



## Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 11:11 AM JST

PDB ID : 5GOA  
EMDB ID : EMD-9529  
Title : Cryo-EM structure of RyR2 in open state  
Authors : Peng, W.; Wu, J.P.; Yan, N.  
Deposited on : 2016-07-26  
Resolution : 4.20 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.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

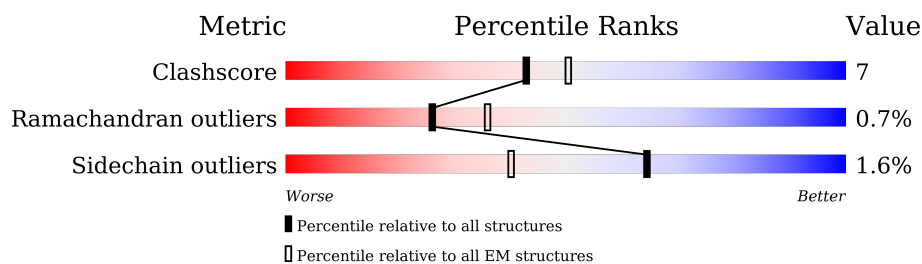
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	4968	 14% 54% 14% • 31%
1	B	4968	 14% 54% 14% • 31%
1	C	4968	 14% 54% 14% • 31%
1	D	4968	 14% 53% 14% • 31%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 105072 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3423	Total	C	N	O	S	0	0
			26267	16741	4498	4874	154		
1	B	3423	Total	C	N	O	S	0	0
			26267	16741	4498	4874	154		
1	C	3423	Total	C	N	O	S	0	0
			26267	16741	4498	4874	154		
1	D	3423	Total	C	N	O	S	0	0
			26267	16741	4498	4874	154		

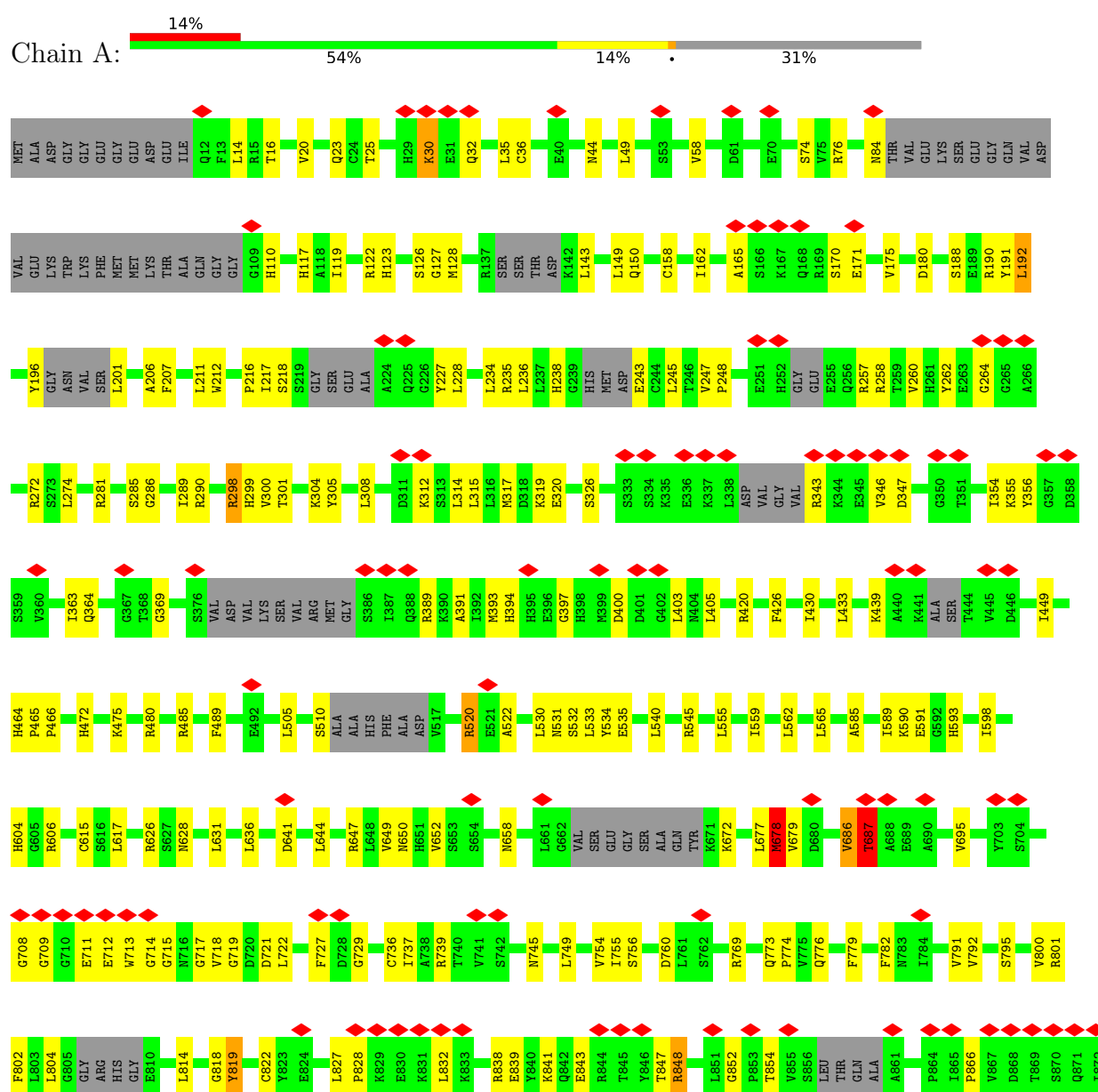
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	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.

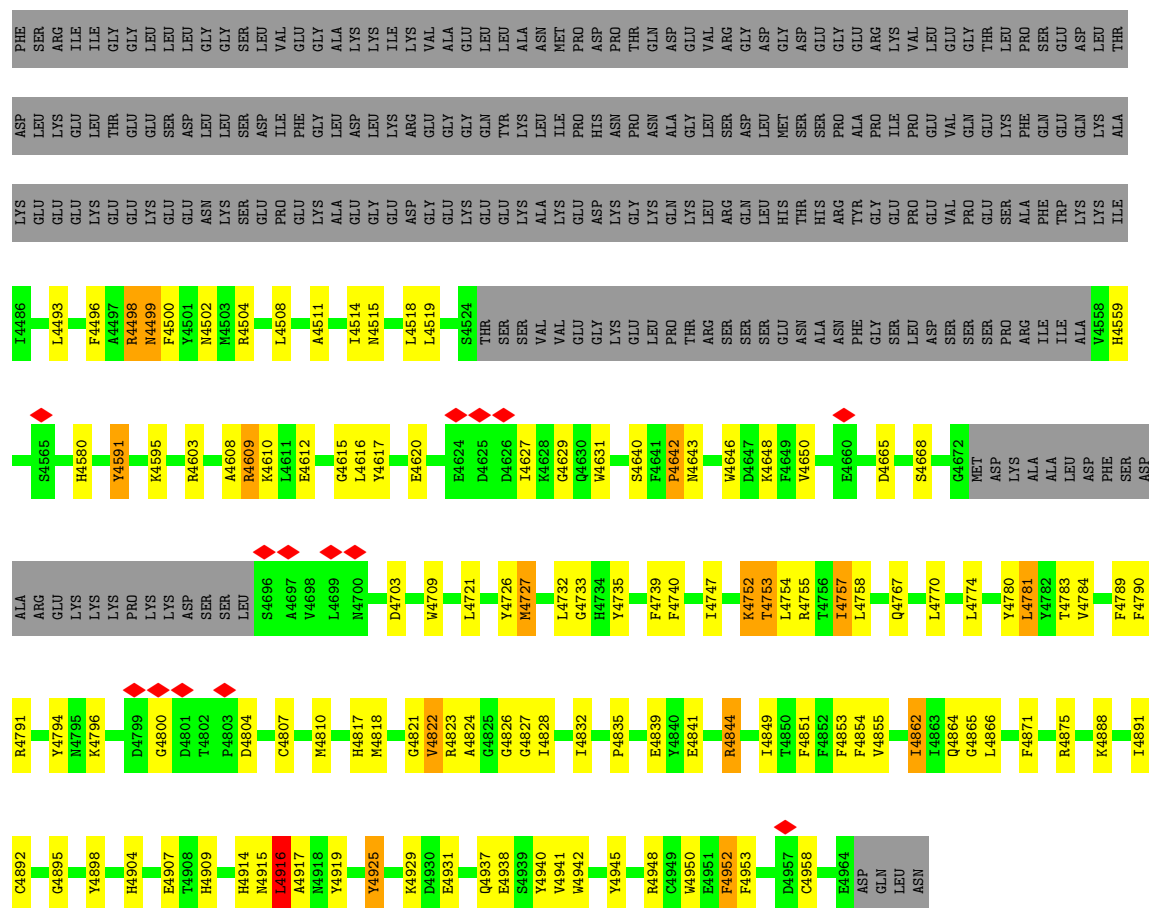
#### • Molecule 1: RyR2



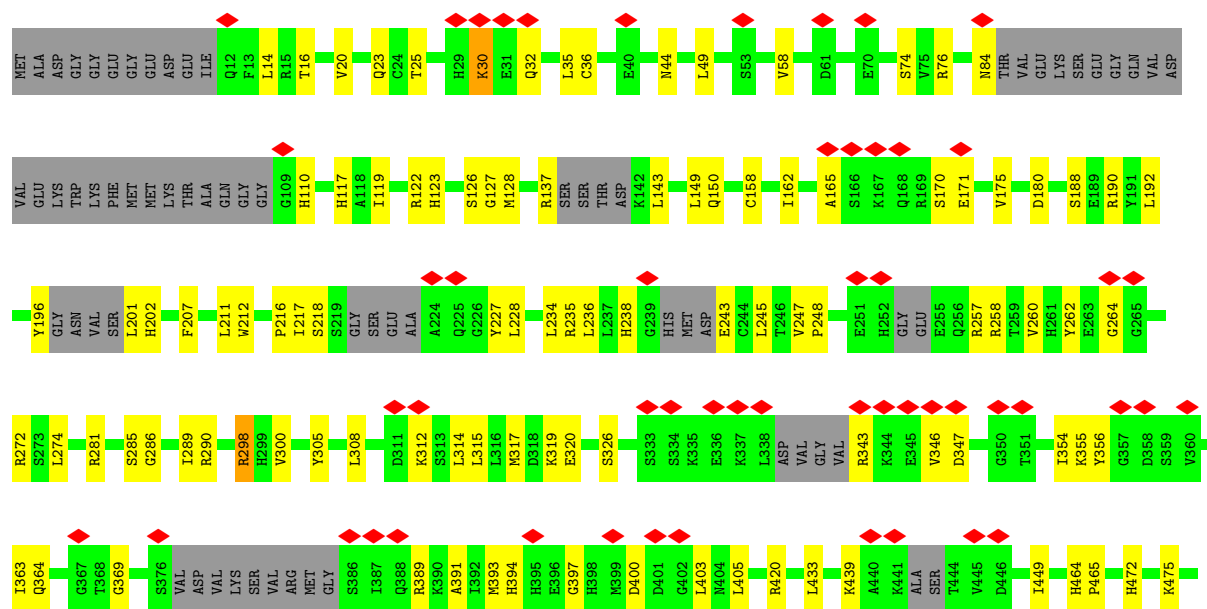




WORLDWIDE  
**PDB**  
PROTEIN DATA BANK



### • Molecule 1: RyR2











A4917	M4918	Y4919	Y4925	K4929	D4930	E4931	Q4937	E4938	S4939	Y4940	V4941	W4942	Y4945	R4948	C4949	W4950	E4951	F4952	F4953	D4957	C4958	E4964	ASP	GLN	LEU	ASN																						
H4817	M4818	W4709	L4721	Y4726	M4727	G4826	G4827	I4828	T4832	P4835	E4839	Y4840	E4841	R4844	I4849	T4850	F4851	F4852	F4853	F4854	V4855	A4861	L4862	T4863	Q4864	C4865	L4866	F4871	R4875	K4888	I4891	C4892	G4895	Y4898	H4904	F4907	T4908	H4909	H4914	N4915	L4916							
L4616	Y4617	E4620	E4624	D4625	D4626	K4628	G4629	Q4630	W4631	S4640	F4641	P4642	N4643	W4646	K4647	K4648	F4649	V4650	E4660	D4665	S4668	G4672	MET	ASP	LYS	ALA	LEU	ASP	PHE	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY					
I4514	N4515	L4518	L4519	S4524	THR	SER	VAL	VAL	GLY	LYS	GLY	GLY	GLY	GLY	SER	SER	GLY	ASN	ALA	PHE	LEU	ASP	SER	LYS	PRO	PRO	VAL	VAL	ARG	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY					
L4616	Y4617	E4620	E4624	D4625	D4626	K4628	G4629	Q4630	W4631	S4640	F4641	P4642	N4643	W4646	K4647	K4648	F4649	V4650	E4660	D4665	S4668	G4672	MET	ASP	LYS	ALA	LEU	ASP	PHE	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY				
D4703	W4709	L4721	Y4726	M4727	L4732	G4733	H4734	Y4735	F4739	F4740	I4747	K4752	T4753	L4754	R4755	T4756	L4757	L4758	Q4767	L4770	L4774	Y4780	L4781	Y4782	T4783	V4784	F4789	F4790	R4791	Y4794	K4795	S4796	S4797	E4798	D4799	G4800	T4802	P4803	D4804	M4805	K4806	C4807	M4810					
H4817	M4818	W4709	L4721	Y4726	M4727	G4826	G4827	I4828	T4832	P4835	E4839	Y4840	E4841	R4844	I4849	T4850	F4851	F4852	F4853	F4854	V4855	A4861	L4862	T4863	Q4864	C4865	L4866	F4871	R4875	K4888	I4891	C4892	G4895	Y4898	H4904	F4907	T4908	H4909	H4914	N4915	L4916							
L4616	Y4617	E4620	E4624	D4625	D4626	K4628	G4629	Q4630	W4631	S4640	F4641	P4642	N4643	W4646	K4647	K4648	F4649	V4650	E4660	D4665	S4668	G4672	MET	ASP	LYS	ALA	LEU	ASP	PHE	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY				
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L4616	Y4617	E4620	E4624	D4625	D4626	K4628	G4629	Q4630	W4631	S4640	F4641	P4642	N4643	W4646	K4647	K4648	F4649	V4650	E4660	D4665	S4668	G4672	MET	ASP	LYS	ALA	LEU	ASP	PHE	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY			
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L4616	Y4617	E4620	E4624	D4625	D4626	K4628	G4629	Q4630	W4631	S4640	F4641	P4642	N4643	W4646	K4647	K4648	F4649	V4650	E4660	D4665	S4668	G4672	MET	ASP	LYS	ALA	LEU	ASP	PHE	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY		
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L4616	Y4617	E4620	E4624	D4625	D4626	K4628	G4629	Q4630	W4631	S4640	F4641	P4642	N4643	W4646	K4647	K4648	F4649	V4650	E4660	D4665	S4668	G4672	MET	ASP	LYS	ALA	LEU	ASP	PHE	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
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L4616	Y4617	E4620	E4624	D4625	D4626	K4628	G4629	Q4630	W4631	S4640	F4641	P4642	N4643	W4646	K4647	K4648	F4649	V4650	E4660	D4665	S4668	G4672	MET	ASP	LYS	ALA	LEU	ASP	PHE	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
I4514	N4515	L4518	L4519	S4524	THR	SER	VAL	VAL	GLY	LYS	GLY	GLY	GLY	GLY	SER	SER	GLY	ASN	ALA	PHE	LEU	ASP	SER	LYS	PRO	PRO																						

• Molecule 1: RyR2

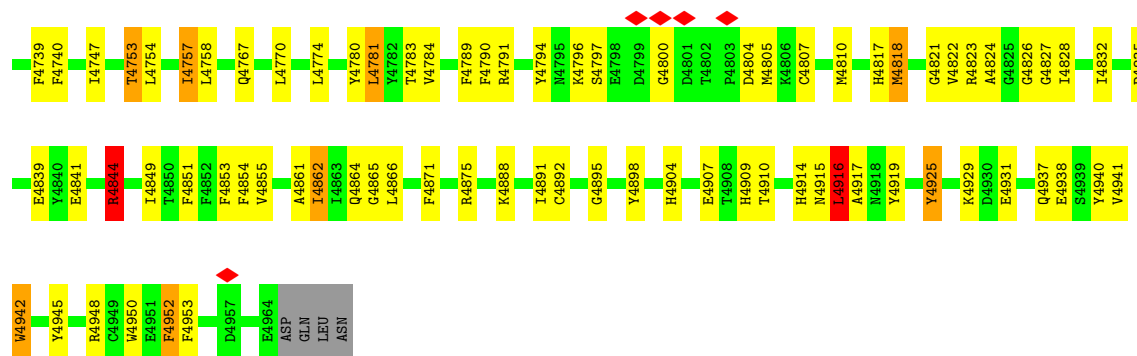




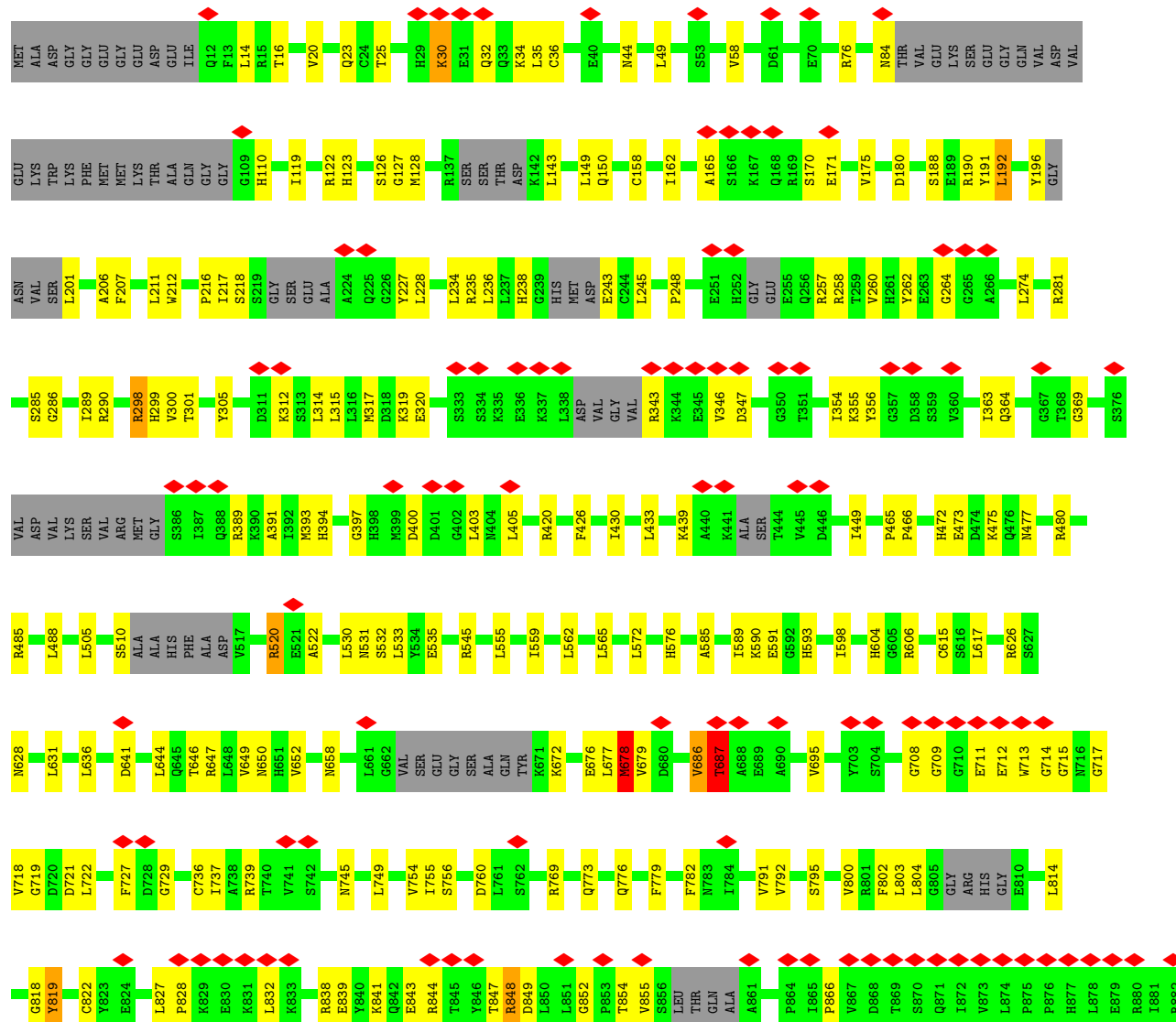








• Molecule 1: RyR2











## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133196	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.155	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	546.0, 546.0, 546.0	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	1.09	70/26752 (0.3%)	1.00	96/36151 (0.3%)
1	B	1.09	66/26752 (0.2%)	1.00	95/36151 (0.3%)
1	C	1.08	67/26752 (0.3%)	1.00	95/36151 (0.3%)
1	D	1.09	67/26752 (0.3%)	1.00	99/36151 (0.3%)
All	All	1.08	270/107008 (0.3%)	1.00	385/144604 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	23
1	B	0	23
1	C	0	24
1	D	0	23
All	All	0	93

All (270) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3700	CYS	CB-SG	13.49	2.05	1.82
1	D	3700	CYS	CB-SG	13.43	2.05	1.82
1	A	3700	CYS	CB-SG	13.37	2.04	1.82
1	C	3700	CYS	CB-SG	13.08	2.04	1.82
1	B	3878	TYR	CG-CD1	-12.72	1.22	1.39
1	C	3878	TYR	CG-CD1	-12.50	1.22	1.39
1	A	3878	TYR	CG-CD1	-12.34	1.23	1.39
1	D	3878	TYR	CG-CD1	-12.33	1.23	1.39
1	C	4849	ILE	C-O	10.92	1.44	1.23
1	A	4849	ILE	C-O	10.87	1.44	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4849	ILE	C-O	10.86	1.44	1.23
1	B	4849	ILE	C-O	10.81	1.43	1.23
1	B	4646	TRP	CZ3-CH2	9.99	1.56	1.40
1	A	4646	TRP	CZ3-CH2	9.96	1.55	1.40
1	C	4646	TRP	CZ3-CH2	9.86	1.55	1.40
1	D	4646	TRP	CZ3-CH2	9.54	1.55	1.40
1	A	4940	TYR	CE1-CZ	-9.18	1.26	1.38
1	B	4940	TYR	CE1-CZ	-8.95	1.26	1.38
1	D	4940	TYR	CE1-CZ	-8.94	1.26	1.38
1	C	4940	TYR	CE1-CZ	-8.90	1.26	1.38
1	B	4953	PHE	CG-CD1	-8.71	1.25	1.38
1	A	4940	TYR	CG-CD2	-8.64	1.27	1.39
1	C	4940	TYR	CG-CD2	-8.63	1.27	1.39
1	A	4953	PHE	CG-CD1	-8.52	1.25	1.38
1	D	4940	TYR	CG-CD2	-8.52	1.28	1.39
1	B	4940	TYR	CG-CD2	-8.47	1.28	1.39
1	D	4919	TYR	CE1-CZ	-8.46	1.27	1.38
1	C	4919	TYR	CE1-CZ	-8.33	1.27	1.38
1	C	4953	PHE	CG-CD1	-8.32	1.26	1.38
1	D	4953	PHE	CG-CD1	-8.31	1.26	1.38
1	B	3858	TYR	CG-CD2	-8.30	1.28	1.39
1	D	887	GLU	CG-CD	8.25	1.64	1.51
1	C	3878	TYR	CE2-CZ	-8.15	1.27	1.38
1	A	3858	TYR	CG-CD2	-8.03	1.28	1.39
1	B	3878	TYR	CE2-CZ	-7.99	1.28	1.38
1	D	3858	TYR	CG-CD2	-7.95	1.28	1.39
1	D	4818	MET	CG-SD	7.94	2.01	1.81
1	A	3878	TYR	CE2-CZ	-7.93	1.28	1.38
1	D	3878	TYR	CE2-CZ	-7.90	1.28	1.38
1	C	3858	TYR	CG-CD2	-7.88	1.28	1.39
1	B	4646	TRP	CG-CD1	-7.88	1.25	1.36
1	A	4646	TRP	CG-CD1	-7.86	1.25	1.36
1	C	4818	MET	CG-SD	7.83	2.01	1.81
1	A	4818	MET	CG-SD	7.68	2.01	1.81
1	A	887	GLU	CG-CD	7.60	1.63	1.51
1	D	4646	TRP	CG-CD1	-7.55	1.26	1.36
1	B	4953	PHE	CG-CD2	-7.52	1.27	1.38
1	A	3699	SER	CB-OG	-7.51	1.32	1.42
1	B	3699	SER	CB-OG	-7.51	1.32	1.42
1	C	4646	TRP	CG-CD1	-7.51	1.26	1.36
1	A	4612	GLU	CD-OE2	7.50	1.33	1.25
1	B	4818	MET	CG-SD	7.50	2.00	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4919	TYR	CE1-CZ	-7.48	1.28	1.38
1	B	4919	TYR	CE1-CZ	-7.44	1.28	1.38
1	A	4953	PHE	CG-CD2	-7.43	1.27	1.38
1	C	4953	PHE	CG-CD2	-7.41	1.27	1.38
1	C	4853	PHE	CD1-CE1	7.36	1.53	1.39
1	D	3699	SER	CB-OG	-7.36	1.32	1.42
1	D	4953	PHE	CG-CD2	-7.32	1.27	1.38
1	C	4612	GLU	CD-OE2	7.31	1.33	1.25
1	C	3699	SER	CB-OG	-7.31	1.32	1.42
1	B	4612	GLU	CD-OE2	7.28	1.33	1.25
1	D	4853	PHE	CD1-CE1	7.28	1.53	1.39
1	A	4952	PHE	CG-CD1	-7.20	1.27	1.38
1	C	4161	TRP	CG-CD2	-7.14	1.31	1.43
1	B	4161	TRP	CG-CD2	-7.12	1.31	1.43
1	C	4945	TYR	CE2-CZ	-7.12	1.29	1.38
1	B	4952	PHE	CG-CD1	-7.11	1.28	1.38
1	D	4161	TRP	CG-CD2	-7.09	1.31	1.43
1	D	4952	PHE	CG-CD1	-7.08	1.28	1.38
1	A	4161	TRP	CG-CD2	-7.04	1.31	1.43
1	D	4612	GLU	CD-OE2	7.04	1.33	1.25
1	B	4709	TRP	CE3-CZ3	-7.01	1.26	1.38
1	C	3841	PHE	CG-CD2	-7.00	1.28	1.38
1	A	3924	TYR	CE1-CZ	-6.99	1.29	1.38
1	B	4945	TYR	CE2-CZ	-6.98	1.29	1.38
1	B	4789	PHE	CG-CD2	6.95	1.49	1.38
1	A	4853	PHE	CD1-CE1	6.91	1.53	1.39
1	C	4709	TRP	CE3-CZ3	-6.88	1.26	1.38
1	A	4945	TYR	CE2-CZ	-6.87	1.29	1.38
1	C	4952	PHE	CG-CD1	-6.85	1.28	1.38
1	D	4945	TYR	CE2-CZ	-6.85	1.29	1.38
1	D	3924	TYR	CE1-CZ	-6.82	1.29	1.38
1	A	4709	TRP	CE3-CZ3	-6.81	1.26	1.38
1	B	4853	PHE	CD1-CE1	6.79	1.52	1.39
1	B	3841	PHE	CG-CD2	-6.79	1.28	1.38
1	D	3841	PHE	CG-CD2	-6.76	1.28	1.38
1	B	4952	PHE	CE2-CZ	-6.75	1.24	1.37
1	D	4709	TRP	CE3-CZ3	-6.72	1.27	1.38
1	A	4952	PHE	CE2-CZ	-6.70	1.24	1.37
1	A	4953	PHE	CE1-CZ	-6.68	1.24	1.37
1	A	3841	PHE	CG-CD2	-6.67	1.28	1.38
1	B	1778	TYR	CB-CG	-6.67	1.41	1.51
1	C	4853	PHE	CD2-CE2	6.66	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4853	PHE	CD2-CE2	6.63	1.52	1.39
1	A	1778	TYR	CB-CG	-6.63	1.41	1.51
1	A	4789	PHE	CG-CD2	6.62	1.48	1.38
1	D	4952	PHE	CG-CD2	-6.60	1.28	1.38
1	A	4925	TYR	CD1-CE1	-6.55	1.29	1.39
1	C	4952	PHE	CE2-CZ	-6.50	1.25	1.37
1	C	4150	TYR	C-O	-6.46	1.11	1.23
1	B	4150	TYR	C-O	-6.46	1.11	1.23
1	D	4150	TYR	C-O	-6.46	1.11	1.23
1	B	4952	PHE	CG-CD2	-6.44	1.29	1.38
1	B	2192	LYS	N-CA	6.42	1.59	1.46
1	B	3924	TYR	CE1-CZ	-6.42	1.30	1.38
1	A	4150	TYR	C-O	-6.42	1.11	1.23
1	B	4591	TYR	CG-CD1	-6.40	1.30	1.39
1	C	3924	TYR	CE1-CZ	-6.40	1.30	1.38
1	D	4952	PHE	CE2-CZ	-6.40	1.25	1.37
1	C	4789	PHE	CG-CD2	6.36	1.48	1.38
1	A	4952	PHE	CG-CD2	-6.34	1.29	1.38
1	B	4138	GLU	CD-OE1	-6.34	1.18	1.25
1	A	2192	LYS	N-CA	6.32	1.58	1.46
1	D	4925	TYR	CD1-CE1	-6.31	1.29	1.39
1	D	4789	PHE	CG-CD2	6.30	1.48	1.38
1	C	4138	GLU	CD-OE1	-6.29	1.18	1.25
1	C	4925	TYR	CD1-CE1	-6.28	1.29	1.39
1	D	4138	GLU	CD-OE1	-6.27	1.18	1.25
1	A	4853	PHE	CD2-CE2	6.27	1.51	1.39
1	C	4952	PHE	CG-CD2	-6.24	1.29	1.38
1	C	4591	TYR	CG-CD1	-6.23	1.31	1.39
1	D	1778	TYR	CB-CG	-6.22	1.42	1.51
1	C	1778	TYR	CB-CG	-6.21	1.42	1.51
1	B	4853	PHE	CD2-CE2	6.20	1.51	1.39
1	B	4925	TYR	CD1-CE1	-6.20	1.30	1.39
1	A	4138	GLU	CD-OE1	-6.20	1.18	1.25
1	C	4839	GLU	CG-CD	6.19	1.61	1.51
1	A	4591	TYR	CG-CD1	-6.16	1.31	1.39
1	B	615	CYS	CB-SG	-6.15	1.71	1.82
1	D	2192	LYS	N-CA	6.15	1.58	1.46
1	C	2192	LYS	N-CA	6.12	1.58	1.46
1	A	3893	TYR	CE1-CZ	-6.11	1.30	1.38
1	D	4195	GLU	CG-CD	6.10	1.61	1.51
1	A	4925	TYR	CD2-CE2	-6.07	1.30	1.39
1	B	2080	GLU	CG-CD	6.04	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4953	PHE	CE1-CZ	-6.04	1.25	1.37
1	A	3755	MET	N-CA	-6.04	1.34	1.46
1	C	4945	TYR	CG-CD1	-6.04	1.31	1.39
1	A	615	CYS	CB-SG	-6.02	1.72	1.82
1	D	4591	TYR	CG-CD1	-6.01	1.31	1.39
1	B	4898	TYR	CG-CD2	-5.99	1.31	1.39
1	C	3850	GLY	N-CA	-5.99	1.37	1.46
1	D	4925	TYR	CD2-CE2	-5.99	1.30	1.39
1	B	3850	GLY	N-CA	-5.99	1.37	1.46
1	A	4195	GLU	CG-CD	5.95	1.60	1.51
1	D	4735	TYR	CE1-CZ	5.92	1.46	1.38
1	C	4925	TYR	CD2-CE2	-5.91	1.30	1.39
1	D	4945	TYR	CG-CD1	-5.91	1.31	1.39
1	B	4735	TYR	CE1-CZ	5.90	1.46	1.38
1	C	4195	GLU	CG-CD	5.89	1.60	1.51
1	B	4938	GLU	CD-OE2	-5.89	1.19	1.25
1	A	4898	TYR	CG-CD2	-5.88	1.31	1.39
1	B	4945	TYR	CG-CD1	-5.88	1.31	1.39
1	A	4938	GLU	CD-OE2	-5.88	1.19	1.25
1	B	4925	TYR	CD2-CE2	-5.87	1.30	1.39
1	C	615	CYS	CB-SG	-5.84	1.72	1.81
1	A	4735	TYR	CE1-CZ	5.83	1.46	1.38
1	A	3850	GLY	N-CA	-5.83	1.37	1.46
1	D	615	CYS	CB-SG	-5.83	1.72	1.81
1	B	3755	MET	N-CA	-5.81	1.34	1.46
1	D	3850	GLY	N-CA	-5.80	1.37	1.46
1	A	4945	TYR	CG-CD1	-5.78	1.31	1.39
1	C	2080	GLU	CG-CD	5.77	1.60	1.51
1	C	4735	TYR	CE1-CZ	5.77	1.46	1.38
1	D	3755	MET	N-CA	-5.77	1.34	1.46
1	D	4953	PHE	CE1-CZ	-5.76	1.26	1.37
1	C	3988	GLU	CD-OE2	-5.74	1.19	1.25
1	C	4919	TYR	CG-CD2	-5.74	1.31	1.39
1	C	4953	PHE	CE1-CZ	-5.73	1.26	1.37
1	B	4195	GLU	CG-CD	5.72	1.60	1.51
1	B	4853	PHE	N-CA	5.71	1.57	1.46
1	C	4726	TYR	CE1-CZ	-5.70	1.31	1.38
1	B	3988	GLU	CD-OE2	-5.70	1.19	1.25
1	C	4938	GLU	CD-OE2	-5.70	1.19	1.25
1	A	4853	PHE	N-CA	5.69	1.57	1.46
1	D	3893	TYR	CE1-CZ	-5.69	1.31	1.38
1	D	4919	TYR	CG-CD2	-5.67	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4938	GLU	CD-OE2	-5.67	1.19	1.25
1	C	4865	GLY	CA-C	-5.66	1.42	1.51
1	D	4898	TYR	CG-CD2	-5.66	1.31	1.39
1	B	4726	TYR	CE1-CZ	-5.65	1.31	1.38
1	B	4790	PHE	CG-CD2	-5.63	1.30	1.38
1	C	4853	PHE	N-CA	5.62	1.57	1.46
1	C	3755	MET	N-CA	-5.60	1.35	1.46
1	C	4898	TYR	CG-CD2	-5.59	1.31	1.39
1	A	3854	ASP	CG-OD1	-5.58	1.12	1.25
1	B	4865	GLY	CA-C	-5.58	1.43	1.51
1	C	2253	GLU	CG-CD	5.57	1.60	1.51
1	D	4865	GLY	CA-C	-5.57	1.43	1.51
1	D	2080	GLU	CB-CG	5.57	1.62	1.52
1	B	4839	GLU	CG-CD	5.56	1.60	1.51
1	B	4646	TRP	CE3-CZ3	-5.55	1.29	1.38
1	B	3893	TYR	CE1-CZ	-5.54	1.31	1.38
1	C	4950	TRP	CD2-CE3	-5.53	1.32	1.40
1	D	3907	PHE	CG-CD2	-5.53	1.30	1.38
1	B	4950	TRP	CD2-CE3	-5.52	1.32	1.40
1	C	4591	TYR	CE2-CZ	-5.51	1.31	1.38
1	C	3907	PHE	CG-CD2	-5.51	1.30	1.38
1	D	4591	TYR	CE2-CZ	-5.51	1.31	1.38
1	D	3988	GLU	CD-OE2	-5.51	1.19	1.25
1	D	4790	PHE	CG-CD2	-5.50	1.30	1.38
1	B	3854	ASP	CG-OD1	-5.50	1.12	1.25
1	A	4790	PHE	CG-CD2	-5.50	1.30	1.38
1	D	2253	GLU	CG-CD	5.49	1.60	1.51
1	D	4853	PHE	N-CA	5.49	1.57	1.46
1	C	4790	PHE	CG-CD2	-5.48	1.30	1.38
1	C	3854	ASP	CG-OD1	-5.48	1.12	1.25
1	A	4839	GLU	CG-CD	5.47	1.60	1.51
1	B	4919	TYR	CG-CD1	-5.47	1.32	1.39
1	D	4950	TRP	CD2-CE3	-5.46	1.32	1.40
1	A	2080	GLU	CB-CG	5.46	1.62	1.52
1	C	3770	GLY	C-O	-5.46	1.15	1.23
1	A	4865	GLY	CA-C	-5.45	1.43	1.51
1	C	3811	ARG	CZ-NH1	5.44	1.40	1.33
1	A	4646	TRP	CE3-CZ3	-5.41	1.29	1.38
1	C	4753	THR	C-O	-5.40	1.13	1.23
1	A	4591	TYR	CE2-CZ	-5.39	1.31	1.38
1	D	4839	GLU	CG-CD	5.39	1.60	1.51
1	D	4726	TYR	CE1-CZ	-5.38	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4950	TRP	CD2-CE3	-5.38	1.32	1.40
1	C	4919	TYR	CG-CD1	-5.37	1.32	1.39
1	A	3791	PHE	CG-CD1	-5.36	1.30	1.38
1	C	4862	ILE	CA-CB	-5.35	1.42	1.54
1	B	4591	TYR	CE2-CZ	-5.35	1.31	1.38
1	D	3854	ASP	CG-OD1	-5.35	1.13	1.25
1	B	3790	PHE	CG-CD2	-5.35	1.30	1.38
1	A	3907	PHE	CG-CD2	-5.35	1.30	1.38
1	B	4919	TYR	CG-CD2	-5.35	1.32	1.39
1	A	4862	ILE	CA-CB	-5.33	1.42	1.54
1	C	2077	GLU	CG-CD	5.33	1.59	1.51
1	D	4862	ILE	CA-CB	-5.33	1.42	1.54
1	A	2077	GLU	CG-CD	5.32	1.59	1.51
1	A	3988	GLU	CD-OE2	-5.31	1.19	1.25
1	D	4753	THR	C-O	-5.31	1.13	1.23
1	D	3770	GLY	C-O	-5.30	1.15	1.23
1	D	2077	GLU	CG-CD	5.29	1.59	1.51
1	B	2253	GLU	CG-CD	5.28	1.59	1.51
1	B	3907	PHE	CG-CD2	-5.28	1.30	1.38
1	D	3811	ARG	CZ-NH1	5.26	1.39	1.33
1	C	3893	TYR	CE1-CZ	-5.26	1.31	1.38
1	B	3811	ARG	CZ-NH1	5.25	1.39	1.33
1	B	4753	THR	C-O	-5.25	1.13	1.23
1	A	3790	PHE	CG-CD2	-5.24	1.30	1.38
1	C	3790	PHE	CG-CD2	-5.24	1.30	1.38
1	A	4753	THR	C-O	-5.23	1.13	1.23
1	D	2080	GLU	CG-CD	5.22	1.59	1.51
1	A	3811	ARG	CZ-NH1	5.21	1.39	1.33
1	B	4862	ILE	CA-CB	-5.21	1.42	1.54
1	B	3770	GLY	C-O	-5.21	1.15	1.23
1	A	3770	GLY	C-O	-5.18	1.15	1.23
1	B	2077	GLU	CG-CD	5.18	1.59	1.51
1	C	3791	PHE	CG-CD1	-5.12	1.31	1.38
1	C	4925	TYR	CE2-CZ	-5.11	1.31	1.38
1	A	2253	GLU	CG-CD	5.11	1.59	1.51
1	D	3791	PHE	CG-CD1	-5.09	1.31	1.38
1	A	4919	TYR	CG-CD2	-5.08	1.32	1.39
1	A	4726	TYR	CE1-CZ	-5.07	1.31	1.38
1	B	4754	LEU	N-CA	-5.07	1.36	1.46
1	D	4921	PHE	CG-CD1	-5.07	1.31	1.38
1	D	4136	ARG	C-O	-5.07	1.13	1.23
1	C	534	TYR	CE1-CZ	-5.05	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3753	GLY	N-CA	-5.05	1.38	1.46
1	A	4925	TYR	CE2-CZ	-5.05	1.31	1.38
1	C	4942	TRP	CG-CD2	-5.04	1.35	1.43
1	B	534	TYR	CE1-CZ	-5.03	1.32	1.38
1	A	534	TYR	CE1-CZ	-5.02	1.32	1.38
1	A	4136	ARG	C-O	-5.02	1.13	1.23
1	D	4925	TYR	CE2-CZ	-5.02	1.32	1.38
1	A	4919	TYR	CG-CD1	-5.01	1.32	1.39

All (385) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4948	ARG	NE-CZ-NH2	13.56	127.08	120.30
1	D	4948	ARG	NE-CZ-NH2	13.25	126.92	120.30
1	B	4948	ARG	NE-CZ-NH2	13.09	126.84	120.30
1	C	4948	ARG	NE-CZ-NH2	12.28	126.44	120.30
1	A	1089	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	B	1089	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	A	4818	MET	CG-SD-CE	9.16	114.86	100.20
1	B	4853	PHE	N-CA-CB	9.15	127.06	110.60
1	D	4853	PHE	N-CA-CB	9.12	127.01	110.60
1	A	4853	PHE	N-CA-CB	9.10	126.99	110.60
1	D	1089	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	C	4853	PHE	N-CA-CB	9.02	126.84	110.60
1	A	3854	ASP	CB-CG-OD2	8.98	126.38	118.30
1	D	4948	ARG	NE-CZ-NH1	-8.92	115.84	120.30
1	C	1089	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	D	4818	MET	CG-SD-CE	8.78	114.25	100.20
1	B	4818	MET	CG-SD-CE	8.76	114.21	100.20
1	C	4818	MET	CG-SD-CE	8.76	114.21	100.20
1	C	3854	ASP	CB-CG-OD2	8.74	126.17	118.30
1	B	3854	ASP	CB-CG-OD2	8.73	126.15	118.30
1	D	3854	ASP	CB-CG-OD2	8.73	126.15	118.30
1	A	4948	ARG	NE-CZ-NH1	-8.69	115.96	120.30
1	D	4818	MET	CA-CB-CG	8.49	127.73	113.30
1	C	4818	MET	CA-CB-CG	8.32	127.44	113.30
1	B	4727	MET	CG-SD-CE	8.24	113.39	100.20
1	C	4727	MET	CG-SD-CE	8.23	113.36	100.20
1	C	4948	ARG	NE-CZ-NH1	-8.19	116.20	120.30
1	D	2239	THR	N-CA-CB	-8.13	94.85	110.30
1	D	2495	PRO	N-CA-CB	8.12	113.04	103.30
1	A	4818	MET	CA-CB-CG	8.12	127.10	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4727	MET	CG-SD-CE	8.09	113.14	100.20
1	A	2495	PRO	N-CA-CB	8.08	112.99	103.30
1	D	4875	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	C	2495	PRO	N-CA-CB	8.05	112.96	103.30
1	B	2495	PRO	N-CA-CB	8.05	112.96	103.30
1	B	3878	TYR	CB-CG-CD2	7.95	125.77	121.00
1	A	347	ASP	CB-CG-OD1	7.93	125.44	118.30
1	B	4948	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	B	4818	MET	CA-CB-CG	7.86	126.65	113.30
1	C	2239	THR	N-CA-CB	-7.85	95.38	110.30
1	C	3878	TYR	CB-CG-CD2	7.84	125.70	121.00
1	A	2239	THR	N-CA-CB	-7.79	95.49	110.30
1	D	3878	TYR	CB-CG-CD2	7.78	125.67	121.00
1	A	3878	TYR	CB-CG-CD2	7.77	125.66	121.00
1	A	4727	MET	CG-SD-CE	7.74	112.58	100.20
1	B	1758	ARG	NE-CZ-NH1	-7.69	116.46	120.30
1	D	1758	ARG	NE-CZ-NH1	-7.59	116.50	120.30
1	D	347	ASP	CB-CG-OD1	7.57	125.11	118.30
1	B	2583	PRO	N-CA-CB	7.52	112.33	103.30
1	B	4781	LEU	CB-CG-CD1	7.44	123.65	111.00
1	A	2583	PRO	N-CA-CB	7.44	112.22	103.30
1	A	1758	ARG	NE-CZ-NH1	-7.43	116.58	120.30
1	C	1758	ARG	NE-CZ-NH1	-7.43	116.58	120.30
1	C	347	ASP	CB-CG-OD1	7.38	124.94	118.30
1	B	485	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	C	4781	LEU	CB-CG-CD1	7.31	123.43	111.00
1	B	347	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	3896	LYS	CD-CE-NZ	7.28	128.45	111.70
1	C	2583	PRO	N-CA-CB	7.27	112.02	103.30
1	C	2607	PRO	N-CA-CB	7.24	111.99	103.30
1	C	4875	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	D	2598	PRO	N-CA-CB	7.21	111.95	103.30
1	B	2239	THR	N-CA-CB	-7.19	96.65	110.30
1	A	2607	PRO	N-CA-CB	7.18	111.92	103.30
1	B	2598	PRO	N-CA-CB	7.17	111.90	103.30
1	D	3896	LYS	CD-CE-NZ	7.17	128.18	111.70
1	B	2607	PRO	N-CA-CB	7.17	111.90	103.30
1	D	2583	PRO	N-CA-CB	7.16	111.89	103.30
1	D	2607	PRO	N-CA-CB	7.14	111.86	103.30
1	A	4781	LEU	CB-CG-CD1	7.13	123.13	111.00
1	A	2598	PRO	N-CA-CB	7.12	111.84	103.30
1	C	2598	PRO	N-CA-CB	7.11	111.84	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3896	LYS	CD-CE-NZ	7.08	128.00	111.70
1	C	3896	LYS	CD-CE-NZ	6.97	127.73	111.70
1	A	4875	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	B	4875	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	D	4952	PHE	CB-CG-CD2	-6.91	115.96	120.80
1	A	2625	PRO	N-CA-CB	6.90	111.58	103.30
1	B	2625	PRO	N-CA-CB	6.90	111.58	103.30
1	D	2173	MET	CG-SD-CE	-6.89	89.17	100.20
1	B	4498	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	C	3882	VAL	CG1-CB-CG2	-6.88	99.90	110.90
1	D	2625	PRO	N-CA-CB	6.86	111.53	103.30
1	B	3882	VAL	CG1-CB-CG2	-6.86	99.93	110.90
1	C	545	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	B	3948	PHE	CB-CG-CD2	-6.81	116.03	120.80
1	B	2736	ASP	CB-CG-OD2	6.79	124.41	118.30
1	C	3948	PHE	CB-CG-CD2	-6.79	116.05	120.80
1	D	545	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	3104	PRO	N-CA-CB	6.76	111.41	103.30
1	D	4781	LEU	CB-CG-CD1	6.76	122.49	111.00
1	A	3104	PRO	N-CA-CB	6.75	111.41	103.30
1	A	3882	VAL	CG1-CB-CG2	-6.75	100.10	110.90
1	C	2625	PRO	N-CA-CB	6.75	111.40	103.30
1	A	2173	MET	CG-SD-CE	-6.73	89.43	100.20
1	D	3882	VAL	CG1-CB-CG2	-6.72	100.15	110.90
1	A	4739	PHE	CB-CG-CD2	6.71	125.50	120.80
1	D	4498	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	B	4789	PHE	CB-CG-CD1	6.69	125.48	120.80
1	C	4139	ILE	CG1-CB-CG2	-6.67	96.73	111.40
1	D	4139	ILE	CG1-CB-CG2	-6.67	96.73	111.40
1	B	3858	TYR	CB-CG-CD1	6.67	125.00	121.00
1	A	545	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	C	4498	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	485	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	2173	MET	CG-SD-CE	-6.64	89.58	100.20
1	A	4941	VAL	CG1-CB-CG2	-6.63	100.29	110.90
1	C	2736	ASP	CB-CG-OD2	6.63	124.27	118.30
1	A	4498	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	B	4139	ILE	CG1-CB-CG2	-6.62	96.83	111.40
1	C	1610	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	D	721	ASP	CB-CG-OD1	6.62	124.26	118.30
1	C	3104	PRO	N-CA-CB	6.61	111.23	103.30
1	C	4941	VAL	CG1-CB-CG2	-6.61	100.33	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2668	PRO	N-CA-CB	6.61	111.23	103.30
1	C	485	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	4952	PHE	CB-CG-CD2	-6.59	116.19	120.80
1	D	2668	PRO	N-CA-CB	6.59	111.21	103.30
1	A	3948	PHE	CB-CG-CD2	-6.58	116.19	120.80
1	D	2736	ASP	CB-CG-OD2	6.58	124.22	118.30
1	B	4739	PHE	CB-CG-CD2	6.57	125.40	120.80
1	B	4941	VAL	CG1-CB-CG2	-6.57	100.39	110.90
1	C	4789	PHE	CB-CG-CD1	6.56	125.39	120.80
1	C	2173	MET	CG-SD-CE	-6.55	89.72	100.20
1	A	2668	PRO	N-CA-CB	6.55	111.16	103.30
1	A	4139	ILE	CG1-CB-CG2	-6.55	97.00	111.40
1	A	4789	PHE	CB-CG-CD1	6.55	125.38	120.80
1	D	3104	PRO	N-CA-CB	6.54	111.15	103.30
1	C	721	ASP	CB-CG-OD1	6.53	124.18	118.30
1	D	485	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	C	4952	PHE	CB-CG-CD2	-6.52	116.23	120.80
1	A	2736	ASP	CB-CG-OD2	6.51	124.16	118.30
1	B	545	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	D	4941	VAL	CG1-CB-CG2	-6.49	100.52	110.90
1	D	3700	CYS	N-CA-CB	-6.48	98.94	110.60
1	A	3858	TYR	CB-CG-CD1	6.45	124.87	121.00
1	D	4739	PHE	CB-CG-CD2	6.45	125.31	120.80
1	B	2668	PRO	N-CA-CB	6.45	111.03	103.30
1	D	3948	PHE	CB-CG-CD2	-6.45	116.29	120.80
1	A	4916	LEU	CB-CG-CD1	-6.42	100.08	111.00
1	B	2396	LEU	CB-CG-CD2	6.41	121.90	111.00
1	B	4952	PHE	CB-CG-CD2	-6.40	116.32	120.80
1	A	2678	PRO	N-CA-CB	6.40	110.98	103.30
1	D	2679	PRO	N-CA-CB	6.40	110.98	103.30
1	C	3690	MET	CG-SD-CE	-6.38	90.00	100.20
1	D	4789	PHE	CB-CG-CD1	6.37	125.26	120.80
1	B	3982	MET	CG-SD-CE	-6.37	90.02	100.20
1	D	1610	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	C	2678	PRO	N-CA-CB	6.36	110.93	103.30
1	D	2678	PRO	N-CA-CB	6.36	110.93	103.30
1	B	2678	PRO	N-CA-CB	6.35	110.92	103.30
1	A	4774	LEU	CB-CG-CD2	6.35	121.80	111.00
1	D	2990	PRO	N-CA-CB	6.34	110.91	103.30
1	C	2679	PRO	N-CA-CB	6.33	110.90	103.30
1	A	2679	PRO	N-CA-CB	6.31	110.87	103.30
1	A	2990	PRO	N-CA-CB	6.30	110.86	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4758	LEU	CB-CG-CD2	6.30	121.72	111.00
1	C	2990	PRO	N-CA-CB	6.30	110.86	103.30
1	C	3700	CYS	N-CA-CB	-6.29	99.29	110.60
1	C	4739	PHE	CB-CG-CD2	6.28	125.19	120.80
1	B	3700	CYS	N-CA-CB	-6.27	99.31	110.60
1	C	3858	TYR	CB-CG-CD1	6.27	124.76	121.00
1	D	4871	PHE	CB-CG-CD1	-6.25	116.42	120.80
1	A	3982	MET	CG-SD-CE	-6.25	90.20	100.20
1	C	4871	PHE	CB-CG-CD1	-6.25	116.42	120.80
1	B	2990	PRO	N-CA-CB	6.24	110.79	103.30
1	A	721	ASP	CB-CG-OD1	6.22	123.89	118.30
1	B	3690	MET	CG-SD-CE	-6.21	90.26	100.20
1	D	3858	TYR	CB-CG-CD1	6.21	124.73	121.00
1	B	2139	GLU	OE1-CD-OE2	-6.21	115.85	123.30
1	C	2139	GLU	OE1-CD-OE2	-6.21	115.85	123.30
1	A	4871	PHE	CB-CG-CD1	-6.21	116.46	120.80
1	D	3982	MET	CG-SD-CE	-6.20	90.28	100.20
1	B	2679	PRO	N-CA-CB	6.20	110.73	103.30
1	B	4871	PHE	CB-CG-CD1	-6.18	116.47	120.80
1	C	3982	MET	CG-SD-CE	-6.18	90.31	100.20
1	D	3690	MET	CG-SD-CE	-6.18	90.31	100.20
1	D	4916	LEU	CB-CG-CD1	-6.15	100.54	111.00
1	A	1610	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	3700	CYS	N-CA-CB	-6.13	99.56	110.60
1	B	1457	PHE	CB-CG-CD1	-6.13	116.51	120.80
1	C	848	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	B	1610	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	D	4195	GLU	OE1-CD-OE2	-6.01	116.09	123.30
1	A	4603	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	848	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	C	4758	LEU	CB-CG-CD2	6.00	121.19	111.00
1	B	4758	LEU	CB-CG-CD2	5.99	121.19	111.00
1	A	2396	LEU	CB-CG-CD2	5.98	121.16	111.00
1	A	4940	TYR	CB-CG-CD2	5.97	124.58	121.00
1	B	721	ASP	CB-CG-OD1	5.95	123.66	118.30
1	C	1457	PHE	CB-CG-CD1	-5.93	116.65	120.80
1	C	3700	CYS	CB-CA-C	5.92	122.25	110.40
1	A	4854	PHE	CB-CG-CD2	-5.92	116.66	120.80
1	B	1303	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	4195	GLU	OE1-CD-OE2	-5.91	116.21	123.30
1	A	1303	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	C	687	THR	CA-CB-CG2	-5.88	104.16	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3690	MET	CG-SD-CE	-5.87	90.81	100.20
1	A	520	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	4102	LEU	CA-CB-CG	5.85	128.75	115.30
1	D	687	THR	CA-CB-CG2	-5.84	104.22	112.40
1	B	3700	CYS	CB-CA-C	5.83	122.07	110.40
1	B	4774	LEU	CB-CG-CD2	5.82	120.90	111.00
1	B	4940	TYR	CB-CG-CD2	5.82	124.49	121.00
1	D	3700	CYS	CB-CA-C	5.82	122.03	110.40
1	D	4102	LEU	CA-CB-CG	5.81	128.67	115.30
1	D	2140	GLU	OE1-CD-OE2	-5.81	116.33	123.30
1	D	4854	PHE	CB-CG-CD2	-5.81	116.73	120.80
1	B	4102	LEU	CA-CB-CG	5.80	128.65	115.30
1	B	520	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	687	THR	CA-CB-CG2	-5.79	104.29	112.40
1	B	4195	GLU	OE1-CD-OE2	-5.79	116.35	123.30
1	D	4758	LEU	CB-CG-CD2	5.79	120.85	111.00
1	A	3700	CYS	CB-CA-C	5.79	121.98	110.40
1	B	4721	LEU	CA-CB-CG	5.78	128.60	115.30
1	C	1089	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	4721	LEU	CA-CB-CG	5.77	128.56	115.30
1	A	4735	TYR	CB-CG-CD1	5.76	124.46	121.00
1	B	4854	PHE	CB-CG-CD2	-5.76	116.77	120.80
1	D	4940	TYR	CB-CG-CD2	5.75	124.45	121.00
1	C	3811	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	D	4774	LEU	CB-CG-CD2	5.75	120.78	111.00
1	A	687	THR	CA-CB-CG2	-5.75	104.35	112.40
1	D	4721	LEU	CA-CB-CG	5.75	128.52	115.30
1	C	4102	LEU	CA-CB-CG	5.74	128.50	115.30
1	C	4721	LEU	CA-CB-CG	5.74	128.49	115.30
1	B	4916	LEU	CB-CG-CD1	-5.73	101.25	111.00
1	B	4735	TYR	CB-CG-CD1	5.71	124.43	121.00
1	A	4822	VAL	CA-CB-CG1	5.71	119.47	110.90
1	A	2083	ARG	CG-CD-NE	-5.70	99.83	111.80
1	D	4822	VAL	CA-CB-CG1	5.69	119.44	110.90
1	C	520	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	D	1457	PHE	CB-CG-CD1	-5.68	116.83	120.80
1	B	3726	LEU	CA-CB-CG	5.68	128.36	115.30
1	C	4940	TYR	CB-CG-CD2	5.67	124.40	121.00
1	C	4822	VAL	CA-CB-CG1	5.65	119.37	110.90
1	A	4087	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	2396	LEU	CB-CG-CD2	5.64	120.59	111.00
1	B	4822	VAL	CA-CB-CG1	5.64	119.36	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4195	GLU	OE1-CD-OE2	-5.64	116.54	123.30
1	B	678	MET	CB-CG-SD	5.63	129.29	112.40
1	B	4757	ILE	CG1-CB-CG2	-5.63	99.02	111.40
1	C	678	MET	CB-CG-SD	5.63	129.28	112.40
1	D	4087	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	4757	ILE	CG1-CB-CG2	-5.62	99.04	111.40
1	D	4603	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	B	4844	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	C	4854	PHE	CB-CG-CD2	-5.60	116.88	120.80
1	D	2083	ARG	CG-CD-NE	-5.58	100.09	111.80
1	B	1089	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	D	3642	ILE	CG1-CB-CG2	-5.57	99.14	111.40
1	C	814	LEU	CA-CB-CG	5.57	128.10	115.30
1	A	678	MET	CB-CG-SD	5.56	129.08	112.40
1	C	1303	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	C	4603	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	D	678	MET	CB-CG-SD	5.56	129.07	112.40
1	B	1652	LYS	CD-CE-NZ	5.55	124.46	111.70
1	C	2140	GLU	OE1-CD-OE2	-5.55	116.64	123.30
1	B	3940	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	1089	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	A	2139	GLU	OE1-CD-OE2	-5.53	116.67	123.30
1	D	2396	LEU	CB-CG-CD2	5.53	120.40	111.00
1	B	3811	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	B	2083	ARG	CG-CD-NE	-5.51	100.22	111.80
1	C	4916	LEU	CB-CG-CD1	-5.51	101.64	111.00
1	D	1089	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	C	3642	ILE	CG1-CB-CG2	-5.49	99.33	111.40
1	D	4757	ILE	CG1-CB-CG2	-5.49	99.33	111.40
1	D	814	LEU	CA-CB-CG	5.48	127.91	115.30
1	D	3726	LEU	CA-CB-CG	5.48	127.91	115.30
1	C	4732	LEU	CB-CG-CD2	5.48	120.31	111.00
1	C	3726	LEU	CA-CB-CG	5.48	127.90	115.30
1	A	3726	LEU	CA-CB-CG	5.48	127.90	115.30
1	D	4735	TYR	CB-CG-CD1	5.47	124.28	121.00
1	D	1303	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	C	4087	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	B	4087	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	814	LEU	CA-CB-CG	5.43	127.78	115.30
1	B	814	LEU	CA-CB-CG	5.42	127.77	115.30
1	C	2083	ARG	CG-CD-NE	-5.42	100.42	111.80
1	D	4732	LEU	CB-CG-CD2	5.42	120.21	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1652	LYS	CD-CE-NZ	5.41	124.15	111.70
1	A	1457	PHE	CB-CG-CD1	-5.41	117.02	120.80
1	B	4115	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	B	1905	LEU	CB-CG-CD1	5.40	120.18	111.00
1	B	3878	TYR	OH-CZ-CE2	5.39	134.66	120.10
1	B	4732	LEU	CB-CG-CD2	5.39	120.17	111.00
1	A	3878	TYR	OH-CZ-CE2	5.37	134.60	120.10
1	A	2140	GLU	OE1-CD-OE2	-5.37	116.86	123.30
1	D	3878	TYR	OH-CZ-CE2	5.37	134.59	120.10
1	A	1905	LEU	CA-CB-CG	5.36	127.63	115.30
1	B	1778	TYR	CB-CG-CD1	-5.36	117.79	121.00
1	A	4735	TYR	CG-CD2-CE2	5.34	125.57	121.30
1	D	1905	LEU	CA-CB-CG	5.34	127.57	115.30
1	A	30	LYS	CA-CB-CG	5.33	125.12	113.40
1	D	1112	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	A	801	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	A	4732	LEU	CB-CG-CD2	5.31	120.02	111.00
1	D	520	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	4727	MET	CB-CG-SD	5.29	128.28	112.40
1	A	1652	LYS	CD-CE-NZ	5.29	123.87	111.70
1	C	1944	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	D	4189	LEU	CB-CG-CD1	5.29	119.99	111.00
1	A	3940	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	C	3940	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	D	678	MET	CG-SD-CE	5.28	108.65	100.20
1	D	30	LYS	CA-CB-CG	5.28	125.01	113.40
1	A	1644	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	30	LYS	CA-CB-CG	5.28	125.00	113.40
1	D	1644	LEU	CA-CB-CG	5.28	127.44	115.30
1	D	848	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	3642	ILE	CG1-CB-CG2	-5.27	99.80	111.40
1	C	2534	PRO	N-CA-CB	5.26	109.62	103.30
1	A	3642	ILE	CG1-CB-CG2	-5.26	99.83	111.40
1	B	678	MET	CG-SD-CE	5.25	108.60	100.20
1	A	1112	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	D	4862	ILE	CA-CB-CG1	-5.23	101.05	111.00
1	B	801	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	A	678	MET	CG-SD-CE	5.23	108.57	100.20
1	C	3878	TYR	OH-CZ-CE2	5.23	134.22	120.10
1	D	3940	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	C	678	MET	CG-SD-CE	5.23	108.56	100.20
1	C	4844	ARG	NE-CZ-NH2	5.23	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1942	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	A	848	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	1644	LEU	CA-CB-CG	5.22	127.31	115.30
1	D	1905	LEU	CB-CG-CD1	5.22	119.87	111.00
1	B	1185	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	4853	PHE	CE1-CZ-CE2	-5.21	110.61	120.00
1	C	1905	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	4757	ILE	CG1-CB-CG2	-5.21	99.94	111.40
1	B	4735	TYR	CG-CD2-CE2	5.21	125.47	121.30
1	B	1644	LEU	CA-CB-CG	5.20	127.27	115.30
1	C	4115	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	C	1905	LEU	CB-CG-CD1	5.20	119.84	111.00
1	D	3811	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	2173	MET	CB-CG-SD	5.20	127.99	112.40
1	A	4862	ILE	CA-CB-CG1	-5.19	101.13	111.00
1	D	2534	PRO	N-CA-CB	5.19	109.53	103.30
1	C	30	LYS	CA-CB-CG	5.19	124.82	113.40
1	D	4134	LEU	CA-CB-CG	5.19	127.24	115.30
1	C	4774	LEU	CB-CG-CD2	5.19	119.82	111.00
1	A	1303	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	4134	LEU	CA-CB-CG	5.18	127.20	115.30
1	C	4853	PHE	CE1-CZ-CE2	-5.16	110.71	120.00
1	A	4115	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	B	1303	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	4189	LEU	CB-CG-CD1	5.14	119.74	111.00
1	D	4115	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	A	2534	PRO	N-CA-CB	5.13	109.46	103.30
1	B	1905	LEU	CA-CB-CG	5.13	127.09	115.30
1	B	2534	PRO	N-CA-CB	5.12	109.45	103.30
1	B	4134	LEU	CA-CB-CG	5.12	127.08	115.30
1	D	1652	LYS	CD-CE-NZ	5.11	123.45	111.70
1	D	4004	LEU	CB-CG-CD2	5.11	119.69	111.00
1	D	4174	ILE	CG1-CB-CG2	-5.11	100.16	111.40
1	C	4189	LEU	CB-CG-CD1	5.10	119.67	111.00
1	A	887	GLU	OE1-CD-OE2	-5.10	117.18	123.30
1	C	1778	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	D	2432	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	D	2203	TYR	CB-CG-CD2	-5.09	117.94	121.00
1	D	1778	TYR	CB-CG-CD1	-5.09	117.95	121.00
1	A	2173	MET	CB-CG-SD	5.08	127.65	112.40
1	C	4134	LEU	CA-CB-CG	5.08	126.99	115.30
1	D	2139	GLU	OE1-CD-OE2	-5.08	117.20	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4174	ILE	CG1-CB-CG2	-5.08	100.23	111.40
1	B	4603	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	D	4735	TYR	CG-CD2-CE2	5.07	125.36	121.30
1	A	3700	CYS	CA-CB-SG	5.07	123.12	114.00
1	C	4004	LEU	CB-CG-CD2	5.06	119.61	111.00
1	A	4518	LEU	CB-CG-CD2	5.06	119.60	111.00
1	A	4174	ILE	CG1-CB-CG2	-5.05	100.28	111.40
1	B	2173	MET	CB-CG-SD	5.05	127.56	112.40
1	D	4518	LEU	CB-CG-CD2	5.05	119.58	111.00
1	B	4518	LEU	CB-CG-CD2	5.04	119.57	111.00
1	C	2392	PHE	CB-CG-CD2	-5.04	117.27	120.80
1	C	4518	LEU	CB-CG-CD2	5.04	119.56	111.00
1	D	4853	PHE	CB-CG-CD1	5.04	124.33	120.80
1	A	2203	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	C	4853	PHE	CB-CG-CD1	5.03	124.32	120.80
1	D	4561	VAL	CG1-CB-CG2	5.03	118.94	110.90
1	B	2140	GLU	OE1-CD-OE2	-5.01	117.29	123.30
1	B	4174	ILE	CG1-CB-CG2	-5.01	100.38	111.40
1	A	1905	LEU	CB-CG-CD1	5.00	119.50	111.00

There are no chirality outliers.

All (93) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1475	LYS	Peptide
1	A	1579	VAL	Peptide
1	A	1635	GLU	Peptide
1	A	1736	ILE	Peptide
1	A	1755	THR	Peptide
1	A	1808	ASP	Peptide
1	A	1835	HIS	Peptide
1	A	1847	GLU	Peptide
1	A	2075	VAL	Peptide
1	A	2329	PRO	Peptide,Mainchain
1	A	3800	SER	Peptide
1	A	4163	LYS	Peptide
1	A	4952	PHE	Sidechain
1	A	641	ASP	Peptide
1	A	686	VAL	Peptide
1	A	791	VAL	Peptide
1	A	818	GLY	Peptide
1	A	819	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	A	827	LEU	Peptide
1	A	838	ARG	Peptide
1	A	852	GLY	Peptide,Mainchain
1	B	1475	LYS	Peptide
1	B	1579	VAL	Peptide
1	B	1635	GLU	Peptide
1	B	1736	ILE	Peptide
1	B	1755	THR	Peptide
1	B	1808	ASP	Peptide
1	B	1835	HIS	Peptide
1	B	1847	GLU	Peptide
1	B	2075	VAL	Peptide
1	B	2329	PRO	Peptide,Mainchain
1	B	3800	SER	Peptide
1	B	4163	LYS	Peptide
1	B	4952	PHE	Sidechain
1	B	641	ASP	Peptide
1	B	686	VAL	Peptide
1	B	791	VAL	Peptide
1	B	818	GLY	Peptide
1	B	819	TYR	Peptide
1	B	827	LEU	Peptide
1	B	838	ARG	Peptide
1	B	852	GLY	Peptide,Mainchain
1	C	1475	LYS	Peptide
1	C	1579	VAL	Peptide
1	C	1635	GLU	Peptide
1	C	1736	ILE	Peptide
1	C	1755	THR	Peptide
1	C	1756	SER	Peptide
1	C	1808	ASP	Peptide
1	C	1835	HIS	Peptide
1	C	1847	GLU	Peptide
1	C	2075	VAL	Peptide
1	C	2329	PRO	Peptide,Mainchain
1	C	3800	SER	Peptide
1	C	4163	LYS	Peptide
1	C	4952	PHE	Sidechain
1	C	641	ASP	Peptide
1	C	686	VAL	Peptide
1	C	791	VAL	Peptide
1	C	818	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	C	819	TYR	Peptide
1	C	827	LEU	Peptide
1	C	838	ARG	Peptide
1	C	852	GLY	Peptide,Mainchain
1	D	1475	LYS	Peptide
1	D	1579	VAL	Peptide
1	D	1635	GLU	Peptide
1	D	1736	ILE	Peptide
1	D	1755	THR	Peptide
1	D	1808	ASP	Peptide
1	D	1835	HIS	Peptide
1	D	1847	GLU	Peptide
1	D	2075	VAL	Peptide
1	D	2329	PRO	Peptide,Mainchain
1	D	3800	SER	Peptide
1	D	4163	LYS	Peptide
1	D	4952	PHE	Sidechain
1	D	641	ASP	Peptide
1	D	686	VAL	Peptide
1	D	791	VAL	Peptide
1	D	818	GLY	Peptide
1	D	819	TYR	Peptide
1	D	827	LEU	Peptide
1	D	838	ARG	Peptide
1	D	852	GLY	Peptide,Mainchain

## 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	26267	0	24896	381	0
1	B	26267	0	24897	372	0
1	C	26267	0	24897	370	0
1	D	26267	0	24896	377	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	105072	0	99586	1447	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1447) 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:D:4818:MET:CG	1:D:4818:MET:SD	2.01	1.49
1:C:4818:MET:CG	1:C:4818:MET:SD	2.01	1.48
1:C:3700:CYS:CB	1:C:3700:CYS:SG	2.04	1.45
1:B:3700:CYS:CB	1:B:3700:CYS:SG	2.05	1.43
1:D:3700:CYS:SG	1:D:3700:CYS:CB	2.05	1.43
1:A:3700:CYS:CB	1:A:3700:CYS:SG	2.05	1.43
1:A:4171:ARG:NH1	1:A:4752:LYS:HD3	1.63	1.12
1:D:4171:ARG:NH1	1:D:4752:LYS:HE3	1.76	1.00
1:A:4171:ARG:HH12	1:A:4752:LYS:HD3	1.28	0.94
1:A:4767:GLN:HE22	1:B:4753:THR:HB	1.29	0.94
1:B:4767:GLN:HE22	1:C:4753:THR:HB	1.31	0.93
1:A:4767:GLN:NE2	1:B:4753:THR:HB	1.84	0.93
1:C:4767:GLN:HE22	1:D:4753:THR:HB	1.32	0.93
1:D:4171:ARG:HH11	1:D:4752:LYS:HE3	1.30	0.93
1:B:4767:GLN:NE2	1:C:4753:THR:HB	1.84	0.92
1:A:4753:THR:HB	1:D:4767:GLN:HE22	1.32	0.92
1:A:4753:THR:HB	1:D:4767:GLN:NE2	1.85	0.91
1:C:4767:GLN:NE2	1:D:4753:THR:HB	1.85	0.91
1:A:76:ARG:HD2	1:B:3891:TRP:HB3	1.54	0.89
1:C:76:ARG:HD2	1:D:3891:TRP:HB3	1.54	0.89
1:A:3891:TRP:HB3	1:D:76:ARG:HD2	1.52	0.88
1:B:76:ARG:HD2	1:C:3891:TRP:HB3	1.53	0.87
1:A:4754:LEU:HD11	1:D:4770:LEU:HB3	1.66	0.78
1:C:4770:LEU:HB3	1:D:4754:LEU:HD11	1.67	0.77
1:B:4791:ARG:HH12	1:C:4559:HIS:CE1	2.04	0.76
1:C:4791:ARG:HH12	1:D:4559:HIS:CE1	2.04	0.75
1:A:4791:ARG:HH12	1:B:4559:HIS:CE1	2.04	0.75
1:B:4770:LEU:HB3	1:C:4754:LEU:HD11	1.68	0.75
1:C:4171:ARG:HG3	1:C:4171:ARG:HH21	1.50	0.74
1:A:4770:LEU:HB3	1:B:4754:LEU:HD11	1.69	0.74
1:A:4559:HIS:CE1	1:D:4791:ARG:HH12	2.05	0.73
1:A:4171:ARG:NH1	1:A:4752:LYS:CD	2.49	0.71
1:D:2349:GLU:HG2	1:D:2439:ILE:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2349:GLU:HG2	1:C:2439:ILE:HD11	1.72	0.71
1:C:1011:ARG:HB3	1:C:1032:LEU:HD21	1.73	0.71
1:D:1011:ARG:HB3	1:D:1032:LEU:HD21	1.72	0.70
1:A:2349:GLU:HG2	1:A:2439:ILE:HD11	1.72	0.70
1:B:2349:GLU:HG2	1:B:2439:ILE:HD11	1.72	0.70
1:B:4832:ILE:HG21	1:B:4844:ARG:HH21	1.57	0.69
1:A:4832:ILE:HG21	1:A:4844:ARG:HH21	1.58	0.69
1:B:1011:ARG:HB3	1:B:1032:LEU:HD21	1.74	0.69
1:B:986:ILE:HD12	1:B:1059:GLY:HA2	1.74	0.69
1:B:1645:THR:HG22	1:B:1695:PRO:HG3	1.73	0.69
1:C:4817:HIS:HE1	1:C:4828:ILE:HD12	1.57	0.68
1:C:4832:ILE:HG21	1:C:4844:ARG:HH21	1.58	0.68
1:A:1011:ARG:HB3	1:A:1032:LEU:HD21	1.75	0.68
1:B:4817:HIS:HE1	1:B:4828:ILE:HD12	1.57	0.68
1:C:1645:THR:HG22	1:C:1695:PRO:HG3	1.73	0.68
1:A:4817:HIS:HE1	1:A:4828:ILE:HD12	1.57	0.68
1:A:4642:PRO:HG2	1:A:4648:LYS:HD2	1.76	0.68
1:B:4642:PRO:HG2	1:B:4648:LYS:HD2	1.76	0.68
1:D:4832:ILE:HG21	1:D:4844:ARG:HH21	1.57	0.68
1:B:4511:ALA:HA	1:B:4514:ILE:HD12	1.77	0.67
1:D:1645:THR:HG22	1:D:1695:PRO:HG3	1.75	0.67
1:A:4511:ALA:HA	1:A:4514:ILE:HD12	1.77	0.67
1:C:1620:GLN:HE21	1:C:1622:LEU:HD21	1.60	0.67
1:D:4817:HIS:HE1	1:D:4828:ILE:HD12	1.58	0.67
1:A:143:LEU:HD23	1:B:2426:SER:HB3	1.77	0.67
1:B:2463:PRO:HB2	1:B:2519:ARG:HD2	1.76	0.67
1:D:644:LEU:HB2	1:D:1654:HIS:HD2	1.60	0.67
1:A:1645:THR:HG22	1:A:1695:PRO:HG3	1.75	0.66
1:C:4642:PRO:HG2	1:C:4648:LYS:HD2	1.77	0.66
1:D:2463:PRO:HB2	1:D:2519:ARG:HD2	1.77	0.66
1:B:1620:GLN:HE21	1:B:1622:LEU:HD21	1.60	0.66
1:D:4642:PRO:HG2	1:D:4648:LYS:HD2	1.77	0.66
1:C:644:LEU:HB2	1:C:1654:HIS:HD2	1.60	0.66
1:D:4511:ALA:HA	1:D:4514:ILE:HD12	1.78	0.66
1:A:1620:GLN:HE21	1:A:1622:LEU:HD21	1.60	0.66
1:A:986:ILE:HD12	1:A:1059:GLY:HA2	1.78	0.65
1:C:4511:ALA:HA	1:C:4514:ILE:HD12	1.78	0.65
1:D:3802:SER:OG	1:D:3833:ASP:O	2.14	0.65
1:D:1620:GLN:HE21	1:D:1622:LEU:HD21	1.60	0.65
1:B:1304:LEU:HB3	1:B:1541:PRO:HG2	1.79	0.65
1:B:1258:PHE:HB2	1:B:1593:HIS:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3802:SER:OG	1:B:3833:ASP:O	2.15	0.65
1:A:2463:PRO:HB2	1:A:2519:ARG:HD2	1.76	0.65
1:A:3802:SER:OG	1:A:3833:ASP:O	2.14	0.65
1:B:644:LEU:HB2	1:B:1654:HIS:HD2	1.60	0.65
1:C:143:LEU:HD23	1:D:2426:SER:HB3	1.79	0.64
1:C:2463:PRO:HB2	1:C:2519:ARG:HD2	1.77	0.64
1:A:644:LEU:HB2	1:A:1654:HIS:HD2	1.61	0.64
1:A:1304:LEU:HB3	1:A:1541:PRO:HG2	1.79	0.64
1:A:4171:ARG:HH11	1:A:4752:LYS:HD3	1.59	0.64
1:D:1602:GLN:HE22	1:D:1642:LEU:HB3	1.63	0.64
1:B:3911:ILE:HG21	1:B:3971:GLU:HB3	1.80	0.64
1:C:986:ILE:HD12	1:C:1059:GLY:HA2	1.79	0.63
1:D:1258:PHE:HB2	1:D:1593:HIS:HB3	1.80	0.63
1:A:1602:GLN:HE22	1:A:1642:LEU:HB3	1.63	0.63
1:B:143:LEU:HD23	1:C:2426:SER:HB3	1.80	0.63
1:D:986:ILE:HD12	1:D:1059:GLY:HA2	1.79	0.63
1:A:1258:PHE:HB2	1:A:1593:HIS:HB3	1.80	0.63
1:C:1258:PHE:HB2	1:C:1593:HIS:HB3	1.79	0.63
1:C:4002:ASP:HA	1:C:4115:ARG:HH22	1.63	0.63
1:C:647:ARG:NH1	1:C:1681:ASP:OD2	2.32	0.63
1:D:1286:THR:HA	1:D:1586:LEU:HD11	1.80	0.63
1:D:1304:LEU:HB3	1:D:1541:PRO:HG2	1.80	0.63
1:C:1304:LEU:HB3	1:C:1541:PRO:HG2	1.79	0.62
1:C:1602:GLN:HE22	1:C:1642:LEU:HB3	1.63	0.62
1:A:3911:ILE:HG21	1:A:3971:GLU:HB3	1.81	0.62
1:A:3925:ILE:HG23	1:A:3933:GLN:HG2	1.82	0.62
1:B:1602:GLN:HE22	1:B:1642:LEU:HB3	1.63	0.62
1:A:1286:THR:HA	1:A:1586:LEU:HD11	1.80	0.62
1:A:4002:ASP:HA	1:A:4115:ARG:HH22	1.64	0.62
1:C:2256:LEU:O	1:C:3811:ARG:NH1	2.32	0.62
1:A:238:HIS:HE1	1:A:400:ASP:HB3	1.65	0.62
1:B:1286:THR:HA	1:B:1586:LEU:HD11	1.80	0.62
1:D:647:ARG:NH1	1:D:1681:ASP:OD2	2.33	0.62
1:D:1605:LYS:HD3	1:D:1606:VAL:HG23	1.81	0.62
1:D:3925:ILE:HG23	1:D:3933:GLN:HG2	1.82	0.62
1:B:2256:LEU:O	1:B:3811:ARG:NH1	2.32	0.62
1:D:228:LEU:HB3	1:D:289:ILE:HD12	1.82	0.62
1:A:228:LEU:HB3	1:A:289:ILE:HD12	1.82	0.62
1:A:647:ARG:NH1	1:A:1681:ASP:OD2	2.33	0.62
1:A:708:GLY:HA2	1:A:714:GLY:HA3	1.82	0.62
1:C:228:LEU:HB3	1:C:289:ILE:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3911:ILE:HG21	1:C:3971:GLU:HB3	1.82	0.62
1:B:228:LEU:HB3	1:B:289:ILE:HD12	1.82	0.61
1:B:647:ARG:NH1	1:B:1681:ASP:OD2	2.32	0.61
1:C:3802:SER:OG	1:C:3833:ASP:O	2.15	0.61
1:D:238:HIS:HE1	1:D:400:ASP:HB3	1.65	0.61
1:A:1605:LYS:HD3	1:A:1606:VAL:HG23	1.82	0.61
1:B:4002:ASP:HA	1:B:4115:ARG:HH22	1.64	0.61
1:A:2426:SER:HB3	1:D:143:LEU:HD23	1.81	0.61
1:C:1286:THR:HA	1:C:1586:LEU:HD11	1.80	0.61
1:C:1605:LYS:HD3	1:C:1606:VAL:HG23	1.81	0.61
1:D:4002:ASP:HA	1:D:4115:ARG:HH22	1.63	0.61
1:A:2256:LEU:O	1:A:3811:ARG:NH1	2.32	0.61
1:B:3925:ILE:HG23	1:B:3933:GLN:HG2	1.83	0.61
1:C:238:HIS:HE1	1:C:400:ASP:HB3	1.66	0.61
1:B:238:HIS:HE1	1:B:400:ASP:HB3	1.66	0.61
1:B:708:GLY:HA2	1:B:714:GLY:HA3	1.82	0.61
1:C:192:LEU:O	1:C:212:TRP:NE1	2.33	0.61
1:D:3922:THR:O	1:D:3926:GLN:N	2.34	0.61
1:B:1605:LYS:HD3	1:B:1606:VAL:HG23	1.82	0.61
1:C:3922:THR:O	1:C:3926:GLN:N	2.34	0.61
1:C:3925:ILE:HG23	1:C:3933:GLN:HG2	1.83	0.61
1:D:192:LEU:O	1:D:212:TRP:NE1	2.33	0.61
1:A:4170:LYS:HE2	1:A:4916:LEU:HD23	1.82	0.60
1:B:1445:TRP:HE1	1:B:1508:GLY:HA3	1.66	0.60
1:D:3911:ILE:HG21	1:D:3971:GLU:HB3	1.82	0.60
1:D:644:LEU:HD22	1:D:1632:ILE:HG22	1.83	0.60
1:D:2256:LEU:O	1:D:3811:ARG:NH1	2.32	0.60
1:A:4085:VAL:HG12	1:A:4090:GLU:HG3	1.84	0.60
1:C:3914:ALA:HB3	1:C:3975:LEU:HD11	1.82	0.60
1:C:4171:ARG:HH21	1:C:4171:ARG:CG	2.14	0.60
1:D:708:GLY:HA2	1:D:714:GLY:HA3	1.83	0.60
1:D:3914:ALA:HB3	1:D:3975:LEU:HD11	1.83	0.60
1:A:192:LEU:O	1:A:212:TRP:NE1	2.33	0.60
1:A:644:LEU:HD22	1:A:1632:ILE:HG22	1.83	0.60
1:A:3914:ALA:HB3	1:A:3975:LEU:HD11	1.84	0.60
1:C:708:GLY:HA2	1:C:714:GLY:HA3	1.83	0.60
1:A:4170:LYS:HE2	1:A:4916:LEU:CD2	2.32	0.60
1:B:300:VAL:HG13	1:B:420:ARG:HH21	1.67	0.60
1:C:300:VAL:HG13	1:C:420:ARG:HH21	1.66	0.60
1:D:4085:VAL:HG12	1:D:4090:GLU:HG3	1.84	0.60
1:C:4085:VAL:HG12	1:C:4090:GLU:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:SER:HB2	1:B:190:ARG:HH21	1.67	0.59
1:C:779:PHE:HB3	1:C:782:PHE:HE2	1.67	0.59
1:A:1445:TRP:HE1	1:A:1508:GLY:HA3	1.67	0.59
1:B:3914:ALA:HB3	1:B:3975:LEU:HD11	1.84	0.59
1:A:188:SER:HB2	1:A:190:ARG:HH21	1.67	0.59
1:B:779:PHE:HB3	1:B:782:PHE:HE2	1.67	0.59
1:B:1444:GLY:HA2	1:B:1487:MET:HB2	1.83	0.59
1:B:192:LEU:O	1:B:212:TRP:NE1	2.33	0.59
1:C:644:LEU:HD22	1:C:1632:ILE:HG22	1.83	0.59
1:C:711:GLU:HG3	1:C:1449:ASP:HB3	1.85	0.59
1:D:1272:ARG:NH1	1:D:1587:HIS:O	2.36	0.59
1:A:779:PHE:HB3	1:A:782:PHE:HE2	1.67	0.59
1:A:1444:GLY:HA2	1:A:1487:MET:HB2	1.83	0.59
1:D:779:PHE:HB3	1:D:782:PHE:HE2	1.67	0.59
1:D:1762:GLN:O	1:D:1779:SER:OG	2.21	0.59
1:A:650:ASN:HA	1:A:1626:GLN:HG2	1.85	0.59
1:C:4170:LYS:HE3	1:C:4916:LEU:HD23	1.85	0.59
1:D:300:VAL:HG13	1:D:420:ARG:HH21	1.67	0.59
1:D:2204:PHE:O	1:D:2211:ASN:ND2	2.36	0.59
1:A:300:VAL:HG13	1:A:420:ARG:HH21	1.67	0.59
1:B:644:LEU:HD22	1:B:1632:ILE:HG22	1.84	0.59
1:C:227:TYR:HE1	1:C:355:LYS:HG2	1.68	0.59
1:C:1445:TRP:HE1	1:C:1508:GLY:HA3	1.67	0.59
1:A:677:LEU:HB2	1:A:755:ILE:HB	1.85	0.59
1:C:1272:ARG:NH1	1:C:1587:HIS:O	2.36	0.58
1:C:1762:GLN:O	1:C:1779:SER:OG	2.21	0.58
1:C:2204:PHE:O	1:C:2211:ASN:ND2	2.36	0.58
1:A:1272:ARG:NH1	1:A:1587:HIS:O	2.36	0.58
1:B:3922:THR:O	1:B:3926:GLN:N	2.34	0.58
1:A:35:LEU:HD13	1:A:49:LEU:HD22	1.85	0.58
1:D:1444:GLY:HA2	1:D:1487:MET:HB2	1.84	0.58
1:D:1445:TRP:HE1	1:D:1508:GLY:HA3	1.68	0.58
1:B:711:GLU:HG3	1:B:1449:ASP:HB3	1.85	0.58
1:A:711:GLU:HG3	1:A:1449:ASP:HB3	1.84	0.58
1:A:2204:PHE:O	1:A:2211:ASN:ND2	2.36	0.58
1:A:1086:ARG:HB2	1:A:1207:LEU:HB2	1.86	0.58
1:B:4085:VAL:HG12	1:B:4090:GLU:HG3	1.84	0.58
1:C:677:LEU:HB2	1:C:755:ILE:HB	1.86	0.58
1:C:1444:GLY:HA2	1:C:1487:MET:HB2	1.84	0.58
1:B:58:VAL:HG22	1:B:320:GLU:HA	1.86	0.58
1:D:188:SER:HB2	1:D:190:ARG:HH21	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:650:ASN:HA	1:D:1626:GLN:HG2	1.86	0.58
1:D:1726:ILE:HD11	1:D:2121:LEU:HD11	1.86	0.58
1:B:2204:PHE:O	1:B:2211:ASN:ND2	2.37	0.58
1:A:1762:GLN:O	1:A:1779:SER:OG	2.22	0.58
1:C:3879:LEU:HD12	1:C:3917:VAL:HG13	1.86	0.58
1:D:35:LEU:HD13	1:D:49:LEU:HD22	1.85	0.58
1:B:3879:LEU:HD12	1:B:3917:VAL:HG13	1.85	0.57
1:C:58:VAL:HG22	1:C:320:GLU:HA	1.86	0.57
1:C:188:SER:HB2	1:C:190:ARG:HH21	1.69	0.57
1:B:1086:ARG:HB2	1:B:1207:LEU:HB2	1.85	0.57
1:D:227:TYR:HE1	1:D:355:LYS:HG2	1.68	0.57
1:D:711:GLU:HG3	1:D:1449:ASP:HB3	1.84	0.57
1:B:1272:ARG:NH1	1:B:1587:HIS:O	2.36	0.57
1:C:35:LEU:HD13	1:C:49:LEU:HD22	1.86	0.57
1:A:1726:ILE:HD11	1:A:2121:LEU:HD11	1.87	0.57
1:C:4617:TYR:OH	1:C:4629:GLY:O	2.23	0.57
1:A:3922:THR:O	1:A:3926:GLN:N	2.34	0.57
1:C:1086:ARG:HB2	1:C:1207:LEU:HB2	1.86	0.57
1:B:672:LYS:HA	1:B:760:ASP:HA	1.87	0.57
1:B:897:LYS:HD3	1:B:918:LEU:HD21	1.86	0.57
1:C:897:LYS:HD3	1:C:918:LEU:HD21	1.86	0.57
1:D:58:VAL:HG22	1:D:320:GLU:HA	1.86	0.57
1:A:58:VAL:HG22	1:A:320:GLU:HA	1.87	0.57
1:B:650:ASN:HA	1:B:1626:GLN:HG2	1.85	0.57
1:B:677:LEU:HB2	1:B:755:ILE:HB	1.85	0.57
1:A:3879:LEU:HD12	1:A:3917:VAL:HG13	1.87	0.57
1:B:227:TYR:HE1	1:B:355:LYS:HG2	1.70	0.57
1:B:4617:TYR:OH	1:B:4629:GLY:O	2.23	0.57
1:C:672:LYS:HA	1:C:760:ASP:HA	1.87	0.57
1:D:672:LYS:HA	1:D:760:ASP:HA	1.87	0.57
1:A:672:LYS:HA	1:A:760:ASP:HA	1.87	0.56
1:B:3914:ALA:HA	1:B:3917:VAL:HG12	1.87	0.56
1:D:1086:ARG:HB2	1:D:1207:LEU:HB2	1.86	0.56
1:C:650:ASN:HA	1:C:1626:GLN:HG2	1.86	0.56
1:D:4800:GLY:HA2	1:D:4804:ASP:HB3	1.87	0.56
1:A:2737:LYS:HB3	1:A:2742:TRP:HB2	1.88	0.56
1:B:756:SER:HB3	1:B:769:ARG:HB2	1.87	0.56
1:C:1726:ILE:HD11	1:C:2121:LEU:HD11	1.87	0.56
1:C:4045:SER:HA	1:C:4078:THR:HA	1.87	0.56
1:D:258:ARG:NH1	1:D:317:MET:SD	2.79	0.56
1:D:677:LEU:HB2	1:D:755:ILE:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2071:ALA:HA	1:D:2076:ILE:HD11	1.87	0.56
1:B:1762:GLN:O	1:B:1779:SER:OG	2.22	0.56
1:B:2737:LYS:HB3	1:B:2742:TRP:HB2	1.88	0.56
1:C:905:GLY:HA3	1:C:914:GLN:HB3	1.88	0.56
1:C:4888:LYS:HA	1:C:4895:GLY:HA2	1.88	0.56
1:D:4617:TYR:OH	1:D:4629:GLY:O	2.23	0.56
1:A:364:GLN:HE21	1:A:369:GLY:HA2	1.71	0.56
1:B:905:GLY:HA3	1:B:914:GLN:HB3	1.87	0.56
1:D:897:LYS:HD3	1:D:918:LEU:HD21	1.87	0.56
1:B:35:LEU:HD13	1:B:49:LEU:HD22	1.87	0.56
1:B:258:ARG:NH1	1:B:317:MET:SD	2.78	0.56
1:B:4888:LYS:HA	1:B:4895:GLY:HA2	1.87	0.56
1:A:258:ARG:NH1	1:A:317:MET:SD	2.79	0.56
1:A:897:LYS:HD3	1:A:918:LEU:HD21	1.87	0.56
1:A:905:GLY:HA3	1:A:914:GLN:HB3	1.88	0.56
1:A:3804:LEU:HD13	1:A:3910:ALA:HB2	1.88	0.56
1:B:3804:LEU:HD13	1:B:3910:ALA:HB2	1.88	0.56
1:C:258:ARG:NH1	1:C:317:MET:SD	2.78	0.56
1:C:4800:GLY:HA2	1:C:4804:ASP:HB3	1.88	0.56
1:D:3879:LEU:HD12	1:D:3917:VAL:HG13	1.87	0.56
1:D:905:GLY:HA3	1:D:914:GLN:HB3	1.88	0.56
1:D:4045:SER:HA	1:D:4078:THR:HA	1.87	0.56
1:B:364:GLN:HE21	1:B:369:GLY:HA2	1.71	0.56
1:C:4835:PRO:HB2	1:C:4841:GLU:HG3	1.87	0.56
1:D:364:GLN:HE21	1:D:369:GLY:HA2	1.71	0.56
1:D:1137:PHE:HA	1:D:1144:ARG:HA	1.88	0.55
1:A:227:TYR:HE1	1:A:355:LYS:HG2	1.70	0.55
1:A:228:LEU:HD12	1:A:354:ILE:HB	1.89	0.55
1:A:4045:SER:HA	1:A:4078:THR:HA	1.87	0.55
1:A:4617:TYR:OH	1:A:4629:GLY:O	2.23	0.55
1:C:1137:PHE:HA	1:C:1144:ARG:HA	1.89	0.55
1:C:2737:LYS:HB3	1:C:2742:TRP:HB2	1.88	0.55
1:D:559:ILE:HD13	1:D:593:HIS:HB3	1.88	0.55
1:D:756:SER:HB3	1:D:769:ARG:HB2	1.87	0.55
1:A:756:SER:HB3	1:A:769:ARG:HB2	1.87	0.55
1:B:4780:TYR:HA	1:B:4783:THR:HG22	1.89	0.55
1:C:756:SER:HB3	1:C:769:ARG:HB2	1.88	0.55
1:C:4791:ARG:HH12	1:D:4559:HIS:HE1	1.53	0.55
1:D:3804:LEU:HD13	1:D:3910:ALA:HB2	1.88	0.55
1:A:1137:PHE:HA	1:A:1144:ARG:HA	1.88	0.55
1:B:4045:SER:HA	1:B:4078:THR:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3914:ALA:HA	1:D:3917:VAL:HG12	1.88	0.55
1:C:364:GLN:HE21	1:C:369:GLY:HA2	1.71	0.55
1:D:4817:HIS:CE1	1:D:4828:ILE:HD12	2.40	0.55
1:A:1245:ARG:HE	1:A:1692:LYS:HG2	1.72	0.55
1:D:776:GLN:HB3	1:D:1470:GLY:HA3	1.89	0.55
1:D:2737:LYS:HB3	1:D:2742:TRP:HB2	1.88	0.55
1:A:2404:ALA:HB3	1:A:2475:ARG:HH21	1.72	0.54
1:A:4888:LYS:HA	1:A:4895:GLY:HA2	1.89	0.54
1:B:1726:ILE:HD11	1:B:2121:LEU:HD11	1.88	0.54
1:B:4835:PRO:HB2	1:B:4841:GLU:HG3	1.88	0.54
1:C:4817:HIS:CE1	1:C:4828:ILE:HD12	2.40	0.54
1:C:4915:ASN:O	1:C:4917:ALA:N	2.41	0.54
1:A:1607:ASP:HB3	1:A:1608:VAL:HG23	1.89	0.54
1:B:4817:HIS:CE1	1:B:4828:ILE:HD12	2.39	0.54
1:C:3804:LEU:HD13	1:C:3910:ALA:HB2	1.88	0.54
1:A:559:ILE:HD13	1:A:593:HIS:HB3	1.88	0.54
1:B:1137:PHE:HA	1:B:1144:ARG:HA	1.89	0.54
1:B:1245:ARG:HE	1:B:1692:LYS:HG2	1.72	0.54
1:B:4915:ASN:O	1:B:4917:ALA:N	2.40	0.54
1:C:3914:ALA:HA	1:C:3917:VAL:HG12	1.88	0.54
1:A:123:HIS:HD2	1:A:126:SER:H	1.55	0.54
1:A:1601:ASN:ND2	1:A:1643:GLU:OE2	2.41	0.54
1:A:3914:ALA:HA	1:A:3917:VAL:HG12	1.88	0.54
1:A:4754:LEU:CD1	1:D:4770:LEU:HB3	2.36	0.54
1:A:4791:ARG:HH12	1:B:4559:HIS:HE1	1.54	0.54
1:B:1607:ASP:HB3	1:B:1608:VAL:HG23	1.88	0.54
1:C:559:ILE:HD13	1:C:593:HIS:HB3	1.89	0.54
1:C:4780:TYR:HA	1:C:4783:THR:HG22	1.89	0.54
1:D:4835:PRO:HB2	1:D:4841:GLU:HG3	1.89	0.54
1:A:4817:HIS:CE1	1:A:4828:ILE:HD12	2.40	0.54
1:B:123:HIS:HD2	1:B:126:SER:H	1.56	0.54
1:B:1510:VAL:HG12	1:B:1511:VAL:HG23	1.90	0.54
1:A:1629:SER:HA	1:A:1640:ASP:HA	1.90	0.54
1:A:4915:ASN:O	1:A:4917:ALA:N	2.41	0.54
1:C:1252:SER:HB2	1:C:1598:ARG:HB2	1.90	0.54
1:C:1607:ASP:HB3	1:C:1608:VAL:HG23	1.89	0.54
1:C:2071:ALA:HA	1:C:2076:ILE:HD11	1.88	0.54
1:B:228:LEU:HD12	1:B:354:ILE:HB	1.90	0.54
1:C:2404:ALA:HB3	1:C:2475:ARG:HH21	1.73	0.54
1:A:3670:LEU:HD22	1:A:3674:ARG:HH21	1.73	0.54
1:B:281:ARG:NH1	1:B:346:VAL:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:652:VAL:HG11	1:C:715:GLY:HA2	1.90	0.54
1:C:1601:ASN:ND2	1:C:1643:GLU:OE2	2.41	0.54
1:C:2489:LEU:O	1:C:2492:GLY:N	2.41	0.54
1:D:228:LEU:HD12	1:D:354:ILE:HB	1.89	0.54
1:D:4915:ASN:O	1:D:4917:ALA:N	2.41	0.54
1:A:4835:PRO:HB2	1:A:4841:GLU:HG3	1.89	0.54
1:B:1601:ASN:ND2	1:B:1643:GLU:OE2	2.41	0.54
1:B:4800:GLY:HA2	1:B:4804:ASP:HB3	1.90	0.54
1:D:2404:ALA:HB3	1:D:2475:ARG:HH21	1.73	0.54
1:A:2489:LEU:O	1:A:2492:GLY:N	2.41	0.54
1:A:4823:ARG:NH1	1:D:4826:GLY:O	2.41	0.54
1:B:1267:HIS:HB3	1:B:1294:ASN:HD21	1.73	0.54
1:C:123:HIS:HD2	1:C:126:SER:H	1.56	0.54
1:C:1267:HIS:HB3	1:C:1294:ASN:HD21	1.73	0.54
1:C:1629:SER:HA	1:C:1640:ASP:HA	1.90	0.54
1:D:1601:ASN:ND2	1:D:1643:GLU:OE2	2.41	0.54
1:D:1629:SER:HA	1:D:1640:ASP:HA	1.90	0.54
1:A:243:GLU:HA	1:A:264:GLY:HA2	1.89	0.53
1:A:776:GLN:HB3	1:A:1470:GLY:HA3	1.89	0.53
1:B:1431:ARG:HB3	1:B:1554:GLN:HB2	1.90	0.53
1:B:2489:LEU:O	1:B:2492:GLY:N	2.41	0.53
1:B:4171:ARG:HH21	1:B:4171:ARG:HG3	1.72	0.53
1:D:1267:HIS:HB3	1:D:1294:ASN:HD21	1.73	0.53
1:A:800:VAL:HG23	1:A:1619:VAL:HG13	1.90	0.53
1:A:1510:VAL:HG12	1:A:1511:VAL:HG23	1.90	0.53
1:A:2071:ALA:HA	1:A:2076:ILE:HD11	1.90	0.53
1:B:3670:LEU:HD22	1:B:3674:ARG:HH21	1.73	0.53
1:B:4810:MET:HB3	1:C:4519:LEU:O	2.08	0.53
1:A:4780:TYR:HA	1:A:4783:THR:HG22	1.89	0.53
1:B:800:VAL:HG23	1:B:1619:VAL:HG13	1.90	0.53
1:C:1510:VAL:HG12	1:C:1511:VAL:HG23	1.90	0.53
1:D:123:HIS:HD2	1:D:126:SER:H	1.55	0.53
1:D:1690:GLU:OE2	1:D:1790:LYS:NZ	2.39	0.53
1:A:1690:GLU:OE2	1:A:1790:LYS:NZ	2.39	0.53
1:B:1252:SER:HB2	1:B:1598:ARG:HB2	1.90	0.53
1:B:4191:VAL:HA	1:B:4194:CYS:HB2	1.91	0.53
1:D:3670:LEU:HD22	1:D:3674:ARG:HH21	1.74	0.53
1:A:4800:GLY:HA2	1:A:4804:ASP:HB3	1.90	0.53
1:B:1629:SER:HA	1:B:1640:ASP:HA	1.90	0.53
1:B:4188:GLU:O	1:B:4192:ASN:ND2	2.42	0.53
1:A:1442:TRP:HD1	1:A:1488:VAL:HG13	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4826:GLY:O	1:B:4823:ARG:NH1	2.42	0.53
1:D:800:VAL:HG23	1:D:1619:VAL:HG13	1.91	0.53
1:A:1267:HIS:HB3	1:A:1294:ASN:HD21	1.74	0.53
1:B:1128:LEU:HD13	1:B:1206:SER:HB2	1.90	0.53
1:C:1128:LEU:HD13	1:C:1206:SER:HB2	1.91	0.53
1:D:2489:LEU:O	1:D:2492:GLY:N	2.41	0.53
1:D:4888:LYS:HA	1:D:4895:GLY:HA2	1.90	0.53
1:B:559:ILE:HD13	1:B:593:HIS:HB3	1.89	0.53
1:B:4752:LYS:HG3	1:B:4755:ARG:HE	1.74	0.53
1:B:4791:ARG:HH12	1:C:4559:HIS:HE1	1.53	0.53
1:C:228:LEU:HD12	1:C:354:ILE:HB	1.89	0.53
1:C:243:GLU:HA	1:C:264:GLY:HA2	1.90	0.53
1:D:243:GLU:HA	1:D:264:GLY:HA2	1.89	0.53
1:D:1607:ASP:HB3	1:D:1608:VAL:HG23	1.90	0.53
1:A:1128:LEU:HD13	1:A:1206:SER:HB2	1.90	0.53
1:A:1431:ARG:HB3	1:A:1554:GLN:HB2	1.90	0.53
1:C:3670:LEU:HD22	1:C:3674:ARG:HH21	1.72	0.53
1:D:1442:TRP:HB2	1:D:1544:PHE:HB2	1.91	0.53
1:A:1442:TRP:HB2	1:A:1544:PHE:HB2	1.91	0.53
1:D:1245:ARG:HE	1:D:1692:LYS:HG2	1.74	0.53
1:D:4780:TYR:HA	1:D:4783:THR:HG22	1.90	0.53
1:C:800:VAL:HG23	1:C:1619:VAL:HG13	1.91	0.52
1:C:1431:ARG:HB3	1:C:1554:GLN:HB2	1.91	0.52
1:D:1510:VAL:HG12	1:D:1511:VAL:HG23	1.91	0.52
1:B:652:VAL:HG11	1:B:715:GLY:HA2	1.90	0.52
1:C:3645:LEU:HB2	1:C:3665:LEU:HD12	1.91	0.52
1:C:4810:MET:HB3	1:D:4519:LEU:O	2.09	0.52
1:D:1431:ARG:HB3	1:D:1554:GLN:HB2	1.91	0.52
1:B:243:GLU:HA	1:B:264:GLY:HA2	1.90	0.52
1:B:776:GLN:HB3	1:B:1470:GLY:HA3	1.90	0.52
1:C:712:GLU:OE2	1:C:1636:ASN:ND2	2.43	0.52
1:C:4014:ILE:HA	1:C:4017:PHE:HB3	1.92	0.52
1:D:1128:LEU:HD13	1:D:1206:SER:HB2	1.91	0.52
1:D:1266:GLU:O	1:D:1294:ASN:ND2	2.43	0.52
1:D:4014:ILE:HA	1:D:4017:PHE:HB3	1.92	0.52
1:D:4188:GLU:O	1:D:4192:ASN:ND2	2.43	0.52
1:A:4519:LEU:O	1:D:4810:MET:HB3	2.09	0.52
1:C:4191:VAL:HA	1:C:4194:CYS:HB2	1.92	0.52
1:B:2794:ARG:HB2	1:B:2901:GLY:HA3	1.92	0.52
1:B:3645:LEU:HB2	1:B:3665:LEU:HD12	1.92	0.52
1:C:1442:TRP:HB2	1:C:1544:PHE:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:TYR:CE1	1:B:355:LYS:HG2	2.45	0.52
1:B:1442:TRP:HB2	1:B:1544:PHE:HB2	1.92	0.52
1:B:2130:LEU:HD12	1:B:2133:VAL:HG21	1.92	0.52
1:B:2404:ALA:HB3	1:B:2475:ARG:HH21	1.74	0.52
1:C:2130:LEU:HD12	1:C:2133:VAL:HG21	1.92	0.52
1:D:3924:TYR:O	1:D:3932:ASN:ND2	2.43	0.52
1:A:4188:GLU:O	1:A:4192:ASN:ND2	2.42	0.52
1:A:4810:MET:HB3	1:B:4519:LEU:O	2.09	0.52
1:C:776:GLN:HB3	1:C:1470:GLY:HA3	1.90	0.52
1:D:281:ARG:NH1	1:D:346:VAL:O	2.42	0.52
1:A:4559:HIS:HE1	1:D:4791:ARG:HH12	1.54	0.52
1:C:2794:ARG:HB2	1:C:2901:GLY:HA3	1.92	0.52
1:C:4817:HIS:HA	1:C:4821:GLY:H	1.75	0.52
1:D:1252:SER:HB2	1:D:1598:ARG:HB2	1.91	0.52
1:D:3730:ALA:HA	1:D:3733:HIS:CE1	2.45	0.52
1:A:3665:LEU:HD22	1:A:3735:ARG:HH11	1.75	0.52
1:A:4608:ALA:HB1	1:A:4650:VAL:HG11	1.92	0.52
1:C:4770:LEU:HB3	1:D:4754:LEU:CD1	2.37	0.52
1:D:652:VAL:HG11	1:D:715:GLY:HA2	1.92	0.52
1:D:1272:ARG:NH2	1:D:1590:PHE:O	2.43	0.52
1:D:3645:LEU:HB2	1:D:3665:LEU:HD12	1.92	0.52
1:D:4817:HIS:HA	1:D:4821:GLY:H	1.74	0.52
1:A:2794:ARG:HB2	1:A:2901:GLY:HA3	1.92	0.52
1:B:1442:TRP:HD1	1:B:1488:VAL:HG13	1.75	0.52
1:C:227:TYR:CE1	1:C:355:LYS:HG2	2.44	0.52
1:C:3665:LEU:HD22	1:C:3735:ARG:HH11	1.75	0.52
1:C:4188:GLU:O	1:C:4192:ASN:ND2	2.42	0.52
1:D:598:ILE:HG23	1:D:636:LEU:HD12	1.92	0.52
1:A:3730:ALA:HA	1:A:3733:HIS:CE1	2.45	0.51
1:B:2071:ALA:HA	1:B:2076:ILE:HD11	1.91	0.51
1:D:1442:TRP:HD1	1:D:1488:VAL:HG13	1.75	0.51
1:D:1703:TYR:HD2	1:D:1820:PRO:HB2	1.75	0.51
1:D:2076:ILE:HG21	1:D:2081:LEU:HD22	1.92	0.51
1:D:4170:LYS:HE2	1:D:4916:LEU:HD23	1.91	0.51
1:A:227:TYR:CE1	1:A:355:LYS:HG2	2.45	0.51
1:A:4752:LYS:HG3	1:A:4755:ARG:HE	1.76	0.51
1:B:3665:LEU:HD22	1:B:3735:ARG:HH11	1.75	0.51
1:B:3730:ALA:HA	1:B:3733:HIS:CE1	2.46	0.51
1:C:2076:ILE:HG21	1:C:2081:LEU:HD22	1.92	0.51
1:C:2083:ARG:HG3	1:C:3688:LEU:HD22	1.92	0.51
1:D:3665:LEU:HD22	1:D:3735:ARG:HH11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4608:ALA:HB1	1:D:4650:VAL:HG11	1.91	0.51
1:A:2130:LEU:HD12	1:A:2133:VAL:HG21	1.93	0.51
1:A:3645:LEU:HB2	1:A:3665:LEU:HD12	1.93	0.51
1:A:4014:ILE:HA	1:A:4017:PHE:HB3	1.91	0.51
1:A:4191:VAL:HA	1:A:4194:CYS:HB2	1.93	0.51
1:B:3742:LEU:HD23	1:B:3781:TYR:HB3	1.92	0.51
1:D:227:TYR:CE1	1:D:355:LYS:HG2	2.45	0.51
1:A:1266:GLU:O	1:A:1294:ASN:ND2	2.43	0.51
1:B:4824:ALA:HB3	1:B:4827:GLY:H	1.75	0.51
1:C:1124:PRO:HB2	1:C:1252:SER:HB3	1.93	0.51
1:C:1272:ARG:NH2	1:C:1590:PHE:O	2.44	0.51
1:D:866:PRO:HD2	1:D:1009:ARG:HD2	1.92	0.51
1:D:2083:ARG:HG3	1:D:3688:LEU:HD22	1.92	0.51
1:D:2794:ARG:HB2	1:D:2901:GLY:HA3	1.92	0.51
1:A:1252:SER:HB2	1:A:1598:ARG:HB2	1.91	0.51
1:A:1272:ARG:NH2	1:A:1590:PHE:O	2.44	0.51
1:C:866:PRO:HD2	1:C:1009:ARG:HD2	1.92	0.51
1:C:1266:GLU:O	1:C:1294:ASN:ND2	2.43	0.51
1:C:3730:ALA:HA	1:C:3733:HIS:CE1	2.45	0.51
1:C:3924:TYR:O	1:C:3932:ASN:ND2	2.43	0.51
1:A:281:ARG:NH1	1:A:346:VAL:O	2.42	0.51
1:A:4817:HIS:HA	1:A:4821:GLY:H	1.74	0.51
1:D:1124:PRO:HB2	1:D:1252:SER:HB3	1.93	0.51
1:A:866:PRO:HD2	1:A:1009:ARG:HD2	1.92	0.51
1:B:1272:ARG:NH2	1:B:1590:PHE:O	2.44	0.51
1:B:2076:ILE:HG21	1:B:2081:LEU:HD22	1.91	0.51
1:C:598:ILE:HG23	1:C:636:LEU:HD12	1.93	0.51
1:A:1124:PRO:HB2	1:A:1252:SER:HB3	1.93	0.51
1:B:1124:PRO:HB2	1:B:1252:SER:HB3	1.93	0.51
1:C:1245:ARG:HE	1:C:1692:LYS:HG2	1.75	0.51
1:C:1442:TRP:HD1	1:C:1488:VAL:HG13	1.75	0.51
1:D:712:GLU:OE2	1:D:1636:ASN:ND2	2.43	0.51
1:A:677:LEU:HD23	1:A:802:PHE:HA	1.93	0.51
1:B:598:ILE:HG23	1:B:636:LEU:HD12	1.93	0.51
1:B:866:PRO:HD2	1:B:1009:ARG:HD2	1.93	0.51
1:B:4817:HIS:HA	1:B:4821:GLY:H	1.75	0.51
1:D:2226:SER:HB2	1:D:2241:LEU:HB2	1.93	0.51
1:A:394:HIS:HD2	1:A:397:GLY:H	1.59	0.51
1:A:1184:ASP:OD2	1:A:1188:SER:OG	2.29	0.51
1:A:3924:TYR:O	1:A:3932:ASN:ND2	2.44	0.51
1:D:2130:LEU:HD12	1:D:2133:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1703:TYR:HD2	1:A:1820:PRO:HB2	1.76	0.50
1:A:2076:ILE:HG21	1:A:2081:LEU:HD22	1.92	0.50
1:A:2083:ARG:HG3	1:A:3688:LEU:HD22	1.93	0.50
1:B:394:HIS:HD2	1:B:397:GLY:H	1.59	0.50
1:B:2163:MET:HA	1:B:2166:LEU:HD12	1.93	0.50
1:B:4014:ILE:HA	1:B:4017:PHE:HB3	1.91	0.50
1:B:4170:LYS:HE2	1:B:4174:ILE:HD11	1.93	0.50
1:C:1690:GLU:OE2	1:C:1790:LYS:NZ	2.39	0.50
1:C:2226:SER:HB2	1:C:2241:LEU:HB2	1.94	0.50
1:C:4891:ILE:HD13	1:C:4914:HIS:HB3	1.92	0.50
1:A:2226:SER:HB2	1:A:2241:LEU:HB2	1.93	0.50
1:B:1703:TYR:HD2	1:B:1820:PRO:HB2	1.76	0.50
1:B:3924:TYR:O	1:B:3932:ASN:ND2	2.44	0.50
1:A:598:ILE:HG23	1:A:636:LEU:HD12	1.92	0.50
1:B:1266:GLU:O	1:B:1294:ASN:ND2	2.44	0.50
1:B:2083:ARG:HG3	1:B:3688:LEU:HD22	1.93	0.50
1:C:598:ILE:HD13	1:C:636:LEU:HB2	1.94	0.50
1:D:2163:MET:HA	1:D:2166:LEU:HD12	1.93	0.50
1:B:712:GLU:OE2	1:B:1636:ASN:ND2	2.44	0.50
1:A:3779:LEU:HD11	1:A:3783:LYS:HE2	1.94	0.50
1:A:4780:TYR:O	1:A:4784:VAL:HG23	2.12	0.50
1:C:281:ARG:NH1	1:C:346:VAL:O	2.41	0.50
1:C:1703:TYR:HD2	1:C:1820:PRO:HB2	1.76	0.50
1:C:2163:MET:HA	1:C:2166:LEU:HD12	1.94	0.50
1:D:677:LEU:HD23	1:D:802:PHE:HA	1.93	0.50
1:D:4191:VAL:HA	1:D:4194:CYS:HB2	1.93	0.50
1:A:652:VAL:HG11	1:A:715:GLY:HA2	1.92	0.50
1:B:4608:ALA:HB1	1:B:4650:VAL:HG11	1.93	0.50
1:D:394:HIS:HD2	1:D:397:GLY:H	1.60	0.50
1:D:3779:LEU:HD11	1:D:3783:LYS:HE2	1.94	0.50
1:D:4891:ILE:HD13	1:D:4914:HIS:HB3	1.93	0.50
1:A:2521:LEU:HD22	1:A:2565:ALA:HB2	1.94	0.50
1:B:1690:GLU:OE2	1:B:1790:LYS:NZ	2.39	0.50
1:B:3779:LEU:HD11	1:B:3783:LYS:HE2	1.94	0.50
1:C:2723:ASN:OD1	1:C:2773:ARG:NH2	2.45	0.50
1:D:1706:LEU:HD21	1:D:1787:LEU:HD21	1.94	0.50
1:A:2163:MET:HA	1:A:2166:LEU:HD12	1.92	0.50
1:A:4824:ALA:HB3	1:A:4827:GLY:H	1.77	0.50
1:C:3742:LEU:HD23	1:C:3781:TYR:HB3	1.93	0.50
1:A:3879:LEU:HD13	1:A:3921:LEU:HD12	1.94	0.49
1:C:677:LEU:HD23	1:C:802:PHE:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3779:LEU:HD11	1:C:3783:LYS:HE2	1.94	0.49
1:C:4060:THR:OG1	1:C:4063:GLU:OE1	2.26	0.49
1:C:4780:TYR:O	1:C:4784:VAL:HG23	2.12	0.49
1:D:1184:ASP:HB3	1:D:1186:SER:H	1.77	0.49
1:D:2723:ASN:OD1	1:D:2773:ARG:NH2	2.45	0.49
1:B:677:LEU:HD23	1:B:802:PHE:HA	1.93	0.49
1:B:1160:ASP:OD1	1:B:1178:ASN:ND2	2.43	0.49
1:C:1184:ASP:OD2	1:C:1188:SER:OG	2.29	0.49
1:C:3990:ASN:ND2	1:C:3991:VAL:O	2.45	0.49
1:A:4627:ILE:O	1:A:4631:TRP:N	2.46	0.49
1:A:4640:SER:OG	1:A:4703:ASP:OD2	2.29	0.49
1:A:4891:ILE:HD13	1:A:4914:HIS:HB3	1.93	0.49
1:C:1706:LEU:HD21	1:C:1787:LEU:HD21	1.95	0.49
1:D:598:ILE:HD13	1:D:636:LEU:HB2	1.94	0.49
1:D:4114:THR:HA	1:D:4117:GLN:HB2	1.95	0.49
1:D:4780:TYR:O	1:D:4784:VAL:HG23	2.11	0.49
1:D:4824:ALA:HB3	1:D:4827:GLY:H	1.77	0.49
1:A:235:ARG:HE	1:A:274:LEU:HD21	1.77	0.49
1:A:2222:LEU:HD21	1:A:2243:VAL:HB	1.94	0.49
1:B:2226:SER:HB2	1:B:2241:LEU:HB2	1.94	0.49
1:B:2723:ASN:OD1	1:B:2773:ARG:NH2	2.45	0.49
1:B:4780:TYR:O	1:B:4784:VAL:HG23	2.13	0.49
1:C:4824:ALA:HB3	1:C:4827:GLY:H	1.77	0.49
1:D:2521:LEU:HD22	1:D:2565:ALA:HB2	1.94	0.49
1:A:4114:THR:HA	1:A:4117:GLN:HB2	1.95	0.49
1:A:4189:LEU:HA	1:A:4192:ASN:HD22	1.77	0.49
1:B:4060:THR:OG1	1:B:4063:GLU:OE1	2.26	0.49
1:D:3879:LEU:HD13	1:D:3921:LEU:HD12	1.95	0.49
1:A:712:GLU:OE2	1:A:1636:ASN:ND2	2.44	0.49
1:A:1706:LEU:HD21	1:A:1787:LEU:HD21	1.93	0.49
1:C:1184:ASP:HB3	1:C:1186:SER:H	1.77	0.49
1:D:2222:LEU:HD21	1:D:2243:VAL:HB	1.94	0.49
1:A:1716:THR:HA	1:A:1719:LEU:HD12	1.95	0.49
1:B:218:SER:HB3	1:B:286:GLY:HA3	1.94	0.49
1:B:2222:LEU:HD21	1:B:2243:VAL:HB	1.94	0.49
1:B:4627:ILE:O	1:B:4631:TRP:N	2.46	0.49
1:C:1938:GLN:HE22	1:C:3614:ARG:HA	1.77	0.49
1:B:298:ARG:HA	1:B:305:TYR:HA	1.94	0.49
1:C:843:GLU:HA	1:C:848:ARG:HG2	1.95	0.49
1:C:1244:ASN:HD22	1:C:1801:GLU:HG2	1.78	0.49
1:C:4608:ALA:HB1	1:C:4650:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1692:LYS:HA	1:D:1810:VAL:HG13	1.95	0.49
1:D:4189:LEU:HA	1:D:4192:ASN:HD22	1.78	0.49
1:A:1160:ASP:OD1	1:A:1178:ASN:ND2	2.43	0.49
1:A:1654:HIS:O	1:A:1657:THR:OG1	2.27	0.49
1:A:2723:ASN:OD1	1:A:2773:ARG:NH2	2.45	0.49
1:B:843:GLU:HA	1:B:848:ARG:HG2	1.94	0.49
1:B:4189:LEU:HA	1:B:4192:ASN:HD22	1.78	0.49
1:C:2213:LYS:HA	1:C:2254:LEU:HD21	1.94	0.49
1:C:4627:ILE:O	1:C:4631:TRP:N	2.45	0.49
1:A:218:SER:HB3	1:A:286:GLY:HA3	1.95	0.49
1:A:3990:ASN:ND2	1:A:3991:VAL:O	2.46	0.49
1:B:4891:ILE:HD13	1:B:4914:HIS:HB3	1.94	0.49
1:C:2222:LEU:HD21	1:C:2243:VAL:HB	1.95	0.49
1:C:4171:ARG:CG	1:C:4171:ARG:NH2	2.73	0.49
1:D:2857:LYS:HE3	1:D:2861:LEU:HD11	1.95	0.49
1:D:3742:LEU:HD23	1:D:3781:TYR:HB3	1.95	0.49
1:A:3729:GLN:NE2	1:A:3767:LEU:O	2.47	0.48
1:A:4796:LYS:NZ	1:A:4807:CYS:SG	2.82	0.48
1:B:598:ILE:HD13	1:B:636:LEU:HB2	1.95	0.48
1:B:678:MET:HG3	1:B:754:VAL:HG22	1.94	0.48
1:B:1121:GLY:O	1:B:1133:ARG:NH1	2.43	0.48
1:B:1184:ASP:OD2	1:B:1188:SER:OG	2.29	0.48
1:B:3990:ASN:ND2	1:B:3991:VAL:O	2.46	0.48
1:C:218:SER:HB3	1:C:286:GLY:HA3	1.95	0.48
1:C:1121:GLY:O	1:C:1133:ARG:NH1	2.43	0.48
1:C:1692:LYS:HA	1:C:1810:VAL:HG13	1.95	0.48
1:A:843:GLU:HA	1:A:848:ARG:HG2	1.94	0.48
1:B:290:ARG:HH22	1:B:343:ARG:HG3	1.78	0.48
1:B:4114:THR:HA	1:B:4117:GLN:HB2	1.95	0.48
1:D:128:MET:HB3	1:D:149:LEU:HB3	1.95	0.48
1:D:1160:ASP:OD1	1:D:1178:ASN:ND2	2.42	0.48
1:A:4770:LEU:HB3	1:B:4754:LEU:CD1	2.40	0.48
1:C:4826:GLY:O	1:D:4823:ARG:NH1	2.46	0.48
1:D:1184:ASP:OD2	1:D:1188:SER:OG	2.29	0.48
1:D:1931:ASP:O	1:D:3614:ARG:NH1	2.42	0.48
1:D:3990:ASN:ND2	1:D:3991:VAL:O	2.46	0.48
1:D:4060:THR:OG1	1:D:4063:GLU:OE1	2.26	0.48
1:D:4627:ILE:O	1:D:4631:TRP:N	2.45	0.48
1:D:4796:LYS:NZ	1:D:4807:CYS:SG	2.82	0.48
1:A:1184:ASP:HB3	1:A:1186:SER:H	1.78	0.48
1:C:128:MET:HB3	1:C:149:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:678:MET:HG3	1:C:754:VAL:HG22	1.96	0.48
1:C:1160:ASP:OD1	1:C:1178:ASN:ND2	2.43	0.48
1:D:2213:LYS:HA	1:D:2254:LEU:HD21	1.95	0.48
1:A:2857:LYS:HE3	1:A:2861:LEU:HD11	1.95	0.48
1:B:4826:GLY:O	1:C:4823:ARG:NH1	2.46	0.48
1:C:394:HIS:HD2	1:C:397:GLY:H	1.60	0.48
1:D:218:SER:HB3	1:D:286:GLY:HA3	1.96	0.48
1:D:843:GLU:HA	1:D:848:ARG:HG2	1.94	0.48
1:B:1184:ASP:HB3	1:B:1186:SER:H	1.77	0.48
1:D:235:ARG:HE	1:D:274:LEU:HD21	1.78	0.48
1:D:3690:MET:HE1	1:D:3754:PRO:HB2	1.96	0.48
1:D:4794:TYR:HB3	1:D:4807:CYS:HB2	1.95	0.48
1:A:4931:GLU:OE2	1:A:4942:TRP:NE1	2.46	0.48
1:B:4770:LEU:HB3	1:C:4754:LEU:CD1	2.39	0.48
1:C:2521:LEU:HD22	1:C:2565:ALA:HB2	1.95	0.48
1:A:2843:GLU:OE1	1:A:2887:ARG:NH2	2.47	0.48
1:B:1706:LEU:HD21	1:B:1787:LEU:HD21	1.94	0.48
1:D:1716:THR:HA	1:D:1719:LEU:HD12	1.95	0.48
1:D:3729:GLN:NE2	1:D:3767:LEU:O	2.47	0.48
1:D:4610:LYS:O	1:D:4615:GLY:N	2.46	0.48
1:A:678:MET:HG3	1:A:754:VAL:HG22	1.95	0.48
1:A:4794:TYR:HB3	1:A:4807:CYS:HB2	1.96	0.48
1:B:235:ARG:HE	1:B:274:LEU:HD21	1.79	0.48
1:B:1654:HIS:O	1:B:1657:THR:OG1	2.28	0.48
1:B:1716:THR:HA	1:B:1719:LEU:HD12	1.96	0.48
1:B:3729:GLN:NE2	1:B:3767:LEU:O	2.47	0.48
1:C:2857:LYS:HE3	1:C:2861:LEU:HD11	1.95	0.48
1:D:2528:LEU:HD11	1:D:2568:ASP:HA	1.96	0.48
1:B:1611:ILE:N	1:B:1620:GLN:O	2.43	0.48
1:B:1664:VAL:HG12	1:B:1672:VAL:HG11	1.96	0.48
1:C:235:ARG:HE	1:C:274:LEU:HD21	1.79	0.48
1:C:4114:THR:HA	1:C:4117:GLN:HB2	1.96	0.48
1:C:4610:LYS:O	1:C:4615:GLY:N	2.46	0.48
1:A:128:MET:HB3	1:A:149:LEU:HB3	1.96	0.47
1:B:1726:ILE:HB	1:B:2109:ILE:HD11	1.96	0.47
1:B:2521:LEU:HD22	1:B:2565:ALA:HB2	1.95	0.47
1:C:650:ASN:ND2	1:C:795:SER:O	2.47	0.47
1:C:2843:GLU:OE1	1:C:2887:ARG:NH2	2.47	0.47
1:C:3729:GLN:NE2	1:C:3767:LEU:O	2.47	0.47
1:D:2843:GLU:OE1	1:D:2887:ARG:NH2	2.47	0.47
1:A:298:ARG:HA	1:A:305:TYR:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:LEU:HD22	1:A:822:CYS:HB3	1.96	0.47
1:A:3748:SER:HB2	1:A:3751:GLU:HB2	1.96	0.47
1:B:165:ALA:HB3	1:B:211:LEU:HD21	1.96	0.47
1:D:678:MET:HG3	1:D:754:VAL:HG22	1.96	0.47
1:B:2857:LYS:HE3	1:B:2861:LEU:HD11	1.95	0.47
1:B:3875:THR:HG21	1:B:3924:TYR:HE2	1.79	0.47
1:C:1716:THR:HA	1:C:1719:LEU:HD12	1.95	0.47
1:C:1931:ASP:O	1:C:3614:ARG:NH1	2.42	0.47
1:C:3952:PHE:HZ	1:C:3975:LEU:HD22	1.78	0.47
1:C:4931:GLU:OE2	1:C:4942:TRP:NE1	2.47	0.47
1:B:4046:LYS:HG3	1:B:4068:LEU:HD22	1.96	0.47
1:C:3875:THR:HG21	1:C:3924:TYR:HE2	1.79	0.47
1:D:718:VAL:HA	1:D:736:CYS:HB2	1.96	0.47
1:D:3748:SER:HB2	1:D:3751:GLU:HB2	1.96	0.47
1:D:4931:GLU:OE2	1:D:4942:TRP:NE1	2.46	0.47
1:A:718:VAL:HA	1:A:736:CYS:HB2	1.96	0.47
1:A:3742:LEU:HD23	1:A:3781:TYR:HB3	1.95	0.47
1:B:128:MET:HB3	1:B:149:LEU:HB3	1.96	0.47
1:B:4733:GLY:HA3	1:B:4740:PHE:CD1	2.50	0.47
1:C:165:ALA:HB3	1:C:211:LEU:HD21	1.96	0.47
1:C:3879:LEU:HD13	1:C:3921:LEU:HD12	1.96	0.47
1:C:4189:LEU:HA	1:C:4192:ASN:HD22	1.79	0.47
1:D:298:ARG:HA	1:D:305:TYR:HA	1.95	0.47
1:B:718:VAL:HA	1:B:736:CYS:HB2	1.97	0.47
1:B:2843:GLU:OE1	1:B:2887:ARG:NH2	2.47	0.47
1:C:25:THR:HB	1:C:32:GLN:HB3	1.97	0.47
1:C:1654:HIS:O	1:C:1657:THR:OG1	2.28	0.47
1:C:1707:ILE:HA	1:C:1711:LEU:HB2	1.96	0.47
1:C:2528:LEU:HD11	1:C:2568:ASP:HA	1.97	0.47
1:D:1121:GLY:O	1:D:1133:ARG:NH1	2.43	0.47
1:A:260:VAL:HG12	1:A:391:ALA:HB3	1.97	0.47
1:A:290:ARG:HH22	1:A:343:ARG:HG3	1.79	0.47
1:A:598:ILE:HD13	1:A:636:LEU:HB2	1.96	0.47
1:A:1132:GLU:HG2	1:A:1133:ARG:HG3	1.97	0.47
1:A:1611:ILE:N	1:A:1620:GLN:O	2.43	0.47
1:A:1664:VAL:HG12	1:A:1672:VAL:HG11	1.97	0.47
1:C:4796:LYS:NZ	1:C:4807:CYS:SG	2.82	0.47
1:D:25:THR:HB	1:D:32:GLN:HB3	1.97	0.47
1:D:260:VAL:HG12	1:D:391:ALA:HB3	1.97	0.47
1:B:1244:ASN:HD22	1:B:1801:GLU:HG2	1.79	0.47
1:B:2213:LYS:HA	1:B:2254:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:ARG:HA	1:C:305:TYR:HA	1.95	0.47
1:C:718:VAL:HA	1:C:736:CYS:HB2	1.97	0.47
1:C:804:LEU:HD22	1:C:822:CYS:HB3	1.97	0.47
1:C:4046:LYS:HG3	1:C:4068:LEU:HD22	1.96	0.47
1:D:165:ALA:HB3	1:D:211:LEU:HD21	1.96	0.47
1:D:3797:LEU:O	1:D:3800:SER:OG	2.32	0.47
1:B:207:PHE:CE2	1:C:2326:ILE:HG21	2.50	0.47
1:B:4931:GLU:OE2	1:B:4942:TRP:NE1	2.46	0.47
1:C:1726:ILE:HB	1:C:2109:ILE:HD11	1.97	0.47
1:C:1833:ILE:HG22	1:C:1834:PHE:H	1.79	0.47
1:D:1132:GLU:HG2	1:D:1133:ARG:HG3	1.97	0.47
1:D:1432:ILE:HD13	1:D:1441:VAL:HG21	1.97	0.47
1:D:1611:ILE:N	1:D:1620:GLN:O	2.43	0.47
1:D:3952:PHE:HZ	1:D:3975:LEU:HD22	1.80	0.47
1:D:4733:GLY:HA3	1:D:4740:PHE:CD1	2.50	0.47
1:A:1692:LYS:HA	1:A:1810:VAL:HG13	1.98	0.47
1:A:1707:ILE:HA	1:A:1711:LEU:HB2	1.96	0.47
1:A:2213:LYS:HA	1:A:2254:LEU:HD21	1.96	0.47
1:A:2390:MET:HG3	1:A:2465:HIS:CE1	2.50	0.47
1:A:4046:LYS:HG3	1:A:4068:LEU:HD22	1.96	0.47
1:B:260:VAL:HG12	1:B:391:ALA:HB3	1.96	0.47
1:B:559:ILE:HA	1:B:562:LEU:HB2	1.98	0.47
1:C:260:VAL:HG12	1:C:391:ALA:HB3	1.97	0.47
1:D:650:ASN:ND2	1:D:795:SER:O	2.47	0.47
1:D:1172:THR:HG21	1:D:1190:LEU:HD13	1.97	0.47
1:D:1833:ILE:HG22	1:D:1834:PHE:H	1.79	0.47
1:D:2264:GLU:OE2	1:D:2268:ARG:NH2	2.47	0.47
1:D:4046:LYS:HG3	1:D:4068:LEU:HD22	1.96	0.47
1:A:207:PHE:CE2	1:B:2326:ILE:HG21	2.51	0.46
1:A:1833:ILE:HG22	1:A:1834:PHE:H	1.79	0.46
1:A:2528:LEU:HD11	1:A:2568:ASP:HA	1.97	0.46
1:A:4610:LYS:O	1:A:4615:GLY:N	2.46	0.46
1:B:802:PHE:HB2	1:B:1617:TRP:HB2	1.97	0.46
1:B:804:LEU:HD22	1:B:822:CYS:HB3	1.96	0.46
1:B:1707:ILE:HA	1:B:1711:LEU:HB2	1.96	0.46
1:B:3879:LEU:HD13	1:B:3921:LEU:HD12	1.96	0.46
1:D:170:SER:OG	1:D:171:GLU:N	2.49	0.46
1:D:1244:ASN:HD22	1:D:1801:GLU:HG2	1.79	0.46
1:D:4170:LYS:HE2	1:D:4916:LEU:CD2	2.45	0.46
1:A:314:LEU:HB2	1:A:393:MET:HG2	1.98	0.46
1:A:1219:LYS:NZ	1:A:1244:ASN:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4733:GLY:HA3	1:A:4740:PHE:CD1	2.50	0.46
1:B:4794:TYR:HB3	1:B:4807:CYS:HB2	1.97	0.46
1:C:2390:MET:HG3	1:C:2465:HIS:CE1	2.50	0.46
1:C:3748:SER:HB2	1:C:3751:GLU:HB2	1.97	0.46
1:B:25:THR:HB	1:B:32:GLN:HB3	1.97	0.46
1:B:1833:ILE:HG22	1:B:1834:PHE:H	1.79	0.46
1:B:2773:ARG:HA	1:B:2776:ILE:HD12	1.97	0.46
1:C:1132:GLU:HG2	1:C:1133:ARG:HG3	1.97	0.46
1:C:4018:PHE:O	1:C:4022:LEU:N	2.40	0.46
1:C:4733:GLY:HA3	1:C:4740:PHE:CD1	2.50	0.46
1:A:25:THR:HB	1:A:32:GLN:HB3	1.97	0.46
1:A:2773:ARG:HA	1:A:2776:ILE:HD12	1.97	0.46
1:B:1172:THR:HG21	1:B:1190:LEU:HD13	1.96	0.46
1:B:2390:MET:HG3	1:B:2465:HIS:CE1	2.51	0.46
1:C:180:ASP:HB3	1:C:211:LEU:HD22	1.98	0.46
1:C:1172:THR:HG21	1:C:1190:LEU:HD13	1.96	0.46
1:D:14:LEU:HD12	1:D:175:VAL:HG12	1.97	0.46
1:D:1707:ILE:HA	1:D:1711:LEU:HB2	1.96	0.46
1:D:2390:MET:HG3	1:D:2465:HIS:CE1	2.50	0.46
1:A:165:ALA:HB3	1:A:211:LEU:HD21	1.97	0.46
1:A:3904:GLN:NE2	1:A:3965:GLN:OE1	2.47	0.46
1:A:4018:PHE:O	1:A:4022:LEU:N	2.40	0.46
1:B:1692:LYS:HA	1:B:1810:VAL:HG13	1.98	0.46
1:C:20:VAL:HG12	1:C:216:PRO:HA	1.97	0.46
1:C:170:SER:OG	1:C:171:GLU:N	2.48	0.46
1:C:2264:GLU:OE2	1:C:2268:ARG:NH2	2.48	0.46
1:D:649:VAL:HG21	1:D:713:TRP:HB3	1.98	0.46
1:D:2773:ARG:HA	1:D:2776:ILE:HD12	1.98	0.46
1:A:1172:THR:HG21	1:A:1190:LEU:HD13	1.97	0.46
1:B:1165:MET:HB2	1:B:1174:MET:HB2	1.98	0.46
1:B:1219:LYS:H	1:B:1240:ALA:HB3	1.80	0.46
1:B:2264:GLU:OE2	1:B:2268:ARG:NH2	2.47	0.46
1:B:2897:LEU:HB3	1:B:2904:VAL:HG21	1.98	0.46
1:B:4052:ALA:O	1:B:4056:HIS:ND1	2.48	0.46
1:B:4640:SER:OG	1:B:4703:ASP:OD2	2.30	0.46
1:B:4796:LYS:NZ	1:B:4807:CYS:SG	2.82	0.46
1:C:290:ARG:HH22	1:C:343:ARG:HG3	1.81	0.46
1:D:686:VAL:O	1:D:687:THR:OG1	2.33	0.46
1:D:804:LEU:HD22	1:D:822:CYS:HB3	1.97	0.46
1:A:3875:THR:HG21	1:A:3924:TYR:HE2	1.81	0.46
1:B:1432:ILE:HD13	1:B:1441:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1449:ASP:N	1:B:1449:ASP:OD1	2.49	0.46
1:B:1689:ILE:HA	1:B:1703:TYR:HE1	1.81	0.46
1:C:695:VAL:HG21	1:C:755:ILE:HD13	1.98	0.46
1:C:4616:LEU:HA	1:C:4620:GLU:HB2	1.98	0.46
1:D:695:VAL:HG21	1:D:755:ILE:HD13	1.98	0.46
1:D:717:GLY:O	1:D:736:CYS:N	2.45	0.46
1:A:650:ASN:ND2	1:A:795:SER:O	2.48	0.46
1:A:1165:MET:HB2	1:A:1174:MET:HB2	1.97	0.46
1:A:1258:PHE:HB3	1:A:1303:ARG:NH2	2.31	0.46
1:A:4171:ARG:HH11	1:A:4752:LYS:CD	2.23	0.46
1:B:14:LEU:HD12	1:B:175:VAL:HG12	1.98	0.46
1:B:20:VAL:HG12	1:B:216:PRO:HA	1.97	0.46
1:B:1938:GLN:HE22	1:B:3614:ARG:HA	1.81	0.46
1:B:2528:LEU:HD11	1:B:2568:ASP:HA	1.97	0.46
1:C:3904:GLN:NE2	1:C:3965:GLN:OE1	2.48	0.46
1:D:20:VAL:HG12	1:D:216:PRO:HA	1.98	0.46
1:A:2897:LEU:HB3	1:A:2904:VAL:HG21	1.98	0.46
1:B:650:ASN:ND2	1:B:795:SER:O	2.48	0.46
1:B:3794:LEU:HA	1:B:3797:LEU:HD12	1.97	0.46
1:C:1091:GLU:HA	1:C:1250:TRP:CZ3	2.51	0.46
1:D:238:HIS:HB3	1:D:243:GLU:HB3	1.98	0.46
1:D:1219:LYS:NZ	1:D:1244:ASN:O	2.49	0.46
1:D:3919:ASN:O	1:D:3922:THR:OG1	2.32	0.46
1:D:4018:PHE:O	1:D:4022:LEU:N	2.40	0.46
1:A:1219:LYS:H	1:A:1240:ALA:HB3	1.81	0.46
1:A:3952:PHE:HZ	1:A:3975:LEU:HD22	1.81	0.46
1:B:1132:GLU:HG2	1:B:1133:ARG:HG3	1.97	0.46
1:B:4018:PHE:O	1:B:4022:LEU:N	2.40	0.46
1:C:1219:LYS:H	1:C:1240:ALA:HB3	1.81	0.46
1:C:1449:ASP:OD1	1:C:1449:ASP:N	2.49	0.46
1:C:1664:VAL:HG12	1:C:1672:VAL:HG11	1.97	0.46
1:C:4794:TYR:HB3	1:C:4807:CYS:HB2	1.97	0.46
1:D:1219:LYS:H	1:D:1240:ALA:HB3	1.81	0.46
1:D:2897:LEU:HB3	1:D:2904:VAL:HG21	1.98	0.46
1:A:14:LEU:HD12	1:A:175:VAL:HG12	1.97	0.45
1:A:649:VAL:HG21	1:A:713:TRP:HB3	1.98	0.45
1:A:686:VAL:O	1:A:687:THR:OG1	2.33	0.45
1:B:449:ILE:HG13	1:B:522:ALA:HB1	1.98	0.45
1:B:1091:GLU:HA	1:B:1250:TRP:CZ3	2.51	0.45
1:B:3748:SER:HB2	1:B:3751:GLU:HB2	1.97	0.45
1:B:3952:PHE:HZ	1:B:3975:LEU:HD22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4610:LYS:O	1:B:4615:GLY:N	2.46	0.45
1:C:3794:LEU:HA	1:C:3797:LEU:HD12	1.98	0.45
1:D:954:ASP:HB3	1:D:1061:GLY:HA3	1.98	0.45
1:D:1258:PHE:HB3	1:D:1303:ARG:NH2	2.32	0.45
1:D:1938:GLN:HE22	1:D:3614:ARG:HA	1.81	0.45
1:A:1432:ILE:HD13	1:A:1441:VAL:HG21	1.98	0.45
1:A:4616:LEU:HA	1:A:4620:GLU:HB2	1.99	0.45
1:B:1611:ILE:HB	1:B:1620:GLN:HB3	1.98	0.45
1:C:23:GLN:HA	1:C:36:CYS:HA	1.99	0.45
1:C:1570:LEU:HD13	1:C:1584:PRO:HG3	1.98	0.45
1:C:1611:ILE:N	1:C:1620:GLN:O	2.44	0.45
1:C:4130:PHE:O	1:C:4134:LEU:N	2.50	0.45
1:D:3875:THR:HG21	1:D:3924:TYR:HE2	1.81	0.45
1:A:1570:LEU:HD13	1:A:1584:PRO:HG3	1.98	0.45
1:A:4757:ILE:HG21	1:A:4757:ILE:HD13	1.71	0.45
1:B:180:ASP:HB3	1:B:211:LEU:HD22	1.98	0.45
1:B:480:ARG:NH2	1:B:3677:LEU:O	2.50	0.45
1:C:14:LEU:HD12	1:C:175:VAL:HG12	1.97	0.45
1:C:234:LEU:HD13	1:C:405:LEU:HD22	1.98	0.45
1:C:238:HIS:HB3	1:C:243:GLU:HB3	1.98	0.45
1:C:954:ASP:HB3	1:C:1061:GLY:HA3	1.99	0.45
1:C:1089:ARG:HH21	1:C:1600:PRO:HG3	1.81	0.45
1:C:1219:LYS:NZ	1:C:1244:ASN:O	2.49	0.45
1:C:1689:ILE:HA	1:C:1703:TYR:HE1	1.81	0.45
1:A:954:ASP:HB3	1:A:1061:GLY:HA3	1.98	0.45
1:A:3794:LEU:HA	1:A:3797:LEU:HD12	1.98	0.45
1:C:207:PHE:CE2	1:D:2326:ILE:HG21	2.51	0.45
1:C:433:LEU:HD21	1:C:505:LEU:HG	1.99	0.45
1:C:2773:ARG:HA	1:C:2776:ILE:HD12	1.98	0.45
1:D:472:HIS:CE1	1:D:3674:ARG:HB2	2.52	0.45
1:D:2436:VAL:HG21	1:D:2469:MET:HE3	1.98	0.45
1:A:20:VAL:HG12	1:A:216:PRO:HA	1.97	0.45
1:A:472:HIS:CE1	1:A:3674:ARG:HB2	2.52	0.45
1:A:802:PHE:HB2	1:A:1617:TRP:HB2	1.97	0.45
1:A:1611:ILE:HB	1:A:1620:GLN:HB3	1.99	0.45
1:C:1432:ILE:HD13	1:C:1441:VAL:HG21	1.97	0.45
1:C:1899:LEU:O	1:C:1904:LYS:NZ	2.37	0.45
1:D:1664:VAL:HG12	1:D:1672:VAL:HG11	1.98	0.45
1:A:23:GLN:HA	1:A:36:CYS:HA	1.98	0.45
1:A:1244:ASN:HD22	1:A:1801:GLU:HG2	1.79	0.45
1:A:2264:GLU:OE2	1:A:2268:ARG:NH2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3919:ASN:O	1:A:3922:THR:OG1	2.32	0.45
1:B:170:SER:OG	1:B:171:GLU:N	2.48	0.45
1:B:472:HIS:CE1	1:B:3674:ARG:HB2	2.51	0.45
1:B:1219:LYS:NZ	1:B:1244:ASN:O	2.49	0.45
1:B:1258:PHE:HB3	1:B:1303:ARG:NH2	2.32	0.45
1:B:1570:LEU:HD13	1:B:1584:PRO:HG3	1.98	0.45
1:B:1931:ASP:O	1:B:3614:ARG:NH1	2.41	0.45
1:C:248:PRO:HG2	1:C:257:ARG:HA	1.98	0.45
1:C:472:HIS:CE1	1:C:3674:ARG:HB2	2.51	0.45
1:C:1165:MET:HB2	1:C:1174:MET:HB2	1.98	0.45
1:C:2436:VAL:HG21	1:C:2469:MET:HE3	1.97	0.45
1:C:3696:MET:O	1:C:3699:SER:OG	2.32	0.45
1:D:23:GLN:HA	1:D:36:CYS:HA	1.99	0.45
1:D:737:ILE:HG22	1:D:739:ARG:HG3	1.99	0.45
1:D:1091:GLU:HA	1:D:1250:TRP:CZ3	2.52	0.45
1:D:1689:ILE:HA	1:D:1703:TYR:HE1	1.81	0.45
1:D:3794:LEU:HA	1:D:3797:LEU:HD12	1.99	0.45
1:D:4196:ASP:O	1:D:4200:GLU:N	2.49	0.45
1:A:1938:GLN:HE22	1:A:3614:ARG:HA	1.82	0.45
1:B:23:GLN:HA	1:B:36:CYS:HA	1.98	0.45
1:B:262:TYR:N	1:B:389:ARG:O	2.49	0.45
1:C:2897:LEU:HB3	1:C:2904:VAL:HG21	1.98	0.45
1:C:3729:GLN:O	1:C:3733:HIS:ND1	2.47	0.45
1:D:480:ARG:NH2	1:D:3677:LEU:O	2.49	0.45
1:D:1174:MET:SD	1:D:1236:TYR:OH	2.74	0.45
1:D:1469:LEU:HG	1:D:1480:ILE:HD11	1.98	0.45
1:D:1726:ILE:HB	1:D:2109:ILE:HD11	1.99	0.45
1:D:3729:GLN:O	1:D:3733:HIS:ND1	2.47	0.45
1:B:248:PRO:HG2	1:B:257:ARG:HA	1.99	0.45
1:B:3919:ASN:O	1:B:3922:THR:OG1	2.32	0.45
1:C:559:ILE:HA	1:C:562:LEU:HB2	1.99	0.45
1:D:1449:ASP:N	1:D:1449:ASP:OD1	2.49	0.45
1:D:4616:LEU:HA	1:D:4620:GLU:HB2	1.99	0.45
1:D:4851:PHE:O	1:D:4855:VAL:HB	2.17	0.45
1:A:1091:GLU:HA	1:A:1250:TRP:CZ3	2.52	0.45
1:A:1689:ILE:HA	1:A:1703:TYR:HE1	1.81	0.45
1:A:1726:ILE:HB	1:A:2109:ILE:HD11	1.99	0.45
1:A:3737:ALA:O	1:A:3740:MET:HG2	2.17	0.45
1:A:4904:HIS:NE2	1:A:4907:GLU:OE1	2.50	0.45
1:B:4616:LEU:HA	1:B:4620:GLU:HB2	1.99	0.45
1:C:480:ARG:NH2	1:C:3677:LEU:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1699:ARG:NH1	1:C:1816:PHE:O	2.48	0.45
1:C:3737:ALA:O	1:C:3740:MET:HG2	2.17	0.45
1:A:217:ILE:HG23	1:A:285:SER:HB3	1.99	0.45
1:A:480:ARG:NH2	1:A:3677:LEU:O	2.49	0.45
1:A:559:ILE:HA	1:A:562:LEU:HB2	1.99	0.45
1:A:1087:ILE:HG23	1:A:1128:LEU:HD12	1.98	0.45
1:A:1640:ASP:OD1	1:A:1640:ASP:N	2.49	0.45
1:A:4060:THR:OG1	1:A:4063:GLU:OE1	2.26	0.45
1:B:532:SER:HA	1:B:535:GLU:HB2	1.99	0.45
1:B:3904:GLN:NE2	1:B:3965:GLN:OE1	2.48	0.45
1:B:4904:HIS:NE2	1:B:4907:GLU:OE1	2.50	0.45
1:C:314:LEU:HB2	1:C:393:MET:HG2	1.98	0.45
1:C:649:VAL:HG21	1:C:713:TRP:HB3	1.98	0.45
1:C:1258:PHE:HB3	1:C:1303:ARG:NH2	2.32	0.45
1:C:1736:ILE:HG23	1:C:1753:LEU:HD12	1.99	0.45
1:D:290:ARG:HH22	1:D:343:ARG:HG3	1.81	0.45
1:D:709:GLY:O	1:D:1253:LYS:NZ	2.50	0.45
1:D:802:PHE:HB2	1:D:1617:TRP:HB2	1.98	0.45
1:D:1165:MET:HB2	1:D:1174:MET:HB2	1.98	0.45
1:D:1570:LEU:HD13	1:D:1584:PRO:HG3	1.98	0.45
1:A:433:LEU:HD21	1:A:505:LEU:HG	1.98	0.44
1:A:449:ILE:HG13	1:A:522:ALA:HB1	1.98	0.44
1:A:2326:ILE:HG21	1:D:207:PHE:CE2	2.52	0.44
1:B:16:THR:HB	1:B:110:HIS:HA	1.99	0.44
1:D:1699:ARG:NH1	1:D:1816:PHE:O	2.48	0.44
1:D:1926:ILE:HD11	1:D:3625:TYR:CE2	2.53	0.44
1:D:3737:ALA:O	1:D:3740:MET:HG2	2.17	0.44
1:A:248:PRO:HG2	1:A:257:ARG:HA	1.98	0.44
1:A:4052:ALA:O	1:A:4056:HIS:ND1	2.48	0.44
1:A:4832:ILE:HG21	1:A:4844:ARG:NH2	2.30	0.44
1:B:4892:CYS:SG	1:B:4909:HIS:NE2	2.80	0.44
1:C:510:SER:O	1:C:520:ARG:NH2	2.51	0.44
1:C:802:PHE:HB2	1:C:1617:TRP:HB2	1.99	0.44
1:C:1613:GLU:HB2	1:C:1618:LEU:H	1.82	0.44
1:C:4196:ASP:O	1:C:4200:GLU:N	2.49	0.44
1:C:4904:HIS:NE2	1:C:4907:GLU:OE1	2.50	0.44
1:D:234:LEU:HD13	1:D:405:LEU:HD22	1.98	0.44
1:D:248:PRO:HG2	1:D:257:ARG:HA	1.98	0.44
1:D:532:SER:HA	1:D:535:GLU:HB2	1.99	0.44
1:A:238:HIS:HB3	1:A:243:GLU:HB3	1.98	0.44
1:A:1174:MET:SD	1:A:1236:TYR:OH	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4153:ILE:HD13	1:A:4158:ARG:HH11	1.82	0.44
1:A:4196:ASP:O	1:A:4200:GLU:N	2.49	0.44
1:B:234:LEU:HD13	1:B:405:LEU:HD22	2.00	0.44
1:B:954:ASP:HB3	1:B:1061:GLY:HA3	1.99	0.44
1:C:16:THR:HB	1:C:110:HIS:HA	2.00	0.44
1:C:737:ILE:HG22	1:C:739:ARG:HG3	2.00	0.44
1:C:1611:ILE:HB	1:C:1620:GLN:HB3	1.99	0.44
1:C:3919:ASN:O	1:C:3922:THR:OG1	2.32	0.44
1:D:449:ILE:HG13	1:D:522:ALA:HB1	1.99	0.44
1:D:4153:ILE:HD13	1:D:4158:ARG:HH11	1.83	0.44
1:D:4904:HIS:NE2	1:D:4907:GLU:OE1	2.50	0.44
1:A:262:TYR:N	1:A:389:ARG:O	2.49	0.44
1:A:555:LEU:HD13	1:A:585:ALA:HB1	1.99	0.44
1:A:1736:ILE:HG23	1:A:1753:LEU:HD12	1.99	0.44
1:A:1931:ASP:O	1:A:3614:ARG:NH1	2.42	0.44
1:A:3729:GLN:O	1:A:3733:HIS:ND1	2.48	0.44
1:B:305:TYR:HE1	1:B:319:LYS:HG2	1.83	0.44
1:B:590:LYS:HB2	1:B:593:HIS:HD2	1.82	0.44
1:B:1089:ARG:HH21	1:B:1600:PRO:HG3	1.83	0.44
1:B:4130:PHE:O	1:B:4134:LEU:N	2.50	0.44
1:B:4153:ILE:HD13	1:B:4158:ARG:HH11	1.82	0.44
1:C:262:TYR:N	1:C:389:ARG:O	2.49	0.44
1:C:591:GLU:HA	1:C:631:LEU:HD21	1.99	0.44
1:D:555:LEU:HD13	1:D:585:ALA:HB1	1.99	0.44
1:D:3904:GLN:NE2	1:D:3965:GLN:OE1	2.48	0.44
1:D:4130:PHE:O	1:D:4134:LEU:N	2.50	0.44
1:A:695:VAL:HG21	1:A:755:ILE:HD13	1.99	0.44
1:A:1469:LEU:HG	1:A:1480:ILE:HD11	1.98	0.44
1:A:3893:TYR:CE2	1:A:3899:ILE:HG23	2.53	0.44
1:A:4130:PHE:O	1:A:4134:LEU:N	2.50	0.44
1:A:4817:HIS:O	1:A:4822:VAL:N	2.45	0.44
1:B:150:GLN:NE2	1:B:158:CYS:SG	2.72	0.44
1:B:314:LEU:HB2	1:B:393:MET:HG2	1.98	0.44
1:B:510:SER:O	1:B:520:ARG:NH2	2.50	0.44
1:D:217:ILE:HG23	1:D:285:SER:HB3	1.99	0.44
1:D:4804:ASP:OD1	1:D:4804:ASP:N	2.50	0.44
1:A:299:HIS:CD2	1:A:301:THR:HG1	2.34	0.44
1:A:510:SER:O	1:A:520:ARG:NH2	2.51	0.44
1:A:1219:LYS:N	1:A:1240:ALA:HB3	2.33	0.44
1:A:3642:ILE:HD12	1:A:3642:ILE:HG23	1.79	0.44
1:B:433:LEU:HD21	1:B:505:LEU:HG	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:LEU:HG	1:B:604:HIS:CE1	2.53	0.44
1:B:3696:MET:O	1:B:3699:SER:OG	2.32	0.44
1:B:3936:LEU:HD21	1:B:3941:LEU:HD13	1.99	0.44
1:B:4752:LYS:HG2	1:B:4755:ARG:HH21	1.83	0.44
1:C:1174:MET:SD	1:C:1236:TYR:OH	2.74	0.44
1:D:30:LYS:HB2	1:D:30:LYS:HE3	1.82	0.44
1:A:16:THR:HB	1:A:110:HIS:HA	1.99	0.44
1:A:565:LEU:HD23	1:A:1588:VAL:HG23	1.99	0.44
1:A:1272:ARG:HH12	1:A:1588:VAL:HA	1.83	0.44
1:A:2436:VAL:HG21	1:A:2469:MET:HE3	1.99	0.44
1:A:3921:LEU:HD23	1:A:3921:LEU:HA	1.78	0.44
1:B:236:LEU:HD23	1:B:245:LEU:HD22	2.00	0.44
1:B:238:HIS:HB3	1:B:243:GLU:HB3	1.99	0.44
1:B:695:VAL:HG21	1:B:755:ILE:HD13	1.99	0.44
1:B:1753:LEU:HD23	1:B:1753:LEU:HA	1.84	0.44
1:B:3737:ALA:O	1:B:3740:MET:HG2	2.17	0.44
1:C:305:TYR:HE1	1:C:319:LYS:HG2	1.83	0.44
1:D:433:LEU:HD21	1:D:505:LEU:HG	1.99	0.44
1:A:4804:ASP:N	1:A:4804:ASP:OD1	2.50	0.44
1:B:1219:LYS:N	1:B:1240:ALA:HB3	2.33	0.44
1:B:4862:ILE:O	1:B:4866:LEU:N	2.50	0.44
1:C:1899:LEU:HD23	1:C:1903:VAL:HG12	2.00	0.44
1:C:4052:ALA:O	1:C:4056:HIS:ND1	2.48	0.44
1:C:4851:PHE:O	1:C:4855:VAL:HB	2.18	0.44
1:D:180:ASP:HB3	1:D:211:LEU:HD22	1.98	0.44
1:D:510:SER:O	1:D:520:ARG:NH2	2.51	0.44
1:D:1219:LYS:N	1:D:1240:ALA:HB3	2.33	0.44
1:D:3893:TYR:CE2	1:D:3899:ILE:HG23	2.53	0.44
1:A:1926:ILE:HD11	1:A:3625:TYR:CE2	2.52	0.44
1:B:464:HIS:HA	1:B:465:PRO:HD3	1.86	0.44
1:B:591:GLU:HA	1:B:631:LEU:HD21	1.99	0.44
1:B:709:GLY:O	1:B:1253:LYS:NZ	2.51	0.44
1:B:1613:GLU:HB2	1:B:1618:LEU:H	1.82	0.44
1:B:2301:ASP:OD1	1:B:2304:ARG:NH2	2.51	0.44
1:B:3642:ILE:HD12	1:B:3642:ILE:HG23	1.78	0.44
1:C:709:GLY:O	1:C:1253:LYS:NZ	2.50	0.44
1:C:1087:ILE:HG23	1:C:1128:LEU:HD12	1.98	0.44
1:C:2770:GLU:HA	1:C:2773:ARG:HB2	2.00	0.44
1:C:4153:ILE:HD13	1:C:4158:ARG:HH11	1.82	0.44
1:C:4862:ILE:O	1:C:4866:LEU:N	2.50	0.44
1:D:314:LEU:HB2	1:D:393:MET:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1087:ILE:HG23	1:D:1128:LEU:HD12	1.99	0.44
1:A:1089:ARG:HH21	1:A:1600:PRO:HG3	1.83	0.43
1:A:1613:GLU:HB2	1:A:1618:LEU:H	1.82	0.43
1:B:649:VAL:HG21	1:B:713:TRP:HB3	1.98	0.43
1:B:1736:ILE:HG23	1:B:1753:LEU:HD12	1.99	0.43
1:C:565:LEU:HD23	1:C:1588:VAL:HG23	2.00	0.43
1:C:565:LEU:HG	1:C:604:HIS:CE1	2.53	0.43
1:D:1611:ILE:HB	1:D:1620:GLN:HB3	1.99	0.43
1:D:2738:LEU:HD22	1:D:2819:ALA:HB3	2.00	0.43
1:A:305:TYR:HE1	1:A:319:LYS:HG2	1.83	0.43
1:A:2770:GLU:HA	1:A:2773:ARG:HB2	2.00	0.43
1:B:565:LEU:HD23	1:B:1588:VAL:HG23	1.99	0.43
1:B:1170:GLU:O	1:B:1172:THR:N	2.51	0.43
1:B:1699:ARG:HH22	1:B:1821:LEU:HD11	1.83	0.43
1:B:4187:MET:SD	1:B:4187:MET:N	2.91	0.43
1:C:1219:LYS:N	1:C:1240:ALA:HB3	2.33	0.43
1:C:2738:LEU:HD22	1:C:2819:ALA:HB3	2.00	0.43
1:C:2887:ARG:O	1:C:2891:GLN:N	2.49	0.43
1:D:305:TYR:HE1	1:D:319:LYS:HG2	1.83	0.43
1:D:1089:ARG:HH21	1:D:1600:PRO:HG3	1.82	0.43
1:D:1736:ILE:HG23	1:D:1753:LEU:HD12	1.99	0.43
1:A:234:LEU:HD13	1:A:405:LEU:HD22	1.99	0.43
1:A:3936:LEU:HD21	1:A:3941:LEU:HD13	1.99	0.43
1:B:1899:LEU:HD23	1:B:1903:VAL:HG12	2.00	0.43
1:C:1469:LEU:HG	1:C:1480:ILE:HD11	1.99	0.43
1:D:1613:GLU:HB2	1:D:1618:LEU:H	1.83	0.43
1:A:532:SER:HA	1:A:535:GLU:HB2	1.99	0.43
1:A:565:LEU:HG	1:A:604:HIS:CE1	2.53	0.43
1:B:4925:TYR:CZ	1:B:4929:LYS:HD2	2.54	0.43
1:C:4187:MET:SD	1:C:4187:MET:N	2.91	0.43
1:D:559:ILE:HA	1:D:562:LEU:HB2	2.00	0.43
1:D:1445:TRP:H	1:D:1487:MET:HB2	1.83	0.43
1:D:2435:GLY:O	1:D:2438:SER:OG	2.29	0.43
1:A:122:ARG:HE	1:A:127:GLY:HA2	1.83	0.43
1:A:180:ASP:HB3	1:A:211:LEU:HD22	2.00	0.43
1:A:1647:GLN:O	1:A:1651:LEU:N	2.52	0.43
1:A:2301:ASP:OD1	1:A:2304:ARG:NH2	2.51	0.43
1:A:4851:PHE:O	1:A:4855:VAL:HB	2.18	0.43
1:B:572:LEU:O	1:B:576:HIS:N	2.51	0.43
1:C:532:SER:HA	1:C:535:GLU:HB2	1.99	0.43
1:C:4804:ASP:N	1:C:4804:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4892:CYS:SG	1:C:4909:HIS:NE2	2.79	0.43
1:D:16:THR:HB	1:D:110:HIS:HA	2.00	0.43
1:D:4665:ASP:HA	1:D:4668:SER:HB2	2.00	0.43
1:A:464:HIS:HA	1:A:465:PRO:HD3	1.87	0.43
1:A:4862:ILE:O	1:A:4866:LEU:N	2.50	0.43
1:A:4925:TYR:CZ	1:A:4929:LYS:HD2	2.53	0.43
1:B:1104:GLU:HA	1:B:1163:GLY:HA2	2.00	0.43
1:B:1136:ALA:HB3	1:B:1145:TRP:HB2	2.01	0.43
1:B:1272:ARG:HH12	1:B:1588:VAL:HA	1.83	0.43
1:C:217:ILE:HG23	1:C:285:SER:HB3	2.00	0.43
1:C:679:VAL:HA	1:C:800:VAL:HG12	2.00	0.43
1:C:920:GLU:HG2	1:C:976:TYR:CE1	2.54	0.43
1:C:2301:ASP:OD1	1:C:2304:ARG:NH2	2.51	0.43
1:D:565:LEU:HD23	1:D:1588:VAL:HG23	2.00	0.43
1:D:679:VAL:HA	1:D:800:VAL:HG12	2.00	0.43
1:D:1899:LEU:HD23	1:D:1903:VAL:HG12	2.00	0.43
1:D:4862:ILE:O	1:D:4866:LEU:N	2.50	0.43
1:A:170:SER:OG	1:A:171:GLU:N	2.49	0.43
1:A:1699:ARG:HH22	1:A:1821:LEU:HD11	1.82	0.43
1:A:3891:TRP:CB	1:D:76:ARG:HD2	2.37	0.43
1:A:4892:CYS:SG	1:A:4909:HIS:NE2	2.80	0.43
1:B:119:ILE:HD13	1:B:162:ILE:HD11	2.01	0.43
1:C:590:LYS:HB2	1:C:593:HIS:HD2	1.83	0.43
1:C:1640:ASP:OD1	1:C:1640:ASP:N	2.49	0.43
1:C:1764:SER:N	1:C:1779:SER:O	2.51	0.43
1:C:1926:ILE:HD11	1:C:3625:TYR:CE2	2.54	0.43
1:D:1699:ARG:HH22	1:D:1821:LEU:HD11	1.83	0.43
1:A:590:LYS:HB2	1:A:593:HIS:HD2	1.83	0.43
1:A:717:GLY:O	1:A:736:CYS:N	2.45	0.43
1:A:1104:GLU:HA	1:A:1163:GLY:HA2	1.99	0.43
1:A:1753:LEU:HD23	1:A:1753:LEU:HA	1.85	0.43
1:A:4508:LEU:HD11	1:A:4747:ILE:HD12	2.00	0.43
1:B:217:ILE:HG23	1:B:285:SER:HB3	2.00	0.43
1:B:737:ILE:HG22	1:B:739:ARG:HG3	2.00	0.43
1:B:2436:VAL:HG21	1:B:2469:MET:HE3	2.00	0.43
1:B:2770:GLU:HA	1:B:2773:ARG:HB2	2.00	0.43
1:B:3729:GLN:O	1:B:3733:HIS:ND1	2.48	0.43
1:B:4851:PHE:O	1:B:4855:VAL:HB	2.18	0.43
1:C:449:ILE:HG13	1:C:522:ALA:HB1	1.99	0.43
1:C:473:GLU:OE2	1:C:477:ASN:ND2	2.50	0.43
1:C:1104:GLU:HA	1:C:1163:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4072:GLU:HB3	1:C:4074:ASP:HB2	2.01	0.43
1:C:4591:TYR:HE1	1:C:4595:LYS:HD2	1.84	0.43
1:D:565:LEU:HG	1:D:604:HIS:CE1	2.53	0.43
1:D:4187:MET:SD	1:D:4187:MET:N	2.91	0.43
1:A:1121:GLY:O	1:A:1133:ARG:NH1	2.43	0.43
1:B:1172:THR:HG22	1:B:1193:LYS:HG3	2.01	0.43
1:B:4804:ASP:OD1	1:B:4804:ASP:N	2.51	0.43
1:C:119:ILE:HD13	1:C:162:ILE:HD11	2.01	0.43
1:C:1647:GLN:O	1:C:1651:LEU:N	2.52	0.43
1:D:920:GLU:HG2	1:D:976:TYR:CE1	2.54	0.43
1:D:2301:ASP:OD1	1:D:2304:ARG:NH2	2.51	0.43
1:A:591:GLU:HA	1:A:631:LEU:HD21	2.00	0.43
1:B:1087:ILE:HG23	1:B:1128:LEU:HD12	1.99	0.43
1:B:1174:MET:SD	1:B:1236:TYR:OH	2.74	0.43
1:B:1727:VAL:HG11	1:B:1927:VAL:HG21	2.00	0.43
1:C:719:GLY:H	1:C:722:LEU:HD12	1.84	0.43
1:C:1170:GLU:O	1:C:1172:THR:N	2.52	0.43
1:C:1172:THR:HG22	1:C:1193:LYS:HG3	2.01	0.43
1:C:3893:TYR:CE2	1:C:3899:ILE:HG23	2.54	0.43
1:D:1272:ARG:HH12	1:D:1588:VAL:HA	1.83	0.43
1:D:3936:LEU:HD21	1:D:3941:LEU:HD13	2.00	0.43
1:D:4508:LEU:HD11	1:D:4747:ILE:HD12	2.01	0.43
1:A:832:LEU:HG	1:A:1617:TRP:HE1	1.83	0.42
1:A:1449:ASP:OD1	1:A:1449:ASP:N	2.49	0.42
1:A:4011:VAL:HG12	1:A:4015:LEU:HG	2.01	0.42
1:B:3893:TYR:CE2	1:B:3899:ILE:HG23	2.54	0.42
1:C:3988:GLU:HB2	1:C:4937:GLN:NE2	2.34	0.42
1:A:2738:LEU:HD22	1:A:2819:ALA:HB3	2.00	0.42
1:A:4187:MET:SD	1:A:4187:MET:N	2.92	0.42
1:B:247:VAL:O	1:B:272:ARG:NH1	2.46	0.42
1:B:717:GLY:O	1:B:736:CYS:N	2.45	0.42
1:B:1469:LEU:HG	1:B:1480:ILE:HD11	2.01	0.42
1:C:1272:ARG:HH12	1:C:1588:VAL:HA	1.83	0.42
1:C:1445:TRP:H	1:C:1487:MET:HB2	1.83	0.42
1:C:4665:ASP:HA	1:C:4668:SER:HB2	2.00	0.42
1:D:676:GLU:HB2	1:D:803:LEU:HB2	2.01	0.42
1:A:119:ILE:HD13	1:A:162:ILE:HD11	2.02	0.42
1:A:1136:ALA:HB3	1:A:1145:TRP:HB2	2.01	0.42
1:A:1300:MET:O	1:A:1545:ALA:N	2.44	0.42
1:B:122:ARG:HE	1:B:127:GLY:HA2	1.84	0.42
1:B:555:LEU:HD13	1:B:585:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:719:GLY:H	1:B:722:LEU:HD12	1.84	0.42
1:B:920:GLU:HG2	1:B:976:TYR:CE1	2.54	0.42
1:B:1094:TYR:OH	1:B:1808:ASP:OD1	2.37	0.42
1:B:2738:LEU:HD22	1:B:2819:ALA:HB3	2.01	0.42
1:B:3642:ILE:HG22	1:B:3731:ARG:HD3	2.01	0.42
1:B:4508:LEU:HD11	1:B:4747:ILE:HD12	2.01	0.42
1:C:1457:PHE:HD1	1:C:1488:VAL:HG21	1.84	0.42
1:C:1699:ARG:HH22	1:C:1821:LEU:HD11	1.83	0.42
1:D:832:LEU:HG	1:D:1617:TRP:HE1	1.84	0.42
1:D:3907:PHE:HD2	1:D:3968:LEU:HD11	1.85	0.42
1:A:150:GLN:NE2	1:A:158:CYS:SG	2.73	0.42
1:A:1727:VAL:HG11	1:A:1927:VAL:HG21	2.01	0.42
1:A:3955:MET:O	1:A:3959:LEU:N	2.48	0.42
1:B:308:LEU:N	1:B:326:SER:O	2.49	0.42
1:B:1926:ILE:HD11	1:B:3625:TYR:CE2	2.54	0.42
1:C:3642:ILE:HG22	1:C:3731:ARG:HD3	2.02	0.42
1:D:119:ILE:HD13	1:D:162:ILE:HD11	2.01	0.42
1:D:1647:GLN:O	1:D:1651:LEU:N	2.52	0.42
1:A:709:GLY:O	1:A:1253:LYS:NZ	2.51	0.42
1:B:679:VAL:HA	1:B:800:VAL:HG12	2.01	0.42
1:B:3718:LYS:O	1:B:3722:LYS:N	2.50	0.42
1:C:1136:ALA:HB3	1:C:1145:TRP:HB2	2.01	0.42
1:D:122:ARG:HE	1:D:127:GLY:HA2	1.84	0.42
1:D:4580:HIS:HB3	1:D:4740:PHE:HZ	1.84	0.42
1:D:4861:ALA:HA	1:D:4864:GLN:HB3	2.02	0.42
1:D:4925:TYR:CZ	1:D:4929:LYS:HD2	2.54	0.42
1:A:236:LEU:HD23	1:A:245:LEU:HD22	2.01	0.42
1:A:530:LEU:HD23	1:A:533:LEU:HD12	2.02	0.42
1:A:679:VAL:HA	1:A:800:VAL:HG12	2.01	0.42
1:A:1445:TRP:H	1:A:1487:MET:HB2	1.84	0.42
1:A:1899:LEU:HD23	1:A:1903:VAL:HG12	2.01	0.42
1:A:4864:GLN:HG3	1:D:4857:VAL:HG13	2.01	0.42
1:B:196:TYR:O	1:B:201:LEU:N	2.52	0.42
1:B:2884:ALA:HA	1:B:2887:ARG:HB3	2.02	0.42
1:B:4665:ASP:HA	1:B:4668:SER:HB2	2.00	0.42
1:C:555:LEU:HD13	1:C:585:ALA:HB1	2.00	0.42
1:C:1753:LEU:HD23	1:C:1753:LEU:HA	1.84	0.42
1:D:262:TYR:N	1:D:389:ARG:O	2.49	0.42
1:D:1104:GLU:HA	1:D:1163:GLY:HA2	1.99	0.42
1:D:1764:SER:N	1:D:1779:SER:O	2.52	0.42
1:A:30:LYS:HB2	1:A:30:LYS:HE3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:ILE:HG22	1:A:739:ARG:HG3	2.01	0.42
1:B:1699:ARG:NH1	1:B:1816:PHE:O	2.48	0.42
1:B:2587:GLN:O	1:B:2591:ARG:N	2.53	0.42
1:B:4207:ILE:O	1:B:4498:ARG:NH1	2.53	0.42
1:B:4580:HIS:HB3	1:B:4740:PHE:HZ	1.85	0.42
1:C:143:LEU:CD2	1:D:2426:SER:HB3	2.48	0.42
1:C:236:LEU:HD23	1:C:245:LEU:HD22	2.01	0.42
1:C:3921:LEU:HD23	1:C:3921:LEU:HA	1.79	0.42
1:C:4580:HIS:HB3	1:C:4740:PHE:HZ	1.85	0.42
1:D:196:TYR:O	1:D:201:LEU:N	2.53	0.42
1:D:238:HIS:N	1:D:243:GLU:O	2.53	0.42
1:D:591:GLU:HA	1:D:631:LEU:HD21	2.00	0.42
1:D:1505:LEU:HB2	1:D:1523:ASN:HA	2.02	0.42
1:D:4591:TYR:HE1	1:D:4595:LYS:HD2	1.85	0.42
1:A:4580:HIS:HB3	1:A:4740:PHE:HZ	1.84	0.42
1:A:4665:ASP:HA	1:A:4668:SER:HB2	2.01	0.42
1:B:4591:TYR:HE1	1:B:4595:LYS:HD2	1.84	0.42
1:C:4207:ILE:O	1:C:4498:ARG:NH1	2.53	0.42
1:D:1137:PHE:HD1	1:D:1144:ARG:HB3	1.85	0.42
1:A:191:TYR:N	1:A:206:ALA:O	2.48	0.42
1:A:1094:TYR:OH	1:A:1808:ASP:OD1	2.38	0.42
1:A:1172:THR:HG22	1:A:1193:LYS:HG3	2.01	0.42
1:A:2587:GLN:O	1:A:2591:ARG:N	2.53	0.42
1:A:4161:TRP:CZ2	1:A:4917:ALA:HB2	2.55	0.42
1:A:4591:TYR:CE1	1:A:4595:LYS:HB2	2.55	0.42
1:B:76:ARG:HD2	1:C:3891:TRP:CB	2.38	0.42
1:B:832:LEU:HG	1:B:1617:TRP:HE1	1.84	0.42
1:B:2143:MET:SD	1:B:2175:VAL:HG11	2.60	0.42
1:B:2796:GLY:HA2	1:B:2900:ASN:HA	2.02	0.42
1:B:4072:GLU:HB3	1:B:4074:ASP:HB2	2.02	0.42
1:C:717:GLY:O	1:C:736:CYS:N	2.45	0.42
1:C:2143:MET:SD	1:C:2175:VAL:HG11	2.60	0.42
1:D:727:PHE:N	1:D:749:LEU:HD13	2.35	0.42
1:D:2770:GLU:HA	1:D:2773:ARG:HB2	2.00	0.42
1:D:4052:ALA:O	1:D:4056:HIS:ND1	2.48	0.42
1:D:4072:GLU:HB3	1:D:4074:ASP:HB2	2.02	0.42
1:D:4640:SER:HB3	1:D:4643:ASN:HD21	1.85	0.42
1:A:626:ARG:HG2	1:A:1669:ASN:HD21	1.84	0.42
1:A:920:GLU:HG2	1:A:976:TYR:CE1	2.54	0.42
1:A:1799:VAL:HG22	1:A:1894:LEU:HD13	2.02	0.42
1:B:238:HIS:CE1	1:B:400:ASP:HB3	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1799:VAL:HG22	1:B:1894:LEU:HD13	2.02	0.42
1:B:4196:ASP:O	1:B:4200:GLU:N	2.49	0.42
1:B:4591:TYR:CE1	1:B:4595:LYS:HB2	2.55	0.42
1:C:196:TYR:O	1:C:201:LEU:N	2.52	0.42
1:C:3936:LEU:HD21	1:C:3941:LEU:HD13	2.00	0.42
1:D:465:PRO:HA	1:D:466:PRO:HD3	1.87	0.42
1:D:590:LYS:HB2	1:D:593:HIS:HD2	1.83	0.42
1:A:1090:ALA:HA	1:A:1249:MET:HG2	2.01	0.41
1:B:30:LYS:HE3	1:B:30:LYS:HB2	1.82	0.41
1:B:1764:SER:N	1:B:1779:SER:O	2.52	0.41
1:C:150:GLN:NE2	1:C:158:CYS:SG	2.72	0.41
1:C:644:LEU:HB2	1:C:1654:HIS:CD2	2.48	0.41
1:C:852:GLY:HA2	1:C:853:PRO:HA	1.82	0.41
1:C:3955:MET:O	1:C:3959:LEU:N	2.48	0.41
1:D:3718:LYS:O	1:D:3722:LYS:N	2.50	0.41
1:D:3988:GLU:HB2	1:D:4937:GLN:NE2	2.35	0.41
1:A:238:HIS:CE1	1:A:400:ASP:HB3	2.51	0.41
1:A:1137:PHE:HD1	1:A:1144:ARG:HB3	1.85	0.41
1:A:1752:GLY:HA3	1:A:1836:ASN:ND2	2.35	0.41
1:A:1764:SER:N	1:A:1779:SER:O	2.52	0.41
1:A:3988:GLU:HB2	1:A:4937:GLN:NE2	2.35	0.41
1:A:4640:SER:HB3	1:A:4643:ASN:HD21	1.85	0.41
1:C:191:TYR:N	1:C:206:ALA:O	2.48	0.41
1:C:1090:ALA:HB3	1:C:1203:PRO:HD2	2.03	0.41
1:C:2435:GLY:O	1:C:2438:SER:OG	2.29	0.41
1:C:3907:PHE:HD2	1:C:3968:LEU:HD11	1.84	0.41
1:D:488:LEU:HD23	1:D:488:LEU:HA	1.93	0.41
1:D:4161:TRP:CZ2	1:D:4917:ALA:HB2	2.55	0.41
1:A:238:HIS:N	1:A:243:GLU:O	2.53	0.41
1:A:719:GLY:H	1:A:722:LEU:HD12	1.84	0.41
1:A:727:PHE:N	1:A:749:LEU:HD13	2.36	0.41
1:A:1505:LEU:HB2	1:A:1523:ASN:HA	2.03	0.41
1:A:4591:TYR:HE1	1:A:4595:LYS:HD2	1.85	0.41
1:B:1445:TRP:H	1:B:1487:MET:HB2	1.85	0.41
1:B:2435:GLY:O	1:B:2438:SER:OG	2.29	0.41
1:C:572:LEU:O	1:C:576:HIS:N	2.52	0.41
1:C:4861:ALA:HA	1:C:4864:GLN:HB3	2.02	0.41
1:D:191:TYR:N	1:D:206:ALA:O	2.48	0.41
1:D:1136:ALA:HB3	1:D:1145:TRP:HB2	2.01	0.41
1:A:773:GLN:HA	1:A:774:PRO:HD3	1.93	0.41
1:A:2123:SER:OG	1:A:2149:ASP:OD2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2435:GLY:O	1:A:2438:SER:OG	2.29	0.41
1:A:3907:PHE:HD2	1:A:3968:LEU:HD11	1.86	0.41
1:A:4011:VAL:HA	1:A:4014:ILE:HG12	2.03	0.41
1:A:4207:ILE:O	1:A:4498:ARG:NH1	2.53	0.41
1:B:855:VAL:HG22	1:B:1209:VAL:HG12	2.02	0.41
1:B:4011:VAL:HG12	1:B:4015:LEU:HG	2.02	0.41
1:C:122:ARG:HE	1:C:127:GLY:HA2	1.84	0.41
1:C:1752:GLY:HA3	1:C:1836:ASN:ND2	2.36	0.41
1:C:4170:LYS:HE3	1:C:4916:LEU:CD2	2.49	0.41
1:C:4757:ILE:HD13	1:C:4757:ILE:HG21	1.69	0.41
1:D:236:LEU:HD23	1:D:245:LEU:HD22	2.01	0.41
1:D:719:GLY:H	1:D:722:LEU:HD12	1.84	0.41
1:D:1727:VAL:HG11	1:D:1927:VAL:HG21	2.01	0.41
1:D:4583:ILE:HD13	1:D:4583:ILE:HG21	1.81	0.41
1:A:196:TYR:O	1:A:201:LEU:N	2.53	0.41
1:A:4500:PHE:O	1:A:4504:ARG:N	2.52	0.41
1:B:717:GLY:H	1:B:722:LEU:HD13	1.85	0.41
1:B:727:PHE:N	1:B:749:LEU:HD13	2.36	0.41
1:B:1647:GLN:O	1:B:1651:LEU:N	2.52	0.41
1:B:1752:GLY:HA3	1:B:1836:ASN:ND2	2.35	0.41
1:C:727:PHE:N	1:C:749:LEU:HD13	2.36	0.41
1:D:473:GLU:OE2	1:D:477:ASN:ND2	2.50	0.41
1:D:626:ARG:HG2	1:D:1669:ASN:HD21	1.85	0.41
1:D:847:THR:HG22	1:D:848:ARG:H	1.86	0.41
1:D:4011:VAL:HG12	1:D:4015:LEU:HG	2.01	0.41
1:A:247:VAL:O	1:A:272:ARG:NH1	2.46	0.41
1:A:4609:ARG:HH11	1:A:4609:ARG:HD3	1.71	0.41
1:B:3907:PHE:HD2	1:B:3968:LEU:HD11	1.86	0.41
1:B:4499:ASN:ND2	1:B:4502:ASN:HB3	2.36	0.41
1:C:832:LEU:HG	1:C:1617:TRP:HE1	1.85	0.41
1:C:1137:PHE:HD1	1:C:1144:ARG:HB3	1.85	0.41
1:C:2587:GLN:O	1:C:2591:ARG:N	2.53	0.41
1:C:4020:MET:HB3	1:C:4067:LEU:HD11	2.02	0.41
1:A:74:SER:HA	1:A:117:HIS:HA	2.03	0.41
1:A:2426:SER:HB3	1:D:143:LEU:CD2	2.47	0.41
1:A:3891:TRP:CG	1:D:76:ARG:CG	3.03	0.41
1:B:626:ARG:HG2	1:B:1669:ASN:HD21	1.85	0.41
1:B:852:GLY:HA2	1:B:853:PRO:HA	1.82	0.41
1:B:4020:MET:HB3	1:B:4067:LEU:HD11	2.01	0.41
1:C:676:GLU:HB2	1:C:803:LEU:HB2	2.01	0.41
1:C:745:ASN:ND2	1:C:773:GLN:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:847:THR:HG22	1:C:848:ARG:H	1.86	0.41
1:C:1090:ALA:HA	1:C:1249:MET:HG2	2.02	0.41
1:C:1094:TYR:OH	1:C:1808:ASP:OD1	2.38	0.41
1:C:1228:THR:HA	1:C:1232:LEU:HD12	2.03	0.41
1:D:589:ILE:HG21	1:D:617:LEU:HD22	2.02	0.41
1:D:3642:ILE:HG22	1:D:3731:ARG:HD3	2.03	0.41
1:A:308:LEU:N	1:A:326:SER:O	2.50	0.41
1:A:465:PRO:HA	1:A:466:PRO:HD3	1.89	0.41
1:B:312:LYS:HD2	1:B:315:LEU:HD11	2.02	0.41
1:B:706:TYR:HA	1:B:707:PRO:HD3	1.91	0.41
1:B:1090:ALA:HA	1:B:1249:MET:HG2	2.02	0.41
1:B:1137:PHE:HD1	1:B:1144:ARG:HB3	1.85	0.41
1:B:4161:TRP:CZ2	1:B:4917:ALA:HB2	2.56	0.41
1:C:589:ILE:HG21	1:C:617:LEU:HD22	2.02	0.41
1:C:1727:VAL:HG11	1:C:1927:VAL:HG21	2.02	0.41
1:C:2273:CYS:HB3	1:C:2293:PRO:HD2	2.02	0.41
1:C:2884:ALA:HA	1:C:2887:ARG:HB3	2.02	0.41
1:C:4925:TYR:CZ	1:C:4929:LYS:HD2	2.55	0.41
1:D:530:LEU:HD23	1:D:533:LEU:HD12	2.02	0.41
1:D:1090:ALA:HB3	1:D:1203:PRO:HD2	2.03	0.41
1:D:1090:ALA:HA	1:D:1249:MET:HG2	2.02	0.41
1:D:2587:GLN:O	1:D:2591:ARG:N	2.53	0.41
1:D:4500:PHE:O	1:D:4504:ARG:N	2.52	0.41
1:D:4892:CYS:SG	1:D:4909:HIS:NE2	2.79	0.41
1:A:76:ARG:CG	1:B:3891:TRP:CG	3.04	0.41
1:A:363:ILE:HD12	1:A:403:LEU:HD12	2.03	0.41
1:A:745:ASN:ND2	1:A:773:GLN:OE1	2.54	0.41
1:A:1137:PHE:CE2	1:A:1139:GLY:HA2	2.56	0.41
1:A:1170:GLU:O	1:A:1172:THR:N	2.52	0.41
1:A:1184:ASP:HB2	1:A:1188:SER:H	1.86	0.41
1:A:3642:ILE:HG22	1:A:3731:ARG:HD3	2.03	0.41
1:A:4072:GLU:HB3	1:A:4074:ASP:HB2	2.03	0.41
1:B:76:ARG:CG	1:C:3891:TRP:CG	3.04	0.41
1:B:137:ARG:HE	1:B:202:HIS:HB3	1.86	0.41
1:B:238:HIS:N	1:B:243:GLU:O	2.53	0.41
1:B:363:ILE:HD12	1:B:403:LEU:HD12	2.03	0.41
1:B:530:LEU:HD23	1:B:533:LEU:HD12	2.02	0.41
1:B:676:GLU:HB2	1:B:803:LEU:HB2	2.02	0.41
1:B:2857:LYS:HE2	1:B:2869:HIS:CD2	2.56	0.41
1:C:363:ILE:HD12	1:C:403:LEU:HD12	2.03	0.41
1:C:1505:LEU:HB2	1:C:1523:ASN:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1799:VAL:HG22	1:C:1894:LEU:HD13	2.02	0.41
1:C:4011:VAL:HG12	1:C:4015:LEU:HG	2.02	0.41
1:C:4508:LEU:HD11	1:C:4747:ILE:HD12	2.03	0.41
1:C:4832:ILE:HG21	1:C:4844:ARG:NH2	2.30	0.41
1:D:150:GLN:NE2	1:D:158:CYS:SG	2.73	0.41
1:D:228:LEU:HD23	1:D:356:TYR:CE1	2.56	0.41
1:D:312:LYS:HD2	1:D:315:LEU:HD11	2.02	0.41
1:D:646:THR:OG1	1:D:1684:GLN:NE2	2.51	0.41
1:D:745:ASN:ND2	1:D:773:GLN:OE1	2.54	0.41
1:D:855:VAL:HG22	1:D:1209:VAL:HG12	2.03	0.41
1:D:1654:HIS:O	1:D:1657:THR:OG1	2.28	0.41
1:D:3841:PHE:HB3	1:D:3920:THR:HG21	2.02	0.41
1:D:4020:MET:HB3	1:D:4067:LEU:HD11	2.03	0.41
1:A:717:GLY:H	1:A:722:LEU:HD13	1.85	0.41
1:A:1699:ARG:NH1	1:A:1816:PHE:O	2.48	0.41
1:A:4499:ASN:ND2	1:A:4502:ASN:HB3	2.36	0.41
1:B:745:ASN:ND2	1:B:773:GLN:OE1	2.54	0.41
1:B:1113:MET:HG3	1:B:1156:TRP:HZ2	1.86	0.41
1:B:1457:PHE:CD1	1:B:1488:VAL:HG21	2.56	0.41
1:B:3988:GLU:HB2	1:B:4937:GLN:NE2	2.35	0.41
1:B:4170:LYS:HE2	1:B:4916:LEU:CD2	2.51	0.41
1:B:4493:LEU:HA	1:B:4496:PHE:HD2	1.86	0.41
1:B:4861:ALA:HA	1:B:4864:GLN:HB3	2.03	0.41
1:C:76:ARG:CG	1:D:3891:TRP:CG	3.04	0.41
1:C:1457:PHE:CD1	1:C:1488:VAL:HG21	2.55	0.41
1:C:2796:GLY:HA2	1:C:2900:ASN:HA	2.03	0.41
1:D:23:GLN:HE21	1:D:34:LYS:HB3	1.86	0.41
1:D:1172:THR:HG22	1:D:1193:LYS:HG3	2.02	0.41
1:D:1457:PHE:CD1	1:D:1488:VAL:HG21	2.56	0.41
1:D:2143:MET:SD	1:D:2175:VAL:HG11	2.61	0.41
1:D:4011:VAL:HA	1:D:4014:ILE:HG12	2.03	0.41
1:D:4171:ARG:HH11	1:D:4752:LYS:CE	2.17	0.41
1:D:4591:TYR:CE1	1:D:4595:LYS:HB2	2.56	0.41
1:A:312:LYS:HD2	1:A:315:LEU:HD11	2.02	0.40
1:A:589:ILE:HG21	1:A:617:LEU:HD22	2.03	0.40
1:A:3760:LEU:HD13	1:A:3840:LEU:HA	2.02	0.40
1:A:4020:MET:HB3	1:A:4067:LEU:HD11	2.03	0.40
1:A:4036:TYR:HE2	1:A:4048:ASP:HB3	1.87	0.40
1:B:773:GLN:HA	1:B:774:PRO:HD3	1.94	0.40
1:B:2424:LEU:HD23	1:B:2476:VAL:HG22	2.02	0.40
1:B:3768:ASN:H	1:B:3846:LEU:HD23	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4640:SER:HB3	1:B:4643:ASN:HD21	1.85	0.40
1:D:1094:TYR:OH	1:D:1808:ASP:OD1	2.38	0.40
1:D:1170:GLU:O	1:D:1172:THR:N	2.52	0.40
1:D:1300:MET:O	1:D:1545:ALA:N	2.45	0.40
1:D:2520:TYR:HA	1:D:2523:THR:HB	2.03	0.40
1:A:228:LEU:HD23	1:A:356:TYR:CE1	2.56	0.40
1:A:426:PHE:O	1:A:430:ILE:N	2.54	0.40
1:A:847:THR:HG22	1:A:848:ARG:H	1.86	0.40
1:B:1505:LEU:HB2	1:B:1523:ASN:HA	2.03	0.40
1:B:4797:SER:HB3	1:B:4805:MET:H	1.85	0.40
1:C:1455:THR:HB	1:C:1546:GLN:NE2	2.36	0.40
1:C:3920:THR:O	1:C:3924:TYR:N	2.52	0.40
1:C:4640:SER:HB3	1:C:4643:ASN:HD21	1.85	0.40
1:C:4797:SER:HB3	1:C:4805:MET:H	1.86	0.40
1:D:1752:GLY:HA3	1:D:1836:ASN:ND2	2.36	0.40
1:D:3983:LEU:HD23	1:D:3983:LEU:H	1.86	0.40
1:D:4207:ILE:O	1:D:4498:ARG:NH1	2.54	0.40
1:A:2884:ALA:HA	1:A:2887:ARG:HB3	2.03	0.40
1:B:1090:ALA:HB3	1:B:1203:PRO:HD2	2.03	0.40
1:B:1220:ASP:O	1:B:1223:THR:N	2.36	0.40
1:C:2520:TYR:HA	1:C:2523:THR:HB	2.03	0.40
1:C:2857:LYS:HE2	1:C:2869:HIS:CD2	2.57	0.40
1:C:3841:PHE:HB3	1:C:3920:THR:HG21	2.03	0.40
1:C:3983:LEU:HD23	1:C:3983:LEU:H	1.86	0.40
1:C:4499:ASN:ND2	1:C:4502:ASN:HB3	2.36	0.40
1:D:644:LEU:HD12	1:D:1654:HIS:HB2	2.04	0.40
1:D:832:LEU:HB3	1:D:1614:ARG:NH1	2.37	0.40
1:D:1799:VAL:HG22	1:D:1894:LEU:HD13	2.03	0.40
1:A:299:HIS:N	1:A:304:LYS:O	2.50	0.40
1:A:1228:THR:HA	1:A:1232:LEU:HD12	2.03	0.40
1:A:1761:MET:SD	1:A:1761:MET:N	2.92	0.40
1:A:4493:LEU:HA	1:A:4496:PHE:HD2	1.86	0.40
1:B:74:SER:HA	1:B:117:HIS:HA	2.03	0.40
1:B:228:LEU:HD23	1:B:356:TYR:CE1	2.57	0.40
1:B:3797:LEU:O	1:B:3800:SER:OG	2.32	0.40
1:C:30:LYS:HB2	1:C:30:LYS:HE3	1.82	0.40
1:C:686:VAL:O	1:C:687:THR:OG1	2.34	0.40
1:D:572:LEU:O	1:D:576:HIS:N	2.51	0.40
1:D:844:ARG:HD2	1:D:849:ASP:OD2	2.22	0.40
1:D:1457:PHE:HD1	1:D:1488:VAL:HG21	1.86	0.40
1:D:1506:GLU:HA	1:D:1522:ALA:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2857:LYS:HE2	1:D:2869:HIS:CD2	2.57	0.40
1:D:3955:MET:O	1:D:3959:LEU:N	2.48	0.40
1:D:4182:GLY:O	1:D:4186:LYS:N	2.55	0.40
1:A:489:PHE:HD2	1:A:540:LEU:HD21	1.87	0.40
1:A:3690:MET:HE3	1:A:3690:MET:HB3	1.90	0.40
1:A:3980:VAL:HA	1:A:3983:LEU:HD23	2.04	0.40
1:B:589:ILE:HG21	1:B:617:LEU:HD22	2.03	0.40
1:B:1184:ASP:HB2	1:B:1188:SER:H	1.86	0.40
1:B:4054:GLU:HG3	1:B:4061:GLN:HG2	2.03	0.40
1:B:4182:GLY:O	1:B:4186:LYS:N	2.54	0.40
1:C:312:LYS:HD2	1:C:315:LEU:HD11	2.03	0.40
1:C:356:TYR:CE1	1:C:407:ARG:HB3	2.57	0.40
1:C:488:LEU:HD23	1:C:488:LEU:HA	1.94	0.40
1:C:1138:ASP:HB2	1:C:1145:TRP:HE1	1.87	0.40
1:C:4591:TYR:CE1	1:C:4595:LYS:HB2	2.56	0.40
1:D:299:HIS:NE2	1:D:301:THR:OG1	2.47	0.40
1:D:363:ILE:HD12	1:D:403:LEU:HD12	2.04	0.40
1:D:426:PHE:O	1:D:430:ILE:N	2.54	0.40
1:D:1113:MET:HG3	1:D:1156:TRP:HZ2	1.86	0.40
1:D:1306:MET:HB3	1:D:1575:HIS:CE1	2.57	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	3289/4968 (66%)	2988 (91%)	279 (8%)	22 (1%)	22	62
1	B	3289/4968 (66%)	2994 (91%)	273 (8%)	22 (1%)	22	62
1	C	3289/4968 (66%)	2988 (91%)	280 (8%)	21 (1%)	25	64
1	D	3289/4968 (66%)	2986 (91%)	282 (9%)	21 (1%)	25	64
All	All	13156/19872 (66%)	11956 (91%)	1114 (8%)	86 (1%)	26	62

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1737	THR
1	A	1756	SER
1	A	4071	ALA
1	B	1737	THR
1	B	1756	SER
1	B	4071	ALA
1	C	1737	THR
1	C	1756	SER
1	C	4071	ALA
1	D	1737	THR
1	D	1756	SER
1	D	4071	ALA
1	A	1580	PRO
1	A	3805	ASP
1	A	4916	LEU
1	B	1580	PRO
1	B	3805	ASP
1	B	4916	LEU
1	C	1580	PRO
1	C	3805	ASP
1	C	4916	LEU
1	D	1580	PRO
1	D	3805	ASP
1	D	4916	LEU
1	A	819	TYR
1	A	4164	PRO
1	B	819	TYR
1	B	4164	PRO
1	C	819	TYR
1	C	4164	PRO
1	D	819	TYR
1	D	4164	PRO
1	A	1738	LEU
1	A	3804	LEU
1	A	4030	SER
1	B	1738	LEU
1	B	2075	VAL
1	B	3804	LEU
1	B	4030	SER
1	C	1738	LEU
1	C	2075	VAL
1	C	3804	LEU

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Mol	Chain	Res	Type
1	C	4030	SER
1	D	1738	LEU
1	D	3804	LEU
1	D	4030	SER
1	A	792	VAL
1	A	839	GLU
1	A	1581	GLN
1	B	792	VAL
1	B	839	GLU
1	B	1581	GLN
1	C	792	VAL
1	C	839	GLU
1	D	792	VAL
1	D	839	GLU
1	D	2075	VAL
1	A	980	PRO
1	A	2075	VAL
1	A	4642	PRO
1	A	4958	CYS
1	B	980	PRO
1	B	4642	PRO
1	B	4958	CYS
1	C	980	PRO
1	C	1581	GLN
1	C	3769	GLY
1	C	4642	PRO
1	D	980	PRO
1	D	1581	GLN
1	D	4642	PRO
1	A	729	GLY
1	A	3769	GLY
1	B	729	GLY
1	B	3769	GLY
1	C	729	GLY
1	D	729	GLY
1	D	3769	GLY
1	A	1476	VAL
1	B	828	PRO
1	B	1476	VAL
1	C	1476	VAL
1	D	1476	VAL
1	A	828	PRO

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Mol	Chain	Res	Type
1	C	828	PRO
1	D	828	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2660/4355 (61%)	2616 (98%)	44 (2%)	60	78
1	B	2657/4355 (61%)	2617 (98%)	40 (2%)	65	80
1	C	2658/4355 (61%)	2615 (98%)	43 (2%)	62	79
1	D	2660/4355 (61%)	2616 (98%)	44 (2%)	60	78
All	All	10635/17420 (61%)	10464 (98%)	171 (2%)	64	79

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	84	ASN
1	A	192	LEU
1	A	298	ARG
1	A	439	LYS
1	A	475	LYS
1	A	531	ASN
1	A	606	ARG
1	A	628	ASN
1	A	658	ASN
1	A	678	MET
1	A	687	THR
1	A	841	LYS
1	A	854	THR
1	A	925	PRO
1	A	950	VAL
1	A	990	PRO
1	A	1089	ARG
1	A	1619	VAL

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Mol	Chain	Res	Type
1	A	1637	ARG
1	A	1739	PHE
1	A	1760	ARG
1	A	2080	GLU
1	A	2126	GLN
1	A	2206	ARG
1	A	2211	ASN
1	A	2293	PRO
1	A	2419	ARG
1	A	3670	LEU
1	A	3813	ASN
1	A	3906	ASN
1	A	3990	ASN
1	A	4032	THR
1	A	4122	LEU
1	A	4179	ASN
1	A	4184	LYS
1	A	4187	MET
1	A	4499	ASN
1	A	4515	ASN
1	A	4609	ARG
1	A	4727	MET
1	A	4752	LYS
1	A	4781	LEU
1	A	4844	ARG
1	B	44	ASN
1	B	84	ASN
1	B	298	ARG
1	B	439	LYS
1	B	475	LYS
1	B	531	ASN
1	B	606	ARG
1	B	628	ASN
1	B	658	ASN
1	B	678	MET
1	B	687	THR
1	B	841	LYS
1	B	854	THR
1	B	925	PRO
1	B	990	PRO
1	B	1089	ARG
1	B	1619	VAL

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Mol	Chain	Res	Type
1	B	1637	ARG
1	B	1739	PHE
1	B	1760	ARG
1	B	2126	GLN
1	B	2206	ARG
1	B	2211	ASN
1	B	2293	PRO
1	B	2419	ARG
1	B	3670	LEU
1	B	3813	ASN
1	B	3906	ASN
1	B	3990	ASN
1	B	4032	THR
1	B	4122	LEU
1	B	4179	ASN
1	B	4184	LYS
1	B	4187	MET
1	B	4499	ASN
1	B	4515	ASN
1	B	4609	ARG
1	B	4727	MET
1	B	4781	LEU
1	B	4844	ARG
1	C	44	ASN
1	C	84	ASN
1	C	192	LEU
1	C	298	ARG
1	C	439	LYS
1	C	531	ASN
1	C	606	ARG
1	C	628	ASN
1	C	658	ASN
1	C	678	MET
1	C	687	THR
1	C	841	LYS
1	C	854	THR
1	C	925	PRO
1	C	990	PRO
1	C	1089	ARG
1	C	1619	VAL
1	C	1637	ARG
1	C	1739	PHE

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Mol	Chain	Res	Type
1	C	1760	ARG
1	C	2126	GLN
1	C	2206	ARG
1	C	2211	ASN
1	C	2293	PRO
1	C	2419	ARG
1	C	3670	LEU
1	C	3813	ASN
1	C	3906	ASN
1	C	3990	ASN
1	C	4032	THR
1	C	4122	LEU
1	C	4168	GLU
1	C	4171	ARG
1	C	4179	ASN
1	C	4184	LYS
1	C	4187	MET
1	C	4499	ASN
1	C	4515	ASN
1	C	4609	ARG
1	C	4727	MET
1	C	4781	LEU
1	C	4844	ARG
1	C	4910	THR
1	D	44	ASN
1	D	84	ASN
1	D	192	LEU
1	D	298	ARG
1	D	439	LYS
1	D	475	LYS
1	D	531	ASN
1	D	606	ARG
1	D	628	ASN
1	D	658	ASN
1	D	678	MET
1	D	687	THR
1	D	841	LYS
1	D	854	THR
1	D	925	PRO
1	D	950	VAL
1	D	990	PRO
1	D	1089	ARG

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Mol	Chain	Res	Type
1	D	1619	VAL
1	D	1637	ARG
1	D	1739	PHE
1	D	1760	ARG
1	D	2080	GLU
1	D	2126	GLN
1	D	2206	ARG
1	D	2211	ASN
1	D	2293	PRO
1	D	2419	ARG
1	D	3670	LEU
1	D	3813	ASN
1	D	3906	ASN
1	D	3990	ASN
1	D	4032	THR
1	D	4122	LEU
1	D	4171	ARG
1	D	4179	ASN
1	D	4184	LYS
1	D	4187	MET
1	D	4499	ASN
1	D	4515	ASN
1	D	4609	ARG
1	D	4727	MET
1	D	4781	LEU
1	D	4844	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (169) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	44	ASN
1	A	84	ASN
1	A	123	HIS
1	A	238	HIS
1	A	293	GLN
1	A	364	GLN
1	A	394	HIS
1	A	486	GLN
1	A	490	GLN
1	A	531	ASN
1	A	544	ASN

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Mol	Chain	Res	Type
1	A	593	HIS
1	A	604	HIS
1	A	628	ASN
1	A	681	HIS
1	A	1244	ASN
1	A	1294	ASN
1	A	1602	GLN
1	A	1620	GLN
1	A	1654	HIS
1	A	1691	ASN
1	A	1938	GLN
1	A	2090	HIS
1	A	2211	ASN
1	A	2212	GLN
1	A	3666	HIS
1	A	3862	GLN
1	A	3906	ASN
1	A	3954	HIS
1	A	3990	ASN
1	A	4160	GLN
1	A	4179	ASN
1	A	4192	ASN
1	A	4499	ASN
1	A	4559	HIS
1	A	4630	GLN
1	A	4737	ASN
1	A	4767	GLN
1	A	4817	HIS
1	A	4880	GLN
1	A	4914	HIS
1	B	23	GLN
1	B	44	ASN
1	B	84	ASN
1	B	123	HIS
1	B	238	HIS
1	B	293	GLN
1	B	364	GLN
1	B	394	HIS
1	B	486	GLN
1	B	490	GLN
1	B	531	ASN
1	B	544	ASN

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Mol	Chain	Res	Type
1	B	593	HIS
1	B	604	HIS
1	B	628	ASN
1	B	681	HIS
1	B	1244	ASN
1	B	1294	ASN
1	B	1602	GLN
1	B	1620	GLN
1	B	1654	HIS
1	B	1691	ASN
1	B	1938	GLN
1	B	2090	HIS
1	B	2211	ASN
1	B	2212	GLN
1	B	3666	HIS
1	B	3862	GLN
1	B	3906	ASN
1	B	3954	HIS
1	B	3990	ASN
1	B	4179	ASN
1	B	4192	ASN
1	B	4499	ASN
1	B	4559	HIS
1	B	4630	GLN
1	B	4737	ASN
1	B	4767	GLN
1	B	4817	HIS
1	B	4880	GLN
1	B	4914	HIS
1	C	23	GLN
1	C	44	ASN
1	C	84	ASN
1	C	123	HIS
1	C	238	HIS
1	C	293	GLN
1	C	364	GLN
1	C	394	HIS
1	C	486	GLN
1	C	490	GLN
1	C	531	ASN
1	C	544	ASN
1	C	593	HIS

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Mol	Chain	Res	Type
1	C	604	HIS
1	C	628	ASN
1	C	681	HIS
1	C	1244	ASN
1	C	1294	ASN
1	C	1602	GLN
1	C	1620	GLN
1	C	1654	HIS
1	C	1691	ASN
1	C	1938	GLN
1	C	2090	HIS
1	C	2152	ASN
1	C	2211	ASN
1	C	2212	GLN
1	C	3666	HIS
1	C	3862	GLN
1	C	3906	ASN
1	C	3919	ASN
1	C	3954	HIS
1	C	3990	ASN
1	C	4179	ASN
1	C	4192	ASN
1	C	4499	ASN
1	C	4559	HIS
1	C	4630	GLN
1	C	4737	ASN
1	C	4767	GLN
1	C	4817	HIS
1	C	4880	GLN
1	C	4914	HIS
1	D	23	GLN
1	D	44	ASN
1	D	84	ASN
1	D	123	HIS
1	D	238	HIS
1	D	293	GLN
1	D	364	GLN
1	D	394	HIS
1	D	490	GLN
1	D	531	ASN
1	D	544	ASN
1	D	593	HIS

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Mol	Chain	Res	Type
1	D	604	HIS
1	D	628	ASN
1	D	681	HIS
1	D	1244	ASN
1	D	1294	ASN
1	D	1602	GLN
1	D	1620	GLN
1	D	1654	HIS
1	D	1691	ASN
1	D	1938	GLN
1	D	2090	HIS
1	D	2211	ASN
1	D	2212	GLN
1	D	2831	ASN
1	D	3666	HIS
1	D	3862	GLN
1	D	3906	ASN
1	D	3919	ASN
1	D	3954	HIS
1	D	3990	ASN
1	D	4179	ASN
1	D	4192	ASN
1	D	4499	ASN
1	D	4515	ASN
1	D	4559	HIS
1	D	4630	GLN
1	D	4737	ASN
1	D	4767	GLN
1	D	4817	HIS
1	D	4880	GLN
1	D	4914	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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](#)

There are no chain breaks in this entry.

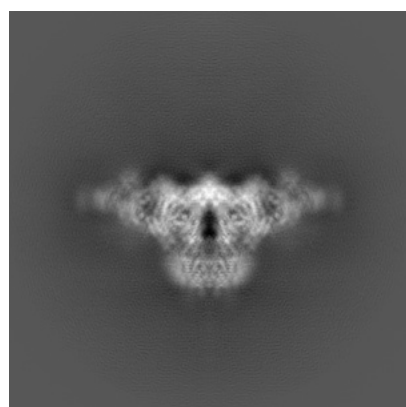
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9529. These allow visual inspection of the internal detail of the map and identification of artifacts.

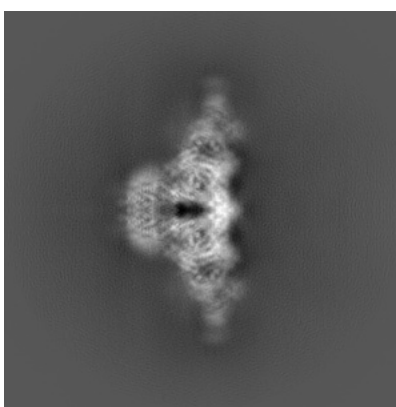
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

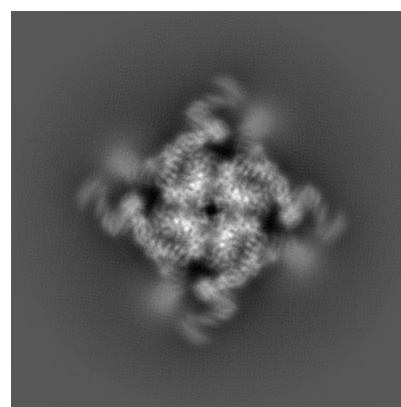
#### 6.1.1 Primary map



X



Y

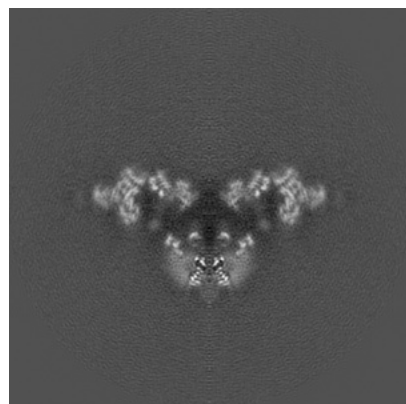


Z

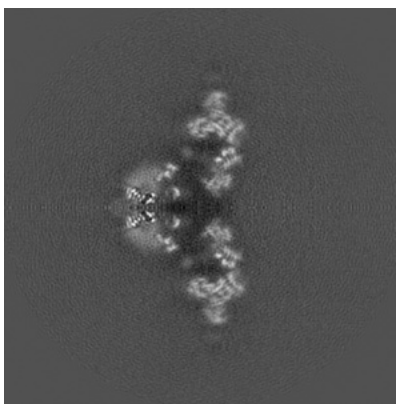
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

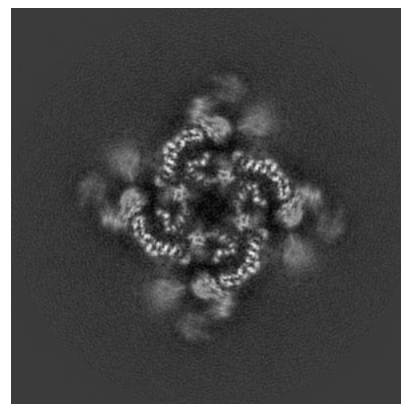
#### 6.2.1 Primary map



X Index: 260



Y Index: 260

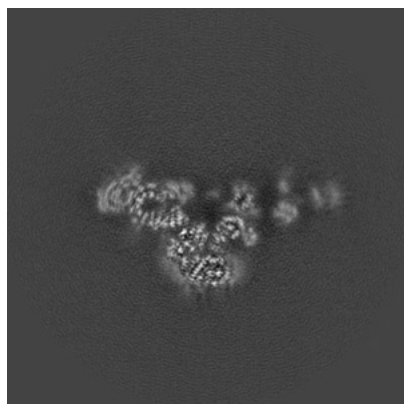


Z Index: 260

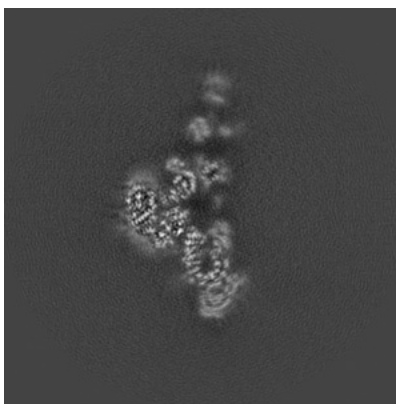
The images above show central slices of the map in three orthogonal directions.

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

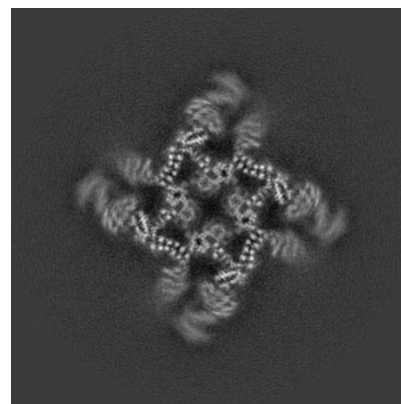
### 6.3.1 Primary map



X Index: 276



Y Index: 244

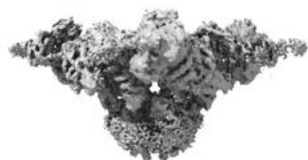


Z Index: 271

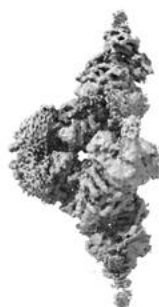
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

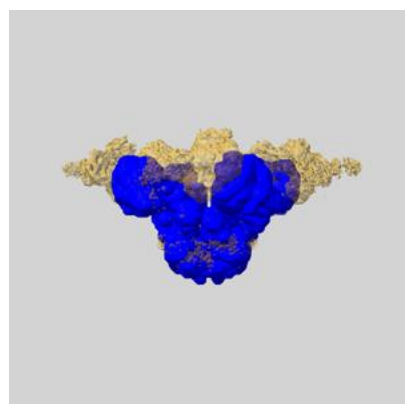
## 6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

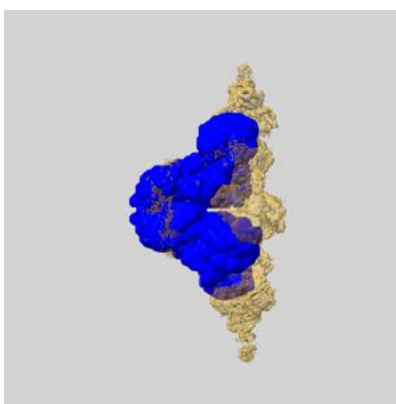
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

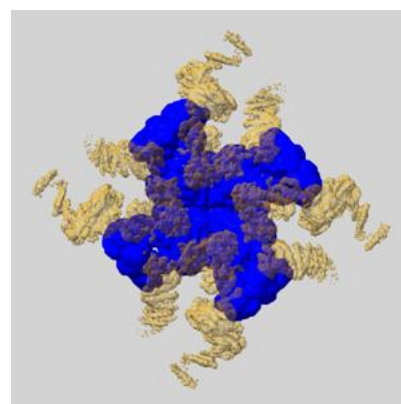
### 6.5.1 emd\_9529\_msk\_1.map [i](#)



X



Y

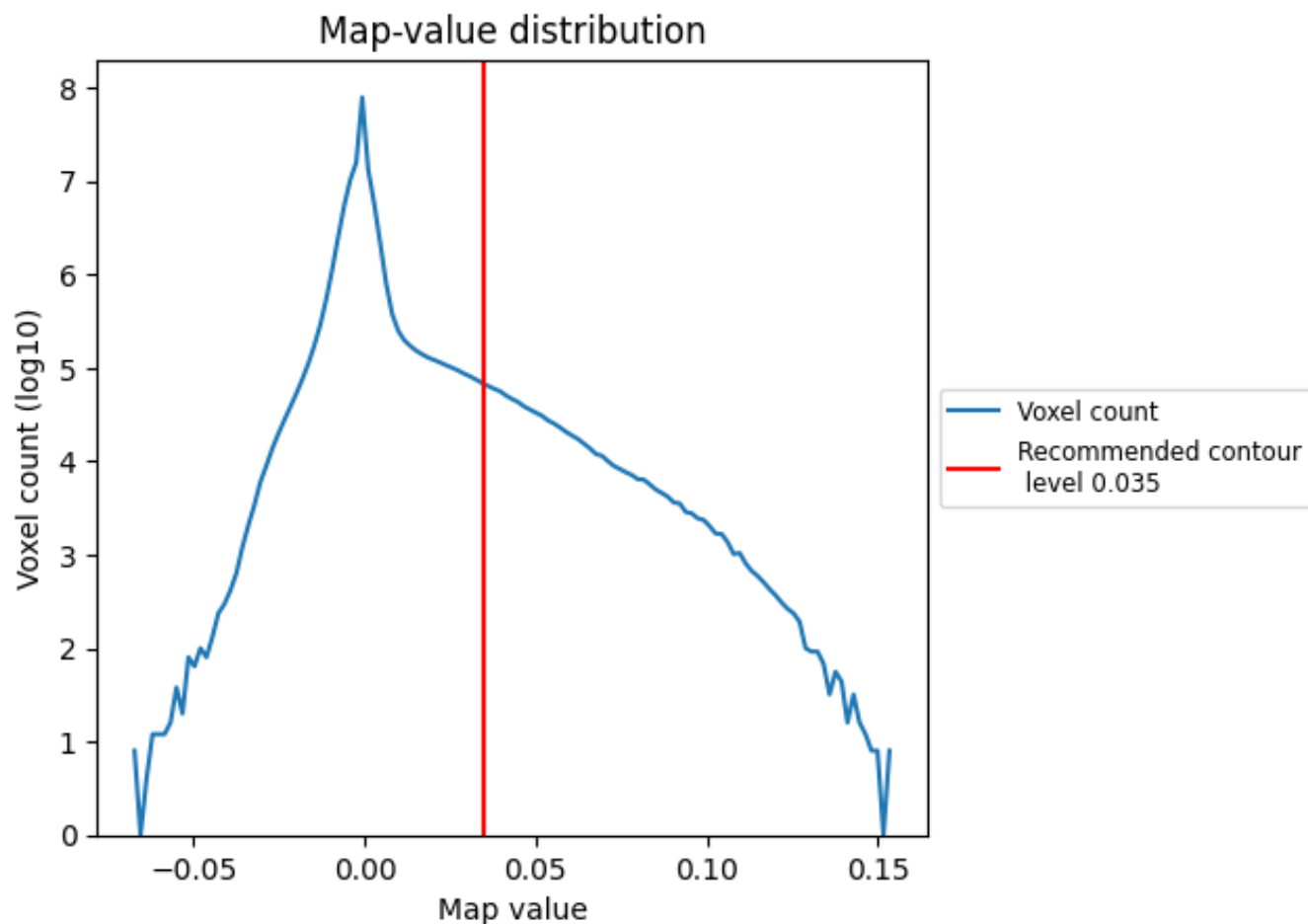


Z

## 7 Map analysis [i](#)

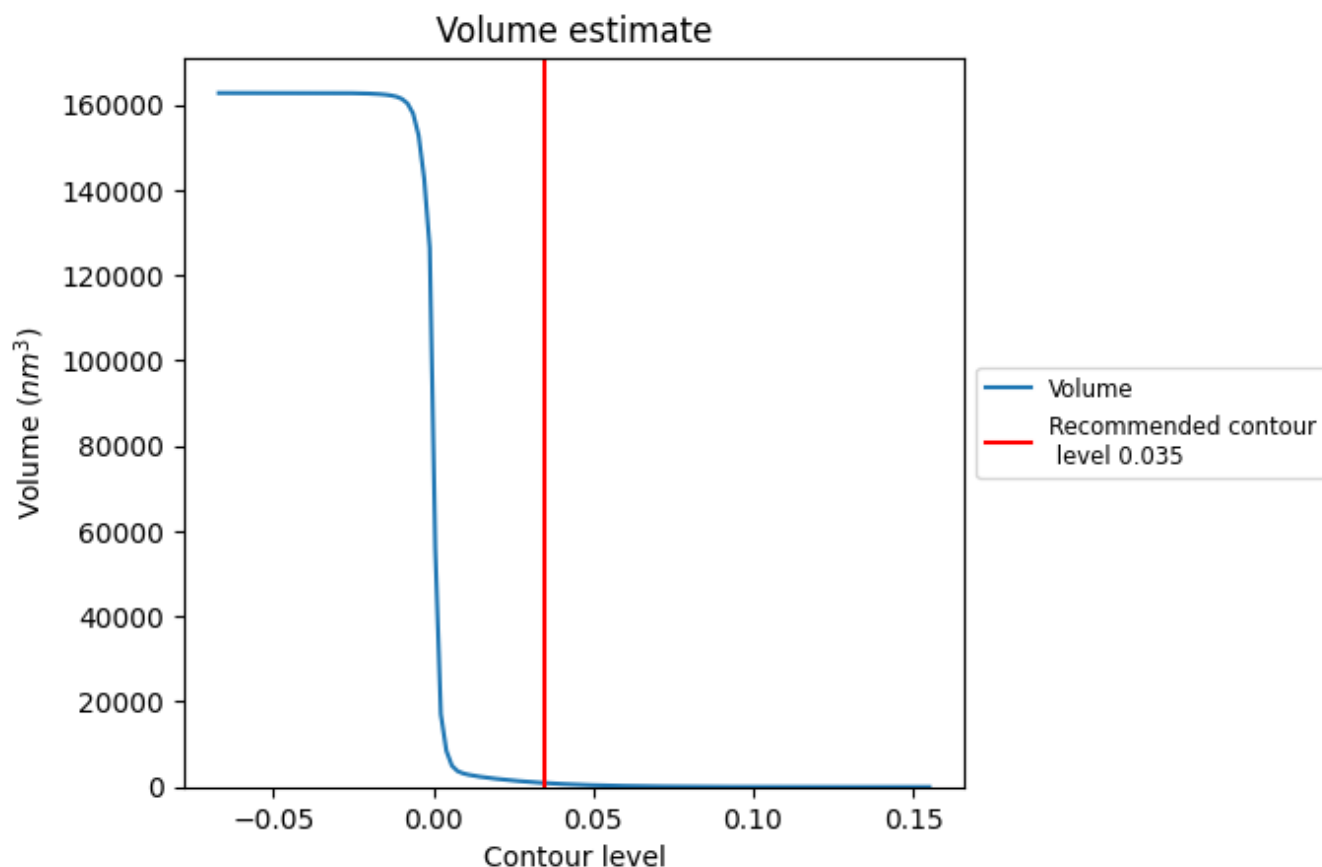
This section contains the results of statistical analysis of the map.

### 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.

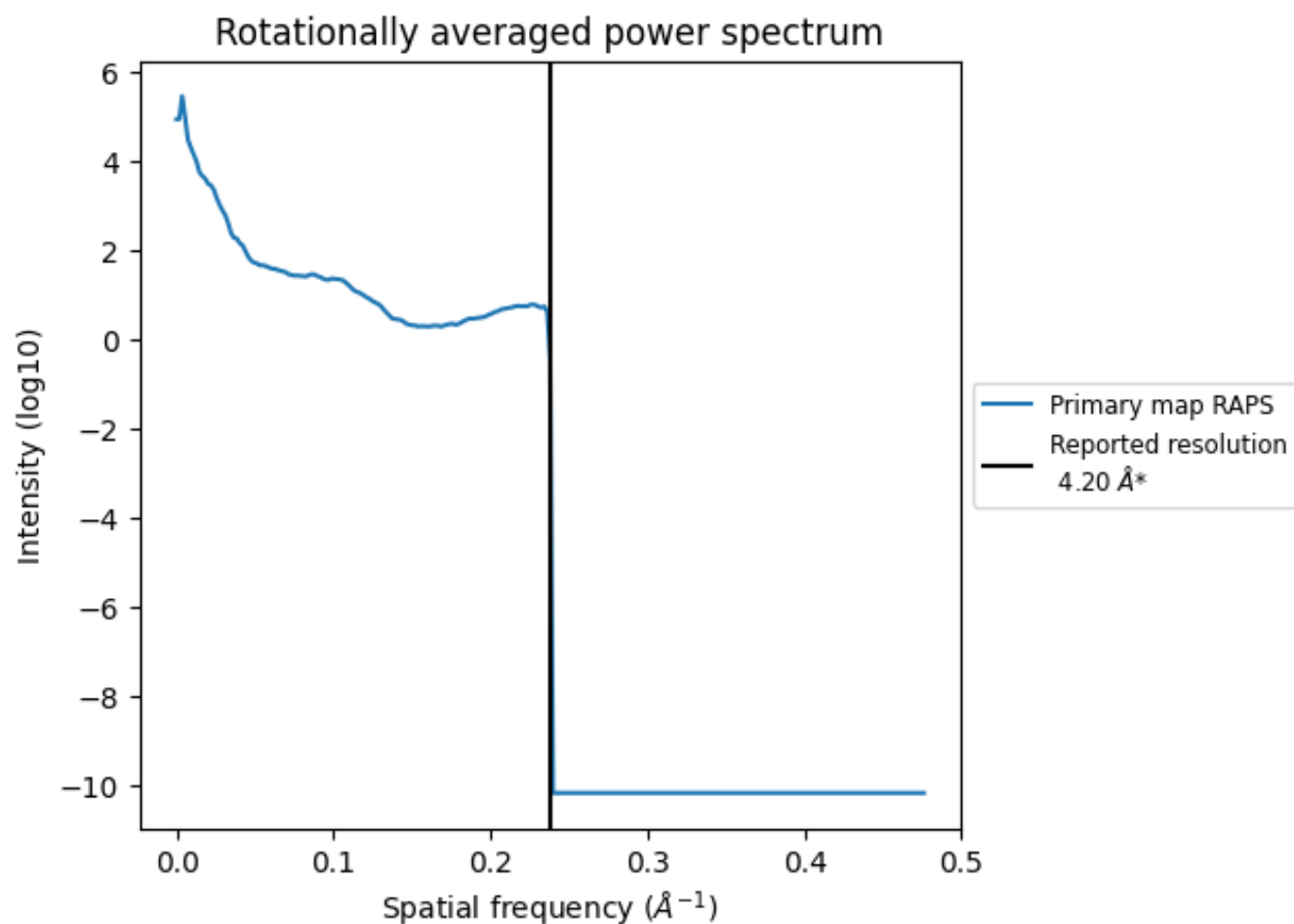
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 919 nm<sup>3</sup>; this corresponds to an approximate mass of 830 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 0.238  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation ⓘ

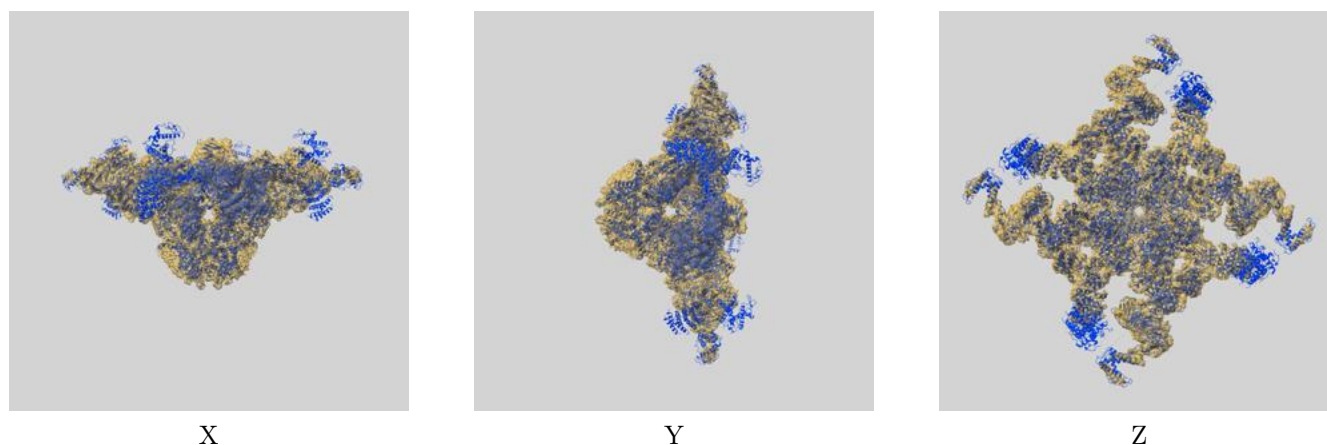
This section was not generated. No FSC curve or half-maps provided.



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

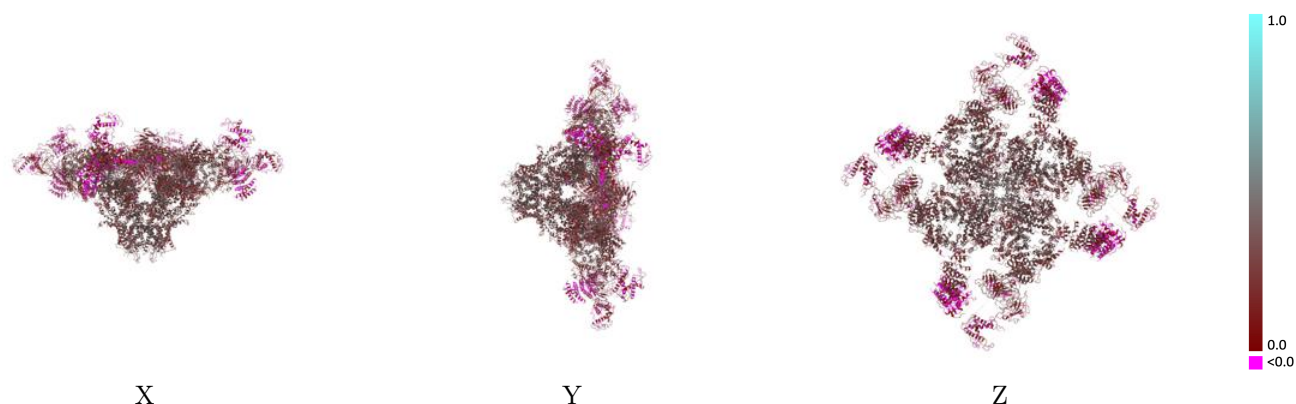
This section contains information regarding the fit between EMDB map EMD-9529 and PDB model 5GOA. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

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



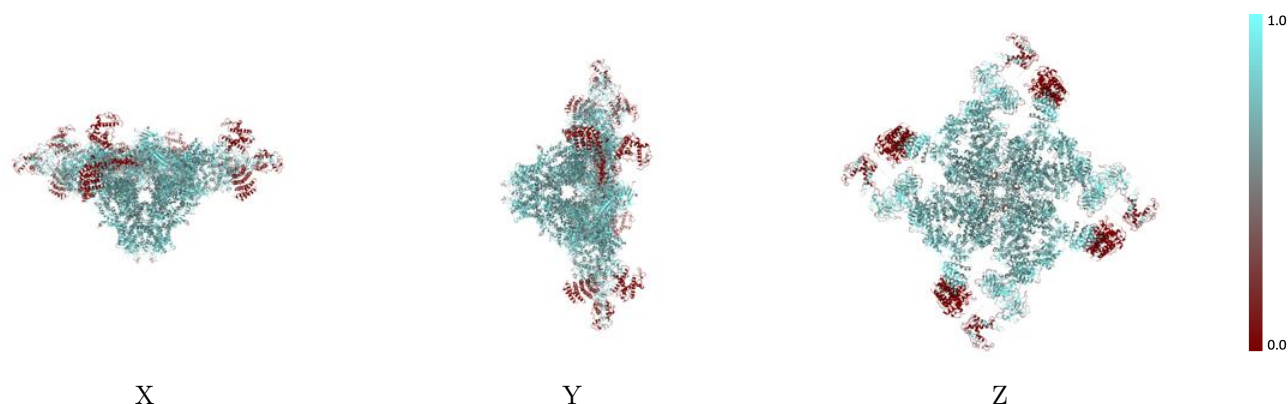
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



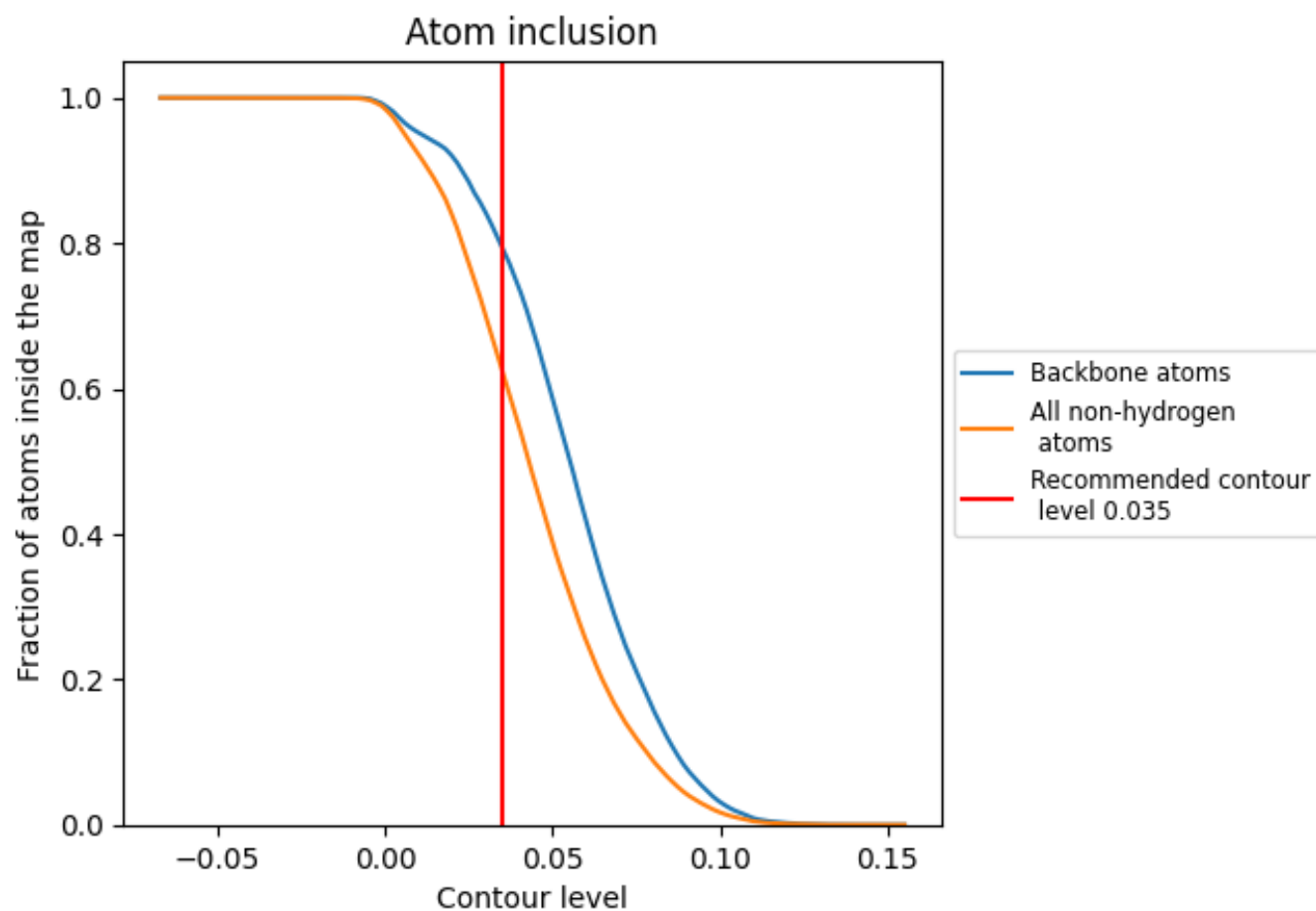
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 62% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6231	<div></div> 0.2450
A	<div></div> 0.6227	<div></div> 0.2450
B	<div></div> 0.6237	<div></div> 0.2440
C	<div></div> 0.6230	<div></div> 0.2440
D	<div></div> 0.6230	<div></div> 0.2440

