	-12.00	1.12	1.52
1	E	356	TYR	CE1-CZ	-12.00	1.09	1.38
1	H	462	ALA	CA-CB	-11.55	1.35	1.53
1	H	303	GLU	CD-OE1	-11.33	1.03	1.25
1	E	403	ARG	CZ-NH2	-11.32	1.18	1.33
1	F	418	GLU	CD-OE2	-11.27	1.03	1.25
1	H	437	ARG	CZ-NH1	-11.01	1.17	1.32
1	B	407	ALA	CA-CB	-11.01	1.36	1.53
1	B	437	ARG	CZ-NH1	-10.97	1.17	1.32
1	H	196	MET	CG-SD	-10.86	1.53	1.80
1	B	161	LEU	CG-CD1	-10.86	1.16	1.52
1	A	98	TYR	CD2-CE2	-10.85	1.06	1.38
1	G	98	TYR	CD2-CE2	-10.82	1.06	1.38
1	E	98	TYR	CD2-CE2	-10.80	1.06	1.38
1	G	114	ARG	NE-CZ	-10.62	1.21	1.33
1	A	407	ALA	CA-CB	-10.58	1.36	1.53
1	F	19	MET	SD-CE	-10.49	1.53	1.79
1	H	46	GLN	C-N	-10.46	1.20	1.33
1	H	19	MET	SD-CE	-10.46	1.53	1.79
1	B	46	GLN	C-N	-10.30	1.20	1.33
1	B	303	GLU	CD-OE1	-10.21	1.05	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	303	GLU	CD-OE1	-10.17	1.06	1.25
1	E	472	TRP	CA-CB	-10.09	1.37	1.53
1	F	46	GLN	C-N	-10.06	1.20	1.33
1	B	161	LEU	N-CA	-10.01	1.31	1.46
1	A	114	ARG	CZ-NH1	9.99	1.46	1.32
1	F	437	ARG	CZ-NH1	-9.94	1.18	1.32
1	H	275	LYS	CD-CE	-9.91	1.22	1.52
1	E	322	LEU	CG-CD2	-9.80	1.20	1.52
1	E	437	ARG	CZ-NH1	-9.80	1.19	1.32
1	G	443	MET	SD-CE	-9.79	1.55	1.79
1	B	49	ARG	CZ-NH2	-9.78	1.20	1.33
1	G	7	SER	CB-OG	-9.78	1.22	1.42
1	H	49	ARG	CZ-NH2	-9.76	1.20	1.33
1	F	453	ARG	CD-NE	-9.76	1.32	1.46
1	A	80	GLU	CB-CG	-9.74	1.23	1.52
1	H	77	MET	SD-CE	-9.69	1.55	1.79
1	F	49	ARG	CZ-NH2	-9.66	1.20	1.33
1	A	84	TRP	CZ2-CH2	-9.63	1.19	1.37
1	E	453	ARG	CZ-NH1	-9.54	1.19	1.32
1	G	407	ALA	CA-CB	-9.52	1.38	1.53
1	G	405	ARG	CZ-NH1	-9.48	1.19	1.32
1	G	353	PRO	CG-CD	-9.43	1.18	1.50
1	A	114	ARG	CZ-NH2	9.42	1.45	1.33
1	A	53	MET	SD-CE	-9.41	1.56	1.79
1	E	353	PRO	CG-CD	-9.41	1.18	1.50
1	F	77	MET	SD-CE	-9.40	1.56	1.79
1	E	53	MET	SD-CE	-9.40	1.56	1.79
1	H	26	GLY	N-CA	-9.39	1.28	1.45
1	A	353	PRO	CG-CD	-9.38	1.18	1.50
1	E	80	GLU	CB-CG	-9.38	1.24	1.52
1	F	26	GLY	N-CA	-9.32	1.28	1.45
1	H	19	MET	C-O	-9.24	1.12	1.24
1	F	19	MET	C-O	-9.23	1.12	1.24
1	G	403	ARG	CZ-NH1	-9.15	1.20	1.32
1	F	562	LEU	CG-CD1	-9.14	1.22	1.52
1	G	216	TRP	CD2-CE2	-9.06	1.25	1.41
1	B	453	ARG	CB-CG	-9.02	1.25	1.52
1	E	157	ARG	CZ-NH1	-8.98	1.20	1.32
1	H	453	ARG	CB-CG	-8.97	1.25	1.52
1	F	72	SER	CA-CB	-8.96	1.38	1.53
1	G	195	ASP	CG-OD2	-8.96	1.08	1.25
1	E	2	ARG	CA-CB	8.89	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	2	ARG	CA-CB	8.89	1.67	1.53
1	A	2	ARG	CA-CB	8.87	1.67	1.53
1	F	403	ARG	CZ-NH1	-8.80	1.20	1.32
1	B	200	GLN	CB-CG	-8.72	1.26	1.52
1	H	453	ARG	CZ-NH2	-8.56	1.22	1.33
1	F	114	ARG	CZ-NH1	8.51	1.44	1.32
1	E	440	ARG	CZ-NH1	-8.42	1.21	1.32
1	B	453	ARG	CZ-NH2	8.40	1.44	1.33
1	E	16	PRO	C-O	-8.39	1.13	1.24
1	G	16	PRO	C-O	-8.35	1.13	1.24
1	H	453	ARG	CD-NE	-8.34	1.34	1.46
1	A	16	PRO	C-O	-8.31	1.13	1.24
1	E	443	MET	SD-CE	-8.30	1.58	1.79
1	E	403	ARG	CZ-NH1	-8.25	1.21	1.32
1	B	120	GLY	CA-C	8.24	1.63	1.51
1	B	275	LYS	CD-CE	-8.24	1.27	1.52
1	E	403	ARG	NE-CZ	-8.22	1.24	1.33
1	H	120	GLY	CA-C	8.21	1.63	1.51
1	F	120	GLY	CA-C	8.12	1.63	1.51
1	H	430	ASP	C-N	-8.11	1.22	1.33
1	B	19	MET	C-O	-8.05	1.13	1.24
1	B	19	MET	SD-CE	-8.04	1.59	1.79
1	A	287	PRO	C-O	-8.03	1.18	1.25
1	H	407	ALA	CA-CB	-8.04	1.40	1.53
1	F	72	SER	C-N	8.01	1.44	1.33
1	B	157	ARG	CZ-NH1	-8.00	1.21	1.32
1	E	161	LEU	CA-CB	7.94	1.63	1.53
1	F	164	GLU	CG-CD	-7.92	1.32	1.52
1	H	164	GLU	CG-CD	-7.91	1.32	1.52
1	B	164	GLU	CG-CD	-7.88	1.32	1.52
1	F	28	ASP	CG-OD2	-7.87	1.10	1.25
1	B	217	GLU	CB-CG	-7.86	1.28	1.52
1	E	114	ARG	CZ-NH1	-7.80	1.21	1.32
1	A	19	MET	SD-CE	-7.71	1.60	1.79
1	H	449	GLU	CA-C	7.70	1.61	1.52
1	H	317	ASN	CG-OD1	-7.66	1.09	1.23
1	A	157	ARG	NE-CZ	7.64	1.41	1.33
1	G	287	PRO	C-O	-7.63	1.18	1.25
1	B	317	ASN	CG-OD1	-7.61	1.09	1.23
1	B	26	GLY	N-CA	-7.58	1.31	1.45
1	F	317	ASN	CG-OD1	-7.58	1.09	1.23
1	G	73	GLU	CB-CG	-7.57	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	157	ARG	CZ-NH2	-7.51	1.23	1.33
1	H	431	LEU	N-CA	-7.49	1.37	1.46
1	H	213	LEU	CB-CG	-7.47	1.38	1.53
1	E	98	TYR	CE1-CZ	-7.47	1.20	1.38
1	B	383	GLU	CG-CD	-7.46	1.33	1.52
1	H	453	ARG	CG-CD	-7.46	1.30	1.52
1	A	98	TYR	CE1-CZ	-7.46	1.20	1.38
1	G	98	TYR	CE1-CZ	-7.46	1.20	1.38
1	F	120	GLY	C-N	7.44	1.44	1.33
1	E	408	ARG	CZ-NH1	-7.41	1.22	1.32
1	G	112	MET	CG-SD	-7.41	1.62	1.80
1	F	46	GLN	CA-C	7.39	1.62	1.52
1	B	120	GLY	C-N	7.37	1.44	1.33
1	H	120	GLY	C-N	7.35	1.44	1.33
1	B	46	GLN	CA-C	7.35	1.62	1.52
1	E	84	TRP	CZ3-CH2	-7.30	1.22	1.40
1	A	157	ARG	CD-NE	7.28	1.56	1.46
1	B	196	MET	C-N	-7.28	1.23	1.33
1	E	161	LEU	N-CA	-7.27	1.38	1.46
1	F	453	ARG	NE-CZ	-7.27	1.25	1.33
1	H	46	GLN	CA-C	7.27	1.62	1.52
1	A	157	ARG	CZ-NH1	-7.22	1.22	1.32
1	G	200	GLN	CB-CG	-7.21	1.30	1.52
1	H	199	ARG	CG-CD	7.21	1.74	1.52
1	F	114	ARG	CD-NE	-7.21	1.36	1.46
1	H	236	ARG	CB-CG	-7.17	1.30	1.52
1	E	196	MET	SD-CE	-7.16	1.61	1.79
1	A	45	GLU	CD-OE1	-7.14	1.11	1.25
1	G	114	ARG	CZ-NH2	7.14	1.42	1.33
1	B	196	MET	C-O	-7.14	1.14	1.23
1	A	435	GLU	CG-CD	-7.13	1.34	1.52
1	G	45	GLU	CD-OE1	-7.12	1.11	1.25
1	G	453	ARG	CZ-NH1	-7.09	1.22	1.32
1	E	435	GLU	CG-CD	-7.08	1.34	1.52
1	G	435	GLU	CG-CD	-7.03	1.34	1.52
1	G	19	MET	SD-CE	-7.03	1.61	1.79
1	E	287	PRO	C-O	-7.00	1.19	1.25
1	E	45	GLU	CD-OE1	-6.99	1.12	1.25
1	E	488	HIS	CA-CB	-6.98	1.43	1.53
1	B	200	GLN	CD-OE1	-6.97	1.10	1.23
1	B	558	THR	C-O	-6.93	1.16	1.24
1	A	73	GLU	CB-CG	-6.90	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	453	ARG	CZ-NH1	-6.88	1.23	1.32
1	A	161	LEU	CG-CD1	-6.88	1.29	1.52
1	G	161	LEU	CB-CG	-6.85	1.39	1.53
1	A	41	SER	CA-C	-6.83	1.44	1.52
1	E	216	TRP	CD2-CE2	-6.83	1.29	1.41
1	E	407	ALA	CA-CB	-6.81	1.42	1.53
1	A	418	GLU	CD-OE2	-6.79	1.12	1.25
1	A	216	TRP	CD2-CE2	-6.79	1.29	1.41
1	G	449	GLU	CD-OE2	-6.78	1.12	1.25
1	G	41	SER	CA-C	-6.75	1.44	1.52
1	E	41	SER	CA-C	-6.75	1.44	1.52
1	E	19	MET	SD-CE	-6.71	1.62	1.79
1	A	200	GLN	CB-CG	-6.71	1.32	1.52
1	H	161	LEU	N-CA	-6.68	1.37	1.46
1	A	196	MET	SD-CE	-6.66	1.62	1.79
1	A	418	GLU	CD-OE1	-6.64	1.12	1.25
1	H	431	LEU	CA-C	6.60	1.61	1.52
1	A	212	ILE	C-O	-6.58	1.16	1.24
1	E	402	ASP	CG-OD1	-6.56	1.12	1.25
1	H	161	LEU	C-N	-6.54	1.23	1.33
1	A	408	ARG	CD-NE	6.53	1.55	1.46
1	E	88	LEU	CB-CG	-6.53	1.40	1.53
1	A	101	LEU	CG-CD1	-6.52	1.31	1.52
1	H	161	LEU	CG-CD1	-6.51	1.31	1.52
1	A	88	LEU	CB-CG	-6.50	1.40	1.53
1	E	212	ILE	C-O	-6.49	1.16	1.24
1	A	453	ARG	CZ-NH2	-6.44	1.25	1.33
1	G	212	ILE	C-O	-6.44	1.16	1.24
1	E	200	GLN	CB-CG	-6.43	1.33	1.52
1	E	41	SER	C-O	-6.42	1.18	1.24
1	H	77	MET	CG-SD	-6.38	1.64	1.80
1	G	216	TRP	CG-CD2	-6.37	1.32	1.43
1	B	437	ARG	NE-CZ	-6.36	1.26	1.33
1	H	437	ARG	NE-CZ	-6.34	1.26	1.33
1	F	71	ARG	C-N	6.33	1.41	1.33
1	F	449	GLU	CD-OE2	-6.32	1.13	1.25
1	A	41	SER	C-O	-6.29	1.18	1.24
1	A	45	GLU	CG-CD	-6.25	1.36	1.52
1	G	41	SER	C-O	-6.25	1.18	1.24
1	F	77	MET	CG-SD	-6.23	1.65	1.80
1	E	45	GLU	CG-CD	-6.21	1.36	1.52
1	G	45	GLU	CG-CD	-6.21	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	434	PHE	CE2-CZ	-6.21	1.20	1.38
1	B	114	ARG	NE-CZ	-6.17	1.26	1.33
1	H	431	LEU	CB-CG	-6.17	1.41	1.53
1	H	275	LYS	CB-CG	-6.16	1.33	1.52
1	E	437	ARG	CG-CD	6.16	1.71	1.52
1	A	84	TRP	CZ3-CH2	-6.14	1.25	1.40
1	B	160	ARG	C-N	-6.12	1.24	1.33
1	B	196	MET	CG-SD	-6.11	1.65	1.80
1	B	72	SER	C-N	6.11	1.42	1.33
1	A	216	TRP	CG-CD2	-6.09	1.32	1.43
1	E	174	SER	CA-CB	-6.05	1.42	1.54
1	A	171	ARG	CZ-NH1	-6.05	1.24	1.32
1	E	437	ARG	NE-CZ	-6.04	1.26	1.33
1	B	161	LEU	CA-C	6.04	1.63	1.52
1	A	174	SER	CA-CB	-6.02	1.42	1.54
1	E	216	TRP	CG-CD2	-6.02	1.32	1.43
1	F	408	ARG	CG-CD	-6.01	1.34	1.52
1	B	275	LYS	CB-CG	-5.97	1.34	1.52
1	B	19	MET	C-N	-5.93	1.25	1.33
1	B	161	LEU	C-N	-5.92	1.24	1.33
1	H	521	LEU	CG-CD1	-5.88	1.33	1.52
1	H	599	ALA	C-N	-5.84	1.25	1.33
1	B	157	ARG	CZ-NH2	-5.80	1.25	1.33
1	E	98	TYR	CG-CD2	-5.76	1.27	1.39
1	G	148	GLU	CD-OE2	-5.76	1.14	1.25
1	G	98	TYR	CG-CD2	-5.76	1.27	1.39
1	E	77	MET	SD-CE	-5.76	1.65	1.79
1	A	98	TYR	CG-CD2	-5.76	1.27	1.39
1	E	196	MET	C-O	-5.73	1.16	1.23
1	E	101	LEU	CG-CD1	-5.72	1.33	1.52
1	B	521	LEU	CG-CD1	-5.71	1.33	1.52
1	B	77	MET	CG-SD	-5.71	1.66	1.80
1	E	161	LEU	C-O	5.67	1.29	1.23
1	A	450	PRO	CG-CD	-5.63	1.31	1.50
1	G	161	LEU	CG-CD1	-5.62	1.33	1.52
1	H	157	ARG	NE-CZ	-5.58	1.26	1.33
1	A	196	MET	C-O	-5.56	1.17	1.23
1	H	243	ASP	CG-OD2	-5.56	1.14	1.25
1	E	76	HIS	CG-ND1	-5.55	1.32	1.38
1	H	199	ARG	CA-C	-5.55	1.45	1.52
1	G	404	SER	C-O	-5.55	1.17	1.24
1	A	212	ILE	C-N	-5.55	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	243	ASP	CG-OD2	-5.52	1.14	1.25
1	E	114	ARG	NE-CZ	-5.51	1.26	1.33
1	H	161	LEU	CA-CB	5.50	1.63	1.53
1	A	161	LEU	CA-CB	-5.47	1.44	1.53
1	A	101	LEU	CG-CD2	-5.47	1.34	1.52
1	B	196	MET	SD-CE	-5.45	1.66	1.79
1	H	114	ARG	NE-CZ	-5.45	1.27	1.33
1	F	19	MET	C-N	-5.42	1.26	1.33
1	G	216	TRP	NE1-CE2	-5.40	1.31	1.37
1	H	19	MET	C-N	-5.39	1.26	1.33
1	A	466	ASP	CG-OD2	-5.38	1.15	1.25
1	B	418	GLU	CD-OE2	-5.38	1.15	1.25
1	E	84	TRP	CD2-CE2	-5.36	1.32	1.41
1	G	212	ILE	C-N	-5.33	1.25	1.33
1	F	72	SER	N-CA	5.33	1.52	1.46
1	F	310	TYR	CZ-OH	-5.32	1.26	1.38
1	H	46	GLN	N-CA	-5.32	1.40	1.46
1	F	217	GLU	CB-CG	-5.31	1.36	1.52
1	G	161	LEU	N-CA	-5.30	1.39	1.46
1	H	271	GLU	CG-CD	-5.30	1.38	1.52
1	F	46	GLN	N-CA	-5.28	1.40	1.46
1	E	440	ARG	NE-CZ	5.28	1.38	1.33
1	B	46	GLN	N-CA	-5.28	1.40	1.46
1	A	73	GLU	CA-CB	5.28	1.61	1.53
1	G	53	MET	SD-CE	-5.26	1.66	1.79
1	A	45	GLU	CB-CG	5.25	1.68	1.52
1	G	526	GLU	C-O	-5.24	1.17	1.24
1	E	212	ILE	C-N	-5.22	1.25	1.33
1	G	45	GLU	CB-CG	5.21	1.68	1.52
1	A	526	GLU	C-O	-5.20	1.17	1.24
1	E	45	GLU	CB-CG	5.20	1.68	1.52
1	G	196	MET	C-N	-5.20	1.26	1.33
1	E	453	ARG	CZ-NH2	-5.20	1.26	1.33
1	G	450	PRO	CG-CD	-5.15	1.33	1.50
1	F	418	GLU	CG-CD	-5.14	1.39	1.52
1	E	85	ARG	CZ-NH1	-5.14	1.25	1.32
1	G	85	ARG	CZ-NH1	-5.14	1.25	1.32
1	A	85	ARG	CZ-NH1	-5.14	1.25	1.32
1	G	488	HIS	CD2-NE2	-5.14	1.32	1.37
1	G	196	MET	SD-CE	-5.13	1.66	1.79
1	F	164	GLU	CB-CG	-5.13	1.37	1.52
1	H	164	GLU	CB-CG	-5.13	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	174	SER	CA-CB	-5.13	1.44	1.54
1	B	164	GLU	CB-CG	-5.12	1.37	1.52
1	E	20	GLN	CD-NE2	-5.10	1.22	1.33
1	E	526	GLU	C-O	-5.10	1.17	1.24
1	H	434	PHE	CB-CG	-5.08	1.39	1.50
1	A	114	ARG	CD-NE	-5.08	1.39	1.46
1	H	434	PHE	CD2-CE2	-5.08	1.23	1.38
1	F	97	ARG	CZ-NH1	-5.07	1.25	1.32
1	E	404	SER	C-O	-5.06	1.17	1.24
1	H	28	ASP	CG-OD2	-5.05	1.15	1.25
1	A	20	GLN	CD-NE2	-5.05	1.22	1.33
1	E	159	VAL	CB-CG2	-5.05	1.35	1.52
1	G	20	GLN	CD-NE2	-5.04	1.22	1.33
1	B	28	ASP	CG-OD2	-5.04	1.15	1.25
1	H	453	ARG	NE-CZ	-5.04	1.27	1.33
1	F	31	HIS	CA-CB	-5.03	1.43	1.54
1	B	562	LEU	CG-CD1	-5.02	1.35	1.52
1	H	97	ARG	CZ-NH1	-5.02	1.25	1.32
1	G	504	ILE	CG1-CD1	-5.01	1.32	1.51
1	G	231	PRO	C-O	-5.00	1.20	1.25

All (275) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	157	ARG	NH1-CZ-NH2	-26.46	84.90	119.30
1	H	196	MET	CG-SD-CE	21.04	147.19	100.90
1	H	199	ARG	CA-CB-CG	18.78	151.66	114.10
1	G	231	PRO	O-C-N	18.39	129.77	121.31
1	A	295	PRO	O-C-N	18.07	129.62	121.31
1	A	287	PRO	O-C-N	17.48	129.35	121.31
1	A	231	PRO	O-C-N	16.75	129.01	121.31
1	E	295	PRO	O-C-N	16.65	128.97	121.31
1	F	231	PRO	O-C-N	15.96	128.65	121.31
1	A	353	PRO	N-CD-CG	-15.89	79.36	103.20
1	G	353	PRO	N-CD-CG	-15.89	79.36	103.20
1	E	353	PRO	N-CD-CG	-15.88	79.38	103.20
1	E	231	PRO	O-C-N	15.88	128.61	121.31
1	G	287	PRO	O-C-N	15.50	128.44	121.31
1	G	295	PRO	O-C-N	14.21	127.85	121.31
1	E	41	SER	CA-C-O	-13.52	106.19	118.63
1	G	41	SER	CA-C-O	-13.52	106.19	118.63
1	A	41	SER	CA-C-O	-13.46	106.25	118.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	287	PRO	O-C-N	12.97	127.28	121.31
1	H	231	PRO	O-C-N	12.88	127.23	121.31
1	H	431	LEU	CB-CA-C	12.24	131.21	110.77
1	E	157	ARG	NE-CZ-NH2	12.13	130.12	119.20
1	A	157	ARG	CD-NE-CZ	12.09	141.33	124.40
1	G	403	ARG	NH1-CZ-NH2	-12.05	103.63	119.30
1	A	45	GLU	CG-CD-OE1	-12.04	90.72	118.40
1	G	45	GLU	CG-CD-OE1	-12.02	90.75	118.40
1	E	45	GLU	CG-CD-OE1	-12.02	90.76	118.40
1	B	231	PRO	O-C-N	11.97	126.82	121.31
1	A	114	ARG	NH1-CZ-NH2	11.53	134.28	119.30
1	A	353	PRO	CA-CB-CG	-11.01	83.58	104.50
1	E	353	PRO	CA-CB-CG	-11.01	83.58	104.50
1	G	353	PRO	CA-CB-CG	-10.99	83.61	104.50
1	F	114	ARG	NH1-CZ-NH2	10.95	133.54	119.30
1	F	453	ARG	NE-CZ-NH2	-10.76	109.52	119.20
1	B	196	MET	O-C-N	-10.68	108.52	122.61
1	G	114	ARG	NE-CZ-NH1	-10.49	111.01	121.50
1	B	383	GLU	CG-CD-OE2	-10.41	94.45	118.40
1	G	403	ARG	NE-CZ-NH2	10.37	128.53	119.20
1	G	114	ARG	NH1-CZ-NH2	10.28	132.66	119.30
1	E	440	ARG	NH1-CZ-NH2	-10.18	106.06	119.30
1	F	453	ARG	NE-CZ-NH1	10.11	131.61	121.50
1	H	453	ARG	NE-CZ-NH2	-9.98	110.22	119.20
1	B	19	MET	O-C-N	-9.95	108.73	122.46
1	E	440	ARG	NE-CZ-NH2	9.65	127.89	119.20
1	H	19	MET	O-C-N	-9.62	109.18	122.46
1	F	19	MET	O-C-N	-9.59	109.22	122.46
1	B	453	ARG	NE-CZ-NH1	-9.53	111.97	121.50
1	G	216	TRP	CH2-CZ2-CE2	9.35	129.65	117.50
1	F	407	ALA	N-CA-CB	-9.29	96.46	110.12
1	B	449	GLU	OE1-CD-OE2	-9.12	101.03	122.90
1	F	114	ARG	NE-CZ-NH2	-8.94	111.15	119.20
1	A	114	ARG	NE-CZ-NH1	-8.89	112.61	121.50
1	H	49	ARG	CG-CD-NE	8.80	131.35	112.00
1	G	403	ARG	CB-CG-CD	8.76	131.45	111.30
1	H	199	ARG	CB-CA-C	-8.74	92.04	110.31
1	F	49	ARG	CG-CD-NE	8.73	131.20	112.00
1	B	49	ARG	CG-CD-NE	8.72	131.19	112.00
1	H	119	PHE	CA-C-N	-8.62	104.51	121.41
1	H	119	PHE	C-N-CA	-8.62	104.51	121.41
1	B	119	PHE	CA-C-N	-8.62	104.52	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	PHE	C-N-CA	-8.62	104.52	121.41
1	F	119	PHE	CA-C-N	-8.60	104.56	121.41
1	F	119	PHE	C-N-CA	-8.60	104.56	121.41
1	B	164	GLU	CG-CD-OE1	8.59	138.16	118.40
1	F	164	GLU	CG-CD-OE1	8.59	138.15	118.40
1	H	164	GLU	CG-CD-OE1	8.56	138.08	118.40
1	E	80	GLU	CB-CG-CD	8.52	127.09	112.60
1	G	216	TRP	CE2-CD2-CE3	-8.49	110.31	118.80
1	H	163	PRO	CA-N-CD	-8.49	100.11	112.00
1	H	431	LEU	CA-CB-CG	8.45	145.89	116.30
1	F	163	PRO	CA-N-CD	-8.44	100.19	112.00
1	B	163	PRO	CA-N-CD	-8.42	100.21	112.00
1	H	199	ARG	N-CA-CB	8.42	124.37	110.39
1	G	216	TRP	CZ3-CH2-CZ2	-8.38	110.60	121.50
1	B	114	ARG	NE-CZ-NH1	-8.38	113.12	121.50
1	H	46	GLN	O-C-N	-8.35	113.27	122.12
1	B	46	GLN	CA-C-O	8.35	129.40	120.55
1	F	46	GLN	O-C-N	-8.30	113.32	122.12
1	H	26	GLY	N-CA-C	8.26	128.07	112.62
1	B	46	GLN	O-C-N	-8.25	113.38	122.12
1	F	46	GLN	CA-C-O	8.24	129.28	120.55
1	F	26	GLY	N-CA-C	8.23	128.00	112.62
1	H	46	GLN	CA-C-O	8.22	129.26	120.55
1	B	378	MET	CG-SD-CE	-8.21	82.84	100.90
1	B	441	ALA	CB-CA-C	-8.19	96.93	110.85
1	H	441	ALA	CB-CA-C	-8.15	97.00	110.85
1	B	161	LEU	N-CA-C	8.05	122.77	113.19
1	B	407	ALA	N-CA-CB	-7.93	98.47	110.12
1	B	164	GLU	CG-CD-OE2	-7.89	100.24	118.40
1	F	164	GLU	CG-CD-OE2	-7.89	100.25	118.40
1	H	77	MET	CG-SD-CE	7.87	118.21	100.90
1	H	164	GLU	CG-CD-OE2	-7.86	100.32	118.40
1	A	72	SER	CA-C-N	7.82	130.76	120.28
1	A	72	SER	C-N-CA	7.82	130.76	120.28
1	F	77	MET	CG-SD-CE	7.76	117.98	100.90
1	A	157	ARG	NH1-CZ-NH2	-7.76	109.21	119.30
1	A	216	TRP	CE2-CD2-CE3	-7.67	111.12	118.80
1	G	161	LEU	CA-CB-CG	7.65	143.06	116.30
1	B	200	GLN	CG-CD-NE2	7.64	127.87	116.40
1	E	216	TRP	CE2-CD2-CE3	-7.63	111.17	118.80
1	B	388	HIS	CA-C-N	7.60	132.62	123.19
1	B	388	HIS	C-N-CA	7.60	132.62	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	403	ARG	NE-CZ-NH2	7.54	125.99	119.20
1	A	80	GLU	CB-CG-CD	7.49	125.33	112.60
1	B	114	ARG	NE-CZ-NH2	7.48	125.93	119.20
1	E	322	LEU	CB-CG-CD1	7.36	132.79	110.70
1	G	73	GLU	CA-CB-CG	7.30	128.70	114.10
1	H	449	GLU	CB-CG-CD	7.29	124.99	112.60
1	H	196	MET	O-C-N	-7.28	113.00	122.61
1	A	171	ARG	NE-CZ-NH1	-7.25	114.25	121.50
1	G	488	HIS	CG-CD2-NE2	7.14	114.34	107.20
1	F	114	ARG	NE-CZ-NH1	-7.12	114.38	121.50
1	H	431	LEU	CA-C-O	7.10	128.62	120.60
1	G	45	GLU	CG-CD-OE2	7.08	134.69	118.40
1	A	45	GLU	CG-CD-OE2	7.08	134.67	118.40
1	E	321	LEU	CA-C-N	-7.06	111.36	122.73
1	E	321	LEU	C-N-CA	-7.06	111.36	122.73
1	E	45	GLU	CG-CD-OE2	7.05	134.62	118.40
1	B	161	LEU	CA-CB-CG	7.03	140.92	116.30
1	A	98	TYR	CZ-CE2-CD2	7.02	132.24	119.60
1	G	98	TYR	CZ-CE2-CD2	7.00	132.20	119.60
1	B	386	ARG	NE-CZ-NH1	-6.99	114.51	121.50
1	E	98	TYR	CZ-CE2-CD2	6.98	132.17	119.60
1	F	288	PRO	CA-N-CD	-6.93	102.30	112.00
1	B	288	PRO	CA-N-CD	-6.93	102.30	112.00
1	A	287	PRO	CA-C-O	-6.92	115.92	120.90
1	G	216	TRP	CE2-CD2-CG	6.91	115.50	107.20
1	E	353	PRO	CA-N-CD	-6.87	102.38	112.00
1	H	288	PRO	CA-N-CD	-6.87	102.39	112.00
1	A	353	PRO	CA-N-CD	-6.86	102.39	112.00
1	G	353	PRO	CA-N-CD	-6.85	102.41	112.00
1	A	114	ARG	NE-CZ-NH2	-6.79	113.09	119.20
1	H	378	MET	CG-SD-CE	-6.78	85.97	100.90
1	E	322	LEU	CA-CB-CG	6.69	139.72	116.30
1	H	114	ARG	NE-CZ-NH2	6.67	125.20	119.20
1	F	25	GLN	CA-C-N	-6.56	109.58	121.32
1	F	25	GLN	C-N-CA	-6.56	109.58	121.32
1	H	25	GLN	CA-C-N	-6.52	109.64	121.32
1	H	25	GLN	C-N-CA	-6.52	109.64	121.32
1	G	161	LEU	CB-CA-C	6.52	122.50	110.56
1	A	453	ARG	NH1-CZ-NH2	-6.51	110.84	119.30
1	G	231	PRO	CA-C-O	-6.47	116.24	120.90
1	A	295	PRO	CA-C-O	-6.45	116.25	120.90
1	B	19	MET	CA-C-O	6.45	127.43	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	TRP	CH2-CZ2-CE2	6.41	125.83	117.50
1	H	200	GLN	CB-CG-CD	6.40	123.48	112.60
1	E	216	TRP	CH2-CZ2-CE2	6.39	125.81	117.50
1	G	287	PRO	CA-C-O	-6.38	116.31	120.90
1	H	599	ALA	O-C-N	-6.38	115.50	122.07
1	G	403	ARG	NE-CZ-NH1	-6.36	115.14	121.50
1	B	463	GLY	N-CA-C	-6.34	105.87	115.00
1	F	230	TRP	CA-CB-CG	6.34	125.65	113.60
1	H	49	ARG	NE-CZ-NH2	-6.31	113.52	119.20
1	A	196	MET	O-C-N	-6.31	114.30	122.56
1	E	161	LEU	CB-CA-C	6.28	121.38	111.39
1	G	197	ARG	CB-CG-CD	6.28	125.74	111.30
1	H	199	ARG	CB-CG-CD	6.27	125.72	111.30
1	B	196	MET	CA-C-O	6.25	130.82	122.44
1	B	161	LEU	CD1-CG-CD2	6.25	124.55	110.80
1	H	161	LEU	O-C-N	-6.25	113.83	122.46
1	B	200	GLN	CB-CG-CD	6.23	123.19	112.60
1	B	49	ARG	NE-CZ-NH2	-6.20	113.62	119.20
1	F	453	ARG	NH1-CZ-NH2	-6.20	111.23	119.30
1	H	161	LEU	CA-C-O	6.19	127.09	119.05
1	F	441	ALA	CB-CA-C	-6.18	100.53	110.79
1	H	463	GLY	N-CA-C	-6.18	106.42	115.63
1	F	403	ARG	NH1-CZ-NH2	-6.17	111.28	119.30
1	F	49	ARG	NE-CZ-NH2	-6.17	113.65	119.20
1	G	196	MET	O-C-N	-6.17	114.47	122.61
1	E	322	LEU	N-CA-C	-6.09	105.78	112.72
1	A	216	TRP	CE2-CD2-CG	6.07	114.48	107.20
1	G	488	HIS	CE1-NE2-CD2	-6.06	102.94	109.00
1	E	216	TRP	CE2-CD2-CG	6.02	114.42	107.20
1	F	121	ALA	N-CA-CB	6.00	120.63	110.49
1	G	488	HIS	ND1-CG-CD2	-5.99	100.11	106.10
1	E	356	TYR	CE1-CZ-CE2	-5.98	108.34	120.30
1	H	407	ALA	N-CA-CB	-5.96	101.35	110.12
1	F	231	PRO	CA-C-O	-5.95	116.61	120.90
1	H	121	ALA	N-CA-CB	5.95	120.55	110.49
1	E	356	TYR	CA-CB-CG	-5.92	103.24	113.90
1	B	121	ALA	N-CA-CB	5.91	120.48	110.49
1	H	449	GLU	CA-CB-CG	5.90	125.91	114.10
1	A	216	TRP	CZ3-CH2-CZ2	-5.88	113.85	121.50
1	E	295	PRO	CA-C-O	-5.88	116.67	120.90
1	A	231	PRO	CA-C-O	-5.86	116.68	120.90
1	E	216	TRP	CZ3-CH2-CZ2	-5.85	113.90	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	437	ARG	NE-CZ-NH1	-5.83	115.67	121.50
1	B	383	GLU	CG-CD-OE1	5.82	131.80	118.40
1	B	161	LEU	CA-C-O	5.77	128.14	118.91
1	B	437	ARG	NE-CZ-NH1	-5.76	115.74	121.50
1	H	431	LEU	N-CA-CB	-5.74	100.75	109.94
1	H	453	ARG	CG-CD-NE	5.71	124.57	112.00
1	F	116	ALA	O-C-N	-5.69	114.66	122.46
1	B	157	ARG	CD-NE-CZ	5.68	132.35	124.40
1	E	196	MET	O-C-N	-5.67	115.12	122.61
1	H	116	ALA	O-C-N	-5.67	114.69	122.46
1	E	84	TRP	CD2-CE2-CZ2	-5.65	116.75	122.40
1	E	231	PRO	CA-C-O	-5.65	116.83	120.90
1	F	378	MET	CG-SD-CE	-5.64	88.49	100.90
1	A	385	ARG	N-CA-C	-5.62	106.10	114.64
1	A	407	ALA	N-CA-CB	-5.59	101.91	110.12
1	E	20	GLN	CG-CD-NE2	-5.56	108.06	116.40
1	H	388	HIS	CA-C-N	5.55	130.07	123.19
1	H	388	HIS	C-N-CA	5.55	130.07	123.19
1	E	212	ILE	CA-C-N	-5.54	111.33	121.52
1	E	212	ILE	C-N-CA	-5.54	111.33	121.52
1	G	547	THR	N-CA-C	-5.54	101.24	109.94
1	E	287	PRO	CA-C-O	-5.54	116.91	120.90
1	A	157	ARG	NE-CZ-NH1	5.53	127.03	121.50
1	E	385	ARG	N-CA-C	-5.53	106.23	114.64
1	G	20	GLN	CG-CD-NE2	-5.53	108.11	116.40
1	A	20	GLN	CG-CD-NE2	-5.52	108.12	116.40
1	G	212	ILE	CA-C-N	-5.52	111.36	121.52
1	G	212	ILE	C-N-CA	-5.52	111.36	121.52
1	E	114	ARG	NE-CZ-NH1	-5.52	115.98	121.50
1	G	385	ARG	N-CA-C	-5.51	106.26	114.64
1	F	408	ARG	CD-NE-CZ	5.51	132.11	124.40
1	A	212	ILE	CA-C-N	-5.49	111.42	121.52
1	A	212	ILE	C-N-CA	-5.49	111.42	121.52
1	F	19	MET	CA-C-O	5.47	126.17	119.05
1	H	19	MET	CA-C-O	5.46	126.15	119.05
1	H	236	ARG	N-CA-C	5.45	117.22	111.28
1	B	72	SER	N-CA-C	5.44	118.31	109.06
1	A	30	VAL	CA-CB-CG2	-5.41	101.20	110.40
1	A	212	ILE	O-C-N	-5.39	115.83	122.57
1	F	196	MET	O-C-N	-5.39	115.49	122.61
1	E	435	GLU	OE1-CD-OE2	5.39	135.83	122.90
1	F	403	ARG	NE-CZ-NH2	5.39	124.05	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	80	GLU	N-CA-C	-5.38	105.50	111.36
1	G	435	GLU	OE1-CD-OE2	5.38	135.81	122.90
1	H	161	LEU	CD1-CG-CD2	5.36	122.60	110.80
1	A	435	GLU	OE1-CD-OE2	5.35	135.73	122.90
1	G	453	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	G	114	ARG	CD-NE-CZ	-5.30	116.97	124.40
1	H	198	LEU	CA-C-N	-5.29	111.88	120.72
1	H	198	LEU	C-N-CA	-5.29	111.88	120.72
1	E	212	ILE	O-C-N	-5.29	115.96	122.57
1	B	116	ALA	O-C-N	-5.28	114.86	122.36
1	G	548	ASP	N-CA-C	-5.27	106.17	113.18
1	G	212	ILE	O-C-N	-5.22	116.04	122.57
1	H	431	LEU	CB-CG-CD2	-5.21	95.08	110.70
1	E	466	ASP	CB-CG-OD1	-5.19	106.46	118.40
1	B	196	MET	CG-SD-CE	-5.18	89.51	100.90
1	E	84	TRP	CE3-CZ3-CH2	5.16	127.80	121.10
1	B	453	ARG	CG-CD-NE	5.16	123.34	112.00
1	E	174	SER	N-CA-CB	5.15	120.65	111.69
1	B	120	GLY	O-C-N	-5.14	116.01	122.70
1	A	174	SER	N-CA-CB	5.13	120.62	111.69
1	G	73	GLU	N-CA-CB	5.13	117.67	110.12
1	E	437	ARG	NE-CZ-NH1	-5.12	116.38	121.50
1	F	71	ARG	CA-C-O	-5.12	113.44	119.48
1	B	71	ARG	CA-C-N	5.10	131.14	122.37
1	B	71	ARG	C-N-CA	5.10	131.14	122.37
1	B	164	GLU	CB-CG-CD	-5.10	103.93	112.60
1	H	120	GLY	O-C-N	-5.09	116.08	122.70
1	F	120	GLY	O-C-N	-5.09	116.08	122.70
1	A	100	CYS	CA-CB-SG	5.08	126.09	114.40
1	G	100	CYS	CA-CB-SG	5.08	126.09	114.40
1	G	295	PRO	CA-C-O	-5.08	117.24	120.90
1	G	407	ALA	N-CA-CB	-5.08	102.65	110.12
1	F	72	SER	CB-CA-C	5.07	119.72	109.68
1	H	434	PHE	CD1-CG-CD2	-5.06	111.01	118.60
1	B	243	ASP	CB-CG-OD2	-5.06	106.77	118.40
1	A	16	PRO	CA-C-O	-5.06	111.86	119.55
1	A	88	LEU	CB-CG-CD2	-5.05	95.55	110.70
1	F	164	GLU	CB-CG-CD	-5.05	104.01	112.60
1	H	243	ASP	CB-CG-OD2	-5.05	106.78	118.40
1	E	88	LEU	CB-CG-CD2	-5.05	95.56	110.70
1	G	88	LEU	CB-CG-CD2	-5.04	95.58	110.70
1	H	164	GLU	CB-CG-CD	-5.04	104.03	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	100	CYS	CA-CB-SG	5.03	125.98	114.40
1	G	16	PRO	CA-C-O	-5.03	111.90	119.55
1	B	207	GLU	CB-CG-CD	5.02	121.14	112.60
1	E	16	PRO	CA-C-O	-5.01	111.93	119.55
1	A	114	ARG	CD-NE-CZ	-5.01	117.39	124.40

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	212	ILE	Mainchain
1	A	41	SER	Mainchain
1	A	98	TYR	Sidechain
1	B	120	GLY	Mainchain
1	B	164	GLU	Sidechain
1	B	453	ARG	Sidechain
1	B	72	SER	Mainchain
1	E	157	ARG	Sidechain
1	E	212	ILE	Mainchain
1	E	356	TYR	Sidechain
1	E	403	ARG	Sidechain
1	E	41	SER	Mainchain
1	E	98	TYR	Sidechain
1	F	120	GLY	Mainchain
1	F	164	GLU	Sidechain
1	F	453	ARG	Sidechain
1	F	72	SER	Mainchain
1	G	212	ILE	Mainchain
1	G	403	ARG	Sidechain
1	G	41	SER	Mainchain
1	G	488	HIS	Sidechain
1	G	98	TYR	Sidechain
1	H	120	GLY	Mainchain
1	H	164	GLU	Sidechain
1	H	434	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	4768	0	4731	269	0
1	B	4760	0	4727	304	0
1	E	4768	0	4731	280	0
1	F	4760	0	4727	265	0
1	G	4768	0	4731	257	0
1	H	4760	0	4727	281	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
All	All	28590	0	28374	1430	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 25.

All (1430) 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:216:TRP:CE3	1:A:216:TRP:CZ3	1.83	1.62
1:G:216:TRP:CZ3	1:G:216:TRP:CE3	1.84	1.55
1:E:216:TRP:CZ3	1:E:216:TRP:CE3	1.83	1.49
1:G:403:ARG:CG	1:G:403:ARG:CA	1.98	1.39
1:E:157:ARG:CD	1:E:157:ARG:CB	2.03	1.34
1:G:403:ARG:CG	1:G:403:ARG:CD	2.10	1.28
1:E:157:ARG:CG	1:E:157:ARG:NE	2.00	1.23
1:A:19:MET:HE1	1:A:30:VAL:HG21	1.20	1.18
1:H:196:MET:CE	1:H:196:MET:CG	2.33	1.07
1:H:157:ARG:HG2	1:G:72:SER:HA	1.37	1.06
1:H:157:ARG:HE	1:G:72:SER:HB2	1.19	1.05
1:H:114:ARG:NH1	1:G:161:LEU:HB3	1.71	1.03
1:B:251:VAL:HG11	1:B:562:LEU:HD11	1.37	1.02
1:E:157:ARG:CG	1:E:157:ARG:HD3	1.52	1.02
1:H:328:LEU:HD21	1:H:370:ILE:HD13	1.37	1.02
1:E:157:ARG:CG	1:E:157:ARG:HD2	1.52	1.01
1:B:157:ARG:HG2	1:A:72:SER:HA	1.40	1.00
1:E:157:ARG:CD	1:E:157:ARG:HG3	1.52	1.00
1:E:157:ARG:CD	1:E:157:ARG:HG2	1.52	1.00
1:H:196:MET:CE	1:H:196:MET:SD	0.89	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ARG:NE	1:A:73:GLU:H	1.60	0.98
1:A:88:LEU:HD11	1:A:174:SER:HA	1.47	0.97
1:E:88:LEU:HD11	1:E:174:SER:HA	1.47	0.97
1:B:157:ARG:HE	1:A:73:GLU:N	1.64	0.96
1:B:72:SER:HA	1:A:157:ARG:HD2	1.49	0.95
1:F:72:SER:HA	1:E:157:ARG:HE	1.31	0.95
1:E:403:ARG:NE	1:H:453:ARG:HD2	1.82	0.95
1:H:196:MET:SD	1:H:196:MET:HE1	1.52	0.94
1:A:444:PHE:HB3	1:A:477:LYS:HZ1	1.33	0.93
1:B:161:LEU:HB3	1:A:114:ARG:NH2	1.83	0.93
1:B:378:MET:HE1	1:B:389:VAL:H	1.31	0.93
1:H:196:MET:SD	1:H:196:MET:HE2	1.52	0.93
1:H:213:LEU:HD11	1:H:236:ARG:HE	1.31	0.93
1:H:196:MET:SD	1:H:196:MET:HE3	1.52	0.93
1:E:575:GLU:HA	1:E:578:LYS:HD3	1.51	0.92
1:G:403:ARG:CG	1:G:403:ARG:HB2	1.41	0.92
1:A:450:PRO:HB3	1:F:407:ALA:HB1	1.50	0.92
1:H:254:LEU:HD12	1:H:255:PRO:HD2	1.51	0.92
1:B:449:GLU:HB3	1:G:403:ARG:CZ	2.00	0.92
1:G:403:ARG:CG	1:G:403:ARG:HB3	1.41	0.91
1:F:397:ARG:HD3	1:F:402:ASP:H	1.34	0.91
1:H:19:MET:HE1	1:H:26:GLY:HA2	1.53	0.91
1:F:397:ARG:HD2	1:F:398:GLU:H	1.33	0.91
1:E:77:MET:HE1	1:E:196:MET:HG3	1.53	0.91
1:F:19:MET:HE1	1:F:26:GLY:HA2	1.53	0.90
1:G:403:ARG:CB	1:G:403:ARG:HG2	1.38	0.90
1:E:157:ARG:CD	1:E:157:ARG:CG	0.90	0.90
1:F:19:MET:O	1:F:19:MET:HE3	1.71	0.90
1:H:19:MET:HE3	1:H:19:MET:O	1.71	0.90
1:G:195:ASP:OD2	1:G:197:ARG:HG3	1.72	0.90
1:B:558:THR:O	1:B:562:LEU:HD13	1.73	0.89
1:H:196:MET:HE3	1:H:196:MET:O	1.73	0.89
1:H:213:LEU:HD21	1:H:236:ARG:HG3	1.55	0.88
1:H:602:ALA:HB3	1:G:216:TRP:HE1	1.38	0.88
1:B:407:ALA:HB1	1:G:450:PRO:HB3	1.54	0.88
1:E:403:ARG:HE	1:H:453:ARG:HD2	1.34	0.88
1:A:196:MET:SD	1:A:200:GLN:HG3	2.13	0.88
1:F:114:ARG:HD2	1:E:161:LEU:HD23	1.55	0.88
1:H:402:ASP:HB2	1:H:405:ARG:HG2	1.54	0.88
1:G:403:ARG:CB	1:G:403:ARG:HG3	1.38	0.88
1:B:254:LEU:HD12	1:B:255:PRO:HD2	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:MET:HE2	1:B:26:GLY:HA2	1.55	0.87
1:B:450:PRO:HB3	1:G:407:ALA:HB1	1.55	0.87
1:F:342:ASP:OD1	1:F:556:SER:HB2	1.75	0.87
1:E:407:ALA:HB1	1:H:450:PRO:HB3	1.57	0.87
1:E:449:GLU:HG2	1:H:403:ARG:HH22	1.37	0.86
1:B:114:ARG:NH1	1:A:161:LEU:HB3	1.91	0.86
1:A:407:ALA:HB1	1:F:450:PRO:HB3	1.56	0.86
1:E:80:GLU:HG2	1:E:84:TRP:CZ2	2.11	0.85
1:H:196:MET:HE3	1:H:200:GLN:HG3	1.60	0.84
1:A:53:MET:HE1	1:A:144:LEU:HD21	1.59	0.84
1:E:450:PRO:HB3	1:H:407:ALA:HB1	1.58	0.84
1:B:161:LEU:HB3	1:A:114:ARG:HH22	1.42	0.84
1:A:375:GLN:HE22	1:A:423:GLY:HA3	1.44	0.83
1:H:19:MET:CE	1:H:26:GLY:HA2	2.09	0.83
1:F:19:MET:CE	1:F:26:GLY:HA2	2.09	0.83
1:E:84:TRP:HH2	1:E:199:ARG:HD3	1.44	0.83
1:E:403:ARG:HH21	1:H:453:ARG:HG3	1.44	0.83
1:A:350:ARG:HH22	1:A:459:THR:HG21	1.44	0.82
1:A:19:MET:CE	1:A:30:VAL:HG21	2.07	0.82
1:E:53:MET:HE1	1:E:144:LEU:HD21	1.59	0.82
1:G:375:GLN:HE22	1:G:423:GLY:HA3	1.44	0.82
1:G:109:SER:HA	1:G:112:MET:HE3	1.63	0.81
1:F:161:LEU:HG	1:E:114:ARG:NH2	1.95	0.81
1:E:375:GLN:HE22	1:E:423:GLY:HA3	1.44	0.81
1:B:403:ARG:NH1	1:G:453:ARG:HH21	1.79	0.81
1:F:73:GLU:N	1:E:157:ARG:HH21	1.78	0.80
1:A:101:LEU:HD21	1:A:126:HIS:HB2	1.61	0.80
1:F:230:TRP:HB2	1:F:235:LEU:HD21	1.61	0.80
1:B:19:MET:HE3	1:B:19:MET:O	1.81	0.80
1:H:453:ARG:HH22	1:G:472:TRP:CD1	1.99	0.80
1:B:453:ARG:HG2	1:G:403:ARG:HH21	1.45	0.79
1:H:196:MET:CE	1:H:200:GLN:HG3	2.12	0.79
1:A:2:ARG:HG3	1:A:98:TYR:CZ	2.17	0.79
1:H:374:PHE:O	1:H:378:MET:HG3	1.83	0.79
1:H:449:GLU:HG2	1:H:450:PRO:HD3	1.62	0.79
1:G:53:MET:HE3	1:G:54:HIS:CE1	2.17	0.79
1:E:2:ARG:HG3	1:E:98:TYR:CZ	2.17	0.79
1:E:403:ARG:CZ	1:H:449:GLU:HB2	2.13	0.79
1:A:132:ARG:HH21	1:A:155:ALA:HB2	1.47	0.79
1:G:132:ARG:HH21	1:G:155:ALA:HB2	1.48	0.79
1:E:19:MET:SD	1:E:27:PHE:HB2	2.22	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:ARG:HH21	1:E:155:ALA:HB2	1.47	0.78
1:E:350:ARG:HH22	1:E:459:THR:HG21	1.46	0.78
1:B:114:ARG:HH12	1:A:161:LEU:HB3	1.45	0.78
1:G:2:ARG:HG3	1:G:98:TYR:CZ	2.17	0.78
1:G:350:ARG:HH22	1:G:459:THR:HG21	1.48	0.78
1:B:76:HIS:HE1	1:B:111:ALA:HB2	1.48	0.78
1:G:403:ARG:CG	1:G:403:ARG:CB	0.78	0.77
1:F:302:GLU:HG2	1:F:303:GLU:OE1	1.84	0.77
1:H:434:PHE:HD2	1:H:462:ALA:CB	1.97	0.77
1:F:196:MET:SD	1:F:199:ARG:HB3	2.24	0.77
1:A:19:MET:SD	1:A:27:PHE:HB2	2.24	0.77
1:H:434:PHE:HD2	1:H:462:ALA:HB2	1.50	0.77
1:F:173:LEU:HD21	1:F:201:HIS:CE1	2.20	0.77
1:E:437:ARG:HE	1:E:440:ARG:HE	1.30	0.76
1:H:196:MET:HE1	1:H:200:GLN:N	2.01	0.76
1:H:161:LEU:HA	1:G:114:ARG:HH12	1.49	0.76
1:H:328:LEU:HD11	1:H:370:ILE:HD11	1.68	0.76
1:B:602:ALA:HB3	1:A:216:TRP:HE1	1.51	0.75
1:F:72:SER:HA	1:E:157:ARG:NE	2.00	0.75
1:B:302:GLU:HG2	1:B:303:GLU:OE1	1.84	0.75
1:H:336:TYR:CD2	1:H:377:ALA:HB1	2.21	0.75
1:B:251:VAL:CG1	1:B:562:LEU:HD11	2.13	0.75
1:A:80:GLU:HG2	1:A:84:TRP:CZ2	2.21	0.75
1:F:602:ALA:HB3	1:E:216:TRP:HE1	1.51	0.75
1:G:488:HIS:HD2	1:G:491:ARG:CZ	1.99	0.75
1:E:449:GLU:HG2	1:H:403:ARG:NH2	2.00	0.75
1:H:437:ARG:HH22	1:H:441:ALA:HB2	1.52	0.75
1:H:161:LEU:HB3	1:G:114:ARG:NH2	2.01	0.74
1:H:342:ASP:OD2	1:H:556:SER:HB2	1.87	0.74
1:B:207:GLU:HA	1:B:210:ARG:HE	1.52	0.74
1:A:19:MET:HE1	1:A:30:VAL:CG2	2.10	0.74
1:H:397:ARG:HH22	1:H:439:THR:HG22	1.53	0.74
1:E:101:LEU:HD21	1:E:126:HIS:HB2	1.69	0.74
1:G:463:GLY:HA3	1:G:486:ALA:HA	1.70	0.73
1:A:444:PHE:HB3	1:A:477:LYS:NZ	2.02	0.73
1:B:70:LEU:HD23	1:A:157:ARG:HH12	1.53	0.73
1:F:31:HIS:CG	1:F:90:ARG:HD3	2.23	0.73
1:H:207:GLU:HA	1:H:210:ARG:HE	1.53	0.73
1:B:437:ARG:HH22	1:B:441:ALA:HB2	1.52	0.73
1:E:84:TRP:CH2	1:E:199:ARG:HD3	2.23	0.73
1:F:254:LEU:HD12	1:F:255:PRO:HD2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:LEU:HD11	1:G:174:SER:HA	1.71	0.73
1:F:397:ARG:HD3	1:F:402:ASP:N	2.04	0.73
1:B:72:SER:HA	1:A:157:ARG:CD	2.19	0.73
1:B:157:ARG:HE	1:A:73:GLU:H	0.83	0.73
1:A:463:GLY:HA3	1:A:486:ALA:HA	1.70	0.72
1:E:468:VAL:HG23	1:E:495:LEU:HD22	1.71	0.72
1:H:294:LEU:HD23	1:H:313:LEU:HD22	1.71	0.72
1:A:196:MET:HE1	1:A:200:GLN:HE21	1.55	0.72
1:H:397:ARG:HG2	1:H:398:GLU:H	1.54	0.72
1:A:196:MET:HE1	1:A:200:GLN:NE2	2.05	0.72
1:F:124:VAL:O	1:F:161:LEU:HB2	1.90	0.72
1:E:80:GLU:HG2	1:E:84:TRP:CE2	2.25	0.71
1:A:407:ALA:CB	1:F:450:PRO:HB3	2.19	0.71
1:E:129:CYS:HB3	1:E:140:GLU:HG3	1.72	0.71
1:B:76:HIS:CE1	1:B:111:ALA:HB2	2.25	0.71
1:E:463:GLY:HA3	1:E:486:ALA:HA	1.70	0.71
1:B:161:LEU:HA	1:A:114:ARG:HH12	1.53	0.71
1:G:403:ARG:CD	1:G:403:ARG:CB	2.68	0.71
1:F:207:GLU:HA	1:F:210:ARG:HE	1.55	0.71
1:B:1:MET:SD	1:B:2:ARG:HG3	2.30	0.70
1:G:129:CYS:HB3	1:G:140:GLU:HG3	1.72	0.70
1:B:157:ARG:NH2	1:A:73:GLU:HB3	2.06	0.70
1:H:213:LEU:CD2	1:H:236:ARG:HG3	2.22	0.70
1:F:1:MET:SD	1:F:2:ARG:HG3	2.31	0.70
1:G:488:HIS:CD2	1:G:491:ARG:NH1	2.59	0.70
1:A:101:LEU:C	1:A:101:LEU:HD12	2.17	0.70
1:F:340:LEU:HD11	1:F:381:THR:HG21	1.73	0.70
1:H:602:ALA:HB3	1:G:216:TRP:NE1	2.06	0.70
1:A:408:ARG:HD3	1:F:418:GLU:OE1	1.90	0.70
1:B:289:VAL:HG13	1:B:316:ASN:HD21	1.57	0.70
1:F:289:VAL:HG13	1:F:316:ASN:HD21	1.57	0.70
1:E:2:ARG:HG3	1:E:98:TYR:OH	1.92	0.70
1:A:2:ARG:HG3	1:A:98:TYR:OH	1.92	0.70
1:A:129:CYS:HB3	1:A:140:GLU:HG3	1.72	0.70
1:F:173:LEU:HD21	1:F:201:HIS:HE1	1.53	0.70
1:H:213:LEU:HD11	1:H:236:ARG:NE	2.07	0.70
1:A:84:TRP:HH2	1:A:199:ARG:HD3	1.56	0.69
1:G:431:LEU:HB3	1:G:443:MET:CE	2.22	0.69
1:B:450:PRO:HB3	1:G:407:ALA:CB	2.21	0.69
1:A:49:ARG:HG3	1:A:53:MET:CE	2.23	0.69
1:A:471:ILE:HG23	1:A:483:LEU:HD21	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ARG:HE	1:G:449:GLU:HG2	1.56	0.69
1:A:305:ILE:HB	1:A:309:ARG:HD3	1.75	0.69
1:G:2:ARG:HG3	1:G:98:TYR:OH	1.93	0.69
1:G:305:ILE:HB	1:G:309:ARG:HD3	1.75	0.69
1:B:562:LEU:HD12	1:B:562:LEU:N	2.08	0.69
1:H:114:ARG:HH11	1:G:161:LEU:HB3	1.53	0.69
1:F:434:PHE:HB3	1:F:462:ALA:HB2	1.75	0.69
1:E:49:ARG:HG3	1:E:53:MET:CE	2.22	0.69
1:H:157:ARG:CZ	1:G:73:GLU:H	2.06	0.69
1:E:305:ILE:HB	1:E:309:ARG:HD3	1.75	0.69
1:B:453:ARG:HE	1:G:403:ARG:NH1	1.91	0.68
1:G:403:ARG:CA	1:G:403:ARG:HG3	1.93	0.68
1:B:434:PHE:HB3	1:B:462:ALA:HB2	1.76	0.68
1:H:289:VAL:HG13	1:H:316:ASN:HD21	1.57	0.68
1:H:114:ARG:HD2	1:G:161:LEU:HD23	1.75	0.68
1:F:161:LEU:HA	1:E:114:ARG:HH12	1.59	0.68
1:H:5:LEU:HD22	1:H:86:TRP:CZ3	2.28	0.68
1:B:414:ILE:HG23	1:B:454:VAL:HG11	1.76	0.68
1:F:453:ARG:NH2	1:E:472:TRP:CG	2.62	0.68
1:B:161:LEU:HB3	1:A:114:ARG:CZ	2.23	0.68
1:F:414:ILE:HG23	1:F:454:VAL:HG11	1.76	0.68
1:G:108:ILE:HG22	1:G:112:MET:CE	2.24	0.68
1:H:414:ILE:HG23	1:H:454:VAL:HG11	1.76	0.67
1:E:439:THR:O	1:E:443:MET:HG2	1.93	0.67
1:G:326:GLY:HA2	1:G:329:ARG:HH12	1.58	0.67
1:B:340:LEU:HD11	1:B:381:THR:HG21	1.76	0.67
1:B:378:MET:CE	1:B:389:VAL:H	2.04	0.67
1:B:418:GLU:OE2	1:G:408:ARG:HG2	1.92	0.67
1:F:434:PHE:HB3	1:F:462:ALA:CB	2.24	0.67
1:A:206:LEU:HD13	1:A:210:ARG:HH22	1.59	0.67
1:F:453:ARG:HH12	1:E:472:TRP:HB3	1.59	0.67
1:G:5:LEU:HD22	1:G:86:TRP:CH2	2.30	0.67
1:B:403:ARG:HE	1:G:449:GLU:CG	2.08	0.67
1:A:53:MET:HG3	1:A:54:HIS:ND1	2.10	0.67
1:G:19:MET:HE1	1:G:27:PHE:HB2	1.75	0.67
1:F:268:THR:HG21	1:F:552:ILE:HG13	1.77	0.66
1:E:53:MET:HG3	1:E:54:HIS:ND1	2.11	0.66
1:G:3:ILE:N	1:G:98:TYR:HE2	1.93	0.66
1:G:439:THR:O	1:G:443:MET:HG2	1.95	0.66
1:E:196:MET:SD	1:E:199:ARG:HB3	2.35	0.66
1:A:3:ILE:N	1:A:98:TYR:HE2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:161:LEU:HB3	1:G:114:ARG:HH22	1.60	0.66
1:A:84:TRP:CH2	1:A:199:ARG:HD3	2.30	0.66
1:B:70:LEU:CD2	1:A:157:ARG:HH22	2.09	0.66
1:E:329:ARG:HG3	1:E:373:HIS:CE1	2.31	0.66
1:H:196:MET:HE1	1:H:199:ARG:HB3	1.76	0.66
1:B:118:LEU:HD11	1:B:206:LEU:HD11	1.77	0.66
1:F:86:TRP:NE1	1:F:90:ARG:HD2	2.11	0.66
1:B:217:GLU:HG2	1:A:171:ARG:HH12	1.61	0.66
1:A:466:ASP:OD2	1:A:491:ARG:HD2	1.95	0.66
1:A:76:HIS:NE2	1:A:111:ALA:HB2	2.11	0.66
1:H:340:LEU:HD11	1:H:381:THR:HG21	1.78	0.66
1:H:397:ARG:NH2	1:H:439:THR:HG22	2.10	0.66
1:G:244:PRO:HG3	1:G:565:ALA:HB3	1.78	0.66
1:F:118:LEU:HD11	1:F:206:LEU:HD11	1.79	0.65
1:E:3:ILE:H	1:E:98:TYR:HE2	1.44	0.65
1:E:3:ILE:N	1:E:98:TYR:HE2	1.94	0.65
1:B:110:ALA:HB1	1:A:161:LEU:HD21	1.78	0.65
1:A:3:ILE:H	1:A:98:TYR:HE2	1.44	0.65
1:A:418:GLU:OE2	1:A:421:LYS:HE2	1.96	0.65
1:B:563:LEU:HG	1:B:567:LEU:HD23	1.78	0.65
1:G:76:HIS:NE2	1:G:111:ALA:HB2	2.11	0.65
1:B:403:ARG:NH2	1:G:453:ARG:HE	1.93	0.65
1:H:462:ALA:HB1	1:H:466:ASP:OD2	1.97	0.65
1:E:244:PRO:HG3	1:E:565:ALA:HB3	1.78	0.65
1:H:302:GLU:HG2	1:H:303:GLU:OE1	1.97	0.65
1:G:488:HIS:CD2	1:G:491:ARG:CZ	2.79	0.65
1:B:157:ARG:HH22	1:A:74:GLN:NE2	1.94	0.65
1:H:161:LEU:CA	1:G:114:ARG:HH12	2.08	0.65
1:F:453:ARG:HH22	1:E:472:TRP:CG	2.13	0.65
1:H:402:ASP:HB2	1:H:405:ARG:CG	2.26	0.65
1:A:5:LEU:HD23	1:A:86:TRP:CZ3	2.32	0.65
1:H:118:LEU:HD11	1:H:206:LEU:HD11	1.79	0.64
1:H:157:ARG:NE	1:G:73:GLU:H	1.95	0.64
1:F:563:LEU:HG	1:F:567:LEU:HD23	1.78	0.64
1:B:19:MET:CE	1:B:26:GLY:HA2	2.27	0.64
1:G:168:PRO:O	1:G:171:ARG:HG2	1.97	0.64
1:F:72:SER:C	1:E:157:ARG:HH21	2.05	0.64
1:B:403:ARG:HH12	1:G:453:ARG:HH21	1.43	0.64
1:A:101:LEU:HD11	1:A:126:HIS:ND1	2.12	0.64
1:A:244:PRO:HG3	1:A:565:ALA:HB3	1.78	0.64
1:H:397:ARG:HD2	1:H:402:ASP:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:196:MET:SD	1:F:200:GLN:HG3	2.38	0.64
1:F:271:GLU:OE2	1:F:275:LYS:HE3	1.97	0.64
1:G:3:ILE:H	1:G:98:TYR:HE2	1.44	0.64
1:G:77:MET:HG2	1:G:199:ARG:NH1	2.13	0.63
1:E:407:ALA:CB	1:H:450:PRO:HB3	2.25	0.63
1:H:453:ARG:HH22	1:G:472:TRP:CG	2.15	0.63
1:G:511:TYR:HE1	1:G:563:LEU:HD13	1.63	0.63
1:A:21:LEU:HB3	1:A:27:PHE:HZ	1.64	0.63
1:F:114:ARG:CZ	1:E:161:LEU:HB3	2.29	0.63
1:B:143:THR:HG22	1:B:144:LEU:HG	1.81	0.63
1:F:31:HIS:CB	1:F:90:ARG:HD3	2.28	0.63
1:E:196:MET:SD	1:E:200:GLN:HG3	2.39	0.63
1:E:437:ARG:NH2	1:E:440:ARG:HH21	1.96	0.63
1:E:511:TYR:HE1	1:E:563:LEU:HD13	1.63	0.63
1:E:5:LEU:HD23	1:E:86:TRP:CZ3	2.33	0.63
1:E:490:SER:HA	1:E:496:LEU:HD11	1.81	0.63
1:G:109:SER:HA	1:G:112:MET:CG	2.29	0.63
1:G:196:MET:SD	1:G:199:ARG:HB3	2.39	0.63
1:E:53:MET:HE1	1:E:144:LEU:CD2	2.29	0.63
1:B:251:VAL:HG11	1:B:562:LEU:CD1	2.22	0.63
1:A:80:GLU:HG2	1:A:84:TRP:CE2	2.33	0.63
1:A:84:TRP:HZ3	1:A:199:ARG:HA	1.64	0.63
1:H:143:THR:HG22	1:H:144:LEU:HG	1.81	0.63
1:A:419:HIS:HD2	1:F:362:SER:OG	1.81	0.62
1:A:594:ARG:HG3	1:A:598:TRP:CD1	2.33	0.62
1:G:21:LEU:HB3	1:G:27:PHE:HZ	1.64	0.62
1:G:490:SER:HA	1:G:496:LEU:HD11	1.81	0.62
1:A:53:MET:HE1	1:A:144:LEU:CD2	2.29	0.62
1:A:511:TYR:HE1	1:A:563:LEU:HD13	1.63	0.62
1:F:46:GLN:O	1:F:49:ARG:HD3	2.00	0.62
1:E:21:LEU:HB3	1:E:27:PHE:HZ	1.64	0.62
1:H:124:VAL:O	1:H:161:LEU:HB2	2.00	0.62
1:A:77:MET:HG2	1:A:199:ARG:NH1	2.14	0.62
1:A:350:ARG:NH2	1:A:459:THR:HG21	2.14	0.62
1:A:114:ARG:O	1:A:118:LEU:HD23	2.00	0.62
1:H:46:GLN:O	1:H:49:ARG:HD3	1.99	0.62
1:H:254:LEU:HD12	1:H:255:PRO:CD	2.28	0.62
1:H:475:VAL:HG13	1:H:504:ILE:HD11	1.81	0.62
1:B:71:ARG:C	1:A:157:ARG:HH11	2.08	0.62
1:B:602:ALA:HB3	1:A:216:TRP:NE1	2.14	0.62
1:H:84:TRP:HA	1:H:87:LEU:CD2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:109:SER:HA	1:G:112:MET:HG2	1.82	0.62
1:B:133:PHE:HA	1:B:137:GLY:HA2	1.82	0.61
1:F:133:PHE:HA	1:F:137:GLY:HA2	1.82	0.61
1:H:397:ARG:HB3	1:H:397:ARG:NH1	2.15	0.61
1:B:84:TRP:HA	1:B:87:LEU:CD2	2.30	0.61
1:A:196:MET:SD	1:A:196:MET:O	2.58	0.61
1:A:490:SER:HA	1:A:496:LEU:HD11	1.81	0.61
1:F:143:THR:HG22	1:F:144:LEU:HG	1.81	0.61
1:F:196:MET:SD	1:F:196:MET:O	2.59	0.61
1:E:50:TYR:HA	1:E:53:MET:HG2	1.83	0.61
1:H:437:ARG:HH12	1:H:441:ALA:N	1.98	0.61
1:F:63:ARG:O	1:F:190:TRP:HA	2.00	0.61
1:F:84:TRP:HA	1:F:87:LEU:CD2	2.30	0.61
1:B:31:HIS:CD2	1:B:90:ARG:HB3	2.36	0.61
1:F:602:ALA:HB3	1:E:216:TRP:NE1	2.14	0.61
1:E:114:ARG:O	1:E:118:LEU:HD23	2.00	0.61
1:H:63:ARG:O	1:H:190:TRP:HA	2.01	0.61
1:H:230:TRP:HB2	1:H:235:LEU:HD21	1.81	0.61
1:B:46:GLN:O	1:B:49:ARG:HD3	1.99	0.61
1:A:450:PRO:CB	1:F:407:ALA:HB1	2.28	0.61
1:B:437:ARG:NH2	1:B:441:ALA:HB2	2.16	0.61
1:E:109:SER:HA	1:E:112:MET:HE3	1.83	0.61
1:G:109:SER:CA	1:G:112:MET:HE3	2.31	0.61
1:F:86:TRP:HE1	1:F:90:ARG:NH1	1.99	0.61
1:E:511:TYR:HD1	1:E:563:LEU:HD22	1.66	0.61
1:B:157:ARG:HH22	1:A:74:GLN:CD	2.09	0.60
1:H:31:HIS:CD2	1:H:90:ARG:HB3	2.36	0.60
1:H:157:ARG:NH2	1:G:73:GLU:HB3	2.16	0.60
1:H:453:ARG:HH12	1:G:472:TRP:HB3	1.66	0.60
1:B:114:ARG:NH1	1:A:161:LEU:HD23	2.16	0.60
1:B:449:GLU:OE1	1:G:403:ARG:NH1	2.34	0.60
1:A:397:ARG:HB3	1:A:397:ARG:CZ	2.31	0.60
1:G:114:ARG:O	1:G:118:LEU:HD23	2.01	0.60
1:B:114:ARG:CZ	1:A:161:LEU:HB3	2.31	0.60
1:B:230:TRP:HB2	1:B:235:LEU:HD21	1.82	0.60
1:A:418:GLU:CD	1:A:418:GLU:O	2.44	0.60
1:E:124:VAL:O	1:E:161:LEU:HB2	2.01	0.60
1:G:346:TYR:HE1	1:G:348:GLU:HG3	1.66	0.60
1:B:63:ARG:O	1:B:190:TRP:HA	2.01	0.60
1:G:511:TYR:HD1	1:G:563:LEU:HD22	1.66	0.60
1:B:437:ARG:HH12	1:B:441:ALA:N	1.98	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:TYR:HA	1:A:53:MET:HG2	1.83	0.60
1:H:453:ARG:NH2	1:G:472:TRP:CD1	2.69	0.60
1:E:157:ARG:NH2	1:E:159:VAL:HG22	2.16	0.60
1:E:346:TYR:HE1	1:E:348:GLU:HG3	1.65	0.60
1:H:133:PHE:HA	1:H:137:GLY:HA2	1.82	0.60
1:G:414:ILE:HG23	1:G:454:VAL:HG11	1.84	0.60
1:B:3:ILE:HD11	1:B:31:HIS:CD2	2.37	0.60
1:A:511:TYR:HD1	1:A:563:LEU:HD22	1.66	0.60
1:E:101:LEU:HD12	1:E:101:LEU:C	2.27	0.60
1:A:6:CYS:CA	1:A:100:CYS:HB3	2.32	0.60
1:A:414:ILE:HG23	1:A:454:VAL:HG11	1.84	0.60
1:F:61:ILE:HG23	1:F:188:VAL:HG22	1.83	0.60
1:B:61:ILE:HG23	1:B:188:VAL:HG22	1.83	0.59
1:H:397:ARG:HH12	1:H:439:THR:HB	1.67	0.59
1:B:170:LEU:HD21	1:B:202:VAL:HG13	1.84	0.59
1:A:109:SER:HA	1:A:112:MET:HE3	1.82	0.59
1:E:31:HIS:CD2	1:E:90:ARG:HB3	2.37	0.59
1:E:414:ILE:HG23	1:E:454:VAL:HG11	1.84	0.59
1:H:3:ILE:HD11	1:H:31:HIS:CD2	2.37	0.59
1:H:157:ARG:HE	1:G:72:SER:CB	2.06	0.59
1:H:170:LEU:HD21	1:H:202:VAL:HG13	1.83	0.59
1:H:397:ARG:HD2	1:H:402:ASP:O	2.02	0.59
1:G:31:HIS:CD2	1:G:90:ARG:HB3	2.37	0.59
1:G:195:ASP:OD2	1:G:197:ARG:CG	2.49	0.59
1:G:403:ARG:CG	1:G:403:ARG:N	2.62	0.59
1:B:161:LEU:CA	1:A:114:ARG:HH12	2.14	0.59
1:H:514:LEU:HD11	1:H:521:LEU:HD11	1.84	0.59
1:H:61:ILE:HG23	1:H:188:VAL:HG22	1.83	0.59
1:H:434:PHE:CE1	1:H:440:ARG:HD3	2.36	0.59
1:B:251:VAL:HG21	1:B:562:LEU:HD11	1.82	0.59
1:G:84:TRP:HZ3	1:G:199:ARG:HA	1.66	0.59
1:B:159:VAL:CG1	1:A:76:HIS:HD1	2.16	0.59
1:B:402:ASP:HB2	1:B:405:ARG:HG2	1.84	0.59
1:B:514:LEU:CD1	1:B:521:LEU:HD11	2.32	0.59
1:B:514:LEU:HD11	1:B:521:LEU:HD11	1.84	0.59
1:H:114:ARG:HH12	1:G:161:LEU:HB3	1.65	0.59
1:A:19:MET:O	1:A:19:MET:HG3	2.03	0.59
1:E:488:HIS:HB3	1:E:491:ARG:HD2	1.84	0.59
1:A:50:TYR:HA	1:A:53:MET:HE3	1.85	0.59
1:F:3:ILE:HD11	1:F:31:HIS:CD2	2.36	0.59
1:F:170:LEU:HD21	1:F:202:VAL:HG13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:397:ARG:HB3	1:E:397:ARG:NH1	2.17	0.59
1:H:514:LEU:CD1	1:H:521:LEU:HD11	2.32	0.59
1:G:6:CYS:HA	1:G:100:CYS:HB3	1.85	0.59
1:B:437:ARG:HH22	1:B:441:ALA:CB	2.16	0.59
1:A:594:ARG:CD	1:A:598:TRP:HE1	2.16	0.59
1:A:31:HIS:CD2	1:A:90:ARG:HB3	2.37	0.58
1:E:6:CYS:CA	1:E:100:CYS:HB3	2.32	0.58
1:E:403:ARG:HH21	1:H:453:ARG:CG	2.15	0.58
1:G:108:ILE:HG22	1:G:112:MET:HE2	1.86	0.58
1:F:431:LEU:HD22	1:F:443:MET:SD	2.43	0.58
1:H:159:VAL:CG1	1:G:76:HIS:HD1	2.16	0.58
1:H:437:ARG:NH2	1:H:441:ALA:HB2	2.15	0.58
1:G:471:ILE:HG23	1:G:483:LEU:HD21	1.85	0.58
1:A:439:THR:O	1:A:443:MET:HG2	2.02	0.58
1:E:50:TYR:HA	1:E:53:MET:HE3	1.85	0.58
1:F:19:MET:HE1	1:F:26:GLY:CA	2.31	0.58
1:F:248:LYS:HA	1:F:562:LEU:HD21	1.86	0.58
1:E:405:ARG:HH11	1:E:405:ARG:HG3	1.68	0.58
1:E:444:PHE:HB3	1:E:477:LYS:NZ	2.18	0.58
1:E:258:GLU:OE1	1:E:546:ASN:HB3	2.03	0.58
1:E:466:ASP:OD1	1:E:488:HIS:CG	2.57	0.58
1:H:196:MET:SD	1:H:199:ARG:HB3	2.43	0.58
1:H:502:ARG:HH12	1:G:479:SER:HB3	1.69	0.58
1:B:431:LEU:HD22	1:B:443:MET:SD	2.43	0.58
1:B:124:VAL:O	1:B:161:LEU:HB2	2.02	0.58
1:H:268:THR:HG23	1:H:314:GLY:HA2	1.85	0.58
1:E:19:MET:HE1	1:E:30:VAL:HG21	1.86	0.58
1:H:251:VAL:HG13	1:H:558:THR:HG23	1.86	0.58
1:H:437:ARG:HH22	1:H:441:ALA:CB	2.16	0.58
1:B:217:GLU:CG	1:A:171:ARG:HH12	2.16	0.58
1:E:49:ARG:C	1:E:53:MET:HE3	2.29	0.58
1:H:434:PHE:CD2	1:H:462:ALA:CB	2.84	0.58
1:A:53:MET:SD	1:A:144:LEU:HD11	2.44	0.57
1:F:161:LEU:HA	1:E:114:ARG:NH1	2.19	0.57
1:F:435:GLU:OE1	1:F:464:GLU:OE2	2.22	0.57
1:E:53:MET:SD	1:E:144:LEU:HD11	2.44	0.57
1:E:361:ARG:HG2	1:E:361:ARG:HH11	1.70	0.57
1:G:444:PHE:HB3	1:G:477:LYS:NZ	2.18	0.57
1:F:268:THR:HG23	1:F:314:GLY:HA2	1.86	0.57
1:F:502:ARG:HH12	1:E:479:SER:HB3	1.69	0.57
1:E:76:HIS:HD2	1:E:76:HIS:O	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:19:MET:CE	1:G:30:VAL:HG21	2.33	0.57
1:A:88:LEU:HD21	1:A:174:SER:C	2.30	0.57
1:A:124:VAL:O	1:A:161:LEU:HB2	2.04	0.57
1:E:88:LEU:HD21	1:E:174:SER:O	2.04	0.57
1:A:594:ARG:HD2	1:A:598:TRP:HE1	1.70	0.57
1:F:203:GLU:O	1:F:207:GLU:HG3	2.05	0.57
1:E:19:MET:CE	1:E:30:VAL:HG21	2.35	0.57
1:H:488:HIS:HB3	1:H:491:ARG:HE	1.70	0.57
1:B:488:HIS:HB3	1:B:491:ARG:HE	1.70	0.57
1:G:196:MET:SD	1:G:200:GLN:HG2	2.45	0.57
1:B:502:ARG:HH12	1:A:479:SER:HB3	1.69	0.57
1:E:451:VAL:HG13	1:E:456:LEU:HB2	1.87	0.57
1:G:19:MET:CE	1:G:27:PHE:HB2	2.35	0.57
1:A:49:ARG:C	1:A:53:MET:HE3	2.29	0.57
1:A:451:VAL:HG13	1:A:456:LEU:HB2	1.87	0.57
1:B:268:THR:HG23	1:B:314:GLY:HA2	1.85	0.57
1:G:108:ILE:C	1:G:112:MET:HE3	2.30	0.57
1:F:433:GLY:O	1:F:462:ALA:HB2	2.04	0.56
1:E:196:MET:HE1	1:E:200:GLN:HG3	1.87	0.56
1:E:468:VAL:HG22	1:E:472:TRP:CD1	2.39	0.56
1:G:109:SER:HA	1:G:112:MET:CE	2.35	0.56
1:F:402:ASP:HB2	1:F:405:ARG:HG2	1.85	0.56
1:E:101:LEU:HD11	1:E:126:HIS:ND1	2.20	0.56
1:B:204:GLY:O	1:B:207:GLU:HG2	2.06	0.56
1:A:84:TRP:HB3	1:A:119:PHE:HE2	1.70	0.56
1:A:88:LEU:HD21	1:A:174:SER:O	2.04	0.56
1:A:196:MET:HG2	1:A:199:ARG:HB3	1.87	0.56
1:E:88:LEU:HD21	1:E:174:SER:C	2.30	0.56
1:E:128:LEU:HB2	1:E:157:ARG:CG	2.35	0.56
1:H:216:TRP:CE3	1:H:239:HIS:HD2	2.22	0.56
1:G:109:SER:HA	1:G:112:MET:SD	2.45	0.56
1:H:161:LEU:HB3	1:G:114:ARG:CZ	2.36	0.56
1:B:157:ARG:CZ	1:A:73:GLU:H	2.18	0.56
1:A:6:CYS:HA	1:A:100:CYS:HB3	1.87	0.56
1:F:488:HIS:HB3	1:F:491:ARG:HE	1.70	0.56
1:G:346:TYR:CE1	1:G:348:GLU:HG3	2.41	0.56
1:E:7:SER:OG	1:E:112:MET:SD	2.63	0.56
1:E:108:ILE:O	1:E:112:MET:HG3	2.06	0.56
1:E:346:TYR:CE1	1:E:348:GLU:HG3	2.41	0.56
1:G:6:CYS:CA	1:G:100:CYS:HB3	2.32	0.56
1:G:170:LEU:CD1	1:G:202:VAL:HG22	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:TRP:CE3	1:B:239:HIS:HD2	2.23	0.56
1:A:84:TRP:CZ3	1:A:199:ARG:HA	2.40	0.56
1:E:405:ARG:O	1:E:409:HIS:CD2	2.59	0.56
1:G:451:VAL:HG13	1:G:456:LEU:HB2	1.87	0.56
1:A:170:LEU:CD1	1:A:202:VAL:HG22	2.36	0.56
1:F:216:TRP:CE3	1:F:239:HIS:HD2	2.23	0.56
1:F:483:LEU:HD23	1:F:504:ILE:HG21	1.88	0.56
1:F:533:LEU:HB3	1:F:568:CYS:SG	2.46	0.56
1:G:326:GLY:HA2	1:G:329:ARG:NH1	2.20	0.56
1:B:403:ARG:NH1	1:G:453:ARG:NH2	2.52	0.56
1:A:453:ARG:HB3	1:F:404:SER:HB3	1.87	0.56
1:E:6:CYS:HA	1:E:100:CYS:HB3	1.87	0.56
1:E:19:MET:HG3	1:E:19:MET:O	2.05	0.56
1:G:361:ARG:HG2	1:G:361:ARG:HH11	1.70	0.56
1:E:350:ARG:NH2	1:E:459:THR:HG21	2.19	0.56
1:A:7:SER:OG	1:A:112:MET:SD	2.63	0.55
1:E:511:TYR:CD1	1:E:563:LEU:HD22	2.41	0.55
1:H:251:VAL:HG11	1:H:562:LEU:HD11	1.88	0.55
1:B:118:LEU:HD13	1:B:167:TRP:CD1	2.42	0.55
1:B:251:VAL:HG11	1:B:562:LEU:HD21	1.88	0.55
1:E:170:LEU:CD1	1:E:202:VAL:HG22	2.36	0.55
1:E:403:ARG:NH2	1:H:449:GLU:HB2	2.20	0.55
1:H:218:GLY:HA2	1:G:171:ARG:HH21	1.71	0.55
1:G:511:TYR:CD1	1:G:563:LEU:HD22	2.41	0.55
1:B:271:GLU:CD	1:B:275:LYS:HG3	2.31	0.55
1:E:84:TRP:HZ3	1:E:199:ARG:HA	1.70	0.55
1:G:64:VAL:HG12	1:G:82:VAL:HG11	1.88	0.55
1:A:64:VAL:HG12	1:A:82:VAL:HG11	1.88	0.55
1:A:511:TYR:CD1	1:A:563:LEU:HD22	2.41	0.55
1:E:74:GLN:O	1:E:77:MET:HG3	2.07	0.55
1:E:403:ARG:NH1	1:H:449:GLU:HB2	2.21	0.55
1:H:118:LEU:HD13	1:H:167:TRP:CD1	2.42	0.55
1:H:328:LEU:HD21	1:H:370:ILE:CD1	2.26	0.55
1:H:472:TRP:CE2	1:H:495:LEU:HD13	2.42	0.55
1:G:53:MET:HE3	1:G:54:HIS:HE1	1.65	0.55
1:G:396:THR:HG23	1:G:397:ARG:HG3	1.89	0.55
1:A:108:ILE:O	1:A:112:MET:HG3	2.06	0.55
1:F:207:GLU:O	1:F:211:HIS:ND1	2.36	0.55
1:E:64:VAL:HG12	1:E:82:VAL:HG11	1.88	0.55
1:E:84:TRP:HZ3	1:E:199:ARG:HB2	1.72	0.55
1:G:109:SER:N	1:G:112:MET:HE3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:118:LEU:HD13	1:F:167:TRP:CD1	2.42	0.55
1:E:437:ARG:HH21	1:E:440:ARG:NH2	2.04	0.55
1:H:76:HIS:HE1	1:H:111:ALA:HB2	1.72	0.55
1:H:533:LEU:HB3	1:H:568:CYS:SG	2.46	0.55
1:F:397:ARG:HD2	1:F:398:GLU:N	2.12	0.55
1:H:196:MET:HE1	1:H:200:GLN:H	1.71	0.55
1:F:114:ARG:HH22	1:E:161:LEU:C	2.14	0.55
1:G:108:ILE:O	1:G:112:MET:HG2	2.07	0.55
1:B:159:VAL:HG13	1:A:76:HIS:HD1	1.72	0.55
1:E:397:ARG:HB3	1:E:397:ARG:CZ	2.38	0.54
1:E:523:GLU:HG2	1:E:569:PRO:HG3	1.88	0.54
1:H:159:VAL:HG13	1:G:76:HIS:HD1	1.72	0.54
1:H:483:LEU:HD23	1:H:504:ILE:HG21	1.89	0.54
1:B:533:LEU:HB3	1:B:568:CYS:SG	2.48	0.54
1:E:21:LEU:HB3	1:E:27:PHE:CZ	2.43	0.54
1:E:196:MET:HE1	1:E:200:GLN:NE2	2.22	0.54
1:A:408:ARG:CD	1:F:418:GLU:OE1	2.55	0.54
1:B:118:LEU:CD1	1:B:206:LEU:HD11	2.38	0.54
1:E:84:TRP:CZ3	1:E:199:ARG:HA	2.42	0.54
1:G:547:THR:HG22	1:G:560:ASN:ND2	2.23	0.54
1:A:21:LEU:HB3	1:A:27:PHE:CZ	2.43	0.54
1:A:362:SER:OG	1:F:419:HIS:HD2	1.91	0.54
1:B:84:TRP:O	1:B:87:LEU:HG	2.07	0.54
1:B:251:VAL:HG21	1:B:562:LEU:CD1	2.37	0.54
1:F:114:ARG:HH22	1:E:162:GLY:HA3	1.71	0.54
1:H:76:HIS:CE1	1:H:111:ALA:HB2	2.43	0.54
1:H:77:MET:SD	1:H:199:ARG:NE	2.80	0.54
1:H:118:LEU:CD1	1:H:206:LEU:HD11	2.38	0.54
1:B:407:ALA:HB1	1:G:450:PRO:CB	2.32	0.54
1:E:84:TRP:HZ3	1:E:199:ARG:CA	2.21	0.54
1:B:520:PRO:HG3	1:B:529:GLU:HG2	1.89	0.54
1:F:483:LEU:HD23	1:F:504:ILE:CG2	2.38	0.54
1:H:483:LEU:HD23	1:H:504:ILE:CG2	2.37	0.54
1:G:21:LEU:HB3	1:G:27:PHE:CZ	2.43	0.54
1:A:203:GLU:O	1:A:207:GLU:HG2	2.08	0.54
1:F:71:ARG:C	1:E:157:ARG:HH11	2.16	0.54
1:F:472:TRP:CE2	1:F:495:LEU:HD13	2.42	0.54
1:G:41:SER:O	1:G:44:VAL:HG12	2.08	0.54
1:B:118:LEU:HD12	1:B:170:LEU:HD22	1.91	0.53
1:B:363:PRO:HD2	1:G:418:GLU:OE1	2.09	0.53
1:A:258:GLU:OE2	1:A:261:CYS:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:TRP:O	1:F:87:LEU:HG	2.09	0.53
1:E:437:ARG:HH11	1:E:437:ARG:CG	2.20	0.53
1:A:87:LEU:HD23	1:A:119:PHE:HD2	1.73	0.53
1:E:41:SER:O	1:E:44:VAL:HG12	2.08	0.53
1:G:79:PHE:CE2	1:G:108:ILE:HD12	2.42	0.53
1:A:41:SER:O	1:A:44:VAL:HG12	2.08	0.53
1:A:594:ARG:O	1:A:598:TRP:HD1	1.92	0.53
1:H:405:ARG:O	1:H:409:HIS:CD2	2.62	0.53
1:B:467:ASP:C	1:B:469:GLU:N	2.65	0.53
1:E:196:MET:HG2	1:E:199:ARG:HB3	1.91	0.53
1:E:254:LEU:HD12	1:E:605:PRO:HD2	1.91	0.53
1:B:483:LEU:HD23	1:B:504:ILE:CG2	2.37	0.53
1:A:203:GLU:CD	1:A:206:LEU:HD21	2.34	0.53
1:A:254:LEU:HD12	1:A:605:PRO:HD2	1.91	0.53
1:H:19:MET:HE1	1:H:26:GLY:CA	2.30	0.53
1:B:70:LEU:HD23	1:A:157:ARG:HH22	1.73	0.53
1:B:157:ARG:HH21	1:A:73:GLU:N	2.06	0.53
1:B:403:ARG:CZ	1:G:453:ARG:HH21	2.21	0.53
1:F:118:LEU:CD1	1:F:206:LEU:HD11	2.38	0.53
1:H:599:ALA:O	1:G:216:TRP:CZ2	2.62	0.53
1:G:19:MET:SD	1:G:27:PHE:HB2	2.48	0.53
1:F:378:MET:CE	1:F:389:VAL:H	2.20	0.53
1:F:520:PRO:HG3	1:F:529:GLU:HG2	1.90	0.53
1:B:76:HIS:CD2	1:A:159:VAL:HG11	2.43	0.53
1:A:33:LEU:CD2	1:A:79:PHE:HE1	2.21	0.53
1:A:411:ALA:HA	1:F:411:ALA:HB1	1.91	0.53
1:B:404:SER:HB3	1:G:453:ARG:HB3	1.90	0.53
1:H:84:TRP:O	1:H:87:LEU:HG	2.09	0.53
1:H:434:PHE:CD2	1:H:462:ALA:HB2	2.37	0.53
1:B:12:TRP:CH2	1:B:49:ARG:NH2	2.77	0.52
1:B:157:ARG:NH2	1:A:74:GLN:NE2	2.56	0.52
1:B:356:TYR:HB2	1:B:366:VAL:HG11	1.92	0.52
1:H:471:ILE:O	1:H:475:VAL:HG23	2.09	0.52
1:B:562:LEU:N	1:B:562:LEU:CD1	2.72	0.52
1:A:227:LEU:O	1:A:235:LEU:HD21	2.10	0.52
1:H:116:ALA:O	1:H:164:GLU:CD	2.52	0.52
1:B:483:LEU:HD23	1:B:504:ILE:HG21	1.91	0.52
1:B:516:ILE:HG22	1:B:517:LYS:HD3	1.91	0.52
1:H:157:ARG:NH2	1:G:74:GLN:NE2	2.58	0.52
1:H:356:TYR:HB2	1:H:366:VAL:HG11	1.90	0.52
1:G:227:LEU:O	1:G:235:LEU:HD21	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:258:GLU:OE2	1:G:261:CYS:HB2	2.09	0.52
1:F:116:ALA:O	1:F:164:GLU:CD	2.52	0.52
1:F:217:GLU:HG2	1:E:171:ARG:HH12	1.75	0.52
1:H:223:PRO:HB2	1:H:581:VAL:HG21	1.92	0.52
1:B:467:ASP:C	1:B:469:GLU:H	2.17	0.52
1:A:203:GLU:HA	1:A:206:LEU:CD2	2.39	0.52
1:B:116:ALA:O	1:B:164:GLU:CD	2.52	0.52
1:B:453:ARG:HE	1:G:403:ARG:HH11	1.58	0.52
1:E:196:MET:CE	1:E:200:GLN:HG3	2.40	0.52
1:E:227:LEU:O	1:E:235:LEU:HD21	2.10	0.52
1:E:545:LEU:HG	1:E:579:THR:HG21	1.92	0.52
1:E:437:ARG:NH2	1:E:440:ARG:NH2	2.58	0.52
1:G:64:VAL:HG21	1:G:67:PHE:HD2	1.75	0.52
1:G:254:LEU:HD12	1:G:605:PRO:HD2	1.90	0.52
1:B:157:ARG:HH21	1:A:74:GLN:H	1.58	0.52
1:B:403:ARG:NH1	1:H:469:GLU:OE2	2.43	0.52
1:F:309:ARG:O	1:F:313:LEU:HG	2.10	0.52
1:B:251:VAL:HG13	1:B:558:THR:HG23	1.90	0.52
1:A:418:GLU:OE2	1:A:418:GLU:HA	2.09	0.52
1:F:223:PRO:HB2	1:F:581:VAL:HG21	1.92	0.52
1:E:450:PRO:CB	1:H:407:ALA:HB1	2.35	0.52
1:B:35:THR:HA	1:B:64:VAL:HG12	1.92	0.51
1:E:440:ARG:NH1	1:E:444:PHE:HE2	2.07	0.51
1:G:39:LYS:H	1:G:39:LYS:HD2	1.74	0.51
1:B:88:LEU:HD21	1:B:174:SER:C	2.36	0.51
1:F:72:SER:C	1:E:157:ARG:NH2	2.68	0.51
1:F:406:ILE:HD12	1:F:443:MET:HE1	1.93	0.51
1:B:471:ILE:O	1:B:475:VAL:HG23	2.10	0.51
1:A:64:VAL:HG21	1:A:67:PHE:HD2	1.75	0.51
1:A:79:PHE:CE2	1:A:108:ILE:HD12	2.45	0.51
1:A:84:TRP:HZ3	1:A:199:ARG:CA	2.23	0.51
1:A:453:ARG:NH1	1:F:404:SER:H	2.09	0.51
1:F:356:TYR:HB2	1:F:366:VAL:HG11	1.92	0.51
1:H:31:HIS:HB2	1:H:86:TRP:CH2	2.46	0.51
1:H:88:LEU:HD21	1:H:174:SER:C	2.36	0.51
1:B:223:PRO:HB2	1:B:581:VAL:HG21	1.92	0.51
1:A:206:LEU:HD13	1:A:210:ARG:NH2	2.25	0.51
1:E:64:VAL:HG21	1:E:67:PHE:HD2	1.75	0.51
1:H:12:TRP:CH2	1:H:49:ARG:NH2	2.77	0.51
1:H:397:ARG:HH12	1:H:439:THR:CB	2.23	0.51
1:A:545:LEU:HG	1:A:579:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:431:LEU:HB3	1:G:443:MET:HE3	1.93	0.51
1:B:46:GLN:HA	1:B:49:ARG:NE	2.25	0.51
1:B:207:GLU:O	1:B:210:ARG:HG2	2.11	0.51
1:A:418:GLU:OE2	1:A:418:GLU:CA	2.55	0.51
1:F:46:GLN:HA	1:F:49:ARG:NE	2.25	0.51
1:F:88:LEU:HD21	1:F:174:SER:C	2.36	0.51
1:E:19:MET:CE	1:E:57:PRO:HG2	2.41	0.51
1:E:203:GLU:O	1:E:207:GLU:HG2	2.10	0.51
1:H:46:GLN:HA	1:H:49:ARG:NE	2.26	0.51
1:H:114:ARG:HH22	1:G:162:GLY:HA3	1.75	0.51
1:H:472:TRP:CE2	1:G:453:ARG:NH1	2.78	0.51
1:B:77:MET:HA	1:B:199:ARG:NH2	2.25	0.51
1:E:2:ARG:HA	1:E:98:TYR:CE2	2.46	0.51
1:E:39:LYS:H	1:E:39:LYS:HD2	1.74	0.51
1:H:49:ARG:NH1	1:H:50:TYR:HB2	2.26	0.51
1:G:545:LEU:HG	1:G:579:THR:HG21	1.92	0.51
1:B:70:LEU:HD21	1:A:157:ARG:HH22	1.74	0.51
1:B:250:TRP:CH2	1:B:577:LEU:HD21	2.45	0.51
1:F:97:ARG:HB3	1:F:121:ALA:HA	1.93	0.51
1:F:161:LEU:HG	1:E:114:ARG:CZ	2.41	0.51
1:E:157:ARG:CG	1:E:157:ARG:CZ	2.86	0.51
1:A:574:LEU:O	1:A:578:LYS:HG3	2.12	0.51
1:F:35:THR:HA	1:F:64:VAL:HG12	1.93	0.51
1:H:406:ILE:HD12	1:H:443:MET:HE1	1.92	0.51
1:B:19:MET:HE1	1:B:27:PHE:CD2	2.46	0.50
1:B:289:VAL:HG13	1:B:316:ASN:ND2	2.25	0.50
1:A:39:LYS:H	1:A:39:LYS:HD2	1.74	0.50
1:F:460:VAL:CG2	1:F:483:LEU:HD13	2.41	0.50
1:G:397:ARG:NE	1:G:405:ARG:HH12	2.10	0.50
1:F:217:GLU:HG3	1:E:171:ARG:HH22	1.75	0.50
1:E:128:LEU:HB2	1:E:157:ARG:HG3	1.92	0.50
1:G:203:GLU:O	1:G:207:GLU:HG2	2.10	0.50
1:B:309:ARG:O	1:B:313:LEU:HG	2.10	0.50
1:F:93:GLN:H	1:F:96:HIS:HE1	1.60	0.50
1:H:70:LEU:HD21	1:H:76:HIS:HB2	1.93	0.50
1:F:16:PRO:HB3	1:F:50:TYR:CZ	2.47	0.50
1:F:475:VAL:HG23	1:F:476:PHE:CD2	2.47	0.50
1:H:2:ARG:HB3	1:H:98:TYR:HE1	1.76	0.50
1:H:402:ASP:CB	1:H:405:ARG:HG2	2.35	0.50
1:G:2:ARG:HA	1:G:98:TYR:CE2	2.46	0.50
1:B:5:LEU:HB3	1:B:86:TRP:CH2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:TRP:CZ2	1:F:49:ARG:NH2	2.80	0.50
1:F:31:HIS:HB3	1:F:90:ARG:NH1	2.26	0.50
1:F:46:GLN:HA	1:F:49:ARG:HD2	1.94	0.50
1:E:36:ALA:HB2	1:E:63:ARG:HB3	1.94	0.50
1:H:289:VAL:HG13	1:H:316:ASN:ND2	2.25	0.50
1:B:49:ARG:NH1	1:B:50:TYR:HB2	2.26	0.50
1:H:98:TYR:CD2	1:H:123:GLU:HB3	2.47	0.50
1:H:118:LEU:HD12	1:H:170:LEU:HD22	1.93	0.50
1:H:434:PHE:HD2	1:H:462:ALA:HB3	1.75	0.50
1:G:109:SER:CA	1:G:112:MET:HG2	2.42	0.50
1:B:475:VAL:HG13	1:B:504:ILE:HD11	1.94	0.50
1:F:31:HIS:HB3	1:F:90:ARG:HD3	1.93	0.50
1:E:196:MET:HE1	1:E:200:GLN:HE21	1.76	0.50
1:B:224:ILE:HB	1:B:227:LEU:HG	1.94	0.50
1:B:251:VAL:CG2	1:B:562:LEU:HD11	2.41	0.50
1:F:224:ILE:HB	1:F:227:LEU:HG	1.94	0.50
1:F:471:ILE:O	1:F:475:VAL:HG13	2.12	0.50
1:B:80:GLU:HB2	1:B:199:ARG:NH2	2.27	0.50
1:A:403:ARG:HB3	1:F:453:ARG:HD2	1.94	0.50
1:F:599:ALA:O	1:E:216:TRP:CZ2	2.64	0.50
1:B:97:ARG:HB3	1:B:121:ALA:HA	1.93	0.49
1:B:149:GLN:O	1:B:153:THR:HG22	2.12	0.49
1:B:185:GLN:HB2	1:B:190:TRP:CZ3	2.47	0.49
1:B:362:SER:OG	1:G:419:HIS:HD2	1.94	0.49
1:A:203:GLU:O	1:A:206:LEU:HG	2.11	0.49
1:F:289:VAL:HG13	1:F:316:ASN:ND2	2.25	0.49
1:G:196:MET:HG2	1:G:199:ARG:HB3	1.94	0.49
1:B:599:ALA:O	1:A:216:TRP:CZ2	2.65	0.49
1:F:374:PHE:O	1:F:378:MET:HG3	2.12	0.49
1:H:12:TRP:CZ2	1:H:49:ARG:NH2	2.80	0.49
1:H:93:GLN:H	1:H:96:HIS:HE1	1.60	0.49
1:H:149:GLN:O	1:H:153:THR:HG22	2.12	0.49
1:F:118:LEU:HD12	1:F:170:LEU:HD22	1.93	0.49
1:F:453:ARG:CZ	1:E:472:TRP:CD2	2.96	0.49
1:H:46:GLN:HA	1:H:49:ARG:HD2	1.94	0.49
1:H:195:ASP:HB3	1:H:197:ARG:HG3	1.94	0.49
1:G:36:ALA:HB2	1:G:63:ARG:HB3	1.94	0.49
1:G:350:ARG:NH2	1:G:459:THR:HG21	2.22	0.49
1:B:93:GLN:H	1:B:96:HIS:HE1	1.60	0.49
1:B:195:ASP:HB3	1:B:197:ARG:HG3	1.94	0.49
1:A:61:ILE:HB	1:A:188:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:SER:N	1:E:157:ARG:HH11	2.11	0.49
1:H:16:PRO:HB3	1:H:50:TYR:CZ	2.47	0.49
1:B:12:TRP:CZ2	1:B:49:ARG:NH2	2.80	0.49
1:B:16:PRO:HB3	1:B:50:TYR:CZ	2.47	0.49
1:B:79:PHE:HA	1:B:82:VAL:HG22	1.94	0.49
1:B:196:MET:SD	1:B:199:ARG:HD2	2.53	0.49
1:B:248:LYS:HA	1:B:562:LEU:HD21	1.95	0.49
1:A:2:ARG:HA	1:A:98:TYR:CE2	2.46	0.49
1:A:89:GLN:HA	1:A:175:ALA:HB2	1.95	0.49
1:H:97:ARG:HB3	1:H:121:ALA:HA	1.93	0.49
1:G:224:ILE:HD11	1:G:581:VAL:HG22	1.94	0.49
1:B:46:GLN:HA	1:B:49:ARG:HD2	1.94	0.49
1:B:378:MET:HE1	1:B:389:VAL:N	2.13	0.49
1:B:406:ILE:HD12	1:B:443:MET:HE1	1.93	0.49
1:F:72:SER:C	1:F:74:GLN:N	2.71	0.49
1:F:207:GLU:O	1:F:210:ARG:HG2	2.13	0.49
1:E:88:LEU:HD11	1:E:174:SER:CA	2.31	0.49
1:H:185:GLN:HB2	1:H:190:TRP:CZ3	2.47	0.49
1:B:72:SER:C	1:B:74:GLN:N	2.71	0.49
1:A:36:ALA:HB2	1:A:63:ARG:HB3	1.94	0.49
1:F:77:MET:SD	1:F:199:ARG:NH2	2.85	0.49
1:F:196:MET:HE1	1:F:200:GLN:CG	2.43	0.49
1:H:431:LEU:HD11	1:H:448:PHE:CZ	2.47	0.49
1:G:61:ILE:HB	1:G:188:VAL:HG23	1.94	0.49
1:G:89:GLN:HA	1:G:175:ALA:HB2	1.94	0.49
1:G:475:VAL:HG13	1:G:504:ILE:HD11	1.94	0.49
1:B:80:GLU:HB2	1:B:199:ARG:HH21	1.77	0.49
1:A:453:ARG:HH11	1:F:404:SER:HB3	1.76	0.49
1:F:149:GLN:O	1:F:153:THR:HG22	2.12	0.49
1:H:6:CYS:HB2	1:H:15:VAL:HG22	1.95	0.49
1:A:87:LEU:HD11	1:A:97:ARG:HD3	1.95	0.49
1:F:114:ARG:HH12	1:E:161:LEU:HA	1.77	0.49
1:E:61:ILE:HB	1:E:188:VAL:HG23	1.94	0.49
1:E:89:GLN:HA	1:E:175:ALA:HB2	1.95	0.49
1:H:533:LEU:CD1	1:H:543:VAL:HG11	2.43	0.49
1:B:6:CYS:HB2	1:B:15:VAL:HG22	1.95	0.49
1:B:437:ARG:HD2	1:B:440:ARG:CZ	2.43	0.49
1:A:33:LEU:HD22	1:A:79:PHE:HE1	1.78	0.49
1:A:405:ARG:HH11	1:A:405:ARG:HG2	1.78	0.49
1:F:5:LEU:HB3	1:F:86:TRP:CH2	2.47	0.49
1:F:256:LYS:HE2	1:F:558:THR:OG1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:449:GLU:CD	1:F:453:ARG:HH11	2.20	0.49
1:H:317:ASN:CG	1:H:321:LEU:HD23	2.38	0.49
1:G:440:ARG:HG2	1:G:444:PHE:CE2	2.48	0.49
1:B:72:SER:N	1:A:157:ARG:NH1	2.61	0.48
1:B:310:TYR:CD2	1:B:516:ILE:HD11	2.48	0.48
1:B:403:ARG:CZ	1:G:453:ARG:HE	2.25	0.48
1:F:49:ARG:NH1	1:F:50:TYR:HB2	2.27	0.48
1:F:159:VAL:HG11	1:E:76:HIS:ND1	2.28	0.48
1:F:195:ASP:HB3	1:F:197:ARG:HG3	1.94	0.48
1:E:76:HIS:CD2	1:E:76:HIS:C	2.91	0.48
1:H:437:ARG:HD2	1:H:440:ARG:CZ	2.43	0.48
1:G:87:LEU:HD11	1:G:97:ARG:HD3	1.95	0.48
1:A:53:MET:HG3	1:A:54:HIS:CE1	2.48	0.48
1:H:2:ARG:HA	1:H:96:HIS:HB2	1.95	0.48
1:H:449:GLU:CG	1:H:450:PRO:HD3	2.39	0.48
1:G:403:ARG:CG	1:G:403:ARG:C	2.81	0.48
1:A:84:TRP:HB3	1:A:119:PHE:CE2	2.48	0.48
1:A:594:ARG:HG3	1:A:598:TRP:HD1	1.77	0.48
1:H:77:MET:SD	1:H:199:ARG:NH2	2.86	0.48
1:F:79:PHE:HA	1:F:82:VAL:HG22	1.94	0.48
1:F:86:TRP:HE1	1:F:90:ARG:HH11	1.61	0.48
1:F:185:GLN:HB2	1:F:190:TRP:CZ3	2.48	0.48
1:F:469:GLU:O	1:F:473:GLN:HG2	2.13	0.48
1:E:53:MET:HG3	1:E:54:HIS:CE1	2.48	0.48
1:E:437:ARG:HH21	1:E:440:ARG:CZ	2.27	0.48
1:H:403:ARG:HB3	1:H:403:ARG:NH1	2.28	0.48
1:G:492:SER:HB2	1:G:494:ASP:OD1	2.13	0.48
1:B:453:ARG:NH1	1:G:403:ARG:HG3	2.28	0.48
1:A:275:LYS:HA	1:A:278:GLN:HG2	1.96	0.48
1:F:12:TRP:CH2	1:F:49:ARG:NH2	2.77	0.48
1:E:431:LEU:HB3	1:E:443:MET:CE	2.43	0.48
1:H:224:ILE:HB	1:H:227:LEU:HG	1.93	0.48
1:H:256:LYS:HE2	1:H:558:THR:OG1	2.13	0.48
1:B:469:GLU:O	1:B:473:GLN:HG2	2.13	0.48
1:A:109:SER:HA	1:A:112:MET:CE	2.43	0.48
1:A:534:ARG:HG2	1:A:568:CYS:HB3	1.96	0.48
1:F:2:ARG:HA	1:F:96:HIS:HB2	1.96	0.48
1:F:317:ASN:CG	1:F:321:LEU:HD23	2.38	0.48
1:H:405:ARG:HB3	1:H:405:ARG:CZ	2.44	0.48
1:G:3:ILE:N	1:G:98:TYR:CE2	2.78	0.48
1:B:449:GLU:O	1:G:403:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:SER:O	1:A:45:GLU:OE1	2.31	0.48
1:E:41:SER:O	1:E:45:GLU:OE1	2.31	0.48
1:E:86:TRP:NE1	1:E:90:ARG:HG3	2.29	0.48
1:G:86:TRP:NE1	1:G:90:ARG:HG3	2.29	0.48
1:B:256:LYS:HE2	1:B:558:THR:OG1	2.13	0.48
1:B:461:HIS:O	1:B:461:HIS:CD2	2.67	0.48
1:A:471:ILE:O	1:A:475:VAL:HG23	2.14	0.48
1:E:84:TRP:HZ3	1:E:199:ARG:CB	2.26	0.48
1:E:87:LEU:HD11	1:E:97:ARG:HD3	1.95	0.48
1:E:471:ILE:O	1:E:475:VAL:HG23	2.14	0.48
1:H:266:PHE:HB3	1:H:331:GLN:NE2	2.29	0.48
1:G:41:SER:O	1:G:45:GLU:OE1	2.32	0.48
1:G:196:MET:CE	1:G:200:GLN:HG2	2.44	0.48
1:G:275:LYS:HA	1:G:278:GLN:HG2	1.96	0.48
1:B:76:HIS:CE1	1:B:107:THR:O	2.67	0.48
1:A:492:SER:HB2	1:A:494:ASP:OD1	2.13	0.48
1:F:262:HIS:NE2	1:F:461:HIS:CE1	2.81	0.48
1:F:432:ALA:HA	1:F:461:HIS:HB3	1.95	0.48
1:E:108:ILE:HG22	1:E:112:MET:HE2	1.96	0.48
1:G:403:ARG:HG3	1:G:403:ARG:C	2.38	0.48
1:B:46:GLN:HA	1:B:49:ARG:CD	2.44	0.48
1:F:472:TRP:CE2	1:E:453:ARG:NH1	2.82	0.48
1:F:6:CYS:HB2	1:F:15:VAL:HG22	1.95	0.47
1:F:262:HIS:NE2	1:F:461:HIS:HE1	2.12	0.47
1:H:44:VAL:HG21	1:H:63:ARG:HD2	1.96	0.47
1:G:124:VAL:O	1:G:161:LEU:HB2	2.14	0.47
1:B:77:MET:SD	1:B:199:ARG:CZ	3.02	0.47
1:B:320:ALA:C	1:B:323:LYS:HZ1	2.21	0.47
1:B:453:ARG:HD3	1:A:472:TRP:CE3	2.49	0.47
1:E:109:SER:HA	1:E:112:MET:CE	2.44	0.47
1:E:356:TYR:CD2	1:E:356:TYR:N	2.79	0.47
1:H:120:GLY:C	1:H:164:GLU:OE2	2.57	0.47
1:H:121:ALA:N	1:H:164:GLU:OE2	2.47	0.47
1:B:44:VAL:HG21	1:B:63:ARG:HD2	1.96	0.47
1:A:86:TRP:NE1	1:A:90:ARG:HG3	2.29	0.47
1:A:440:ARG:HG2	1:A:444:PHE:CE2	2.48	0.47
1:A:585:GLN:HG3	1:A:598:TRP:CZ2	2.49	0.47
1:F:44:VAL:HG21	1:F:63:ARG:HD2	1.96	0.47
1:F:46:GLN:HA	1:F:49:ARG:CD	2.44	0.47
1:F:120:GLY:C	1:F:164:GLU:OE2	2.58	0.47
1:F:121:ALA:N	1:F:164:GLU:OE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:404:SER:O	1:G:408:ARG:HD2	2.14	0.47
1:A:227:LEU:O	1:A:230:TRP:HB2	2.15	0.47
1:H:460:VAL:CG2	1:H:483:LEU:HD13	2.44	0.47
1:H:469:GLU:O	1:H:473:GLN:HG2	2.13	0.47
1:B:266:PHE:HB3	1:B:331:GLN:NE2	2.29	0.47
1:E:76:HIS:O	1:E:76:HIS:CD2	2.67	0.47
1:E:227:LEU:O	1:E:230:TRP:HB2	2.15	0.47
1:F:19:MET:SD	1:F:27:PHE:HD2	2.38	0.47
1:F:266:PHE:HB3	1:F:331:GLN:NE2	2.29	0.47
1:F:336:TYR:CD2	1:F:377:ALA:HB1	2.50	0.47
1:H:4:LEU:HB3	1:H:30:VAL:HG22	1.97	0.47
1:A:19:MET:HB2	1:A:19:MET:HE2	1.63	0.47
1:A:397:ARG:HB3	1:A:397:ARG:NH1	2.30	0.47
1:F:397:ARG:HH11	1:F:402:ASP:C	2.23	0.47
1:F:402:ASP:HB2	1:F:405:ARG:CG	2.45	0.47
1:F:453:ARG:NH2	1:E:472:TRP:CD1	2.83	0.47
1:F:472:TRP:CD1	1:E:453:ARG:NH1	2.83	0.47
1:E:534:ARG:HG2	1:E:568:CYS:HB3	1.96	0.47
1:H:245:VAL:HG13	1:H:246:GLN:CD	2.40	0.47
1:H:304:PRO:HB3	1:H:517:LYS:O	2.15	0.47
1:H:453:ARG:NH2	1:G:472:TRP:CG	2.82	0.47
1:G:2:ARG:HA	1:G:98:TYR:HE2	1.80	0.47
1:G:397:ARG:CZ	1:G:405:ARG:NH1	2.78	0.47
1:B:2:ARG:HA	1:B:96:HIS:HB2	1.96	0.47
1:B:271:GLU:OE2	1:B:275:LYS:HG3	2.15	0.47
1:A:123:GLU:OE2	1:A:160:ARG:HB3	2.15	0.47
1:F:77:MET:SD	1:F:199:ARG:NE	2.88	0.47
1:E:403:ARG:NH2	1:H:449:GLU:O	2.48	0.47
1:B:114:ARG:HH11	1:A:161:LEU:HD23	1.77	0.47
1:A:108:ILE:HG22	1:A:112:MET:HE2	1.96	0.47
1:A:237:TRP:CE3	1:A:238:LEU:HD23	2.50	0.47
1:E:322:LEU:HD22	1:E:328:LEU:HA	1.96	0.47
1:B:4:LEU:HB3	1:B:30:VAL:HG22	1.97	0.47
1:B:322:LEU:HD12	1:B:328:LEU:HA	1.97	0.47
1:F:196:MET:HE1	1:F:200:GLN:HG2	1.97	0.47
1:F:453:ARG:HH22	1:E:472:TRP:CB	2.27	0.47
1:E:275:LYS:HA	1:E:278:GLN:HG2	1.96	0.47
1:H:463:GLY:O	1:H:486:ALA:HA	2.15	0.47
1:B:120:GLY:C	1:B:164:GLU:OE2	2.57	0.46
1:B:304:PRO:HB3	1:B:517:LYS:O	2.15	0.46
1:B:319:SER:O	1:B:323:LYS:NZ	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:304:PRO:HB3	1:F:517:LYS:O	2.15	0.46
1:F:350:ARG:HD3	1:F:430:ASP:OD2	2.15	0.46
1:E:123:GLU:OE2	1:E:160:ARG:HB3	2.15	0.46
1:E:437:ARG:HH11	1:E:437:ARG:HG3	1.80	0.46
1:E:437:ARG:NE	1:E:440:ARG:HE	2.05	0.46
1:G:19:MET:HE1	1:G:30:VAL:HG21	1.97	0.46
1:E:2:ARG:HA	1:E:98:TYR:HE2	1.80	0.46
1:H:157:ARG:NE	1:G:72:SER:HB2	2.05	0.46
1:B:72:SER:C	1:A:157:ARG:CZ	2.89	0.46
1:B:121:ALA:N	1:B:164:GLU:OE2	2.47	0.46
1:B:204:GLY:HA2	1:B:207:GLU:HG2	1.98	0.46
1:A:88:LEU:HD11	1:A:174:SER:CA	2.31	0.46
1:H:19:MET:SD	1:H:27:PHE:HD2	2.38	0.46
1:G:196:MET:HE1	1:G:200:GLN:HG2	1.97	0.46
1:G:534:ARG:HG2	1:G:568:CYS:HB3	1.96	0.46
1:B:520:PRO:C	1:B:521:LEU:HD12	2.41	0.46
1:E:453:ARG:HB3	1:H:404:SER:HB3	1.98	0.46
1:H:46:GLN:HA	1:H:49:ARG:CD	2.44	0.46
1:G:196:MET:HE1	1:G:200:GLN:CG	2.45	0.46
1:G:398:GLU:CD	1:G:398:GLU:H	2.23	0.46
1:B:80:GLU:HB3	1:B:84:TRP:CZ2	2.50	0.46
1:B:245:VAL:HG13	1:B:246:GLN:CD	2.40	0.46
1:B:463:GLY:O	1:B:486:ALA:HA	2.15	0.46
1:H:432:ALA:HA	1:H:461:HIS:HB3	1.97	0.46
1:G:227:LEU:O	1:G:230:TRP:HB2	2.15	0.46
1:G:471:ILE:O	1:G:475:VAL:HG23	2.16	0.46
1:A:230:TRP:CZ3	1:A:238:LEU:HD21	2.51	0.46
1:E:404:SER:O	1:E:408:ARG:HD2	2.16	0.46
1:H:207:GLU:O	1:H:210:ARG:HG2	2.15	0.46
1:G:123:GLU:OE2	1:G:160:ARG:HB3	2.15	0.46
1:G:196:MET:HE3	1:G:196:MET:HB3	1.62	0.46
1:B:250:TRP:HH2	1:B:577:LEU:HD21	1.81	0.46
1:B:467:ASP:OD1	1:B:470:GLY:N	2.49	0.46
1:F:93:GLN:H	1:F:96:HIS:CE1	2.34	0.46
1:F:322:LEU:HD12	1:F:328:LEU:HA	1.96	0.46
1:E:1:MET:HB3	1:E:28:ASP:OD2	2.16	0.46
1:H:93:GLN:H	1:H:96:HIS:CE1	2.34	0.46
1:H:520:PRO:C	1:H:521:LEU:HD12	2.41	0.46
1:G:397:ARG:NE	1:G:405:ARG:NH1	2.64	0.46
1:B:72:SER:HA	1:A:157:ARG:NE	2.30	0.46
1:B:93:GLN:H	1:B:96:HIS:CE1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ILE:N	1:A:98:TYR:CE2	2.78	0.46
1:A:170:LEU:HD11	1:A:202:VAL:HG22	1.98	0.46
1:A:196:MET:CE	1:A:200:GLN:HG3	2.45	0.46
1:F:4:LEU:HB3	1:F:30:VAL:HG22	1.97	0.46
1:E:196:MET:HE1	1:E:200:GLN:CG	2.46	0.46
1:E:277:ARG:HG2	1:E:321:LEU:HD11	1.98	0.46
1:B:126:HIS:CG	1:A:107:THR:HG22	2.51	0.46
1:B:206:LEU:HB3	1:B:210:ARG:NH2	2.30	0.46
1:B:227:LEU:O	1:B:235:LEU:HD21	2.15	0.46
1:A:196:MET:SD	1:A:199:ARG:HB3	2.56	0.46
1:E:3:ILE:N	1:E:98:TYR:CE2	2.78	0.46
1:H:227:LEU:O	1:H:235:LEU:HD21	2.15	0.46
1:H:322:LEU:HD12	1:H:328:LEU:HA	1.97	0.46
1:B:219:ILE:HD12	1:B:228:ALA:HB1	1.98	0.46
1:B:453:ARG:NE	1:G:403:ARG:NE	2.64	0.46
1:F:114:ARG:NH2	1:E:161:LEU:C	2.74	0.46
1:H:206:LEU:HB3	1:H:210:ARG:NH2	2.30	0.46
1:B:402:ASP:HB2	1:B:405:ARG:CG	2.44	0.45
1:A:2:ARG:HA	1:A:98:TYR:HE2	1.80	0.45
1:A:207:GLU:C	1:A:211:HIS:HD1	2.24	0.45
1:F:206:LEU:HB3	1:F:210:ARG:NH2	2.30	0.45
1:F:395:ALA:HB3	1:F:431:LEU:HD23	1.98	0.45
1:E:492:SER:HB2	1:E:494:ASP:OD1	2.17	0.45
1:H:64:VAL:HG22	1:H:82:VAL:HG11	1.98	0.45
1:B:302:GLU:CG	1:B:303:GLU:OE1	2.60	0.45
1:F:31:HIS:HB3	1:F:90:ARG:HH11	1.82	0.45
1:F:70:LEU:HD21	1:F:76:HIS:HB2	1.96	0.45
1:F:279:GLU:HG2	1:F:330:ALA:HB2	1.98	0.45
1:E:207:GLU:C	1:E:211:HIS:HD1	2.24	0.45
1:B:204:GLY:HA2	1:B:207:GLU:CD	2.42	0.45
1:B:411:ALA:HB1	1:G:411:ALA:HA	1.97	0.45
1:A:101:LEU:CD1	1:A:126:HIS:ND1	2.80	0.45
1:A:585:GLN:HG3	1:A:598:TRP:CH2	2.52	0.45
1:E:170:LEU:HD11	1:E:202:VAL:HG22	1.99	0.45
1:H:397:ARG:HB3	1:H:397:ARG:HH11	1.80	0.45
1:G:207:GLU:C	1:G:211:HIS:HD1	2.24	0.45
1:G:277:ARG:HG2	1:G:321:LEU:HD11	1.98	0.45
1:B:84:TRP:HA	1:B:87:LEU:HG	1.98	0.45
1:A:1:MET:HB3	1:A:28:ASP:OD2	2.16	0.45
1:F:290:ARG:HG2	1:F:290:ARG:HH11	1.82	0.45
1:E:397:ARG:HH21	1:E:401:GLY:HA2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:398:GLU:CD	1:E:398:GLU:H	2.24	0.45
1:H:230:TRP:HB2	1:H:235:LEU:CD2	2.46	0.45
1:G:44:VAL:HG23	1:G:61:ILE:HG21	1.99	0.45
1:B:164:GLU:CD	1:B:164:GLU:O	2.60	0.45
1:B:290:ARG:HG2	1:B:290:ARG:HH11	1.82	0.45
1:F:98:TYR:CD2	1:F:123:GLU:HB3	2.52	0.45
1:E:157:ARG:CB	1:E:157:ARG:NE	2.58	0.45
1:G:1:MET:HB3	1:G:28:ASP:OD2	2.16	0.45
1:F:114:ARG:NH1	1:E:161:LEU:HA	2.31	0.45
1:F:126:HIS:CG	1:E:107:THR:HG22	2.51	0.45
1:E:157:ARG:HH22	1:E:159:VAL:HG22	1.81	0.45
1:H:219:ILE:HD12	1:H:228:ALA:HB1	1.98	0.45
1:B:597:LEU:O	1:B:601:LEU:HB2	2.17	0.45
1:F:84:TRP:HA	1:F:87:LEU:HG	1.99	0.45
1:F:251:VAL:HB	1:F:562:LEU:HD11	1.99	0.45
1:E:304:PRO:HG3	1:E:518:GLY:HA3	1.99	0.45
1:G:322:LEU:HD22	1:G:328:LEU:HA	1.98	0.45
1:F:31:HIS:CD2	1:F:90:ARG:HB3	2.51	0.45
1:F:101:LEU:HD21	1:F:113:GLN:HB2	1.99	0.45
1:F:378:MET:CE	1:F:389:VAL:HB	2.47	0.45
1:E:440:ARG:HG2	1:E:444:PHE:CE2	2.51	0.45
1:G:79:PHE:CE2	1:G:108:ILE:HG23	2.51	0.45
1:G:386:ARG:O	1:G:600:ARG:NH1	2.49	0.45
1:G:475:VAL:HG13	1:G:504:ILE:CD1	2.47	0.45
1:B:84:TRP:HZ3	1:B:199:ARG:HA	1.82	0.45
1:B:453:ARG:HG2	1:G:403:ARG:NH2	2.22	0.45
1:A:339:LEU:HD11	1:A:349:ILE:HD11	1.99	0.45
1:F:164:GLU:CD	1:F:164:GLU:O	2.60	0.45
1:F:397:ARG:CD	1:F:401:GLY:HA3	2.47	0.45
1:H:126:HIS:CG	1:G:107:THR:HG22	2.51	0.45
1:G:304:PRO:HG3	1:G:518:GLY:HA3	1.99	0.45
1:G:472:TRP:CE2	1:G:495:LEU:HD13	2.51	0.45
1:G:575:GLU:HA	1:G:578:LYS:HD3	1.98	0.45
1:B:266:PHE:HB3	1:B:331:GLN:HE21	1.82	0.45
1:A:398:GLU:CD	1:A:398:GLU:H	2.23	0.45
1:F:302:GLU:CG	1:F:303:GLU:OE1	2.60	0.45
1:H:84:TRP:HA	1:H:87:LEU:HG	1.98	0.45
1:H:84:TRP:HA	1:H:87:LEU:CG	2.48	0.44
1:H:266:PHE:HB3	1:H:331:GLN:HE21	1.82	0.44
1:H:434:PHE:CD2	1:H:462:ALA:HB3	2.50	0.44
1:B:101:LEU:HD21	1:B:113:GLN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:HD23	1:A:114:ARG:CZ	2.47	0.44
1:B:247:ASP:O	1:B:251:VAL:HG12	2.17	0.44
1:B:395:ALA:HB3	1:B:431:LEU:HD23	1.98	0.44
1:B:467:ASP:O	1:B:469:GLU:N	2.50	0.44
1:A:230:TRP:HZ3	1:A:238:LEU:HD21	1.82	0.44
1:A:322:LEU:HD22	1:A:328:LEU:HA	1.98	0.44
1:F:36:ALA:HB2	1:F:64:VAL:O	2.17	0.44
1:F:114:ARG:HH22	1:E:162:GLY:CA	2.30	0.44
1:F:121:ALA:O	1:F:164:GLU:HG3	2.18	0.44
1:E:339:LEU:HD11	1:E:349:ILE:HD11	1.99	0.44
1:H:350:ARG:HD3	1:H:430:ASP:OD2	2.16	0.44
1:A:203:GLU:HA	1:A:206:LEU:HD21	1.97	0.44
1:F:196:MET:CE	1:F:200:GLN:HG3	2.48	0.44
1:F:257:VAL:HG22	1:F:597:LEU:HD11	1.99	0.44
1:E:386:ARG:O	1:E:600:ARG:NH1	2.49	0.44
1:H:118:LEU:HB3	1:H:170:LEU:HD22	1.99	0.44
1:G:339:LEU:HD11	1:G:349:ILE:HD11	1.99	0.44
1:B:118:LEU:HB3	1:B:170:LEU:HD22	1.99	0.44
1:B:453:ARG:NE	1:G:403:ARG:CZ	2.81	0.44
1:B:540:GLY:HA3	1:A:591:GLN:NE2	2.33	0.44
1:A:547:THR:O	1:A:548:ASP:HB2	2.17	0.44
1:F:34:THR:O	1:F:63:ARG:HA	2.18	0.44
1:F:84:TRP:HA	1:F:87:LEU:CG	2.48	0.44
1:F:437:ARG:HH11	1:F:440:ARG:HH22	1.65	0.44
1:E:77:MET:HE1	1:E:196:MET:CG	2.37	0.44
1:E:454:VAL:HG23	1:E:456:LEU:HG	1.99	0.44
1:H:101:LEU:HD21	1:H:113:GLN:HB2	1.99	0.44
1:H:121:ALA:O	1:H:164:GLU:HG3	2.18	0.44
1:B:36:ALA:HB2	1:B:64:VAL:O	2.16	0.44
1:B:64:VAL:HG11	1:B:67:PHE:CD2	2.53	0.44
1:B:240:GLU:HB2	1:B:573:ARG:HH12	1.83	0.44
1:A:34:THR:HG21	1:A:40:ILE:HG21	2.00	0.44
1:E:44:VAL:HG23	1:E:61:ILE:HG21	1.99	0.44
1:H:2:ARG:HD3	1:H:98:TYR:OH	2.17	0.44
1:H:4:LEU:HD12	1:H:27:PHE:CE2	2.53	0.44
1:G:34:THR:HG21	1:G:40:ILE:HG21	2.00	0.44
1:G:454:VAL:HG23	1:G:456:LEU:HG	2.00	0.44
1:B:259:LEU:HD22	1:B:482:ARG:NH1	2.33	0.44
1:A:85:ARG:NH1	1:A:179:PRO:O	2.50	0.44
1:F:86:TRP:CD1	1:F:90:ARG:HD2	2.53	0.44
1:H:34:THR:O	1:H:63:ARG:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:36:ALA:HB2	1:H:64:VAL:O	2.18	0.44
1:B:34:THR:O	1:B:63:ARG:HA	2.18	0.44
1:B:84:TRP:CD1	1:B:119:PHE:HE2	2.36	0.44
1:B:350:ARG:HD3	1:B:430:ASP:OD2	2.17	0.44
1:A:50:TYR:HA	1:A:53:MET:SD	2.58	0.44
1:F:19:MET:HE1	1:F:26:GLY:C	2.43	0.44
1:F:217:GLU:HG3	1:E:171:ARG:NH2	2.33	0.44
1:F:219:ILE:HD12	1:F:228:ALA:HB1	1.98	0.44
1:F:240:GLU:HB2	1:F:573:ARG:HH12	1.83	0.44
1:F:558:THR:O	1:F:562:LEU:HD13	2.17	0.44
1:E:34:THR:HG21	1:E:40:ILE:HG21	2.00	0.44
1:E:50:TYR:HA	1:E:53:MET:SD	2.58	0.44
1:E:157:ARG:NE	1:E:157:ARG:HB2	2.32	0.44
1:H:437:ARG:HD2	1:H:440:ARG:NH1	2.33	0.44
1:H:472:TRP:CG	1:G:453:ARG:CZ	3.00	0.44
1:G:170:LEU:HD11	1:G:202:VAL:HG22	1.98	0.44
1:B:98:TYR:CD2	1:B:123:GLU:HB3	2.52	0.44
1:B:472:TRP:CE2	1:B:495:LEU:HD13	2.53	0.44
1:A:304:PRO:HG3	1:A:518:GLY:HA3	1.99	0.44
1:A:453:ARG:CB	1:F:404:SER:HB3	2.48	0.44
1:E:128:LEU:HD13	1:E:157:ARG:NH1	2.33	0.44
1:E:444:PHE:HB3	1:E:477:LYS:HZ1	1.83	0.44
1:H:259:LEU:HD22	1:H:482:ARG:NH1	2.33	0.44
1:H:268:THR:HG21	1:H:552:ILE:HG12	2.00	0.44
1:H:540:GLY:HA3	1:G:591:GLN:NE2	2.33	0.44
1:G:84:TRP:CZ3	1:G:199:ARG:HA	2.52	0.44
1:G:329:ARG:NH1	1:G:329:ARG:HB3	2.32	0.44
1:B:273:LEU:O	1:B:276:VAL:HG12	2.18	0.44
1:A:50:TYR:HA	1:A:53:MET:CG	2.48	0.44
1:F:4:LEU:HD12	1:F:27:PHE:CE2	2.53	0.44
1:F:266:PHE:HB3	1:F:331:GLN:HE21	1.82	0.44
1:E:168:PRO:O	1:E:171:ARG:HG2	2.18	0.44
1:E:488:HIS:HD2	1:E:491:ARG:NH1	2.15	0.44
1:A:44:VAL:HG23	1:A:61:ILE:HG21	1.99	0.43
1:G:3:ILE:HA	1:G:29:GLU:O	2.18	0.43
1:B:268:THR:HG21	1:B:552:ILE:HG12	2.00	0.43
1:B:350:ARG:NH1	1:B:430:ASP:OD2	2.51	0.43
1:B:453:ARG:NH2	1:G:403:ARG:HD3	2.32	0.43
1:A:328:LEU:HD22	1:A:361:ARG:HH22	1.83	0.43
1:F:273:LEU:O	1:F:276:VAL:HG12	2.18	0.43
1:F:520:PRO:CD	1:F:529:GLU:HG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:523:GLU:O	1:F:524:GLU:HG3	2.18	0.43
1:H:164:GLU:CD	1:H:164:GLU:O	2.60	0.43
1:H:294:LEU:HD23	1:H:313:LEU:CD2	2.42	0.43
1:B:73:GLU:N	1:A:157:ARG:NE	2.66	0.43
1:B:159:VAL:HG11	1:A:76:HIS:ND1	2.33	0.43
1:B:474:ALA:HA	1:B:478:LEU:HB2	2.00	0.43
1:A:3:ILE:HA	1:A:29:GLU:O	2.18	0.43
1:E:269:HIS:HE1	1:E:554:GLN:HG3	1.83	0.43
1:H:86:TRP:CE2	1:H:90:ARG:HG3	2.53	0.43
1:G:50:TYR:CE1	1:G:54:HIS:CE1	3.06	0.43
1:G:269:HIS:HE1	1:G:554:GLN:HG3	1.83	0.43
1:B:6:CYS:HA	1:B:100:CYS:HB3	2.00	0.43
1:B:71:ARG:H	1:B:71:ARG:HD3	1.83	0.43
1:B:72:SER:O	1:A:157:ARG:NH2	2.51	0.43
1:B:87:LEU:HD21	1:B:119:PHE:CE2	2.53	0.43
1:B:361:ARG:NH1	1:B:369:GLU:OE2	2.52	0.43
1:A:269:HIS:HE1	1:A:554:GLN:HG3	1.83	0.43
1:A:449:GLU:OE1	1:A:453:ARG:NE	2.52	0.43
1:A:454:VAL:HG23	1:A:456:LEU:HG	1.99	0.43
1:F:114:ARG:HH11	1:F:114:ARG:HD3	1.49	0.43
1:F:118:LEU:HB3	1:F:170:LEU:HD22	1.99	0.43
1:F:279:GLU:HG3	1:F:279:GLU:O	2.19	0.43
1:F:476:PHE:CZ	1:E:452:HIS:HB3	2.54	0.43
1:F:540:GLY:HA3	1:E:591:GLN:NE2	2.33	0.43
1:E:8:VAL:O	1:E:34:THR:HG23	2.18	0.43
1:E:56:GLY:HA3	1:E:57:PRO:HD3	1.90	0.43
1:H:159:VAL:HG11	1:G:76:HIS:ND1	2.33	0.43
1:H:243:ASP:OD2	1:H:246:GLN:OE1	2.36	0.43
1:H:430:ASP:HA	1:H:459:THR:CG2	2.47	0.43
1:B:4:LEU:HD12	1:B:27:PHE:CE2	2.53	0.43
1:B:476:PHE:CZ	1:A:452:HIS:HB3	2.54	0.43
1:H:6:CYS:HA	1:H:100:CYS:HB3	2.00	0.43
1:H:251:VAL:HG11	1:H:562:LEU:HD21	2.01	0.43
1:G:53:MET:HE1	1:G:148:GLU:OE2	2.18	0.43
1:B:77:MET:HA	1:B:199:ARG:HH21	1.83	0.43
1:B:121:ALA:O	1:B:164:GLU:HG3	2.18	0.43
1:B:437:ARG:HD2	1:B:440:ARG:NH1	2.32	0.43
1:B:510:PRO:HA	1:B:531:TYR:OH	2.19	0.43
1:A:386:ARG:O	1:A:600:ARG:NH1	2.49	0.43
1:E:3:ILE:HA	1:E:29:GLU:O	2.18	0.43
1:H:240:GLU:HB2	1:H:573:ARG:HH12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:523:GLU:O	1:H:524:GLU:HG3	2.18	0.43
1:G:242:LEU:HD13	1:G:573:ARG:HG2	2.01	0.43
1:B:243:ASP:OD2	1:B:246:GLN:OE1	2.36	0.43
1:B:257:VAL:HG22	1:B:597:LEU:HD11	2.00	0.43
1:F:131:PRO:HG2	1:F:133:PHE:CD1	2.54	0.43
1:F:463:GLY:HA2	1:F:466:ASP:OD1	2.19	0.43
1:E:12:TRP:HE3	1:E:47:LEU:HD23	1.84	0.43
1:H:114:ARG:HH22	1:G:162:GLY:CA	2.30	0.43
1:G:19:MET:HE2	1:G:19:MET:HB2	1.87	0.43
1:G:140:GLU:HG2	1:G:141:ALA:H	1.84	0.43
1:B:3:ILE:HG22	1:B:97:ARG:HA	2.01	0.43
1:B:130:GLU:HG2	1:A:71:ARG:HB3	2.01	0.43
1:B:157:ARG:HH22	1:A:74:GLN:HE22	1.64	0.43
1:B:405:ARG:CZ	1:B:405:ARG:HB3	2.48	0.43
1:A:417:ALA:HB2	1:A:456:LEU:HD21	2.01	0.43
1:F:378:MET:HE1	1:F:389:VAL:H	1.83	0.43
1:E:217:GLU:HG3	1:E:217:GLU:O	2.19	0.43
1:B:404:SER:HB3	1:G:453:ARG:HG3	2.01	0.43
1:B:520:PRO:CD	1:B:529:GLU:HG2	2.48	0.43
1:A:242:LEU:HD13	1:A:573:ARG:HG2	2.01	0.43
1:H:273:LEU:O	1:H:276:VAL:HG12	2.18	0.43
1:H:397:ARG:HD2	1:H:402:ASP:N	2.29	0.43
1:B:437:ARG:CD	1:B:440:ARG:NH1	2.82	0.43
1:B:461:HIS:O	1:B:461:HIS:HD2	2.01	0.43
1:A:454:VAL:HG12	1:F:408:ARG:NE	2.34	0.43
1:F:324:ASP:HB3	1:F:327:CYS:HB2	2.01	0.43
1:E:84:TRP:CZ3	1:E:199:ARG:HB2	2.53	0.43
1:E:417:ALA:HB2	1:E:456:LEU:HD21	2.01	0.43
1:E:436:ASP:C	1:E:437:ARG:HD2	2.44	0.43
1:H:475:VAL:HG13	1:H:504:ILE:CD1	2.49	0.43
1:G:417:ALA:HB2	1:G:456:LEU:HD21	2.01	0.43
1:B:378:MET:O	1:B:386:ARG:NE	2.52	0.42
1:B:386:ARG:O	1:B:600:ARG:NH1	2.52	0.42
1:A:8:VAL:O	1:A:34:THR:HG23	2.19	0.42
1:A:87:LEU:HD11	1:A:97:ARG:CD	2.49	0.42
1:A:139:ARG:HH22	1:A:142:SER:HB2	1.84	0.42
1:F:361:ARG:NH1	1:F:369:GLU:OE2	2.52	0.42
1:F:386:ARG:O	1:F:600:ARG:NH1	2.53	0.42
1:H:19:MET:HE1	1:H:26:GLY:C	2.43	0.42
1:H:131:PRO:HG2	1:H:133:PHE:CD1	2.54	0.42
1:B:523:GLU:O	1:B:524:GLU:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LEU:HD13	1:A:157:ARG:NH1	2.34	0.42
1:E:139:ARG:HH22	1:E:142:SER:HB2	1.84	0.42
1:H:257:VAL:HG22	1:H:597:LEU:HD11	1.99	0.42
1:H:476:PHE:CZ	1:G:452:HIS:HB3	2.54	0.42
1:G:8:VAL:O	1:G:34:THR:HG23	2.19	0.42
1:G:12:TRP:HE3	1:G:47:LEU:HD23	1.84	0.42
1:G:150:ALA:HB1	1:G:156:LEU:HD21	2.01	0.42
1:B:230:TRP:HB2	1:B:235:LEU:CD2	2.46	0.42
1:A:80:GLU:HG2	1:A:84:TRP:CH2	2.54	0.42
1:F:201:HIS:CD2	1:F:201:HIS:C	2.98	0.42
1:F:328:LEU:HD21	1:F:370:ILE:HG13	2.01	0.42
1:F:452:HIS:HB3	1:E:476:PHE:CZ	2.55	0.42
1:H:110:ALA:HB1	1:G:161:LEU:HD21	2.01	0.42
1:H:324:ASP:HB3	1:H:327:CYS:HB2	2.01	0.42
1:B:84:TRP:HA	1:B:87:LEU:CG	2.48	0.42
1:B:131:PRO:HG2	1:B:133:PHE:CD1	2.54	0.42
1:F:3:ILE:HG22	1:F:97:ARG:HA	2.01	0.42
1:F:130:GLU:HG2	1:E:71:ARG:HB3	2.01	0.42
1:F:562:LEU:HD12	1:F:562:LEU:N	2.33	0.42
1:E:350:ARG:NH1	1:E:430:ASP:OD2	2.52	0.42
1:G:19:MET:SD	1:G:27:PHE:HD2	2.42	0.42
1:G:217:GLU:O	1:G:217:GLU:HG3	2.20	0.42
1:B:229:ALA:O	1:A:209:SER:HA	2.20	0.42
1:B:328:LEU:HD21	1:B:370:ILE:HG13	2.01	0.42
1:B:453:ARG:NE	1:G:403:ARG:NH1	2.63	0.42
1:B:587:ALA:O	1:B:594:ARG:NH2	2.49	0.42
1:A:408:ARG:NE	1:F:418:GLU:OE1	2.53	0.42
1:F:229:ALA:O	1:E:209:SER:HA	2.19	0.42
1:F:280:ALA:CB	1:F:286:LEU:HD21	2.50	0.42
1:E:33:LEU:HD22	1:E:79:PHE:HE1	1.85	0.42
1:E:128:LEU:HD12	1:E:157:ARG:CZ	2.50	0.42
1:G:139:ARG:HH22	1:G:142:SER:HB2	1.84	0.42
1:A:196:MET:HE1	1:A:200:GLN:HG3	2.01	0.42
1:A:329:ARG:HA	1:A:373:HIS:CD2	2.55	0.42
1:F:6:CYS:HA	1:F:100:CYS:HB3	2.00	0.42
1:F:64:VAL:HG11	1:F:67:PHE:CD2	2.54	0.42
1:F:72:SER:N	1:E:157:ARG:NH1	2.67	0.42
1:E:356:TYR:HB2	1:E:366:VAL:HG11	2.02	0.42
1:H:247:ASP:O	1:H:251:VAL:HG12	2.20	0.42
1:B:437:ARG:NH1	1:B:440:ARG:HB3	2.35	0.42
1:F:405:ARG:HB3	1:F:405:ARG:CZ	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:TYR:HA	1:E:53:MET:CG	2.48	0.42
1:E:87:LEU:HD11	1:E:97:ARG:CD	2.49	0.42
1:E:140:GLU:HG2	1:E:141:ALA:H	1.83	0.42
1:H:209:SER:HB3	1:H:236:ARG:HD3	2.02	0.42
1:H:437:ARG:CD	1:H:440:ARG:NH1	2.82	0.42
1:G:33:LEU:HD12	1:G:62:SER:O	2.20	0.42
1:G:484:GLY:HA2	1:G:507:GLU:HB2	2.02	0.42
1:B:159:VAL:HA	1:A:73:GLU:OE1	2.20	0.42
1:B:324:ASP:HB3	1:B:327:CYS:HB2	2.01	0.42
1:A:254:LEU:HD11	1:A:577:LEU:HD21	2.02	0.42
1:F:469:GLU:OE1	1:E:453:ARG:NH2	2.52	0.42
1:E:85:ARG:NH1	1:E:179:PRO:O	2.50	0.42
1:E:449:GLU:O	1:E:453:ARG:HG2	2.20	0.42
1:H:3:ILE:HG22	1:H:97:ARG:HA	2.01	0.42
1:H:386:ARG:O	1:H:600:ARG:NH1	2.53	0.42
1:H:437:ARG:NH1	1:H:440:ARG:HB3	2.34	0.42
1:G:87:LEU:HD11	1:G:97:ARG:CD	2.50	0.42
1:G:145:GLU:OE1	1:G:149:GLN:NE2	2.53	0.42
1:G:254:LEU:HD11	1:G:577:LEU:HD21	2.02	0.42
1:B:157:ARG:NE	1:A:72:SER:HB2	2.34	0.42
1:B:452:HIS:HB3	1:A:476:PHE:CZ	2.55	0.42
1:A:101:LEU:CD2	1:A:126:HIS:HB2	2.43	0.42
1:F:118:LEU:HA	1:F:167:TRP:CD1	2.55	0.42
1:F:474:ALA:HA	1:F:478:LEU:HB2	2.00	0.42
1:E:77:MET:CE	1:E:196:MET:HG3	2.38	0.42
1:E:408:ARG:NH1	1:H:418:GLU:OE1	2.53	0.42
1:H:229:ALA:O	1:G:209:SER:HA	2.20	0.42
1:H:453:ARG:NH1	1:G:472:TRP:CD2	2.88	0.42
1:B:71:ARG:CA	1:A:157:ARG:HH11	2.33	0.42
1:B:118:LEU:HA	1:B:167:TRP:CD1	2.55	0.42
1:A:84:TRP:HZ3	1:A:199:ARG:CB	2.33	0.42
1:A:139:ARG:NH1	1:A:140:GLU:O	2.53	0.42
1:F:34:THR:HG22	1:F:35:THR:O	2.20	0.42
1:G:139:ARG:NH1	1:G:140:GLU:O	2.53	0.42
1:B:34:THR:HG22	1:B:35:THR:O	2.20	0.41
1:A:140:GLU:HG2	1:A:141:ALA:H	1.84	0.41
1:F:3:ILE:HD12	1:F:29:GLU:O	2.20	0.41
1:F:71:ARG:H	1:F:71:ARG:HD3	1.85	0.41
1:F:378:MET:HE2	1:F:389:VAL:H	1.84	0.41
1:F:397:ARG:CD	1:F:398:GLU:H	2.19	0.41
1:E:16:PRO:O	1:E:20:GLN:NE2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:132:ARG:H	1:H:132:ARG:HG2	1.71	0.41
1:H:159:VAL:HA	1:G:73:GLU:OE1	2.20	0.41
1:H:209:SER:HB3	1:H:236:ARG:CD	2.50	0.41
1:B:290:ARG:CZ	1:B:290:ARG:HB3	2.50	0.41
1:A:84:TRP:HZ3	1:A:199:ARG:HB2	1.85	0.41
1:E:254:LEU:HD11	1:E:577:LEU:HD21	2.02	0.41
1:E:547:THR:O	1:E:548:ASP:HB2	2.19	0.41
1:H:361:ARG:NH1	1:H:369:GLU:OE2	2.52	0.41
1:G:85:ARG:NH1	1:G:179:PRO:O	2.50	0.41
1:G:361:ARG:HG2	1:G:361:ARG:NH1	2.34	0.41
1:B:19:MET:HE1	1:B:27:PHE:N	2.35	0.41
1:B:84:TRP:CD1	1:B:119:PHE:CE2	3.09	0.41
1:B:237:TRP:CZ2	1:B:607:PRO:HB3	2.56	0.41
1:A:364:TRP:NE1	1:F:364:TRP:NE1	2.68	0.41
1:A:547:THR:HG22	1:A:560:ASN:ND2	2.34	0.41
1:F:46:GLN:O	1:F:47:LEU:C	2.62	0.41
1:F:494:ASP:OD1	1:F:495:LEU:N	2.52	0.41
1:E:139:ARG:NH1	1:E:140:GLU:O	2.53	0.41
1:H:2:ARG:HB3	1:H:98:TYR:CE1	2.54	0.41
1:H:3:ILE:HD12	1:H:29:GLU:O	2.20	0.41
1:H:237:TRP:CZ2	1:H:607:PRO:HB3	2.56	0.41
1:H:271:GLU:CD	1:H:275:LYS:HG3	2.46	0.41
1:H:452:HIS:HB3	1:G:476:PHE:CZ	2.55	0.41
1:H:453:ARG:HH12	1:G:472:TRP:CG	2.39	0.41
1:H:474:ALA:HA	1:H:478:LEU:HB2	2.00	0.41
1:B:405:ARG:HG3	1:B:405:ARG:HH11	1.85	0.41
1:F:159:VAL:HA	1:E:73:GLU:OE1	2.20	0.41
1:F:340:LEU:HD13	1:F:385:ARG:NH1	2.36	0.41
1:F:350:ARG:NH1	1:F:430:ASP:OD2	2.53	0.41
1:E:128:LEU:CD1	1:E:157:ARG:NH1	2.83	0.41
1:E:145:GLU:OE1	1:E:149:GLN:NE2	2.53	0.41
1:E:157:ARG:HH22	1:E:159:VAL:CG2	2.33	0.41
1:H:19:MET:HE2	1:H:26:GLY:HA2	1.98	0.41
1:H:46:GLN:O	1:H:47:LEU:C	2.62	0.41
1:H:114:ARG:NH2	1:G:162:GLY:HA3	2.35	0.41
1:H:196:MET:SD	1:H:196:MET:O	2.78	0.41
1:G:196:MET:HE1	1:G:200:GLN:CD	2.45	0.41
1:B:280:ALA:CB	1:B:286:LEU:HD21	2.50	0.41
1:A:2:ARG:HA	1:A:98:TYR:CZ	2.55	0.41
1:F:94:ALA:HB1	1:F:120:GLY:C	2.46	0.41
1:F:116:ALA:O	1:F:164:GLU:OE2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:PRO:HD2	1:E:574:LEU:HD11	2.03	0.41
1:H:77:MET:SD	1:H:199:ARG:CZ	3.09	0.41
1:H:116:ALA:O	1:H:164:GLU:OE2	2.38	0.41
1:H:251:VAL:HG11	1:H:562:LEU:CG	2.50	0.41
1:B:340:LEU:HD13	1:B:385:ARG:NH1	2.36	0.41
1:B:410:LEU:HD22	1:B:451:VAL:HG21	2.03	0.41
1:A:145:GLU:OE1	1:A:149:GLN:NE2	2.53	0.41
1:A:350:ARG:NH1	1:A:430:ASP:OD2	2.54	0.41
1:F:597:LEU:O	1:F:601:LEU:HB2	2.20	0.41
1:E:81:GLU:HA	1:E:84:TRP:CE3	2.56	0.41
1:E:419:HIS:HD2	1:H:362:SER:OG	2.03	0.41
1:E:472:TRP:CE2	1:E:495:LEU:HD13	2.56	0.41
1:E:484:GLY:HA2	1:E:507:GLU:HB2	2.02	0.41
1:H:118:LEU:HA	1:H:167:TRP:CD1	2.55	0.41
1:H:130:GLU:HG2	1:G:71:ARG:HB3	2.01	0.41
1:G:2:ARG:HA	1:G:98:TYR:CZ	2.55	0.41
1:G:356:TYR:HB2	1:G:366:VAL:HG11	2.02	0.41
1:B:3:ILE:HD12	1:B:29:GLU:O	2.20	0.41
1:B:94:ALA:HB1	1:B:120:GLY:C	2.45	0.41
1:A:217:GLU:O	1:A:217:GLU:HG3	2.20	0.41
1:F:405:ARG:HH11	1:F:405:ARG:HG3	1.85	0.41
1:F:410:LEU:HD22	1:F:451:VAL:HG21	2.03	0.41
1:E:21:LEU:HD22	1:E:125:PHE:CE1	2.56	0.41
1:E:319:SER:O	1:E:323:LYS:HG3	2.21	0.41
1:E:375:GLN:HG3	1:E:379:GLU:OE2	2.21	0.41
1:H:44:VAL:HG13	1:H:61:ILE:HD13	2.03	0.41
1:H:280:ALA:CB	1:H:286:LEU:HD21	2.50	0.41
1:G:329:ARG:HA	1:G:373:HIS:CD2	2.55	0.41
1:B:84:TRP:HA	1:B:87:LEU:HD21	2.01	0.41
1:B:403:ARG:HE	1:G:449:GLU:CD	2.29	0.41
1:B:419:HIS:HD2	1:G:362:SER:OG	2.03	0.41
1:A:150:ALA:HB1	1:A:156:LEU:HD21	2.01	0.41
1:A:203:GLU:HA	1:A:206:LEU:CG	2.51	0.41
1:A:453:ARG:HH12	1:F:404:SER:H	1.67	0.41
1:F:72:SER:CA	1:E:157:ARG:NE	2.78	0.41
1:F:205:VAL:HG22	1:F:208:ARG:NH1	2.36	0.41
1:F:290:ARG:HB3	1:F:290:ARG:CZ	2.50	0.41
1:E:196:MET:HE3	1:E:196:MET:HB3	1.70	0.41
1:E:286:LEU:HD11	1:E:321:LEU:CD1	2.51	0.41
1:H:104:GLY:HA3	1:H:109:SER:HB2	2.03	0.41
1:H:350:ARG:NH1	1:H:430:ASP:OD2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:LEU:HD22	1:G:125:PHE:CE1	2.56	0.41
1:B:12:TRP:CZ2	1:B:143:THR:HA	2.56	0.41
1:B:85:ARG:NH1	1:B:179:PRO:O	2.53	0.41
1:B:205:VAL:HG22	1:B:208:ARG:NH1	2.36	0.41
1:B:271:GLU:OE1	1:B:271:GLU:C	2.64	0.41
1:B:520:PRO:HD3	1:B:529:GLU:HG2	2.03	0.41
1:A:21:LEU:HD22	1:A:125:PHE:CE1	2.56	0.41
1:A:124:VAL:HG12	1:A:162:GLY:O	2.21	0.41
1:A:128:LEU:CD1	1:A:157:ARG:CZ	2.99	0.41
1:A:196:MET:HE1	1:A:200:GLN:CD	2.46	0.41
1:A:237:TRP:HE3	1:A:238:LEU:HD23	1.86	0.41
1:A:434:PHE:HZ	1:A:470:GLY:O	2.04	0.41
1:F:12:TRP:CZ2	1:F:143:THR:HA	2.56	0.41
1:F:237:TRP:CZ2	1:F:607:PRO:HB3	2.56	0.41
1:E:97:ARG:HB2	1:E:121:ALA:HA	2.03	0.41
1:E:114:ARG:HG3	1:E:118:LEU:HD23	2.02	0.41
1:E:150:ALA:HB1	1:E:156:LEU:HD21	2.02	0.41
1:E:262:HIS:HD2	1:E:548:ASP:O	2.04	0.41
1:E:329:ARG:HA	1:E:373:HIS:CD2	2.56	0.41
1:E:361:ARG:HG2	1:E:361:ARG:NH1	2.34	0.41
1:H:85:ARG:NH1	1:H:179:PRO:O	2.53	0.41
1:H:94:ALA:HB1	1:H:120:GLY:C	2.46	0.41
1:H:410:LEU:HD22	1:H:451:VAL:HG21	2.03	0.41
1:H:465:ASN:HB2	1:H:517:LYS:NZ	2.35	0.41
1:G:88:LEU:HD21	1:G:174:SER:C	2.46	0.41
1:G:350:ARG:NH1	1:G:430:ASP:OD2	2.54	0.41
1:B:46:GLN:O	1:B:47:LEU:C	2.62	0.41
1:B:322:LEU:CD1	1:B:328:LEU:HA	2.51	0.41
1:B:463:GLY:HA3	1:B:486:ALA:HA	2.03	0.41
1:A:237:TRP:CZ3	1:A:607:PRO:HB3	2.56	0.41
1:A:378:MET:CE	1:A:424:CYS:HB2	2.51	0.41
1:F:132:ARG:H	1:F:132:ARG:HG2	1.71	0.41
1:E:329:ARG:O	1:E:333:ARG:HG3	2.21	0.41
1:H:383:GLU:HG3	1:H:386:ARG:NH1	2.36	0.41
1:H:597:LEU:O	1:H:601:LEU:HB2	2.20	0.41
1:G:3:ILE:O	1:G:98:TYR:CD2	2.74	0.41
1:G:97:ARG:HB2	1:G:121:ALA:HA	2.03	0.41
1:G:286:LEU:HD11	1:G:321:LEU:CD1	2.51	0.41
1:B:207:GLU:O	1:B:211:HIS:ND1	2.46	0.40
1:B:404:SER:HB3	1:G:453:ARG:CB	2.51	0.40
1:A:405:ARG:HG3	1:A:409:HIS:HD2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:HIS:CD2	1:F:362:SER:OG	2.69	0.40
1:A:484:GLY:HA2	1:A:507:GLU:HB2	2.02	0.40
1:E:2:ARG:HG3	1:E:98:TYR:HH	1.85	0.40
1:E:19:MET:HE3	1:E:57:PRO:HG2	2.01	0.40
1:H:85:ARG:NH2	1:H:195:ASP:O	2.55	0.40
1:G:223:PRO:HD2	1:G:574:LEU:HD11	2.03	0.40
1:G:511:TYR:CE1	1:G:563:LEU:HB2	2.57	0.40
1:B:157:ARG:HH21	1:A:74:GLN:N	2.19	0.40
1:B:196:MET:HE3	1:B:196:MET:HB3	1.90	0.40
1:B:204:GLY:C	1:B:207:GLU:HG2	2.46	0.40
1:A:33:LEU:C	1:A:33:LEU:HD23	2.47	0.40
1:A:511:TYR:CE1	1:A:563:LEU:HB2	2.57	0.40
1:F:84:TRP:HA	1:F:87:LEU:HD21	2.02	0.40
1:F:280:ALA:HB2	1:F:286:LEU:HD21	2.03	0.40
1:E:237:TRP:CZ3	1:E:607:PRO:HB3	2.56	0.40
1:E:301:PRO:HD3	1:E:515:GLN:HG2	2.04	0.40
1:E:378:MET:HE1	1:E:424:CYS:HB2	2.04	0.40
1:H:218:GLY:HA2	1:G:171:ARG:NH2	2.36	0.40
1:H:437:ARG:HH22	1:H:441:ALA:CA	2.34	0.40
1:G:403:ARG:CG	1:G:403:ARG:NE	2.79	0.40
1:B:53:MET:SD	1:B:53:MET:N	2.93	0.40
1:B:280:ALA:HB2	1:B:286:LEU:HD21	2.03	0.40
1:B:502:ARG:HD2	1:A:481:ARG:HD2	2.03	0.40
1:F:84:TRP:CD2	1:F:119:PHE:HZ	2.40	0.40
1:F:164:GLU:CD	1:F:164:GLU:C	2.89	0.40
1:F:472:TRP:NE1	1:E:453:ARG:NH1	2.69	0.40
1:F:502:ARG:HD2	1:E:481:ARG:HD2	2.04	0.40
1:E:2:ARG:HA	1:E:98:TYR:CZ	2.56	0.40
1:E:196:MET:CG	1:E:199:ARG:HB3	2.51	0.40
1:E:434:PHE:CZ	1:E:474:ALA:HB2	2.56	0.40
1:H:340:LEU:HD13	1:H:385:ARG:NH1	2.36	0.40
1:B:161:LEU:O	1:A:114:ARG:CZ	2.70	0.40
1:B:164:GLU:CD	1:B:164:GLU:C	2.89	0.40
1:B:251:VAL:CB	1:B:562:LEU:HD11	2.50	0.40
1:A:3:ILE:O	1:A:98:TYR:CD2	2.74	0.40
1:A:248:LYS:HG3	1:A:562:LEU:HD11	2.03	0.40
1:A:397:ARG:HH21	1:A:401:GLY:HA2	1.86	0.40
1:F:85:ARG:NH2	1:F:195:ASP:O	2.55	0.40
1:F:322:LEU:CD1	1:F:328:LEU:HA	2.52	0.40
1:F:453:ARG:HA	1:E:472:TRP:CH2	2.56	0.40
1:F:521:LEU:O	1:F:521:LEU:HD12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:378:MET:CE	1:E:424:CYS:HB2	2.51	0.40
1:H:34:THR:HG22	1:H:35:THR:O	2.20	0.40
1:H:219:ILE:HD11	1:G:226:ALA:HA	2.03	0.40
1:G:237:TRP:CZ3	1:G:607:PRO:HB3	2.56	0.40
1:G:403:ARG:HG2	1:G:403:ARG:N	2.34	0.40
1:B:72:SER:C	1:A:157:ARG:NE	2.79	0.40
1:B:437:ARG:HH22	1:B:441:ALA:CA	2.34	0.40
1:A:223:PRO:HD2	1:A:574:LEU:HD11	2.03	0.40
1:A:336:TYR:CD2	1:A:377:ALA:HB1	2.57	0.40
1:F:77:MET:SD	1:F:199:ARG:CZ	3.09	0.40
1:F:437:ARG:HG3	1:F:440:ARG:NH2	2.36	0.40
1:E:157:ARG:NH2	1:E:159:VAL:CG2	2.85	0.40
1:H:405:ARG:NH2	1:H:409:HIS:NE2	2.69	0.40
1:H:463:GLY:HA3	1:H:486:ALA:HA	2.02	0.40
1:H:502:ARG:HD2	1:G:481:ARG:HD2	2.04	0.40
1:G:547:THR:HG22	1:G:560:ASN:HD22	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	607/625 (97%)	572 (94%)	32 (5%)	3 (0%)	24	57
1	B	606/625 (97%)	578 (95%)	23 (4%)	5 (1%)	16	47
1	E	607/625 (97%)	573 (94%)	31 (5%)	3 (0%)	24	57
1	F	606/625 (97%)	580 (96%)	23 (4%)	3 (0%)	24	57
1	G	607/625 (97%)	575 (95%)	30 (5%)	2 (0%)	36	67
1	H	606/625 (97%)	580 (96%)	23 (4%)	3 (0%)	24	57
All	All	3639/3750 (97%)	3458 (95%)	162 (4%)	19 (0%)	26	57

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	548	ASP
1	E	548	ASP
1	A	28	ASP
1	E	28	ASP
1	G	28	ASP
1	B	466	ASP
1	B	143	THR
1	A	485	HIS
1	F	143	THR
1	E	485	HIS
1	H	121	ALA
1	H	143	THR
1	G	485	HIS
1	B	121	ALA
1	B	485	HIS
1	F	121	ALA
1	F	485	HIS
1	H	485	HIS
1	B	468	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	498/511 (98%)	498 (100%)	0	100	100
1	B	497/511 (97%)	497 (100%)	0	100	100
1	E	498/511 (98%)	498 (100%)	0	100	100
1	F	497/511 (97%)	497 (100%)	0	100	100
1	G	498/511 (98%)	498 (100%)	0	100	100
1	H	497/511 (97%)	497 (100%)	0	100	100
All	All	2985/3066 (97%)	2985 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.



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

Mol	Chain	Res	Type
1	B	54	HIS
1	B	76	HIS
1	B	96	HIS
1	B	126	HIS
1	B	234	HIS
1	B	252	GLN
1	B	316	ASN
1	B	461	HIS
1	B	488	HIS
1	B	513	ASN
1	A	74	GLN
1	A	136	GLN
1	A	189	HIS
1	A	200	GLN
1	A	252	GLN
1	A	373	HIS
1	A	375	GLN
1	A	409	HIS
1	A	419	HIS
1	A	473	GLN
1	A	560	ASN
1	A	591	GLN
1	F	54	HIS
1	F	96	HIS
1	F	126	HIS
1	F	201	HIS
1	F	234	HIS
1	F	252	GLN
1	F	316	ASN
1	F	372	ASN
1	F	419	HIS
1	F	461	HIS
1	F	513	ASN
1	F	603	GLN
1	E	76	HIS
1	E	136	GLN
1	E	149	GLN
1	E	189	HIS
1	E	200	GLN
1	E	252	GLN
1	E	373	HIS

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Mol	Chain	Res	Type
1	E	375	GLN
1	E	419	HIS
1	E	488	HIS
1	E	549	ASN
1	E	560	ASN
1	E	591	GLN
1	H	54	HIS
1	H	76	HIS
1	H	96	HIS
1	H	126	HIS
1	H	234	HIS
1	H	252	GLN
1	H	316	ASN
1	H	372	ASN
1	H	485	HIS
1	H	513	ASN
1	H	603	GLN
1	G	54	HIS
1	G	136	GLN
1	G	189	HIS
1	G	252	GLN
1	G	373	HIS
1	G	375	GLN
1	G	419	HIS
1	G	488	HIS
1	G	549	ASN
1	G	560	ASN
1	G	591	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	F	1
1	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	46:GLN	C	47:LEU	N	1.20
1	F	46:GLN	C	47:LEU	N	1.20
1	H	46:GLN	C	47:LEU	N	1.20

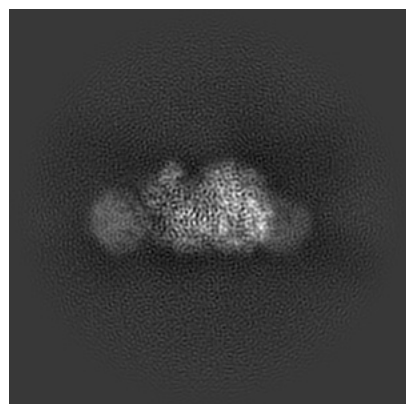
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48116. These allow visual inspection of the internal detail of the map and identification of artifacts.

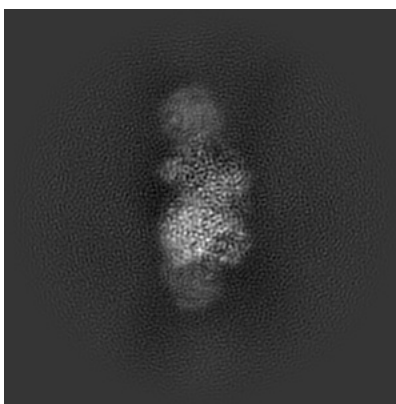
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

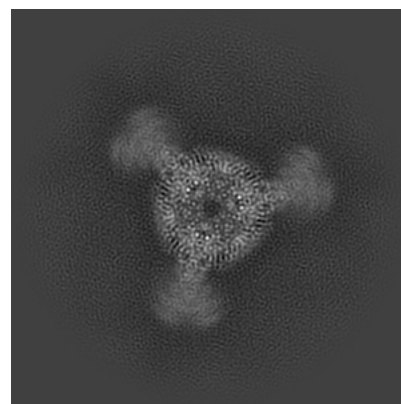
#### 6.1.1 Primary map



X

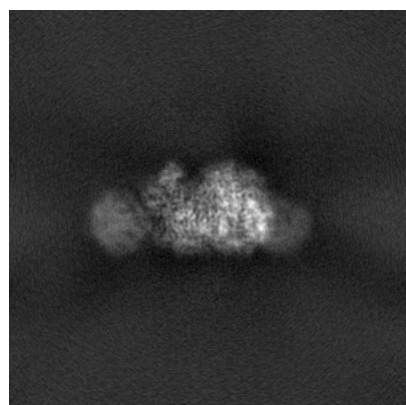


Y

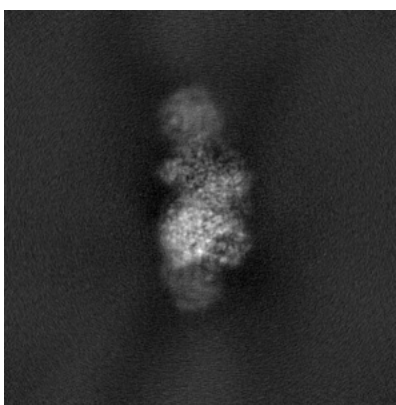


Z

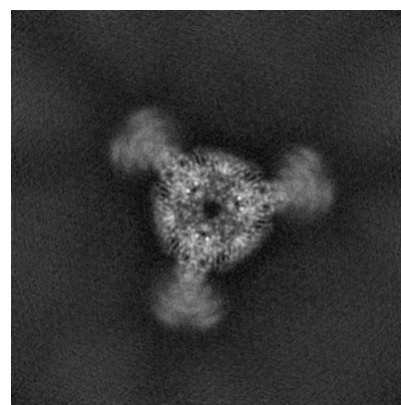
#### 6.1.2 Raw map



X



Y

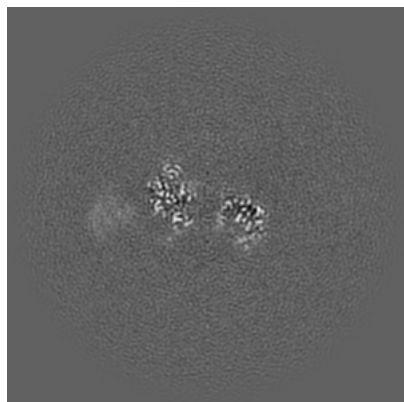


Z

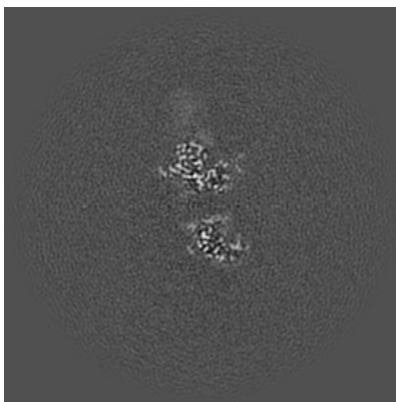
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

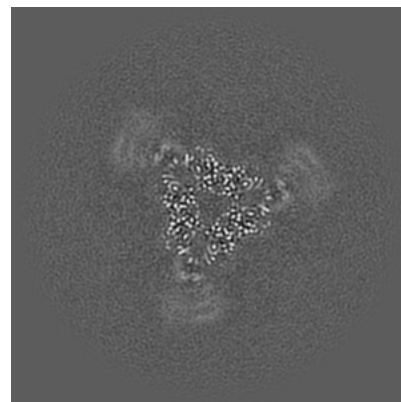
### 6.2.1 Primary map



X Index: 160



Y Index: 160

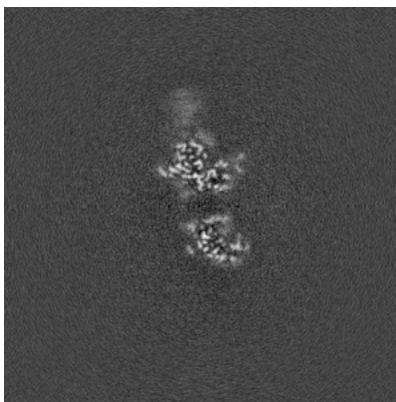


Z Index: 160

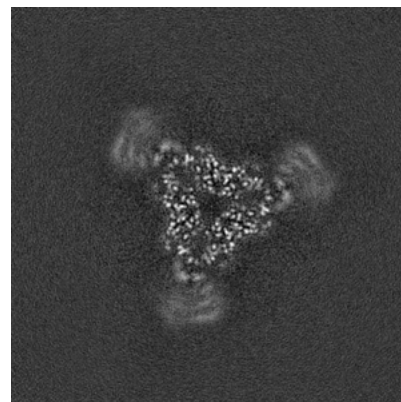
### 6.2.2 Raw map



X Index: 160



Y Index: 160

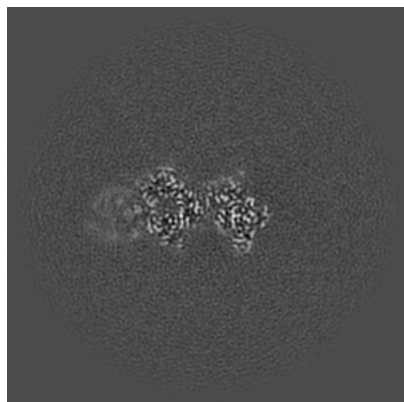


Z Index: 160

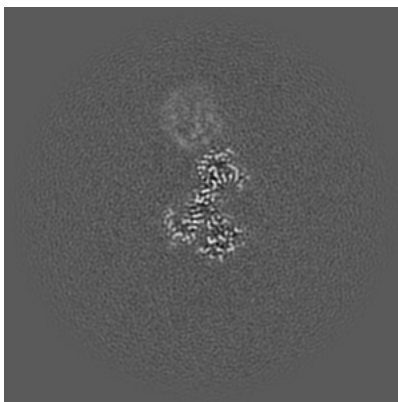
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

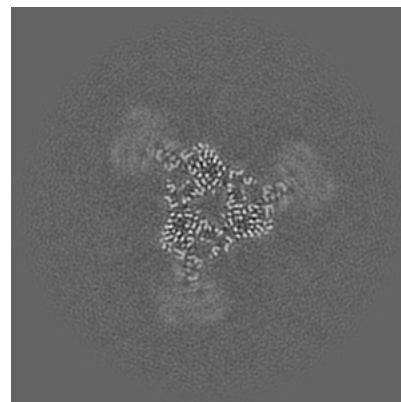
### 6.3.1 Primary map



X Index: 148

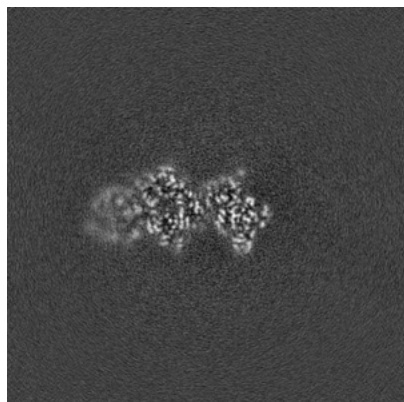


Y Index: 181

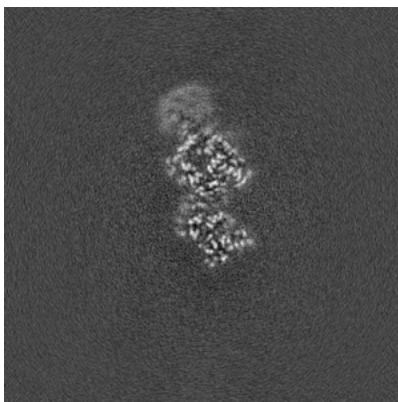


Z Index: 156

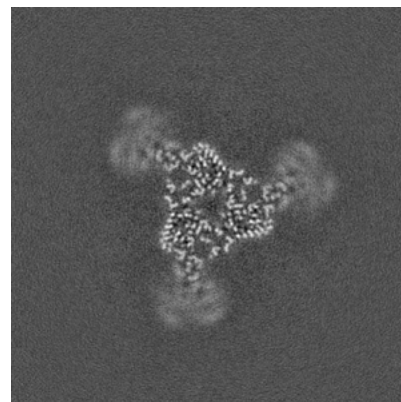
### 6.3.2 Raw map



X Index: 148



Y Index: 172



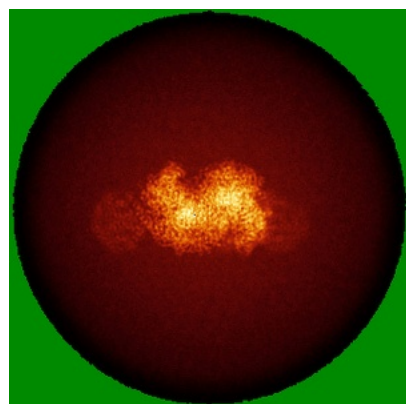
Z Index: 156

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

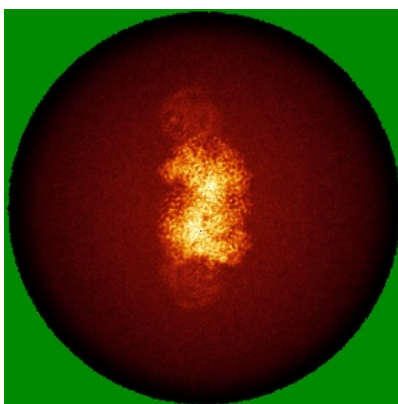


## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

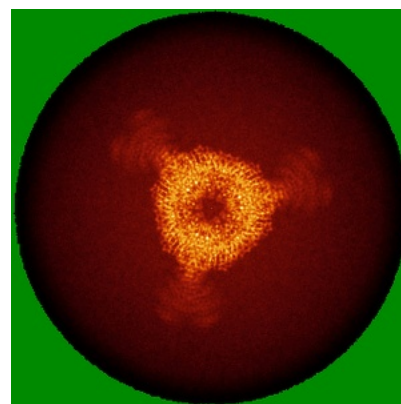
### 6.4.1 Primary map



X

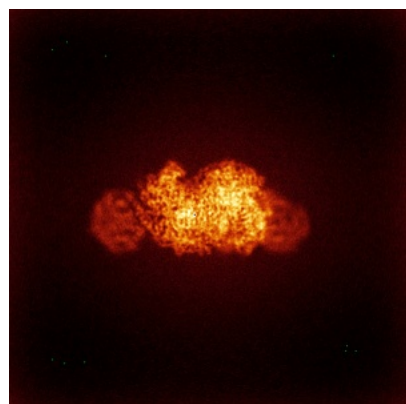


Y

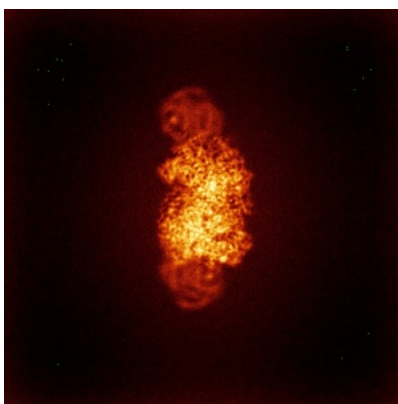


Z

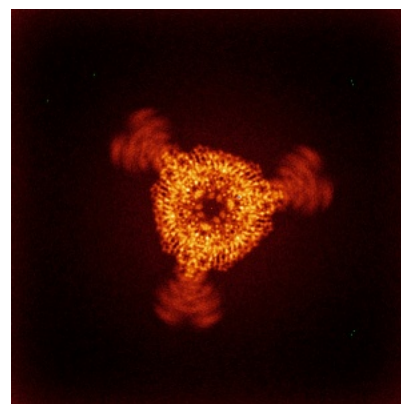
### 6.4.2 Raw map



X



Y

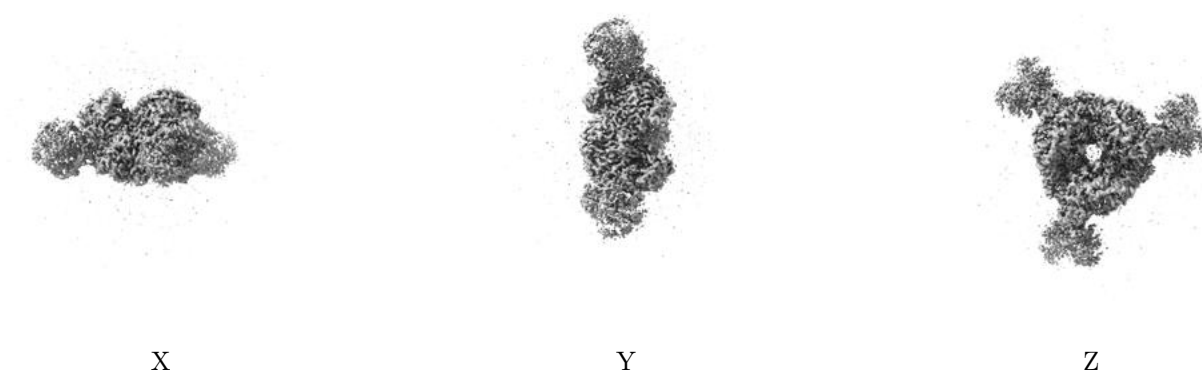


Z

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

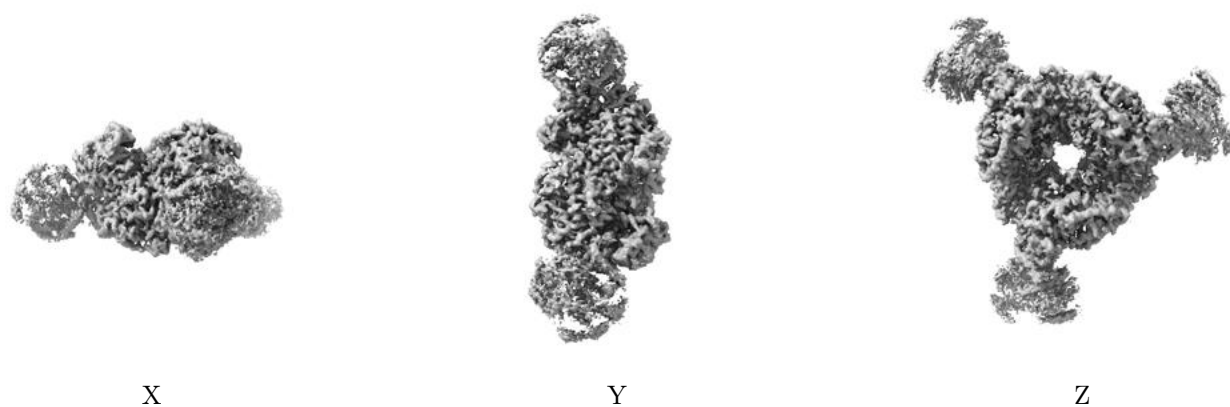
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation [i](#)

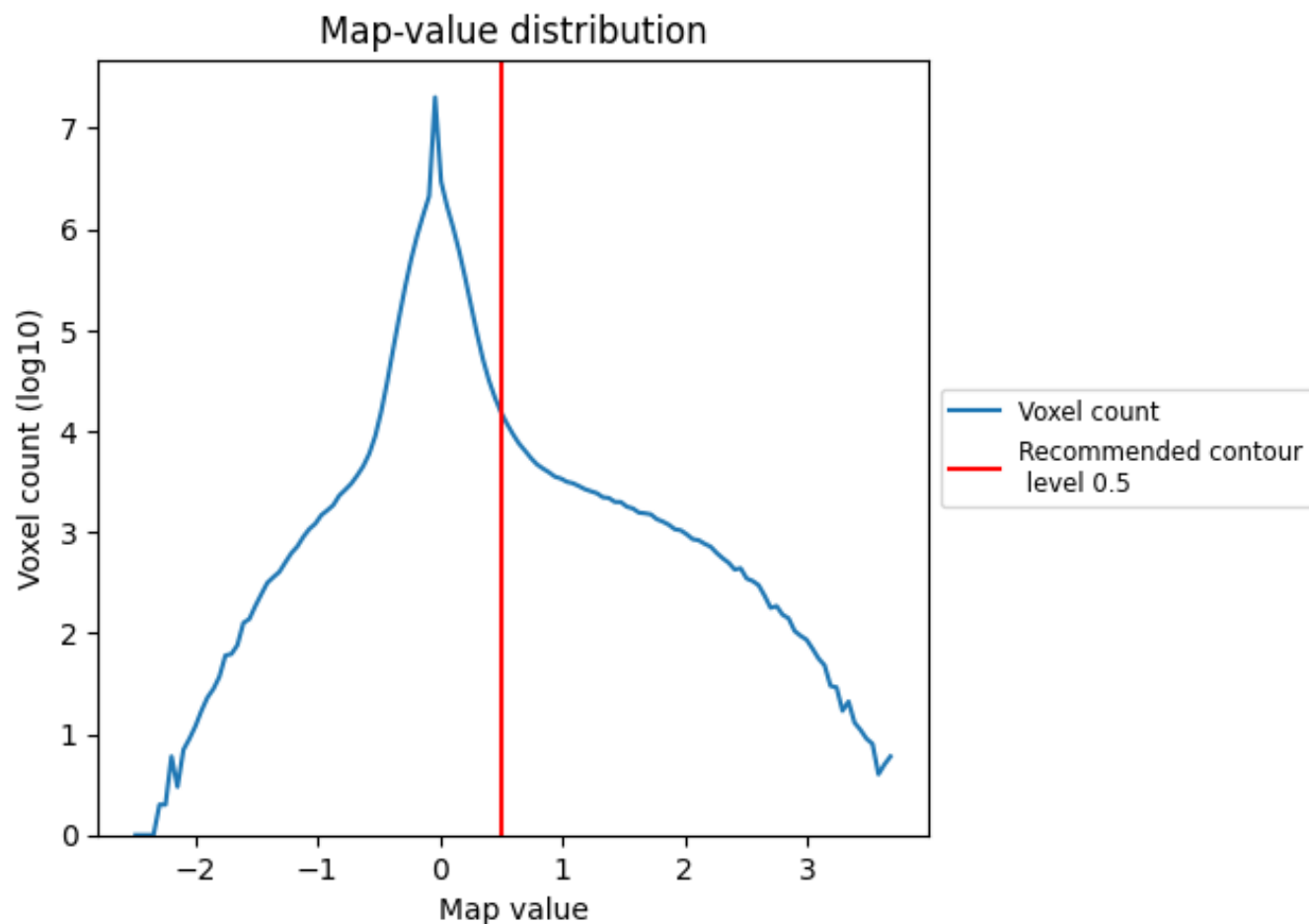
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

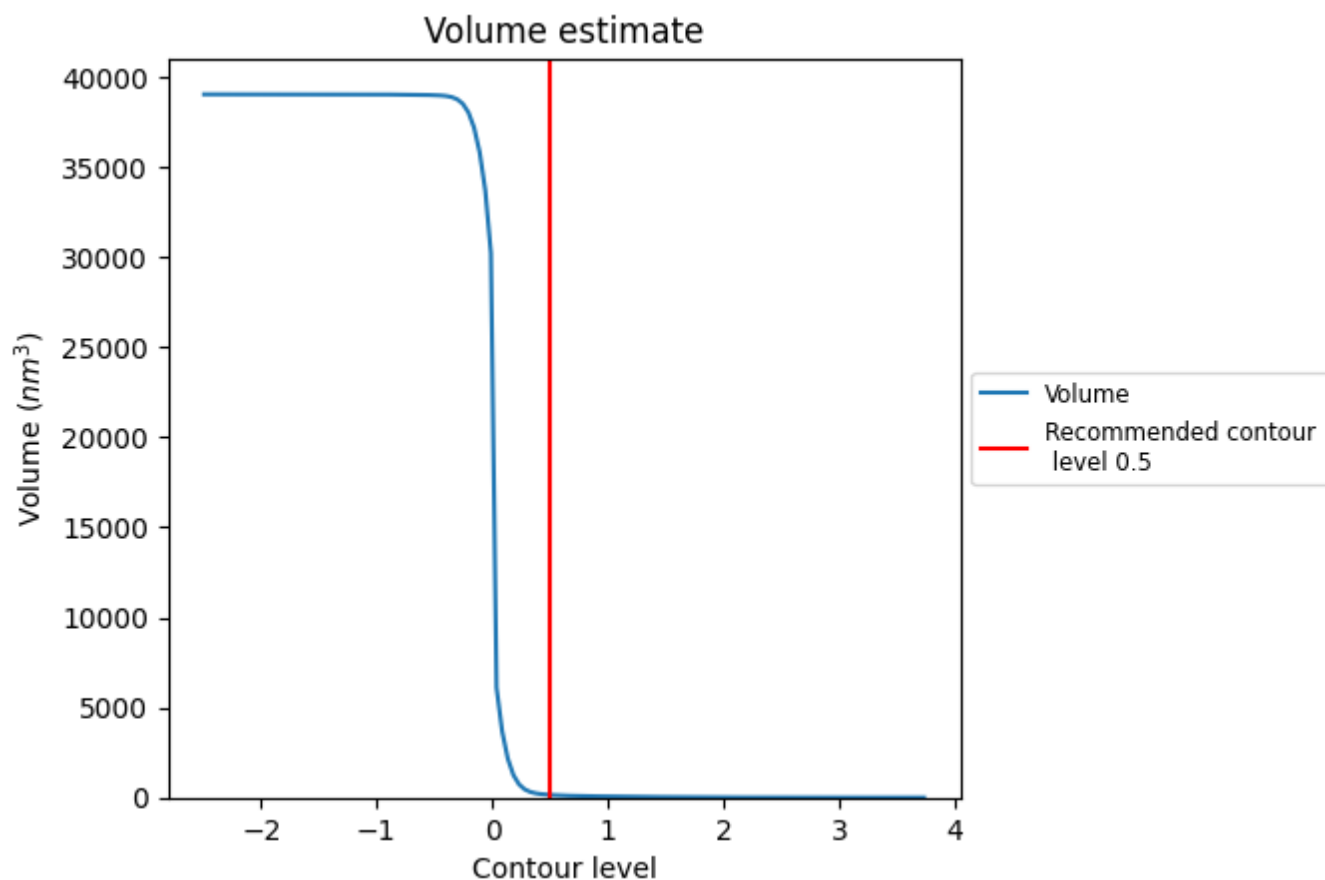
This section contains the results of statistical analysis of the map.

### 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.

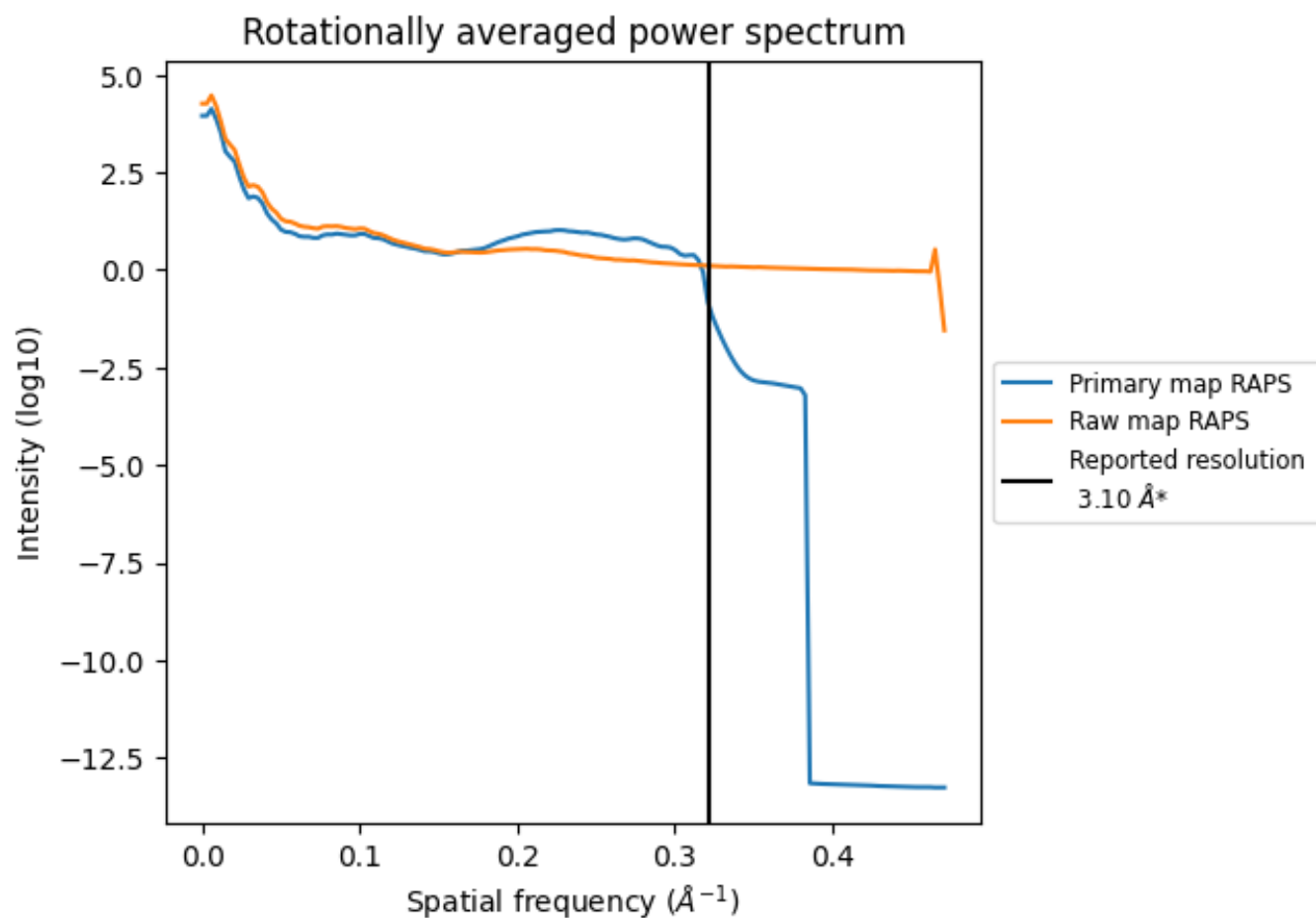
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 148 nm<sup>3</sup>; this corresponds to an approximate mass of 133 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 ⓘ

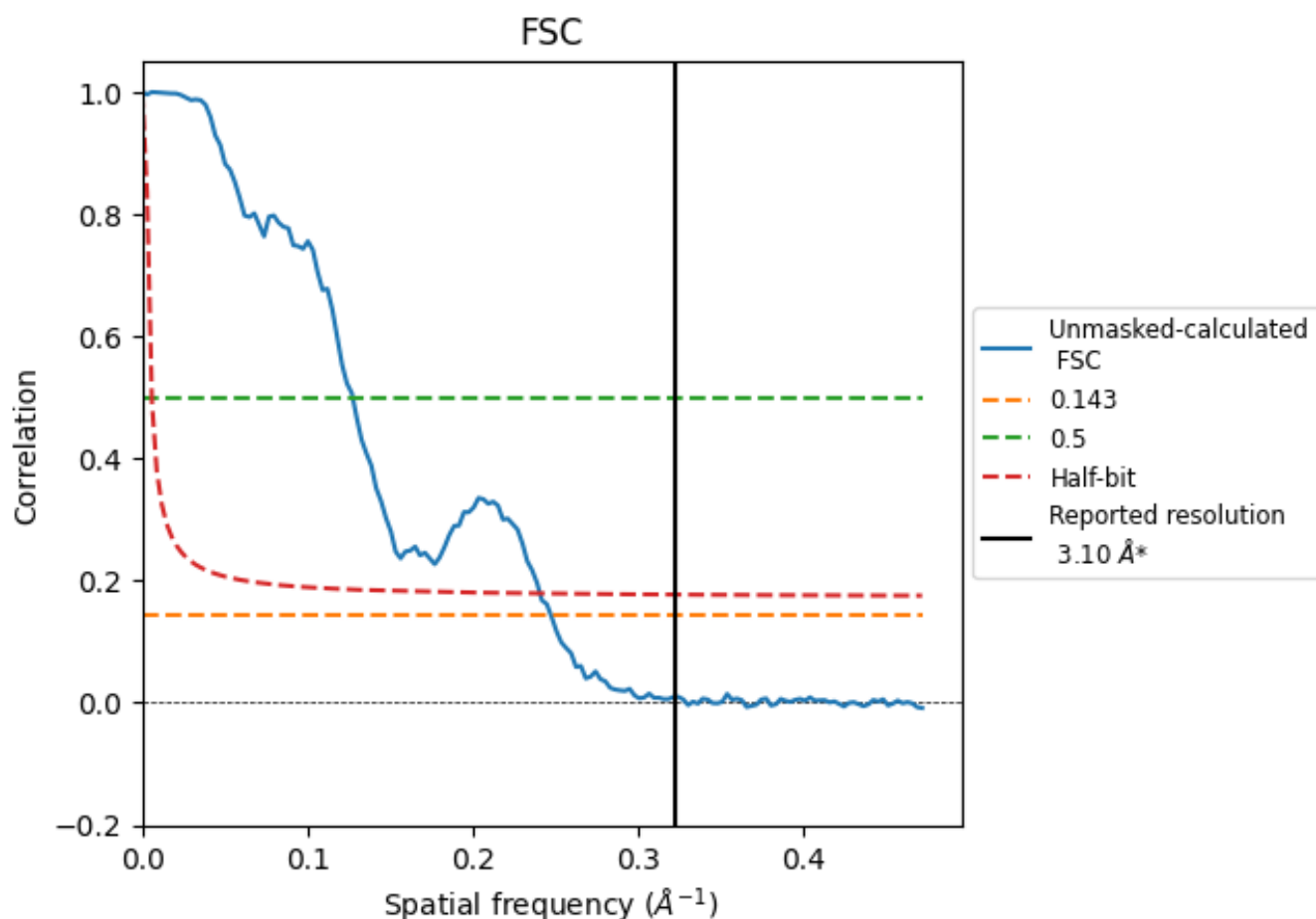


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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 0.323  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

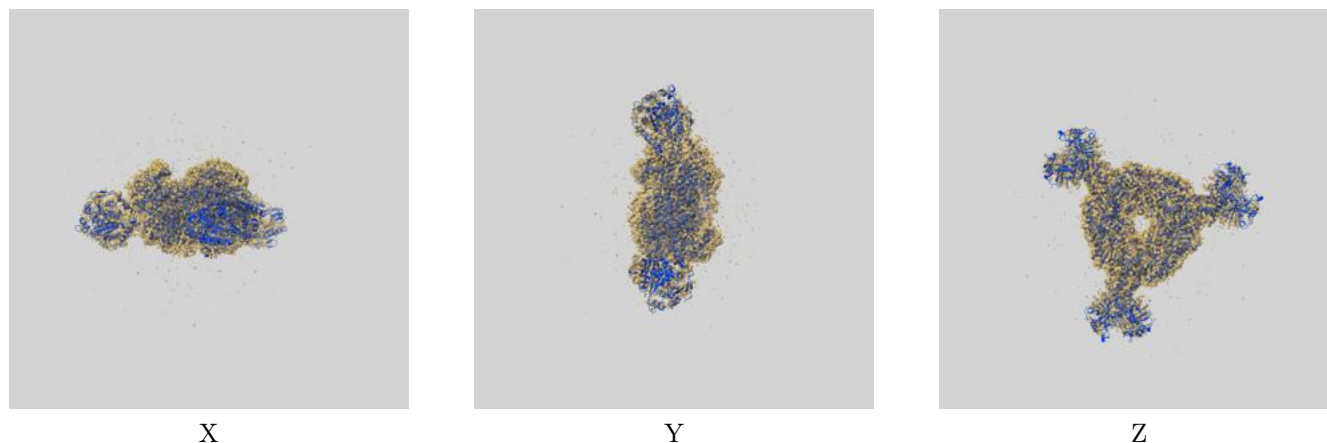
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.04	7.86	4.16

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.04 differs from the reported value 3.1 by more than 10 %

## 9 Map-model fit [i](#)

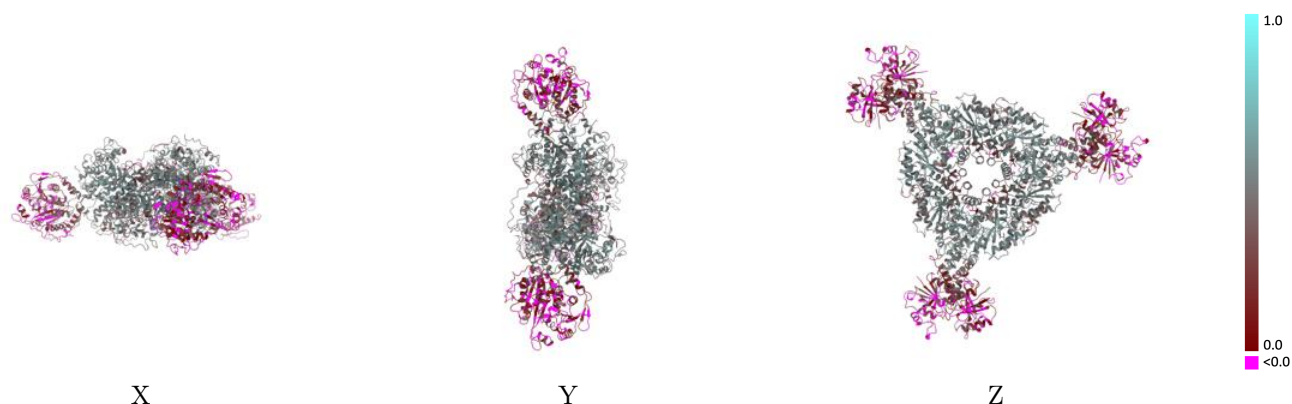
This section contains information regarding the fit between EMDB map EMD-48116 and PDB model 9EKA. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

### 9.1 Map-model overlay [i](#)



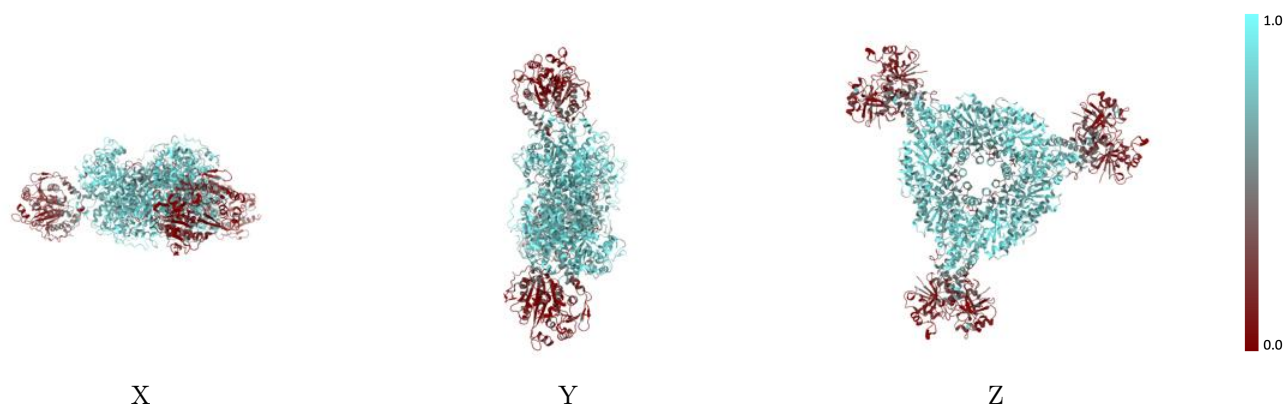
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



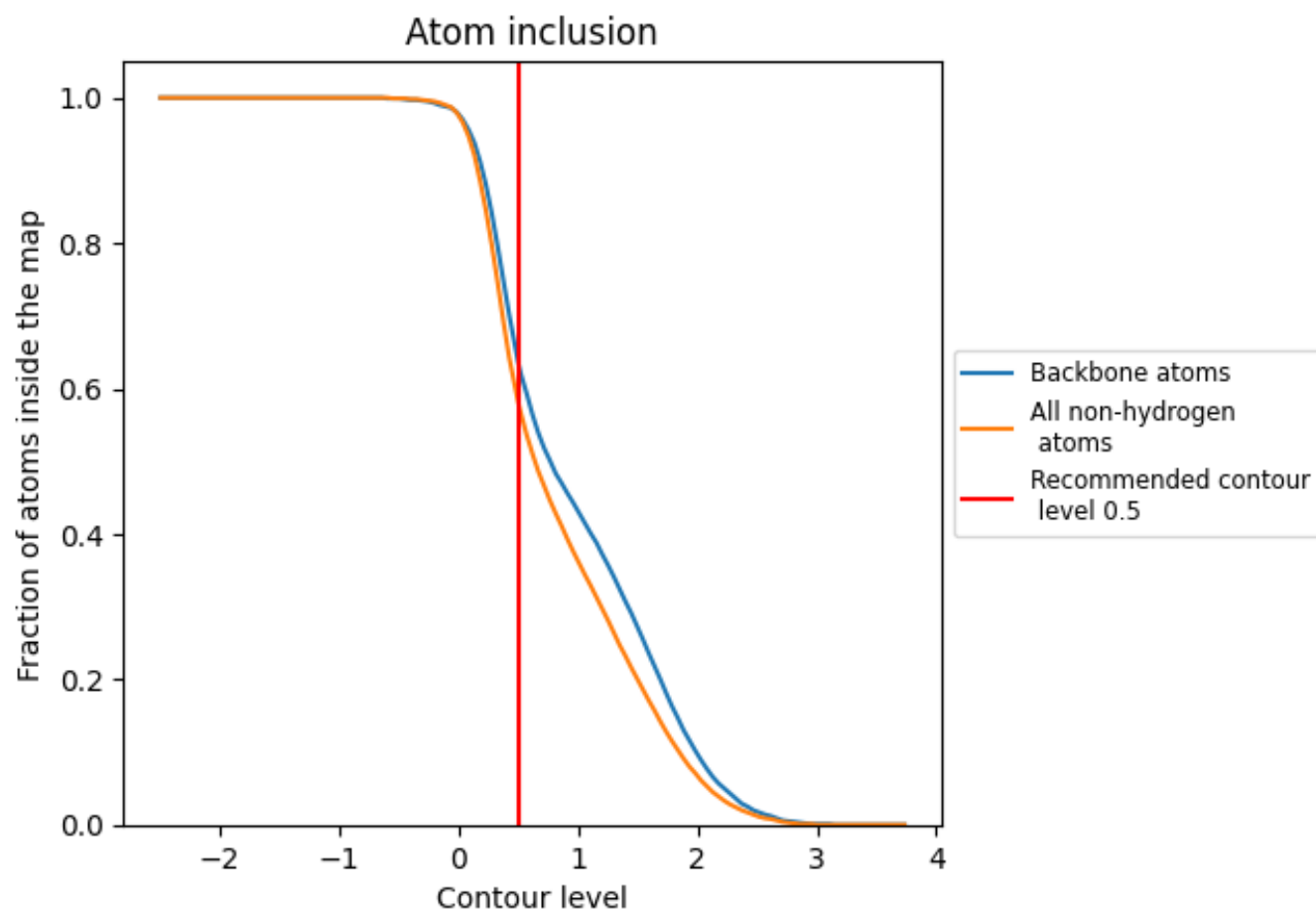
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.5820	<div><div></div></div> 0.3510
A	<div><div></div></div> 0.5890	<div><div></div></div> 0.3610
B	<div><div></div></div> 0.5740	<div><div></div></div> 0.3390
E	<div><div></div></div> 0.5920	<div><div></div></div> 0.3640
F	<div><div></div></div> 0.5760	<div><div></div></div> 0.3420
G	<div><div></div></div> 0.5880	<div><div></div></div> 0.3620
H	<div><div></div></div> 0.5710	<div><div></div></div> 0.3360

1.0

0.0

<0.0