



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:26 PM UTC

PDB ID : 8X4C / pdb_00008x4c
EMDB ID : EMD-38046
Title : Cryo-EM structure of Ryanodine receptor 1 (20 uM Ca²⁺, 2 mM ATP)
Authors : Chen, Q.; Hu, H.
Deposited on : 2023-11-15
Resolution : 3.80 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

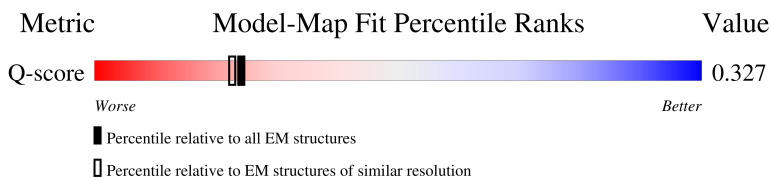
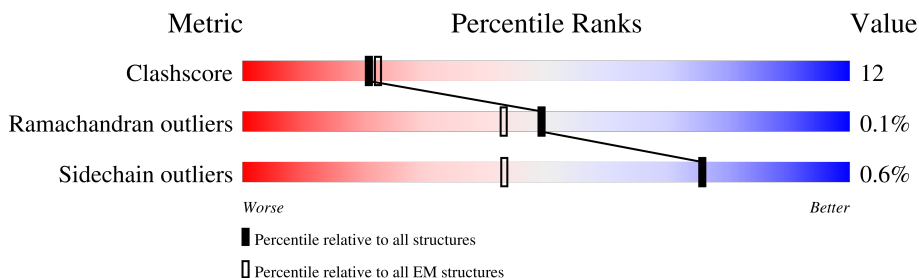
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	5037	
1	B	5037	
1	C	5037	
1	D	5037	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATP	A	5101	-	-	X	-
2	ATP	B	5101	-	-	X	-
2	ATP	C	5101	-	-	X	-
2	ATP	D	5101	-	-	X	-

2 Entry composition [i](#)

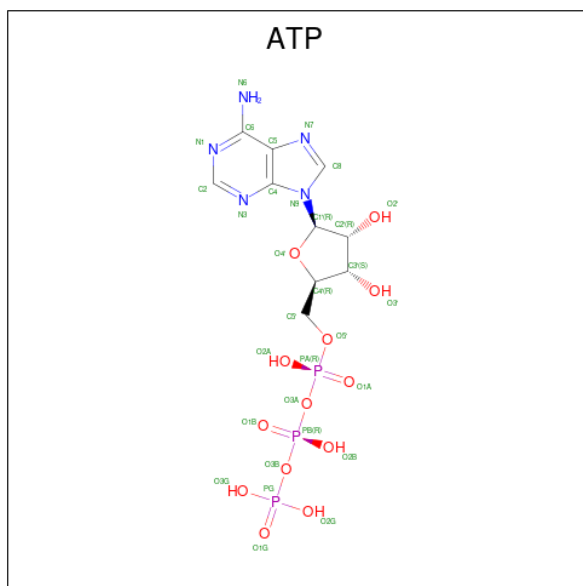
There are 3 unique types of molecules in this entry. The entry contains 95168 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3155	Total	C	N	O	S	0	0
			23760	15222	4111	4274	153		
1	B	3155	Total	C	N	O	S	0	0
			23760	15222	4111	4274	153		
1	C	3155	Total	C	N	O	S	0	0
			23760	15222	4111	4274	153		
1	D	3155	Total	C	N	O	S	0	0
			23760	15222	4111	4274	153		

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Ca	0
			1	1	
3	B	1	Total	Ca	0
			1	1	
3	C	1	Total	Ca	0
			1	1	
3	D	1	Total	Ca	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: Ryanodine receptor 1









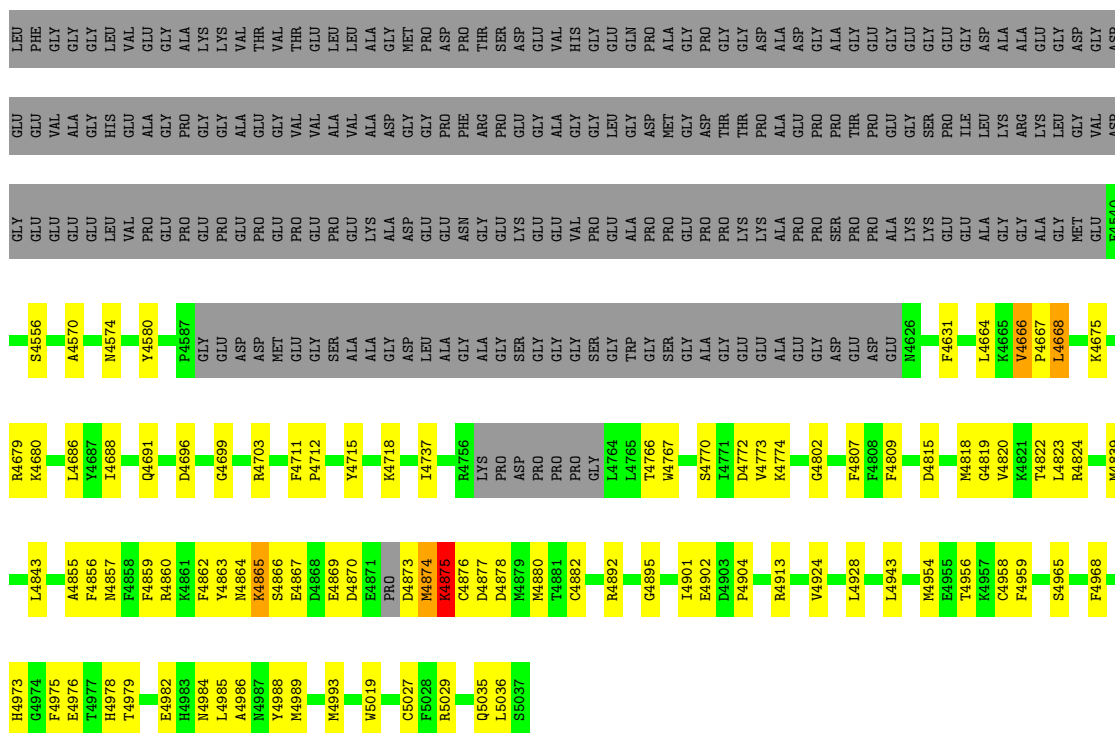
Frequency	Percentage
Often	48%
Sometimes	14%
Rarely	37%



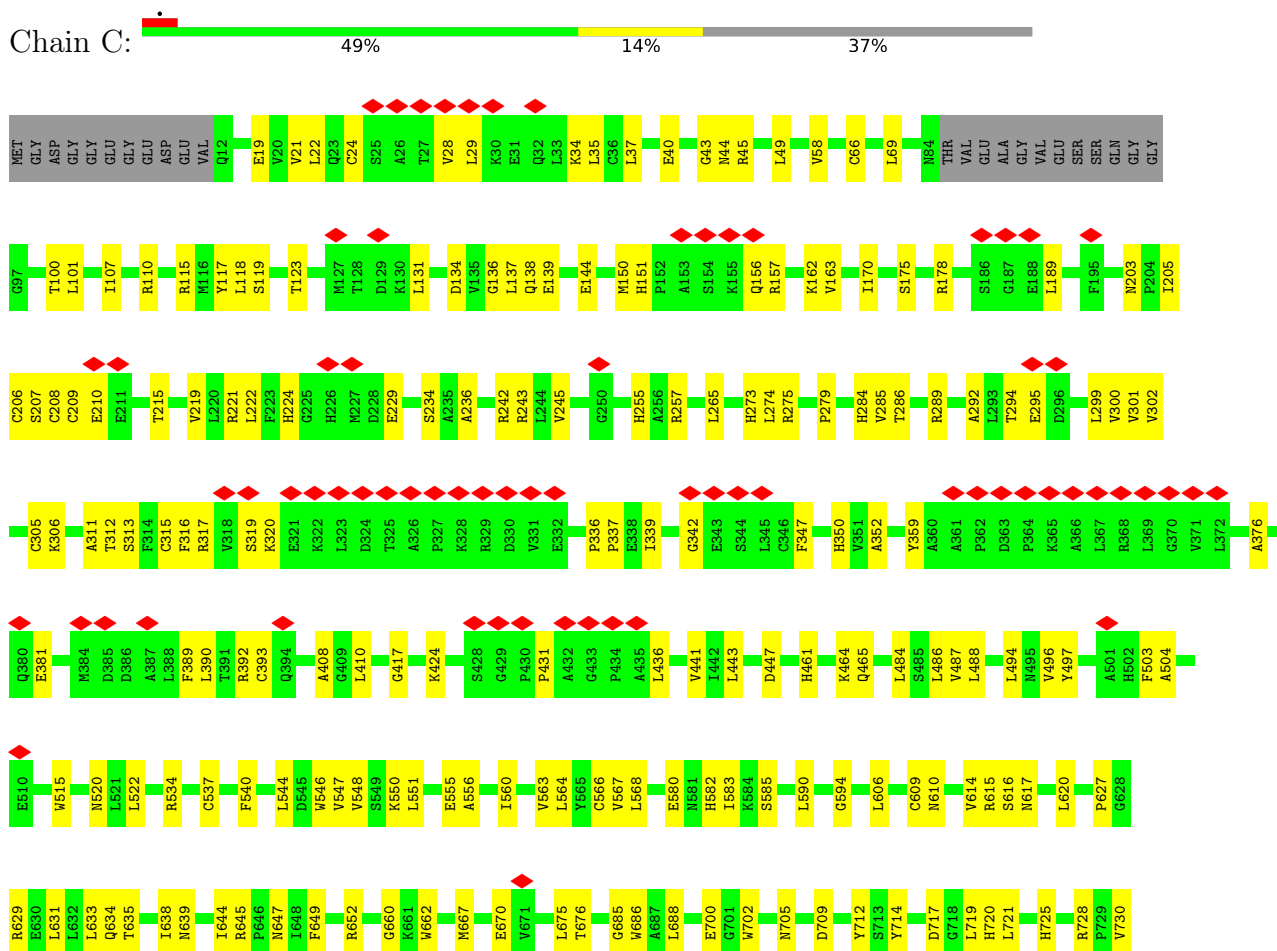








- Molecule 1: Ryanodine receptor 1













A4986	Y4863	S4710	GLU	LYS	ALA	ALA	ARG	ALA	F4103
M4987	K4864	F4711	SER	ASP	ASP	GLY	ARG	GLY	T4104
Y4988	K4865	P4712	GLY	ALA	GLY	MET	LEU	GLU	C4105
M4989	S4866		ALA	GLU	PRO	PRO	THR	ASP	P4106
W5019	D4868	Y4715	GLY	ASN	PHE	PRO	ARG	GLY	M4120
	E4869	K4718	ASP	GLY	ARG	THR	GLU	MET	E4127
C5027	D4870	D4730	LEU	GLU	PRO	PRO	ALA	GLY	
R5029	E4871		ALA	LYS	GLU	ASP	ALA	ALA	R4131
Q5035	P4870	I4737	GLY	GLU	GLY	GLY	THR	ALA	F4132
Q5035	D4873		ALA	VAL	ALA	VAL	ALA	ALA	Q4133
L5036	K4874	R4756	GLY	GLU	GLY	HIS	LEU	ALA	D4138
S5037	K4875		SER	PRO	GLY	GLY	GLY	GLY	
	C4876	LYS	GLY	GLU	LEU	GLU	GLN	ALA	M4142
		PRO	GLY	ALA	GLY	GLY	LEU	GLU	
	M4880	ASP	GLY	PRO	ASP	PRO	ALA	GLY	E4152
	T4881	PRO	SER	GLU	MET	GLY	TPP	ALA	H4153
	C4882	PRO	GLY	GLU	ASP	PRO	VAL	ALA	W4154
		PRO	TRP	GLU	THR	GLY	VAL	GLY	P4155
	M4887	GLY	GLY	PRO	THR	GLY	ARG	ALA	
	R4892	L4764	SER	LYS	PRO	ASP	ALA	GLY	R4175
		L4765	GLY	ALA	ALA	ASP	GLY	GLY	P4176
	T4766	W4767	ALA	ALA	GLY	ASP	ALA	ALA	Y4177
	G4895		GLY	PRO	PRO	GLY	GLY	ALA	
			GLU	PRO	PRO	GLY	ALA	ALA	
	I4901	S4770	GLU	SER	PRO	ALA	ALA	ALA	
	E4902	I4771	ALA	PRO	THR	GLY	GLY	GLY	T4181
	D4903	D4772	GLY	PRO	GLU	GLU	ALA	THR	E4182
	P4904	V4773	GLU	ALA	GLY	GLY	GLY	VAL	T4183
		K4774	ASP	LYS	GLY	GLY	ALA	ALA	M4184
	R4913		GLU	LYS	SER	GLY	ALA	GLY	C4185
		G4802	ASP	GLU	PRO	GLU	GLY	ALA	A4186
	V4924		GLU	GLU	ILE	GLY	GLY	THR	S4187
		F4807	M4526	ALA	ASP	ALA	ALA	THR	
	L4928	F4808		GLY	LYS	ALA	LEU	ARG	I4190
	K4951	F4809	F4631	GLY	ALA	GLY	LEU	ARG	
				ALA	LYS	LYS	LEU	LEU	T4193
	M4954	D4815	L4664	GLY	GLY	GLY	LEU	ALA	Y4194
	E4955	M4818	K4665	MET	GLY	ASP	TPP	ALA	
	T4956	C4819	V4666	GLU	VAL	GLY	GLY	ALA	E4199
	K4957		P4667	F4540	ASP	ASP	SER	ALA	
	C4958	T4822	L4668		GLY	LEU	LEU	ALA	M4205
		L4823		S4556	GLU	GLU	PHE	ARG	E4206
	S4985	R4824	K4875		GLU	VAL	GLY	ALA	M4207
				R4563	GLU	ALA	GLY	LEU	
	F4988	R4839	R4679	A4570	GLY	GLY	GLY	ARG	K4211
			K4680		LEU	HIS	LEU	LEU	
		L4843	L4586	M4574	VAL	VAL	VAL	LEU	E4227
	K4973		Y4587		PRO	ALA	GLY	SER	
	C4974	Y4848	L4688	L4578	PRO	GLY	GLY	TYR	E4232
	F4975			F4579	GLU	GLY	ALA	ARG	
	E4976	A4855	Q4691	Y4580	PRO	GLY	LYS	SER	F4243
	T4977	H4856			GLU	GLY	VAL	ARG	
	H4978	M4857	D4696	F4687	PRO	ALA	THR	ARG	E4253
	T4979			GLY	GLY	GLY	VAL	ARG	PRO
		F4858		GLU	GLY	VAL	THR	ARG	GLU
	E4982	R4859	Q4699	ASP	PRO	VAL	THR	VAL	GLU
	H4983	R4860		ASP	GLU	VAL	GLY	ARG	GLY
	N4984	K4861	R4703	ASP	PRO	GLU	GLY	ARG	GLU
	L4985	F4862		MET	GLU	VAL	LEU	LEU	PRO

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114423	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	5.212	Depositor
Minimum map value	-2.365	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.128	Depositor
Recommended contour level	0.591	Depositor
Map size ($\text{\AA}$)	523.2, 523.2, 523.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.09, 1.09, 1.09	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	1/24282 (0.0%)	0.37	11/32988 (0.0%)
1	B	0.23	1/24282 (0.0%)	0.37	11/32988 (0.0%)
1	C	0.23	1/24282 (0.0%)	0.37	11/32988 (0.0%)
1	D	0.23	1/24282 (0.0%)	0.37	11/32988 (0.0%)
All	All	0.23	4/97128 (0.0%)	0.37	44/131952 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4175	ARG	CA-C	-5.38	1.46	1.52
1	B	4175	ARG	CA-C	-5.38	1.46	1.52
1	C	4175	ARG	CA-C	-5.38	1.46	1.52
1	D	4175	ARG	CA-C	-5.38	1.46	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4175	ARG	CA-C-N	-6.18	112.11	119.84
1	A	4175	ARG	C-N-CA	-6.18	112.11	119.84
1	B	4175	ARG	CA-C-N	-6.18	112.11	119.84
1	B	4175	ARG	C-N-CA	-6.18	112.11	119.84
1	C	4175	ARG	CA-C-N	-6.18	112.11	119.84
1	C	4175	ARG	C-N-CA	-6.18	112.11	119.84
1	D	4175	ARG	CA-C-N	-6.18	112.11	119.84
1	D	4175	ARG	C-N-CA	-6.18	112.11	119.84
1	A	4880	MET	N-CA-C	-5.63	103.79	111.56
1	B	4880	MET	N-CA-C	-5.63	103.79	111.56
1	C	4880	MET	N-CA-C	-5.63	103.79	111.56
1	D	4880	MET	N-CA-C	-5.63	103.79	111.56
1	A	4668	LEU	N-CA-C	-5.56	107.50	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4668	LEU	N-CA-C	-5.56	107.50	114.56
1	C	4668	LEU	N-CA-C	-5.56	107.50	114.56
1	D	4668	LEU	N-CA-C	-5.56	107.50	114.56
1	A	4874	MET	N-CA-C	-5.34	104.02	111.39
1	B	4874	MET	N-CA-C	-5.34	104.02	111.39
1	C	4874	MET	N-CA-C	-5.34	104.02	111.39
1	D	4874	MET	N-CA-C	-5.34	104.02	111.39
1	A	4666	VAL	CA-C-N	-5.10	113.46	119.84
1	A	4666	VAL	C-N-CA	-5.10	113.46	119.84
1	B	4666	VAL	CA-C-N	-5.10	113.46	119.84
1	B	4666	VAL	C-N-CA	-5.10	113.46	119.84
1	C	4666	VAL	CA-C-N	-5.10	113.46	119.84
1	C	4666	VAL	C-N-CA	-5.10	113.46	119.84
1	D	4666	VAL	CA-C-N	-5.10	113.46	119.84
1	D	4666	VAL	C-N-CA	-5.10	113.46	119.84
1	A	1548	LEU	CA-C-N	5.06	131.23	122.28
1	A	1548	LEU	C-N-CA	5.06	131.23	122.28
1	B	1548	LEU	CA-C-N	5.06	131.23	122.28
1	B	1548	LEU	C-N-CA	5.06	131.23	122.28
1	C	1548	LEU	CA-C-N	5.06	131.23	122.28
1	C	1548	LEU	C-N-CA	5.06	131.23	122.28
1	D	1548	LEU	CA-C-N	5.06	131.23	122.28
1	D	1548	LEU	C-N-CA	5.06	131.23	122.28
1	A	1931	LEU	CA-C-N	-5.02	113.57	119.84
1	A	1931	LEU	C-N-CA	-5.02	113.57	119.84
1	B	1931	LEU	CA-C-N	-5.02	113.57	119.84
1	B	1931	LEU	C-N-CA	-5.02	113.57	119.84
1	C	1931	LEU	CA-C-N	-5.02	113.57	119.84
1	C	1931	LEU	C-N-CA	-5.02	113.57	119.84
1	D	1931	LEU	CA-C-N	-5.02	113.57	119.84
1	D	1931	LEU	C-N-CA	-5.02	113.57	119.84

There are no chirality outliers.

There are no planarity outliers.

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	23760	0	22500	563	0
1	B	23760	0	22500	560	0
1	C	23760	0	22500	557	0
1	D	23760	0	22500	550	0
2	A	31	0	12	11	0
2	B	31	0	12	11	0
2	C	31	0	12	10	0
2	D	31	0	12	11	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	95168	0	90048	2214	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 12.

All (2214) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1708:ARG:NE	1:A:1830:VAL:HG11	1.59	1.18
1:D:1708:ARG:NE	1:D:1830:VAL:HG11	1.59	1.17
1:C:1708:ARG:NE	1:C:1830:VAL:HG11	1.59	1.16
1:B:1708:ARG:NE	1:B:1830:VAL:HG11	1.59	1.16
1:B:721:LEU:HD21	1:B:1474:VAL:CG2	1.83	1.08
1:C:1933:GLU:C	1:C:1935:VAL:N	2.12	1.07
1:A:721:LEU:HD21	1:A:1474:VAL:CG2	1.83	1.07
1:D:721:LEU:HD21	1:D:1474:VAL:CG2	1.83	1.07
1:D:1933:GLU:C	1:D:1935:VAL:N	2.12	1.07
1:B:1933:GLU:C	1:B:1935:VAL:N	2.12	1.06
1:C:721:LEU:HD21	1:C:1474:VAL:CG2	1.83	1.06
1:A:721:LEU:CD2	1:A:1474:VAL:HG21	1.86	1.06
1:A:1933:GLU:C	1:A:1935:VAL:N	2.12	1.06
1:B:721:LEU:CD2	1:B:1474:VAL:HG21	1.86	1.06
1:D:721:LEU:CD2	1:D:1474:VAL:HG21	1.86	1.04
1:D:1708:ARG:HE	1:D:1830:VAL:HG11	0.87	1.04
1:C:721:LEU:CD2	1:C:1474:VAL:HG21	1.86	1.03
1:C:1708:ARG:HE	1:C:1830:VAL:HG11	0.87	1.03
1:A:1708:ARG:HE	1:A:1830:VAL:HG11	0.87	1.02
1:B:1708:ARG:HE	1:B:1830:VAL:HG11	0.87	1.01
1:C:721:LEU:HD21	1:C:1474:VAL:HG21	1.00	0.99
1:A:721:LEU:HD21	1:A:1474:VAL:HG21	1.00	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:721:LEU:HD21	1:B:1474:VAL:HG21	1.00	0.97
1:A:1257:VAL:HG11	1:A:1597:VAL:HG11	1.46	0.97
1:D:721:LEU:HD21	1:D:1474:VAL:HG21	1.00	0.97
1:C:1257:VAL:HG11	1:C:1597:VAL:CG1	1.95	0.96
1:D:1257:VAL:HG11	1:D:1597:VAL:HG11	1.46	0.96
1:D:1257:VAL:HG11	1:D:1597:VAL:CG1	1.95	0.95
1:B:1257:VAL:HG11	1:B:1597:VAL:CG1	1.95	0.95
1:A:1257:VAL:HG11	1:A:1597:VAL:CG1	1.95	0.95
1:B:1257:VAL:HG11	1:B:1597:VAL:HG11	1.46	0.95
1:C:1257:VAL:HG11	1:C:1597:VAL:HG11	1.46	0.94
1:A:4876:CYS:HB3	1:A:4882:CYS:SG	2.08	0.94
1:D:4876:CYS:HB3	1:D:4882:CYS:SG	2.08	0.94
1:C:4876:CYS:HB3	1:C:4882:CYS:SG	2.08	0.93
1:B:4876:CYS:HB3	1:B:4882:CYS:SG	2.08	0.93
1:D:743:VAL:H	1:D:760:ASN:HB3	1.39	0.88
1:B:743:VAL:H	1:B:760:ASN:HB3	1.39	0.87
1:C:743:VAL:H	1:C:760:ASN:HB3	1.39	0.86
1:A:743:VAL:H	1:A:760:ASN:HB3	1.39	0.86
1:C:4175:ARG:H	1:C:4176:PRO:HD2	1.41	0.85
1:B:4175:ARG:H	1:B:4176:PRO:HD2	1.41	0.84
1:B:745:SER:O	1:B:757:PHE:HA	1.78	0.84
1:A:3889:GLN:HG3	1:A:3967:GLU:HG3	1.60	0.83
1:A:4175:ARG:H	1:A:4176:PRO:HD2	1.41	0.83
1:D:745:SER:O	1:D:757:PHE:HA	1.78	0.83
1:A:745:SER:O	1:A:757:PHE:HA	1.78	0.83
1:D:3889:GLN:HG3	1:D:3967:GLU:HG3	1.60	0.83
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	1.60	0.82
1:D:4175:ARG:H	1:D:4176:PRO:HD2	1.41	0.82
1:C:745:SER:O	1:C:757:PHE:HA	1.78	0.82
1:C:746:CYS:SG	1:C:746:CYS:O	2.38	0.82
1:C:3889:GLN:HG3	1:C:3967:GLU:HG3	1.60	0.81
1:A:746:CYS:O	1:A:746:CYS:SG	2.38	0.81
1:D:746:CYS:O	1:D:746:CYS:SG	2.38	0.81
1:C:4211:LYS:NZ	1:C:4211:LYS:HB3	1.96	0.81
1:B:4211:LYS:NZ	1:B:4211:LYS:HB3	1.96	0.81
1:B:746:CYS:O	1:B:746:CYS:SG	2.38	0.81
1:C:652:ARG:HD2	1:C:750:LEU:HB3	1.63	0.80
1:A:4211:LYS:HB3	1:A:4211:LYS:NZ	1.96	0.80
1:D:652:ARG:HD2	1:D:750:LEU:HB3	1.63	0.80
1:B:652:ARG:HD2	1:B:750:LEU:HB3	1.63	0.79
1:D:4211:LYS:HB3	1:D:4211:LYS:NZ	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2110:TYR:HA	1:A:3700:GLN:NE2	1.97	0.79
1:B:2110:TYR:HA	1:B:3700:GLN:NE2	1.97	0.79
1:D:2110:TYR:HA	1:D:3700:GLN:NE2	1.97	0.78
1:A:652:ARG:HD2	1:A:750:LEU:HB3	1.63	0.78
1:C:2110:TYR:HA	1:C:3700:GLN:NE2	1.97	0.78
1:C:4207:MET:O	1:C:4211:LYS:HG2	1.87	0.74
1:D:4207:MET:O	1:D:4211:LYS:HG2	1.87	0.74
1:A:4207:MET:O	1:A:4211:LYS:HG2	1.87	0.74
1:B:1293:LEU:CD1	1:B:1580:PHE:CE1	2.70	0.74
1:B:4207:MET:O	1:B:4211:LYS:HG2	1.87	0.74
1:A:1717:SER:HA	1:A:1720:LEU:CD2	2.17	0.74
1:C:417:GLY:HA3	1:C:436:LEU:HD21	1.70	0.74
1:D:1293:LEU:CD1	1:D:1580:PHE:CE1	2.70	0.74
1:A:1293:LEU:CD1	1:A:1580:PHE:CE1	2.70	0.74
1:D:417:GLY:HA3	1:D:436:LEU:HD21	1.70	0.74
1:D:1717:SER:HA	1:D:1720:LEU:CD2	2.17	0.74
1:A:1715:LEU:HD23	1:A:1715:LEU:C	2.13	0.74
1:C:1293:LEU:CD1	1:C:1580:PHE:CE1	2.70	0.74
1:C:1717:SER:HA	1:C:1720:LEU:CD2	2.17	0.74
1:A:417:GLY:HA3	1:A:436:LEU:HD21	1.70	0.74
1:B:4104:THR:HG22	1:B:4106:PRO:HD2	1.70	0.74
1:D:4104:THR:HG22	1:D:4106:PRO:HD2	1.70	0.74
1:B:1717:SER:HA	1:B:1720:LEU:CD2	2.17	0.73
1:C:4104:THR:HG22	1:C:4106:PRO:HD2	1.70	0.73
1:D:746:CYS:HA	1:D:757:PHE:HD1	1.52	0.73
1:A:1293:LEU:HD21	1:A:1579:MET:HB3	1.71	0.73
1:B:417:GLY:HA3	1:B:436:LEU:HD21	1.70	0.73
1:D:1715:LEU:HD23	1:D:1715:LEU:C	2.13	0.73
1:A:746:CYS:HA	1:A:757:PHE:HD1	1.52	0.73
1:B:746:CYS:HA	1:B:757:PHE:HD1	1.52	0.73
1:C:746:CYS:HA	1:C:757:PHE:HD1	1.52	0.73
1:C:1715:LEU:HD23	1:C:1715:LEU:C	2.13	0.73
1:B:1293:LEU:HD21	1:B:1579:MET:HB3	1.71	0.73
1:A:4104:THR:HG22	1:A:4106:PRO:HD2	1.70	0.73
1:B:4979:THR:HG22	1:B:4979:THR:O	1.89	0.73
1:D:1293:LEU:HD21	1:D:1579:MET:HB3	1.71	0.73
1:A:1717:SER:HA	1:A:1720:LEU:HD23	1.71	0.72
1:B:1715:LEU:C	1:B:1715:LEU:HD23	2.13	0.72
1:B:1931:LEU:HD12	1:B:1936:LYS:HG2	1.72	0.72
1:C:1293:LEU:HD21	1:C:1579:MET:HB3	1.71	0.72
1:A:4979:THR:O	1:A:4979:THR:HG22	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:712:TYR:OH	1:B:1491:ASN:ND2	2.23	0.72
1:C:686:TRP:CZ2	1:C:746:CYS:SG	2.83	0.72
1:D:4979:THR:HG22	1:D:4979:THR:O	1.89	0.72
1:B:686:TRP:CZ2	1:B:746:CYS:SG	2.83	0.72
1:D:686:TRP:CZ2	1:D:746:CYS:SG	2.83	0.72
1:D:712:TYR:OH	1:D:1491:ASN:ND2	2.23	0.72
1:A:712:TYR:OH	1:A:1491:ASN:ND2	2.23	0.72
1:D:1931:LEU:HD12	1:D:1936:LYS:HG2	1.72	0.72
1:A:606:LEU:O	1:A:617:ASN:ND2	2.23	0.72
1:B:606:LEU:O	1:B:617:ASN:ND2	2.23	0.72
1:C:712:TYR:OH	1:C:1491:ASN:ND2	2.23	0.72
1:A:686:TRP:CZ2	1:A:746:CYS:SG	2.83	0.72
1:C:1708:ARG:HH22	1:C:1712:TYR:HE1	1.38	0.71
1:C:2107:GLN:NE2	1:C:3680:ALA:O	2.23	0.71
1:A:1708:ARG:HH22	1:A:1712:TYR:HE1	1.38	0.71
1:B:28:VAL:HG13	1:B:29:LEU:HD12	1.73	0.71
1:B:1717:SER:HA	1:B:1720:LEU:HD23	1.71	0.71
1:C:1717:SER:HA	1:C:1720:LEU:HD23	1.71	0.71
1:A:28:VAL:HG13	1:A:29:LEU:HD12	1.73	0.71
1:C:1931:LEU:HD12	1:C:1936:LYS:HG2	1.72	0.71
1:D:2107:GLN:NE2	1:D:3680:ALA:O	2.23	0.71
1:D:4199:GLU:OE2	1:D:4199:GLU:N	2.22	0.71
1:A:1931:LEU:HD12	1:A:1936:LYS:HG2	1.72	0.71
1:D:606:LEU:O	1:D:617:ASN:ND2	2.23	0.71
1:D:1708:ARG:HH22	1:D:1712:TYR:HE1	1.38	0.71
1:B:2107:GLN:NE2	1:B:3680:ALA:O	2.23	0.71
1:C:4979:THR:O	1:C:4979:THR:HG22	1.89	0.71
1:C:606:LEU:O	1:C:617:ASN:ND2	2.23	0.70
1:C:28:VAL:HG13	1:C:29:LEU:HD12	1.73	0.70
1:A:2107:GLN:NE2	1:A:3680:ALA:O	2.23	0.70
1:A:4199:GLU:H	1:A:4199:GLU:CD	2.00	0.70
1:D:1717:SER:HA	1:D:1720:LEU:HD23	1.71	0.70
1:B:1708:ARG:HH22	1:B:1712:TYR:HE1	1.38	0.70
1:B:1719:HIS:CD2	1:B:1802:ILE:HG13	2.27	0.70
1:A:1293:LEU:CD2	1:A:1579:MET:HB3	2.22	0.70
1:D:4199:GLU:H	1:D:4199:GLU:CD	2.00	0.69
1:A:4199:GLU:OE2	1:A:4199:GLU:N	2.22	0.69
1:B:1289:LEU:HD21	1:B:1597:VAL:HG23	1.75	0.69
1:B:3661:TRP:HB3	1:B:3663:LEU:H	1.58	0.69
1:C:1289:LEU:HD21	1:C:1597:VAL:HG23	1.75	0.69
1:C:1719:HIS:CD2	1:C:1802:ILE:HG13	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4199:GLU:OE2	1:B:4199:GLU:N	2.22	0.69
1:D:1708:ARG:NE	1:D:1830:VAL:CG1	2.50	0.69
1:A:3661:TRP:HB3	1:A:3663:LEU:H	1.58	0.69
1:A:1289:LEU:HD21	1:A:1597:VAL:HG23	1.75	0.69
1:A:1719:HIS:CD2	1:A:1802:ILE:HG13	2.27	0.69
1:B:1293:LEU:CD2	1:B:1579:MET:HB3	2.22	0.69
1:B:4199:GLU:H	1:B:4199:GLU:CD	2.00	0.69
1:D:28:VAL:HG13	1:D:29:LEU:HD12	1.73	0.69
1:D:1293:LEU:CD2	1:D:1579:MET:HB3	2.22	0.69
1:A:1152:MET:HB2	1:A:1161:ILE:HB	1.74	0.69
1:A:686:TRP:HZ2	1:A:746:CYS:SG	2.16	0.69
1:C:686:TRP:HZ2	1:C:746:CYS:SG	2.16	0.69
1:D:1719:HIS:CD2	1:D:1802:ILE:HG13	2.27	0.69
1:B:686:TRP:HZ2	1:B:746:CYS:SG	2.16	0.69
1:B:1152:MET:HB2	1:B:1161:ILE:HB	1.74	0.69
1:D:686:TRP:HZ2	1:D:746:CYS:SG	2.16	0.68
1:C:4199:GLU:OE2	1:C:4199:GLU:N	2.22	0.68
1:A:721:LEU:HB3	1:A:728:ARG:HG3	1.75	0.68
1:B:1708:ARG:NE	1:B:1830:VAL:CG1	2.50	0.68
1:C:3661:TRP:HB3	1:C:3663:LEU:H	1.58	0.68
1:C:4199:GLU:CD	1:C:4199:GLU:H	2.00	0.68
1:D:1289:LEU:HD21	1:D:1597:VAL:HG23	1.75	0.68
1:A:1040:CYS:O	1:A:1044:ARG:HG2	1.94	0.68
1:B:4232:GLU:OE1	1:B:5019:TRP:NE1	2.26	0.68
1:C:1839:VAL:HB	1:C:1840:PRO:HD3	1.75	0.68
1:D:721:LEU:HB3	1:D:728:ARG:HG3	1.75	0.68
1:C:1152:MET:HB2	1:C:1161:ILE:HB	1.74	0.68
1:D:1152:MET:HB2	1:D:1161:ILE:HB	1.74	0.68
1:C:1293:LEU:CD2	1:C:1579:MET:HB3	2.22	0.68
1:B:1839:VAL:HB	1:B:1840:PRO:HD3	1.75	0.68
1:D:4901:ILE:HB	1:D:4913:ARG:HH11	1.59	0.68
1:C:4175:ARG:H	1:C:4176:PRO:CD	2.07	0.68
1:D:838:HIS:HA	1:D:1201:HIS:HB3	1.75	0.68
1:A:838:HIS:HA	1:A:1201:HIS:HB3	1.75	0.67
1:C:721:LEU:HB3	1:C:728:ARG:HG3	1.75	0.67
1:B:1040:CYS:O	1:B:1044:ARG:HG2	1.94	0.67
1:C:1040:CYS:O	1:C:1044:ARG:HG2	1.94	0.67
1:D:1040:CYS:O	1:D:1044:ARG:HG2	1.94	0.67
1:B:4901:ILE:HB	1:B:4913:ARG:HH11	1.59	0.67
1:A:1708:ARG:CD	1:A:1830:VAL:HG11	2.24	0.67
1:A:4211:LYS:HB3	1:A:4211:LYS:HZ2	1.56	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4901:ILE:HB	1:A:4913:ARG:HH11	1.59	0.67
1:C:1708:ARG:CD	1:C:1830:VAL:HG11	2.24	0.67
1:A:1839:VAL:HB	1:A:1840:PRO:HD3	1.75	0.67
1:C:838:HIS:HA	1:C:1201:HIS:HB3	1.75	0.67
1:D:3661:TRP:HB3	1:D:3663:LEU:H	1.58	0.67
1:A:4175:ARG:H	1:A:4176:PRO:CD	2.07	0.67
1:A:1708:ARG:NE	1:A:1830:VAL:CG1	2.50	0.67
1:B:728:ARG:NH1	1:B:1474:VAL:HG11	2.10	0.67
1:B:1708:ARG:CD	1:B:1830:VAL:HG11	2.24	0.67
1:B:838:HIS:HA	1:B:1201:HIS:HB3	1.75	0.67
1:B:721:LEU:HB3	1:B:728:ARG:HG3	1.75	0.66
1:C:977:LEU:HD13	1:C:1047:LEU:HD13	1.78	0.66
1:C:219:VAL:O	1:C:392:ARG:NH1	2.29	0.66
1:D:1839:VAL:HB	1:D:1840:PRO:HD3	1.75	0.66
1:B:977:LEU:HD13	1:B:1047:LEU:HD13	1.78	0.66
1:C:4901:ILE:HB	1:C:4913:ARG:HH11	1.59	0.66
1:D:2110:TYR:HD2	1:D:3695:PRO:HG2	1.61	0.66
1:A:2110:TYR:HD2	1:A:3695:PRO:HG2	1.61	0.66
1:D:728:ARG:NH1	1:D:1474:VAL:HG11	2.10	0.66
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.29	0.66
1:B:219:VAL:O	1:B:392:ARG:NH1	2.29	0.66
1:A:728:ARG:NH1	1:A:1474:VAL:HG11	2.10	0.66
1:C:728:ARG:NH1	1:C:1474:VAL:HG11	2.10	0.66
1:D:1708:ARG:CD	1:D:1830:VAL:HG11	2.24	0.66
1:A:219:VAL:O	1:A:392:ARG:NH1	2.29	0.66
1:C:2199:ARG:HA	1:C:2204:HIS:HE1	1.61	0.66
1:C:4570:ALA:O	1:C:4574:ASN:ND2	2.29	0.66
1:B:2199:ARG:HA	1:B:2204:HIS:HE1	1.61	0.65
1:D:2199:ARG:HA	1:D:2204:HIS:HE1	1.61	0.65
1:D:977:LEU:HD13	1:D:1047:LEU:HD13	1.78	0.65
1:D:1653:LEU:HB3	1:D:1660:GLN:HB2	1.79	0.65
1:A:853:PRO:HG3	1:A:1024:TYR:H	1.61	0.65
1:A:4184:MET:HB3	1:A:4190:ILE:HD13	1.79	0.65
1:B:1653:LEU:HB3	1:B:1660:GLN:HB2	1.79	0.65
1:C:151:HIS:HB2	1:C:170:ILE:HB	1.78	0.65
1:D:4184:MET:HB3	1:D:4190:ILE:HD13	1.79	0.65
1:A:2199:ARG:HA	1:A:2204:HIS:HE1	1.61	0.65
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.29	0.65
1:D:219:VAL:O	1:D:392:ARG:NH1	2.29	0.65
1:D:1158:ASN:ND2	1:D:1182:ILE:O	2.30	0.65
1:C:853:PRO:HG3	1:C:1024:TYR:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:855:PRO:HG3	1:C:995:VAL:HA	1.79	0.65
1:A:783:PHE:HB2	1:A:787:VAL:HG21	1.79	0.65
1:A:977:LEU:HD13	1:A:1047:LEU:HD13	1.78	0.65
1:A:1653:LEU:HB3	1:A:1660:GLN:HB2	1.79	0.65
1:B:855:PRO:HG3	1:B:995:VAL:HA	1.79	0.65
1:C:1653:LEU:HB3	1:C:1660:GLN:HB2	1.79	0.65
1:C:4184:MET:HB3	1:C:4190:ILE:HD13	1.79	0.65
1:D:855:PRO:HG3	1:D:995:VAL:HA	1.79	0.65
1:B:151:HIS:HB2	1:B:170:ILE:HB	1.78	0.65
1:B:1158:ASN:ND2	1:B:1182:ILE:O	2.30	0.65
1:B:2110:TYR:HD2	1:B:3695:PRO:HG2	1.61	0.65
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.29	0.65
1:D:4175:ARG:H	1:D:4176:PRO:CD	2.07	0.65
1:A:719:LEU:HA	1:A:730:VAL:HG22	1.79	0.64
1:B:4184:MET:HB3	1:B:4190:ILE:HD13	1.79	0.64
1:C:838:HIS:HB3	1:C:1200:GLY:C	2.22	0.64
1:A:151:HIS:HB2	1:A:170:ILE:HB	1.78	0.64
1:A:855:PRO:HG3	1:A:995:VAL:HA	1.79	0.64
1:A:1208:VAL:HA	1:A:1211:LEU:HD23	1.80	0.64
1:B:783:PHE:HB2	1:B:787:VAL:HG21	1.79	0.64
1:D:746:CYS:HA	1:D:757:PHE:CD1	2.32	0.64
1:D:4232:GLU:OE1	1:D:5019:TRP:NE1	2.26	0.64
1:A:1158:ASN:ND2	1:A:1182:ILE:O	2.30	0.64
1:C:719:LEU:HA	1:C:730:VAL:HG22	1.79	0.64
1:D:719:LEU:HA	1:D:730:VAL:HG22	1.79	0.64
1:D:1208:VAL:HA	1:D:1211:LEU:HD23	1.80	0.64
1:D:151:HIS:HB2	1:D:170:ILE:HB	1.78	0.64
1:A:627:PRO:O	1:A:629:ARG:NH1	2.31	0.64
1:B:627:PRO:O	1:B:629:ARG:NH1	2.31	0.64
1:C:627:PRO:O	1:C:629:ARG:NH1	2.31	0.64
1:C:1208:VAL:HA	1:C:1211:LEU:HD23	1.80	0.64
1:D:4211:LYS:HB3	1:D:4211:LYS:HZ2	1.59	0.64
1:A:2258:LEU:HB3	1:A:2297:LYS:HZ1	1.62	0.64
1:B:838:HIS:HB3	1:B:1200:GLY:C	2.22	0.64
1:D:101:LEU:HB3	1:D:150:MET:HE1	1.80	0.64
1:A:746:CYS:HA	1:A:757:PHE:CD1	2.32	0.64
1:A:877:ASN:ND2	1:A:1045:THR:OG1	2.30	0.64
1:C:2110:TYR:HD2	1:C:3695:PRO:HG2	1.61	0.64
1:D:838:HIS:HB3	1:D:1200:GLY:C	2.22	0.64
1:B:719:LEU:HA	1:B:730:VAL:HG22	1.79	0.64
1:C:1158:ASN:ND2	1:C:1182:ILE:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:877:ASN:ND2	1:D:1045:THR:OG1	2.30	0.64
1:B:853:PRO:HG3	1:B:1024:TYR:H	1.61	0.64
1:C:1708:ARG:NE	1:C:1830:VAL:CG1	2.50	0.64
1:B:520:ASN:ND2	1:B:555:GLU:OE2	2.31	0.63
1:B:3695:PRO:HB3	1:B:3699:HIS:HD2	1.63	0.63
1:A:838:HIS:HB3	1:A:1200:GLY:C	2.22	0.63
1:B:877:ASN:ND2	1:B:1045:THR:OG1	2.30	0.63
1:B:1435:TYR:HB3	1:B:1575:LEU:HD22	1.80	0.63
1:B:4181:ILE:HG22	1:B:4193:ILE:HB	1.81	0.63
1:C:101:LEU:HB3	1:C:150:MET:HE1	1.80	0.63
1:C:877:ASN:ND2	1:C:1045:THR:OG1	2.30	0.63
1:C:3695:PRO:HB3	1:C:3699:HIS:HD2	1.63	0.63
1:D:4181:ILE:HG22	1:D:4193:ILE:HB	1.81	0.63
1:A:3695:PRO:HB3	1:A:3699:HIS:HD2	1.63	0.63
1:C:520:ASN:ND2	1:C:555:GLU:OE2	2.31	0.63
1:B:1208:VAL:HA	1:B:1211:LEU:HD23	1.80	0.63
1:C:746:CYS:HA	1:C:757:PHE:CD1	2.32	0.63
1:A:1743:ARG:O	1:A:1964:ARG:NH2	2.31	0.63
1:D:783:PHE:HB2	1:D:787:VAL:HG21	1.79	0.63
1:D:853:PRO:HG3	1:D:1024:TYR:H	1.61	0.63
1:A:1435:TYR:HB3	1:A:1575:LEU:HD22	1.80	0.63
1:B:1743:ARG:O	1:B:1964:ARG:NH2	2.31	0.63
1:B:4175:ARG:H	1:B:4176:PRO:CD	2.07	0.63
1:C:1743:ARG:O	1:C:1964:ARG:NH2	2.31	0.63
1:A:1144:GLN:HE22	1:A:1164:LEU:HD11	1.64	0.63
1:B:746:CYS:HA	1:B:757:PHE:CD1	2.32	0.63
1:C:4181:ILE:HG22	1:C:4193:ILE:HB	1.81	0.63
1:D:1144:GLN:HE22	1:D:1164:LEU:HD11	1.64	0.63
1:D:3695:PRO:HB3	1:D:3699:HIS:HD2	1.63	0.63
1:B:1144:GLN:HE22	1:B:1164:LEU:HD11	1.64	0.63
1:C:783:PHE:HB2	1:C:787:VAL:HG21	1.79	0.63
1:C:2199:ARG:NE	1:C:2246:ASN:OD1	2.31	0.63
1:D:520:ASN:ND2	1:D:555:GLU:OE2	2.31	0.63
1:D:1743:ARG:O	1:D:1964:ARG:NH2	2.31	0.63
1:A:520:ASN:ND2	1:A:555:GLU:OE2	2.31	0.63
1:A:4181:ILE:HG22	1:A:4193:ILE:HB	1.81	0.63
1:B:101:LEU:HB3	1:B:150:MET:HE1	1.80	0.63
1:A:4895:GLY:O	1:B:4892:ARG:NH2	2.32	0.62
1:B:4895:GLY:O	1:C:4892:ARG:NH2	2.32	0.62
1:C:1243:PRO:HB2	1:C:1600:LEU:HD13	1.81	0.62
1:D:627:PRO:O	1:D:629:ARG:NH1	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:879:HIS:NE2	1:C:908:VAL:O	2.28	0.62
1:C:1144:GLN:HE22	1:C:1164:LEU:HD11	1.64	0.62
1:A:4679:ARG:NH1	1:A:4715:TYR:OH	2.31	0.62
1:B:156:GLN:OE1	1:B:157:ARG:NH1	2.32	0.62
1:C:156:GLN:OE1	1:C:157:ARG:NH1	2.32	0.62
1:C:1164:LEU:HB3	1:C:1169:LEU:HD21	1.81	0.62
1:A:2199:ARG:NE	1:A:2246:ASN:OD1	2.31	0.62
1:A:4892:ARG:NH2	1:D:4895:GLY:O	2.32	0.62
1:B:1932:PRO:O	1:B:1933:GLU:C	2.42	0.62
1:C:1719:HIS:NE2	1:C:1802:ILE:HG13	2.15	0.62
1:A:392:ARG:HH11	1:A:393:CYS:H	1.48	0.62
1:A:1144:GLN:NE2	1:A:1165:ASN:OD1	2.33	0.62
1:D:392:ARG:HH11	1:D:393:CYS:H	1.48	0.62
1:A:156:GLN:OE1	1:A:157:ARG:NH1	2.32	0.62
1:A:1932:PRO:O	1:A:1933:GLU:C	2.42	0.62
1:C:1708:ARG:CD	1:C:1830:VAL:CG1	2.78	0.62
1:A:3767:GLN:OE1	1:A:3809:ASN:ND2	2.31	0.62
1:B:392:ARG:HH11	1:B:393:CYS:H	1.48	0.62
1:C:1144:GLN:NE2	1:C:1165:ASN:OD1	2.33	0.62
1:C:1435:TYR:HB3	1:C:1575:LEU:HD22	1.80	0.62
1:D:1024:TYR:HA	1:D:1032:LYS:HE2	1.82	0.62
1:D:1708:ARG:CD	1:D:1830:VAL:CG1	2.78	0.62
1:A:1243:PRO:HB2	1:A:1600:LEU:HD13	1.81	0.62
1:C:4232:GLU:OE1	1:C:5019:TRP:NE1	2.26	0.62
1:A:4232:GLU:OE1	1:A:5019:TRP:NE1	2.26	0.62
1:C:1024:TYR:HA	1:C:1032:LYS:HE2	1.82	0.62
1:D:1164:LEU:HB3	1:D:1169:LEU:HD21	1.81	0.62
1:A:101:LEU:HB3	1:A:150:MET:HE1	1.80	0.61
1:A:879:HIS:NE2	1:A:908:VAL:O	2.28	0.61
1:B:1164:LEU:HB3	1:B:1169:LEU:HD21	1.81	0.61
1:B:2257:LEU:HD11	1:B:2276:ALA:HB2	1.82	0.61
1:C:4895:GLY:O	1:D:4892:ARG:NH2	2.32	0.61
1:A:2257:LEU:HD11	1:A:2276:ALA:HB2	1.82	0.61
1:B:580:GLU:HG2	1:B:583:ILE:HD11	1.83	0.61
1:B:1144:GLN:NE2	1:B:1165:ASN:OD1	2.33	0.61
1:B:1243:PRO:HB2	1:B:1600:LEU:HD13	1.81	0.61
1:D:1243:PRO:HB2	1:D:1600:LEU:HD13	1.81	0.61
1:A:1024:TYR:HA	1:A:1032:LYS:HE2	1.82	0.61
1:A:1164:LEU:HB3	1:A:1169:LEU:HD21	1.81	0.61
1:A:1719:HIS:NE2	1:A:1802:ILE:HG13	2.15	0.61
1:D:2199:ARG:NE	1:D:2246:ASN:OD1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4856:PHE:O	1:D:4860:ARG:NH2	2.34	0.61
1:A:4856:PHE:O	1:A:4860:ARG:NH2	2.34	0.61
1:D:1719:HIS:NE2	1:D:1802:ILE:HG13	2.15	0.61
1:A:580:GLU:HG2	1:A:583:ILE:HD11	1.83	0.61
1:B:1024:TYR:HA	1:B:1032:LYS:HE2	1.82	0.61
1:B:4680:LYS:HD3	1:B:4686:LEU:HD22	1.83	0.61
1:C:392:ARG:HH11	1:C:393:CYS:H	1.48	0.61
1:D:234:SER:HB2	1:D:242:ARG:HA	1.83	0.61
1:D:1144:GLN:NE2	1:D:1165:ASN:OD1	2.33	0.61
1:D:1435:TYR:HB3	1:D:1575:LEU:HD22	1.80	0.61
1:B:4856:PHE:O	1:B:4860:ARG:NH2	2.34	0.61
1:C:4679:ARG:NH1	1:C:4715:TYR:OH	2.31	0.61
1:D:156:GLN:OE1	1:D:157:ARG:NH1	2.32	0.61
1:A:1160:ILE:HB	1:A:1179:PHE:HB2	1.83	0.61
1:B:1708:ARG:CD	1:B:1830:VAL:CG1	2.78	0.61
1:C:2257:LEU:HD11	1:C:2276:ALA:HB2	1.82	0.61
1:A:1708:ARG:CD	1:A:1830:VAL:CG1	2.78	0.61
1:C:1933:GLU:O	1:C:1935:VAL:N	2.34	0.61
1:D:243:ARG:NH1	1:D:301:VAL:O	2.34	0.61
1:D:3767:GLN:OE1	1:D:3809:ASN:ND2	2.31	0.61
1:A:2042:CYS:SG	1:A:2043:GLY:N	2.75	0.60
1:C:131:LEU:HD12	1:C:178:ARG:HH12	1.66	0.60
1:C:294:THR:HG23	1:C:295:GLU:H	1.66	0.60
1:C:4680:LYS:HD3	1:C:4686:LEU:HD22	1.83	0.60
1:D:1730:MET:O	1:D:1772:ARG:NH1	2.34	0.60
1:A:1933:GLU:O	1:A:1935:VAL:N	2.34	0.60
1:B:1454:THR:HG22	1:B:1456:ASP:H	1.66	0.60
1:C:234:SER:HB2	1:C:242:ARG:HA	1.83	0.60
1:D:1932:PRO:O	1:D:1933:GLU:C	2.42	0.60
1:B:243:ARG:NH1	1:B:301:VAL:O	2.34	0.60
1:B:243:ARG:HA	1:B:301:VAL:HG12	1.84	0.60
1:B:294:THR:HG23	1:B:295:GLU:H	1.66	0.60
1:C:1730:MET:O	1:C:1772:ARG:NH1	2.34	0.60
1:C:1762:LEU:N	1:C:1762:LEU:HD23	2.16	0.60
1:C:1932:PRO:O	1:C:1933:GLU:C	2.42	0.60
1:D:131:LEU:HD12	1:D:178:ARG:HH12	1.66	0.60
1:D:2257:LEU:HD11	1:D:2276:ALA:HB2	1.82	0.60
1:A:4680:LYS:HD3	1:A:4686:LEU:HD22	1.83	0.60
1:B:234:SER:HB2	1:B:242:ARG:HA	1.83	0.60
1:B:1730:MET:O	1:B:1772:ARG:NH1	2.34	0.60
1:B:1933:GLU:O	1:B:1935:VAL:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2042:CYS:SG	1:B:2043:GLY:N	2.75	0.60
1:B:2199:ARG:NE	1:B:2246:ASN:OD1	2.31	0.60
1:B:3767:GLN:OE1	1:B:3809:ASN:ND2	2.31	0.60
1:C:1160:ILE:HB	1:C:1179:PHE:HB2	1.83	0.60
1:C:2042:CYS:SG	1:C:2043:GLY:N	2.75	0.60
1:C:4856:PHE:O	1:C:4860:ARG:NH2	2.34	0.60
1:A:1838:PHE:O	1:A:1839:VAL:C	2.45	0.60
1:B:1719:HIS:NE2	1:B:1802:ILE:HG13	2.15	0.60
1:B:1762:LEU:N	1:B:1762:LEU:HD23	2.16	0.60
1:D:1762:LEU:HD23	1:D:1762:LEU:N	2.16	0.60
1:A:1454:THR:HG22	1:A:1456:ASP:H	1.66	0.60
1:D:243:ARG:HA	1:D:301:VAL:HG12	1.84	0.60
1:A:131:LEU:HD12	1:A:178:ARG:HH12	1.66	0.60
1:C:4666:VAL:C	1:C:4668:LEU:H	2.10	0.60
1:D:44:ASN:O	1:D:45:ARG:NH1	2.35	0.60
1:D:879:HIS:NE2	1:D:908:VAL:O	2.28	0.60
1:D:2042:CYS:SG	1:D:2043:GLY:N	2.75	0.60
1:A:1762:LEU:N	1:A:1762:LEU:HD23	2.16	0.60
1:B:1838:PHE:O	1:B:1839:VAL:C	2.45	0.60
1:B:4679:ARG:NH1	1:B:4715:TYR:OH	2.31	0.60
1:C:1838:PHE:O	1:C:1839:VAL:C	2.45	0.60
1:C:3767:GLN:OE1	1:C:3809:ASN:ND2	2.31	0.60
1:A:1730:MET:O	1:A:1772:ARG:NH1	2.34	0.60
1:B:131:LEU:HD12	1:B:178:ARG:HH12	1.66	0.60
1:B:1160:ILE:HB	1:B:1179:PHE:HB2	1.83	0.60
1:C:580:GLU:HG2	1:C:583:ILE:HD11	1.83	0.60
1:D:4680:LYS:HD3	1:D:4686:LEU:HD22	1.83	0.60
1:A:1716:ILE:O	1:A:1720:LEU:HD23	2.02	0.59
1:C:709:ASP:O	1:C:725:HIS:ND1	2.36	0.59
1:D:1160:ILE:HB	1:D:1179:PHE:HB2	1.83	0.59
1:D:1838:PHE:O	1:D:1839:VAL:C	2.45	0.59
1:B:44:ASN:O	1:B:45:ARG:NH1	2.35	0.59
1:D:580:GLU:HG2	1:D:583:ILE:HD11	1.83	0.59
1:D:4679:ARG:NH1	1:D:4715:TYR:OH	2.31	0.59
1:A:243:ARG:NH1	1:A:301:VAL:O	2.34	0.59
1:A:1103:GLY:HA3	1:A:1123:VAL:HA	1.84	0.59
1:C:44:ASN:O	1:C:45:ARG:NH1	2.35	0.59
1:C:243:ARG:NH1	1:C:301:VAL:O	2.34	0.59
1:A:44:ASN:O	1:A:45:ARG:NH1	2.35	0.59
1:A:243:ARG:HA	1:A:301:VAL:HG12	1.84	0.59
1:B:1716:ILE:O	1:B:1720:LEU:HD23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2165:LEU:HD13	1:A:2178:MET:HE2	1.85	0.59
1:C:320:LYS:NZ	1:C:381:GLU:O	2.35	0.59
1:A:1293:LEU:HD11	1:A:1580:PHE:CE1	2.38	0.59
1:B:1103:GLY:HA3	1:B:1123:VAL:HA	1.84	0.59
1:B:2165:LEU:HD13	1:B:2178:MET:HE2	1.85	0.59
1:B:4666:VAL:C	1:B:4668:LEU:H	2.10	0.59
1:C:2165:LEU:HD13	1:C:2178:MET:HE2	1.85	0.59
1:D:294:THR:HG23	1:D:295:GLU:H	1.66	0.59
1:D:1716:ILE:O	1:D:1720:LEU:HD23	2.02	0.59
1:D:2165:LEU:HD13	1:D:2178:MET:HE2	1.85	0.59
1:A:234:SER:HB2	1:A:242:ARG:HA	1.83	0.59
1:A:320:LYS:NZ	1:A:381:GLU:O	2.35	0.59
1:B:709:ASP:O	1:B:725:HIS:ND1	2.36	0.59
1:C:1155:LEU:HD23	1:C:1184:ILE:HD12	1.85	0.59
1:C:1454:THR:HG22	1:C:1456:ASP:H	1.66	0.59
1:D:320:LYS:NZ	1:D:381:GLU:O	2.35	0.59
1:D:1293:LEU:HD11	1:D:1580:PHE:CE1	2.38	0.59
1:B:4211:LYS:HB3	1:B:4211:LYS:HZ2	1.67	0.59
1:C:652:ARG:NE	1:C:750:LEU:O	2.36	0.59
1:D:709:ASP:O	1:D:725:HIS:ND1	2.36	0.59
1:D:1103:GLY:HA3	1:D:1123:VAL:HA	1.84	0.59
1:D:1738:LEU:HD22	1:D:1963:GLU:HG3	1.85	0.59
1:C:1293:LEU:HD11	1:C:1580:PHE:CE1	2.38	0.58
1:D:4666:VAL:C	1:D:4668:LEU:H	2.10	0.58
1:A:4666:VAL:C	1:A:4668:LEU:H	2.10	0.58
1:B:1155:LEU:HD23	1:B:1184:ILE:HD12	1.85	0.58
1:B:4865:LYS:HA	1:B:4865:LYS:HZ3	1.67	0.58
1:C:1716:ILE:O	1:C:1720:LEU:HD23	2.02	0.58
1:D:243:ARG:HB3	1:D:300:VAL:HG23	1.86	0.58
1:D:1155:LEU:HD23	1:D:1184:ILE:HD12	1.85	0.58
1:D:1454:THR:HG22	1:D:1456:ASP:H	1.66	0.58
1:C:1103:GLY:HA3	1:C:1123:VAL:HA	1.84	0.58
1:D:1933:GLU:O	1:D:1935:VAL:N	2.34	0.58
1:A:709:ASP:O	1:A:725:HIS:ND1	2.36	0.58
1:A:4865:LYS:HZ3	1:A:4865:LYS:HA	1.68	0.58
1:B:4666:VAL:O	1:B:4668:LEU:N	2.37	0.58
1:C:1738:LEU:HD22	1:C:1963:GLU:HG3	1.85	0.58
1:C:2255:SER:O	1:C:2297:LYS:NZ	2.36	0.58
1:D:652:ARG:NE	1:D:750:LEU:O	2.36	0.58
1:A:2255:SER:O	1:A:2297:LYS:NZ	2.36	0.58
1:B:243:ARG:HB3	1:B:300:VAL:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1293:LEU:HD11	1:B:1580:PHE:CE1	2.38	0.58
1:D:4666:VAL:O	1:D:4668:LEU:N	2.37	0.58
1:A:4666:VAL:O	1:A:4668:LEU:N	2.37	0.58
1:B:2255:SER:O	1:B:2297:LYS:NZ	2.36	0.58
1:A:69:LEU:HD22	1:A:107:ILE:HD11	1.86	0.58
1:B:209:CYS:HB2	1:B:215:THR:HG21	1.86	0.58
1:B:879:HIS:NE2	1:B:908:VAL:O	2.28	0.58
1:B:4138:ASP:O	1:B:4142:ASN:ND2	2.37	0.58
1:D:1189:LEU:HD12	1:D:1190:PRO:HD2	1.86	0.58
1:A:243:ARG:HB3	1:A:300:VAL:HG23	1.86	0.58
1:A:294:THR:HG23	1:A:295:GLU:H	1.66	0.58
1:A:2135:LEU:HD13	1:A:3662:ILE:HD11	1.86	0.58
1:A:4138:ASP:O	1:A:4142:ASN:ND2	2.37	0.58
1:B:69:LEU:HD22	1:B:107:ILE:HD11	1.86	0.58
1:B:4211:LYS:HB3	1:B:4211:LYS:HZ3	1.69	0.58
1:C:69:LEU:HD22	1:C:107:ILE:HD11	1.86	0.58
1:D:2255:SER:O	1:D:2297:LYS:NZ	2.36	0.58
1:A:793:LEU:HD22	1:A:821:LEU:HD21	1.86	0.58
1:C:243:ARG:HA	1:C:301:VAL:HG12	1.84	0.58
1:A:1155:LEU:HD23	1:A:1184:ILE:HD12	1.85	0.58
1:B:320:LYS:NZ	1:B:381:GLU:O	2.35	0.58
1:B:652:ARG:NE	1:B:750:LEU:O	2.36	0.58
1:C:1189:LEU:HD12	1:C:1190:PRO:HD2	1.86	0.58
1:C:4666:VAL:O	1:C:4668:LEU:N	2.37	0.58
1:D:69:LEU:HD22	1:D:107:ILE:HD11	1.86	0.58
1:D:2110:TYR:HA	1:D:3700:GLN:HE21	1.69	0.58
1:D:4865:LYS:HZ3	1:D:4865:LYS:HA	1.68	0.58
1:A:209:CYS:HB2	1:A:215:THR:HG21	1.86	0.57
1:A:315:CYS:SG	1:A:316:PHE:N	2.77	0.57
1:A:652:ARG:NE	1:A:750:LEU:O	2.36	0.57
1:A:2110:TYR:CD2	1:A:3695:PRO:HG2	2.39	0.57
1:C:209:CYS:HB2	1:C:215:THR:HG21	1.86	0.57
1:C:2110:TYR:CD2	1:C:3695:PRO:HG2	2.39	0.57
1:C:4138:ASP:O	1:C:4142:ASN:ND2	2.37	0.57
1:A:1189:LEU:HD12	1:A:1190:PRO:HD2	1.86	0.57
1:C:243:ARG:HB3	1:C:300:VAL:HG23	1.86	0.57
1:C:4211:LYS:HB3	1:C:4211:LYS:HZ3	1.67	0.57
1:A:1738:LEU:HD22	1:A:1963:GLU:HG3	1.85	0.57
1:C:4152:GLU:OE1	1:C:4194:TYR:OH	2.22	0.57
1:B:793:LEU:HD22	1:B:821:LEU:HD21	1.86	0.57
1:C:138:GLN:HG2	1:C:139:GLU:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2337:PHE:HA	1:D:2340:PHE:HB2	1.86	0.57
1:D:4138:ASP:O	1:D:4142:ASN:ND2	2.37	0.57
1:A:1160:ILE:HB	1:A:1179:PHE:CD2	2.40	0.57
1:C:315:CYS:SG	1:C:316:PHE:N	2.77	0.57
1:C:2135:LEU:HD13	1:C:3662:ILE:HD11	1.86	0.57
1:C:2337:PHE:HA	1:C:2340:PHE:HB2	1.86	0.57
1:B:2337:PHE:HA	1:B:2340:PHE:HB2	1.86	0.57
1:D:2110:TYR:CD2	1:D:3695:PRO:HG2	2.39	0.57
1:A:2337:PHE:HA	1:A:2340:PHE:HB2	1.86	0.57
1:B:1738:LEU:HD22	1:B:1963:GLU:HG3	1.85	0.57
1:D:2135:LEU:HD13	1:D:3662:ILE:HD11	1.86	0.57
1:B:1160:ILE:HB	1:B:1179:PHE:CD2	2.40	0.57
1:D:315:CYS:SG	1:D:316:PHE:N	2.77	0.57
1:B:138:GLN:HG2	1:B:139:GLU:H	1.70	0.57
1:B:1225:PRO:HG2	1:B:1228:ILE:HB	1.87	0.57
1:B:2110:TYR:CD2	1:B:3695:PRO:HG2	2.39	0.57
1:B:1189:LEU:HD12	1:B:1190:PRO:HD2	1.86	0.57
1:D:209:CYS:HB2	1:D:215:THR:HG21	1.86	0.57
1:A:2110:TYR:HA	1:A:3700:GLN:HE21	1.69	0.56
1:C:4039:MET:HA	1:C:4039:MET:HE2	1.86	0.56
1:D:138:GLN:HG2	1:D:139:GLU:H	1.70	0.56
1:D:793:LEU:HD22	1:D:821:LEU:HD21	1.86	0.56
1:A:138:GLN:HG2	1:A:139:GLU:H	1.70	0.56
1:B:4039:MET:HE2	1:B:4039:MET:HA	1.86	0.56
1:A:998:ARG:O	1:A:1003:GLN:N	2.30	0.56
1:A:3670:GLU:HG2	1:A:3731:LYS:HE3	1.87	0.56
1:A:4152:GLU:OE1	1:A:4194:TYR:OH	2.22	0.56
1:B:1683:HIS:HB3	1:B:1782:PHE:HZ	1.70	0.56
1:B:1699:GLU:OE1	1:B:1813:ARG:NH1	2.38	0.56
1:B:3670:GLU:HG2	1:B:3731:LYS:HE3	1.87	0.56
1:C:793:LEU:HD22	1:C:821:LEU:HD21	1.86	0.56
1:C:1205:GLY:HA2	1:C:1211:LEU:HD21	1.88	0.56
1:C:1683:HIS:HB3	1:C:1782:PHE:HZ	1.70	0.56
1:D:3670:GLU:HG2	1:D:3731:LYS:HE3	1.87	0.56
1:B:315:CYS:SG	1:B:316:PHE:N	2.77	0.56
1:B:1720:LEU:C	1:B:1720:LEU:HD12	2.31	0.56
1:B:4152:GLU:OE1	1:B:4194:TYR:OH	2.22	0.56
1:D:1205:GLY:HA2	1:D:1211:LEU:HD21	1.88	0.56
1:C:686:TRP:NE1	1:C:746:CYS:SG	2.79	0.56
1:C:1160:ILE:HB	1:C:1179:PHE:CD2	2.40	0.56
1:C:3670:GLU:HG2	1:C:3731:LYS:HE3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1225:PRO:HG2	1:D:1228:ILE:HB	1.87	0.56
1:B:686:TRP:NE1	1:B:746:CYS:SG	2.79	0.56
1:D:4039:MET:HE2	1:D:4039:MET:HA	1.86	0.56
1:A:1205:GLY:HA2	1:A:1211:LEU:HD21	1.88	0.56
1:B:998:ARG:O	1:B:1003:GLN:N	2.30	0.56
1:C:1720:LEU:C	1:C:1720:LEU:HD12	2.31	0.56
1:C:4818:MET:O	1:C:4824:ARG:NH1	2.39	0.56
1:D:131:LEU:HB2	1:D:178:ARG:HH22	1.71	0.56
1:A:131:LEU:HB2	1:A:178:ARG:HH22	1.71	0.56
1:B:123:THR:OG1	1:B:134:ASP:OD1	2.24	0.56
1:B:131:LEU:HB2	1:B:178:ARG:HH22	1.71	0.56
1:C:1930:LYS:O	1:C:1931:LEU:C	2.49	0.56
1:D:686:TRP:NE1	1:D:746:CYS:SG	2.79	0.56
1:D:1160:ILE:HB	1:D:1179:PHE:CD2	2.40	0.56
1:B:2135:LEU:HD13	1:B:3662:ILE:HD11	1.86	0.56
1:D:1699:GLU:OE1	1:D:1813:ARG:NH1	2.38	0.56
1:A:1225:PRO:HG2	1:A:1228:ILE:HB	1.87	0.55
1:A:4556:SER:HB2	1:A:4664:LEU:HB2	1.88	0.55
1:A:4818:MET:O	1:A:4824:ARG:NH1	2.39	0.55
1:D:1720:LEU:C	1:D:1720:LEU:HD12	2.31	0.55
1:D:4818:MET:O	1:D:4824:ARG:NH1	2.39	0.55
1:A:4666:VAL:N	1:A:4667:PRO:HD2	2.22	0.55
1:B:1205:GLY:HA2	1:B:1211:LEU:HD21	1.88	0.55
1:B:1930:LYS:O	1:B:1931:LEU:C	2.49	0.55
1:B:4556:SER:HB2	1:B:4664:LEU:HB2	1.88	0.55
1:B:4688:ILE:HD12	1:B:4737:ILE:HD12	1.88	0.55
1:C:4688:ILE:HD12	1:C:4737:ILE:HD12	1.88	0.55
1:D:4666:VAL:N	1:D:4667:PRO:HD2	2.22	0.55
1:A:686:TRP:NE1	1:A:746:CYS:SG	2.79	0.55
1:A:1720:LEU:C	1:A:1720:LEU:HD12	2.31	0.55
1:A:1930:LYS:O	1:A:1931:LEU:C	2.49	0.55
1:A:4039:MET:HE2	1:A:4039:MET:HA	1.86	0.55
1:B:1935:VAL:O	1:B:1936:LYS:C	2.50	0.55
1:A:1717:SER:HA	1:A:1720:LEU:HD21	1.89	0.55
1:C:1225:PRO:HG2	1:C:1228:ILE:HB	1.87	0.55
1:D:4666:VAL:H	1:D:4667:PRO:HD2	1.72	0.55
1:A:221:ARG:NH2	1:A:255:HIS:O	2.40	0.55
1:C:131:LEU:HB2	1:C:178:ARG:HH22	1.71	0.55
1:D:4099:SER:O	1:D:4101:LYS:NZ	2.39	0.55
1:A:1699:GLU:OE1	1:A:1813:ARG:NH1	2.38	0.55
1:B:4818:MET:O	1:B:4824:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4978:HIS:ND1	1:B:4982:GLU:OE1	2.40	0.55
1:D:4152:GLU:OE1	1:D:4194:TYR:OH	2.22	0.55
1:A:4666:VAL:H	1:A:4667:PRO:HD2	1.72	0.55
1:B:2110:TYR:HA	1:B:3700:GLN:HE21	1.69	0.55
1:C:972:LEU:O	1:C:1044:ARG:NH2	2.40	0.55
1:D:221:ARG:NH2	1:D:255:HIS:O	2.40	0.55
1:D:4978:HIS:ND1	1:D:4982:GLU:OE1	2.40	0.55
1:A:1935:VAL:O	1:A:1936:LYS:C	2.50	0.55
1:B:838:HIS:HA	1:B:1201:HIS:CB	2.37	0.55
1:B:4864:ASN:C	1:B:4866:SER:N	2.65	0.55
1:C:838:HIS:HA	1:C:1201:HIS:CB	2.37	0.55
1:C:4666:VAL:N	1:C:4667:PRO:HD2	2.22	0.55
1:D:893:TYR:HD1	1:D:907:LEU:HB2	1.72	0.55
1:D:1683:HIS:HB3	1:D:1782:PHE:HZ	1.70	0.55
1:A:1859:VAL:HA	1:A:1862:ILE:HG12	1.89	0.55
1:A:4978:HIS:ND1	1:A:4982:GLU:OE1	2.40	0.55
1:B:972:LEU:O	1:B:1044:ARG:NH2	2.40	0.55
1:B:1859:VAL:HA	1:B:1862:ILE:HG12	1.89	0.55
1:C:4839:MET:SD	1:D:4822:THR:OG1	2.63	0.55
1:D:1717:SER:HA	1:D:1720:LEU:HD21	1.89	0.55
1:B:1729:SER:O	1:B:2163:ARG:NH1	2.40	0.54
1:B:4666:VAL:N	1:B:4667:PRO:HD2	2.22	0.54
1:C:1699:GLU:OE1	1:C:1813:ARG:NH1	2.38	0.54
1:C:4666:VAL:H	1:C:4667:PRO:HD2	1.72	0.54
1:C:4978:HIS:ND1	1:C:4982:GLU:OE1	2.40	0.54
1:D:675:LEU:HG	1:D:676:THR:H	1.72	0.54
1:D:838:HIS:HA	1:D:1201:HIS:CB	2.37	0.54
1:D:1729:SER:O	1:D:2163:ARG:NH1	2.40	0.54
1:A:972:LEU:O	1:A:1044:ARG:NH2	2.40	0.54
1:B:221:ARG:NH2	1:B:255:HIS:O	2.40	0.54
1:C:1610:ASN:O	1:C:1611:HIS:ND1	2.41	0.54
1:A:1683:HIS:HB3	1:A:1782:PHE:HZ	1.70	0.54
1:A:1729:SER:O	1:A:2163:ARG:NH1	2.40	0.54
1:B:893:TYR:HD1	1:B:907:LEU:HB2	1.72	0.54
1:D:1610:ASN:O	1:D:1611:HIS:ND1	2.41	0.54
1:D:1930:LYS:O	1:D:1931:LEU:C	2.49	0.54
1:D:1935:VAL:O	1:D:1936:LYS:C	2.50	0.54
1:A:4688:ILE:HD12	1:A:4737:ILE:HD12	1.88	0.54
1:B:1717:SER:HA	1:B:1720:LEU:HD21	1.89	0.54
1:D:123:THR:OG1	1:D:134:ASP:OD1	2.24	0.54
1:D:972:LEU:O	1:D:1044:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4864:ASN:C	1:A:4866:SER:N	2.65	0.54
1:C:893:TYR:HD1	1:C:907:LEU:HB2	1.72	0.54
1:C:1717:SER:HA	1:C:1720:LEU:HD21	1.89	0.54
1:A:144:GLU:O	1:A:175:SER:OG	2.20	0.54
1:A:893:TYR:HD1	1:A:907:LEU:HB2	1.72	0.54
1:A:1610:ASN:O	1:A:1611:HIS:ND1	2.41	0.54
1:B:144:GLU:O	1:B:175:SER:OG	2.20	0.54
1:B:4666:VAL:H	1:B:4667:PRO:HD2	1.72	0.54
1:C:144:GLU:O	1:C:175:SER:OG	2.20	0.54
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.90	0.54
1:C:1729:SER:O	1:C:2163:ARG:NH1	2.40	0.54
1:C:1935:VAL:O	1:C:1936:LYS:C	2.50	0.54
1:C:4556:SER:HB2	1:C:4664:LEU:HB2	1.88	0.54
1:D:721:LEU:N	1:D:728:ARG:O	2.40	0.54
1:A:4691:GLN:HE22	1:A:4703:ARG:HH22	1.56	0.54
1:A:4873:ASP:O	1:A:4874:MET:C	2.50	0.54
1:B:1610:ASN:O	1:B:1611:HIS:ND1	2.41	0.54
1:C:675:LEU:HG	1:C:676:THR:H	1.72	0.54
1:C:721:LEU:N	1:C:728:ARG:O	2.40	0.54
1:D:4556:SER:HB2	1:D:4664:LEU:HB2	1.88	0.54
1:D:4688:ILE:HD12	1:D:4737:ILE:HD12	1.88	0.54
1:D:4864:ASN:C	1:D:4866:SER:N	2.65	0.54
1:C:221:ARG:NH2	1:C:255:HIS:O	2.40	0.54
1:C:1859:VAL:HA	1:C:1862:ILE:HG12	1.89	0.54
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.90	0.54
1:B:721:LEU:N	1:B:728:ARG:O	2.40	0.54
1:C:1077:ALA:HB3	1:C:1189:LEU:HD11	1.90	0.54
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.90	0.54
1:C:3874:VAL:HG23	1:C:3875:MET:HG2	1.90	0.54
1:D:49:LEU:HD12	1:D:189:LEU:HB3	1.90	0.54
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.90	0.54
1:D:1859:VAL:HA	1:D:1862:ILE:HG12	1.89	0.54
1:A:1077:ALA:HB3	1:A:1189:LEU:HD11	1.90	0.53
1:C:49:LEU:HD12	1:C:189:LEU:HB3	1.90	0.53
1:C:759:ILE:HG13	1:C:761:GLY:H	1.74	0.53
1:D:998:ARG:O	1:D:1003:GLN:N	2.30	0.53
1:A:1289:LEU:HD21	1:A:1597:VAL:CG2	2.39	0.53
1:A:4839:MET:SD	1:B:4822:THR:OG1	2.63	0.53
1:B:4772:ASP:OD1	1:B:4773:VAL:N	2.42	0.53
1:C:275:ARG:HD2	1:C:336:PRO:HD2	1.90	0.53
1:A:675:LEU:HG	1:A:676:THR:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:LEU:N	1:A:728:ARG:O	2.40	0.53
1:A:4772:ASP:OD1	1:A:4773:VAL:N	2.42	0.53
1:B:274:LEU:HB3	1:B:339:ILE:HD12	1.90	0.53
1:B:881:LEU:O	1:B:885:THR:HG23	2.09	0.53
1:C:123:THR:OG1	1:C:134:ASP:OD1	2.24	0.53
1:C:771:PHE:HA	1:C:1471:ALA:O	2.08	0.53
1:C:4864:ASN:C	1:C:4866:SER:N	2.65	0.53
1:A:838:HIS:HA	1:A:1201:HIS:CB	2.37	0.53
1:B:275:ARG:HD2	1:B:336:PRO:HD2	1.90	0.53
1:B:1077:ALA:HB3	1:B:1189:LEU:HD11	1.90	0.53
1:C:881:LEU:O	1:C:885:THR:HG23	2.09	0.53
1:C:4979:THR:O	1:C:4979:THR:CG2	2.56	0.53
1:D:224:HIS:N	1:D:229:GLU:O	2.42	0.53
1:A:424:LYS:NZ	1:A:431:PRO:O	2.42	0.53
1:A:881:LEU:O	1:A:885:THR:HG23	2.09	0.53
1:B:771:PHE:HA	1:B:1471:ALA:O	2.08	0.53
1:D:4691:GLN:HE22	1:D:4703:ARG:HH22	1.56	0.53
1:A:224:HIS:N	1:A:229:GLU:O	2.42	0.53
1:A:3695:PRO:HB3	1:A:3699:HIS:CD2	2.44	0.53
1:B:424:LYS:NZ	1:B:431:PRO:O	2.42	0.53
1:B:2288:LEU:HD12	1:B:3853:ALA:HB2	1.91	0.53
1:B:4979:THR:O	1:B:4979:THR:CG2	2.56	0.53
1:C:1708:ARG:HD3	1:C:1830:VAL:CG1	2.39	0.53
1:C:2110:TYR:HA	1:C:3700:GLN:HE22	1.74	0.53
1:C:4206:GLU:HA	1:C:4211:LYS:HD3	1.90	0.53
1:C:4865:LYS:HA	1:C:4865:LYS:HZ3	1.73	0.53
1:D:275:ARG:HD2	1:D:336:PRO:HD2	1.90	0.53
1:D:4968:PHE:HD2	1:D:4975:PHE:HD1	1.57	0.53
1:A:4822:THR:OG1	1:D:4839:MET:SD	2.63	0.53
1:B:675:LEU:HG	1:B:676:THR:H	1.72	0.53
1:C:274:LEU:HB3	1:C:339:ILE:HD12	1.90	0.53
1:C:4873:ASP:O	1:C:4874:MET:C	2.50	0.53
1:D:3874:VAL:HG23	1:D:3875:MET:HG2	1.90	0.53
1:A:118:LEU:HA	1:A:137:LEU:HB3	1.91	0.53
1:A:4206:GLU:HA	1:A:4211:LYS:HD3	1.90	0.53
1:B:927:GLU:O	1:B:931:THR:HG23	2.09	0.53
1:B:4205:TRP:CE3	1:B:4989:MET:HE1	2.44	0.53
1:B:4691:GLN:HE22	1:B:4703:ARG:HH22	1.56	0.53
1:C:424:LYS:NZ	1:C:431:PRO:O	2.42	0.53
1:C:2110:TYR:HA	1:C:3700:GLN:HE21	1.69	0.53
1:A:274:LEU:HB3	1:A:339:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ARG:HD2	1:A:336:PRO:HD2	1.90	0.53
1:A:771:PHE:HA	1:A:1471:ALA:O	2.08	0.53
1:B:118:LEU:HA	1:B:137:LEU:HB3	1.91	0.53
1:B:1130:GLN:OE1	1:B:1136:SER:OG	2.27	0.53
1:B:1708:ARG:HD3	1:B:1830:VAL:CG1	2.39	0.53
1:C:4205:TRP:CE3	1:C:4989:MET:HE1	2.44	0.53
1:C:4211:LYS:HB3	1:C:4211:LYS:HZ2	1.69	0.53
1:D:3695:PRO:HB3	1:D:3699:HIS:CD2	2.44	0.53
1:A:927:GLU:O	1:A:931:THR:HG23	2.09	0.53
1:B:4206:GLU:HA	1:B:4211:LYS:HD3	1.90	0.53
1:D:771:PHE:HA	1:D:1471:ALA:O	2.08	0.53
1:D:4979:THR:O	1:D:4979:THR:CG2	2.56	0.53
1:A:123:THR:OG1	1:A:134:ASP:OD1	2.24	0.52
1:A:4205:TRP:CE3	1:A:4989:MET:HE1	2.44	0.52
1:B:660:GLY:HA2	1:B:750:LEU:HD12	1.91	0.52
1:C:4968:PHE:HD2	1:C:4975:PHE:HD1	1.57	0.52
1:D:424:LYS:NZ	1:D:431:PRO:O	2.42	0.52
1:A:759:ILE:HG13	1:A:761:GLY:H	1.74	0.52
1:A:1829:PRO:O	1:A:1830:VAL:C	2.52	0.52
1:A:4979:THR:O	1:A:4979:THR:CG2	2.56	0.52
1:B:1829:PRO:O	1:B:1830:VAL:C	2.52	0.52
1:C:118:LEU:HA	1:C:137:LEU:HB3	1.91	0.52
1:C:660:GLY:HA2	1:C:750:LEU:HD12	1.91	0.52
1:C:786:GLY:HA2	1:C:1631:GLN:HA	1.91	0.52
1:D:759:ILE:HG13	1:D:761:GLY:H	1.74	0.52
1:D:1077:ALA:HB3	1:D:1189:LEU:HD11	1.90	0.52
1:D:2277:ALA:HB1	1:D:2337:PHE:HD2	1.75	0.52
1:D:4175:ARG:C	1:D:4177:TYR:H	2.18	0.52
1:A:4175:ARG:C	1:A:4177:TYR:H	2.18	0.52
1:B:40:GLU:H	1:B:44:ASN:HD22	1.58	0.52
1:C:2107:GLN:HE21	1:C:3683:GLN:CB	2.22	0.52
1:C:2277:ALA:HB1	1:C:2337:PHE:HD2	1.75	0.52
1:D:206:CYS:SG	1:D:207:SER:N	2.82	0.52
1:D:4772:ASP:OD1	1:D:4773:VAL:N	2.42	0.52
1:A:2277:ALA:HB1	1:A:2337:PHE:HD2	1.75	0.52
1:B:49:LEU:HD12	1:B:189:LEU:HB3	1.90	0.52
1:C:4772:ASP:OD1	1:C:4773:VAL:N	2.42	0.52
1:D:1708:ARG:HD3	1:D:1830:VAL:CG1	2.39	0.52
1:D:2288:LEU:HD12	1:D:3853:ALA:HB2	1.91	0.52
1:A:40:GLU:H	1:A:44:ASN:HD22	1.58	0.52
1:A:49:LEU:HD12	1:A:189:LEU:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1158:ASN:HD22	1:B:1182:ILE:HG13	1.75	0.52
1:B:1289:LEU:HD21	1:B:1597:VAL:CG2	2.39	0.52
1:C:1158:ASN:HD22	1:C:1182:ILE:HG13	1.75	0.52
1:D:311:ALA:O	1:D:350:HIS:NE2	2.38	0.52
1:D:927:GLU:O	1:D:931:THR:HG23	2.09	0.52
1:B:206:CYS:SG	1:B:207:SER:N	2.82	0.52
1:B:759:ILE:HG13	1:B:761:GLY:H	1.74	0.52
1:B:1235:THR:HG22	1:B:1607:ARG:HH11	1.75	0.52
1:B:3874:VAL:HG23	1:B:3875:MET:HG2	1.90	0.52
1:B:3893:GLU:OE1	1:B:3893:GLU:HA	2.10	0.52
1:B:4099:SER:O	1:B:4101:LYS:NZ	2.39	0.52
1:C:1130:GLN:OE1	1:C:1136:SER:OG	2.27	0.52
1:C:2288:LEU:HD12	1:C:3853:ALA:HB2	1.91	0.52
1:C:4099:SER:O	1:C:4101:LYS:NZ	2.39	0.52
1:D:274:LEU:HB3	1:D:339:ILE:HD12	1.90	0.52
1:A:1158:ASN:HD22	1:A:1182:ILE:HG13	1.75	0.52
1:B:728:ARG:NH1	1:B:1474:VAL:CG1	2.73	0.52
1:B:2107:GLN:HE21	1:B:3683:GLN:CB	2.22	0.52
1:B:2277:ALA:HB1	1:B:2337:PHE:HD2	1.75	0.52
1:C:1289:LEU:HD21	1:C:1597:VAL:CG2	2.39	0.52
1:D:4206:GLU:HA	1:D:4211:LYS:HD3	1.90	0.52
1:A:206:CYS:SG	1:A:207:SER:N	2.82	0.52
1:A:3874:VAL:HG23	1:A:3875:MET:HG2	1.90	0.52
1:B:4839:MET:SD	1:C:4822:THR:OG1	2.63	0.52
1:C:40:GLU:H	1:C:44:ASN:HD22	1.58	0.52
1:C:206:CYS:SG	1:C:207:SER:N	2.82	0.52
1:C:224:HIS:N	1:C:229:GLU:O	2.42	0.52
1:C:927:GLU:O	1:C:931:THR:HG23	2.09	0.52
1:D:645:ARG:HB3	1:D:780:VAL:HG12	1.91	0.52
1:D:717:ASP:OD1	1:D:720:HIS:ND1	2.41	0.52
1:D:786:GLY:HA2	1:D:1631:GLN:HA	1.91	0.52
1:A:1130:GLN:OE1	1:A:1136:SER:OG	2.27	0.52
1:C:998:ARG:O	1:C:1003:GLN:N	2.30	0.52
1:C:1235:THR:HG22	1:C:1607:ARG:HH11	1.75	0.52
1:C:1476:MET:O	1:C:1484:HIS:N	2.43	0.52
1:D:1829:PRO:O	1:D:1830:VAL:C	2.52	0.52
1:A:645:ARG:HB3	1:A:780:VAL:HG12	1.91	0.52
1:A:660:GLY:HA2	1:A:750:LEU:HD12	1.91	0.52
1:A:2107:GLN:HE21	1:A:3683:GLN:CB	2.22	0.52
1:B:224:HIS:N	1:B:229:GLU:O	2.42	0.52
1:B:837:PRO:O	1:B:1201:HIS:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2110:TYR:HA	1:B:3700:GLN:HE22	1.74	0.52
1:C:645:ARG:HB3	1:C:780:VAL:HG12	1.91	0.52
1:D:359:TYR:HA	1:D:376:ALA:HA	1.92	0.52
1:D:1695:LEU:O	1:D:1810:LYS:NZ	2.43	0.52
1:B:686:TRP:HE3	1:B:777:PHE:HB3	1.75	0.51
1:B:867:LEU:HD11	1:B:929:LEU:HD22	1.92	0.51
1:B:1149:VAL:HB	1:B:1164:LEU:HD13	1.93	0.51
1:C:686:TRP:HE3	1:C:777:PHE:HB3	1.75	0.51
1:C:728:ARG:NH1	1:C:1474:VAL:CG1	2.73	0.51
1:C:4691:GLN:HE22	1:C:4703:ARG:HH22	1.56	0.51
1:D:881:LEU:O	1:D:885:THR:HG23	2.09	0.51
1:D:1158:ASN:HD22	1:D:1182:ILE:HG13	1.75	0.51
1:D:1160:ILE:HB	1:D:1179:PHE:CB	2.40	0.51
1:D:2107:GLN:HE21	1:D:3683:GLN:CB	2.22	0.51
1:D:4205:TRP:CE3	1:D:4989:MET:HE1	2.44	0.51
1:A:837:PRO:O	1:A:1201:HIS:HB2	2.10	0.51
1:A:867:LEU:HD11	1:A:929:LEU:HD22	1.92	0.51
1:A:1160:ILE:HB	1:A:1179:PHE:CB	2.40	0.51
1:A:1235:THR:HG22	1:A:1607:ARG:HH11	1.75	0.51
1:A:1708:ARG:HD3	1:A:1830:VAL:CG1	2.39	0.51
1:A:2288:LEU:HD12	1:A:3853:ALA:HB2	1.91	0.51
1:D:40:GLU:H	1:D:44:ASN:HD22	1.58	0.51
1:D:867:LEU:HD11	1:D:929:LEU:HD22	1.92	0.51
1:D:4081:VAL:HG12	1:D:4088:ILE:HG12	1.92	0.51
1:A:728:ARG:NH1	1:A:1474:VAL:CG1	2.73	0.51
1:A:4081:VAL:HG12	1:A:4088:ILE:HG12	1.92	0.51
1:B:629:ARG:HD3	1:B:634:GLN:HG2	1.93	0.51
1:B:4873:ASP:O	1:B:4874:MET:C	2.50	0.51
1:C:359:TYR:HA	1:C:376:ALA:HA	1.92	0.51
1:C:1149:VAL:HB	1:C:1164:LEU:HD13	1.93	0.51
1:C:1160:ILE:HB	1:C:1179:PHE:CB	2.40	0.51
1:C:3893:GLU:HA	1:C:3893:GLU:OE1	2.10	0.51
1:C:4175:ARG:C	1:C:4177:TYR:H	2.18	0.51
1:D:118:LEU:HA	1:D:137:LEU:HB3	1.91	0.51
1:D:1765:VAL:O	1:D:1768:THR:HG23	2.11	0.51
1:D:3893:GLU:OE1	1:D:3893:GLU:HA	2.10	0.51
1:D:4873:ASP:O	1:D:4874:MET:C	2.50	0.51
1:A:1476:MET:O	1:A:1484:HIS:N	2.43	0.51
1:B:1695:LEU:O	1:B:1810:LYS:NZ	2.43	0.51
1:B:4175:ARG:C	1:B:4177:TYR:H	2.18	0.51
1:C:3695:PRO:HB3	1:C:3699:HIS:CD2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:SER:H	1:A:735:GLN:HE22	1.59	0.51
1:A:2238:TYR:O	1:A:2242:ILE:HG22	2.11	0.51
1:B:1476:MET:O	1:B:1484:HIS:N	2.43	0.51
1:B:4968:PHE:HD2	1:B:4975:PHE:HD1	1.57	0.51
1:C:1257:VAL:CG1	1:C:1597:VAL:HG11	2.31	0.51
1:C:1695:LEU:O	1:C:1810:LYS:NZ	2.43	0.51
1:D:1235:THR:HG22	1:D:1607:ARG:HH11	1.75	0.51
1:B:786:GLY:HA2	1:B:1631:GLN:HA	1.91	0.51
1:C:629:ARG:HD3	1:C:634:GLN:HG2	1.93	0.51
1:C:732:SER:H	1:C:735:GLN:HE22	1.59	0.51
1:C:867:LEU:HD11	1:C:929:LEU:HD22	1.92	0.51
1:D:1289:LEU:HD21	1:D:1597:VAL:CG2	2.39	0.51
1:A:1695:LEU:O	1:A:1810:LYS:NZ	2.43	0.51
1:A:3893:GLU:OE1	1:A:3893:GLU:HA	2.10	0.51
1:B:645:ARG:HB3	1:B:780:VAL:HG12	1.91	0.51
1:B:1160:ILE:HB	1:B:1179:PHE:CB	2.40	0.51
1:B:2238:TYR:O	1:B:2242:ILE:HG22	2.11	0.51
1:C:3787:LYS:N	1:C:3789:GLU:OE1	2.43	0.51
1:D:686:TRP:HE3	1:D:777:PHE:HB3	1.75	0.51
1:D:732:SER:H	1:D:735:GLN:HE22	1.59	0.51
1:D:1476:MET:O	1:D:1484:HIS:N	2.43	0.51
1:A:1149:VAL:HB	1:A:1164:LEU:HD13	1.93	0.51
1:A:4099:SER:O	1:A:4101:LYS:NZ	2.39	0.51
1:B:292:ALA:HB1	1:B:311:ALA:HB1	1.93	0.51
1:B:1719:HIS:CE1	1:B:1800:PRO:HG2	2.46	0.51
1:C:2238:TYR:O	1:C:2242:ILE:HG22	2.11	0.51
1:D:4182:GLU:O	1:D:4988:TYR:OH	2.29	0.51
1:A:292:ALA:HB1	1:A:311:ALA:HB1	1.93	0.51
1:A:786:GLY:HA2	1:A:1631:GLN:HA	1.91	0.51
1:B:317:ARG:O	1:B:347:PHE:N	2.44	0.51
1:B:649:PHE:HB3	1:B:776:LEU:HD22	1.93	0.51
1:B:732:SER:H	1:B:735:GLN:HE22	1.59	0.51
1:C:207:SER:OG	1:C:208:CYS:N	2.44	0.51
1:C:870:ILE:HD11	1:C:1049:TYR:HB3	1.93	0.51
1:C:1829:PRO:O	1:C:1830:VAL:C	2.52	0.51
1:D:660:GLY:HA2	1:D:750:LEU:HD12	1.91	0.51
1:D:837:PRO:O	1:D:1201:HIS:HB2	2.10	0.51
1:A:686:TRP:HE3	1:A:777:PHE:HB3	1.75	0.51
1:B:1652:GLU:OE1	1:B:1656:ARG:NH1	2.39	0.51
1:B:2110:TYR:HB2	1:B:3695:PRO:HD2	1.93	0.51
1:B:4869:GLU:O	1:B:4870:ASP:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4766:THR:HG1	1:D:4767:TRP:CD1	2.29	0.51
1:A:2243:SER:OG	1:A:2244:ARG:N	2.45	0.50
1:B:1765:VAL:O	1:B:1768:THR:HG23	2.11	0.50
1:B:4081:VAL:HG12	1:B:4088:ILE:HG12	1.92	0.50
1:C:667:MET:HE2	1:C:743:VAL:HG22	1.94	0.50
1:C:837:PRO:O	1:C:1201:HIS:HB2	2.10	0.50
1:C:1765:VAL:O	1:C:1768:THR:HG23	2.11	0.50
1:D:629:ARG:HD3	1:D:634:GLN:HG2	1.93	0.50
1:D:743:VAL:O	1:D:760:ASN:N	2.45	0.50
1:A:977:LEU:HG	1:A:1044:ARG:NH1	2.26	0.50
1:C:292:ALA:HB1	1:C:311:ALA:HB1	1.93	0.50
1:C:1101:ARG:HD2	1:C:1115:LEU:HB2	1.93	0.50
1:C:4766:THR:HG1	1:C:4767:TRP:CD1	2.29	0.50
1:C:4864:ASN:C	1:C:4866:SER:H	2.19	0.50
1:A:236:ALA:HA	1:A:242:ARG:HD2	1.93	0.50
1:A:359:TYR:HA	1:A:376:ALA:HA	1.92	0.50
1:A:4766:THR:HG1	1:A:4767:TRP:CD1	2.29	0.50
1:B:635:THR:OG1	1:B:1693:GLN:NE2	2.40	0.50
1:B:2243:SER:OG	1:B:2244:ARG:N	2.45	0.50
1:C:563:VAL:HA	1:C:566:CYS:SG	2.52	0.50
1:C:2110:TYR:HB2	1:C:3695:PRO:HD2	1.93	0.50
1:C:2212:VAL:HA	1:C:2215:LEU:HB2	1.93	0.50
1:D:563:VAL:HA	1:D:566:CYS:SG	2.52	0.50
1:D:728:ARG:NH1	1:D:1474:VAL:CG1	2.73	0.50
1:D:1149:VAL:HB	1:D:1164:LEU:HD13	1.93	0.50
1:D:1927:LEU:HB3	1:D:1939:MET:HE1	1.94	0.50
1:A:647:ASN:HD21	1:A:821:LEU:HA	1.77	0.50
1:A:1653:LEU:HD12	1:A:1660:GLN:N	2.27	0.50
1:A:1927:LEU:HB3	1:A:1939:MET:HE1	1.94	0.50
1:B:977:LEU:HG	1:B:1044:ARG:NH1	2.26	0.50
1:B:4979:THR:HG23	2:B:5101:ATP:N1	2.27	0.50
1:C:236:ALA:HA	1:C:242:ARG:HD2	1.93	0.50
1:D:667:MET:HE2	1:D:743:VAL:HG22	1.94	0.50
1:D:1636:MET:HE2	1:D:1638:ALA:HB2	1.94	0.50
1:D:1653:LEU:HD12	1:D:1660:GLN:N	2.27	0.50
1:D:1835:GLU:O	1:D:1839:VAL:HG23	2.11	0.50
1:D:2238:TYR:O	1:D:2242:ILE:HG22	2.11	0.50
1:A:207:SER:OG	1:A:208:CYS:N	2.44	0.50
1:A:629:ARG:HD3	1:A:634:GLN:HG2	1.93	0.50
1:A:667:MET:HE2	1:A:743:VAL:HG22	1.94	0.50
1:A:1652:GLU:OE1	1:A:1656:ARG:NH1	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1719:HIS:CE1	1:A:1800:PRO:HG2	2.46	0.50
1:B:870:ILE:HD11	1:B:1049:TYR:HB3	1.93	0.50
1:B:4766:THR:HG1	1:B:4767:TRP:CD1	2.29	0.50
1:C:977:LEU:HG	1:C:1044:ARG:NH1	2.26	0.50
1:C:1927:LEU:HB3	1:C:1939:MET:HE1	1.94	0.50
1:D:894:GLY:HA3	1:D:903:LEU:HG	1.94	0.50
1:D:1652:GLU:OE1	1:D:1656:ARG:NH1	2.39	0.50
1:D:1941:ASN:O	1:D:1944:GLU:HG3	2.12	0.50
1:A:743:VAL:O	1:A:760:ASN:N	2.45	0.50
1:A:4968:PHE:HD2	1:A:4975:PHE:HD1	1.57	0.50
1:B:359:TYR:HA	1:B:376:ALA:HA	1.92	0.50
1:B:743:VAL:O	1:B:760:ASN:N	2.45	0.50
1:B:1743:ARG:NH2	1:B:1963:GLU:OE2	2.45	0.50
1:B:1944:GLU:HA	1:B:1947:CYS:SG	2.52	0.50
1:C:894:GLY:HA3	1:C:903:LEU:HG	1.94	0.50
1:C:1652:GLU:OE1	1:C:1656:ARG:NH1	2.39	0.50
1:D:43:GLY:HA2	1:D:443:LEU:HG	1.94	0.50
1:D:207:SER:OG	1:D:208:CYS:N	2.44	0.50
1:D:317:ARG:O	1:D:347:PHE:N	2.44	0.50
1:A:2110:TYR:HB2	1:A:3695:PRO:HD2	1.93	0.50
1:B:667:MET:HE2	1:B:743:VAL:HG22	1.94	0.50
1:B:1835:GLU:O	1:B:1839:VAL:HG23	2.11	0.50
1:B:4864:ASN:C	1:B:4866:SER:H	2.19	0.50
1:C:836:GLY:O	1:C:1201:HIS:CG	2.65	0.50
1:C:4081:VAL:HG12	1:C:4088:ILE:HG12	1.92	0.50
1:C:4182:GLU:O	1:C:4988:TYR:OH	2.29	0.50
1:D:144:GLU:O	1:D:175:SER:OG	2.20	0.50
1:D:292:ALA:HB1	1:D:311:ALA:HB1	1.93	0.50
1:D:649:PHE:HB3	1:D:776:LEU:HD22	1.93	0.50
1:D:977:LEU:HG	1:D:1044:ARG:NH1	2.26	0.50
1:D:1130:GLN:OE1	1:D:1136:SER:OG	2.27	0.50
1:A:836:GLY:O	1:A:1201:HIS:CG	2.65	0.50
1:A:1101:ARG:HD2	1:A:1115:LEU:HB2	1.93	0.50
1:A:1636:MET:HE2	1:A:1638:ALA:HB2	1.94	0.50
1:A:1765:VAL:O	1:A:1768:THR:HG23	2.11	0.50
1:A:2212:VAL:HA	1:A:2215:LEU:HB2	1.93	0.50
1:B:1101:ARG:HD2	1:B:1115:LEU:HB2	1.93	0.50
1:B:3695:PRO:HB2	1:B:3700:GLN:HG3	1.94	0.50
1:C:1743:ARG:NH2	1:C:1963:GLU:OE2	2.45	0.50
1:D:236:ALA:HA	1:D:242:ARG:HD2	1.93	0.50
1:D:1101:ARG:HD2	1:D:1115:LEU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3695:PRO:HB2	1:D:3700:GLN:HG3	1.94	0.50
1:A:43:GLY:HA2	1:A:443:LEU:HG	1.94	0.50
1:A:311:ALA:O	1:A:350:HIS:NE2	2.38	0.50
1:A:633:LEU:HB3	1:A:1639:LEU:HD22	1.94	0.50
1:A:889:GLN:OE1	1:A:891:TRP:NE1	2.29	0.50
1:A:1944:GLU:HA	1:A:1947:CYS:SG	2.52	0.50
1:A:4869:GLU:O	1:A:4870:ASP:C	2.54	0.50
1:B:236:ALA:HA	1:B:242:ARG:HD2	1.93	0.50
1:B:647:ASN:HD21	1:B:821:LEU:HA	1.77	0.50
1:B:836:GLY:O	1:B:1201:HIS:CG	2.65	0.50
1:C:1719:HIS:CE1	1:C:1800:PRO:HG2	2.46	0.50
1:C:2243:SER:OG	1:C:2244:ARG:N	2.45	0.50
1:D:4864:ASN:C	1:D:4866:SER:H	2.19	0.50
1:A:649:PHE:HB3	1:A:776:LEU:HD22	1.93	0.49
1:B:207:SER:OG	1:B:208:CYS:N	2.44	0.49
1:B:1653:LEU:HD12	1:B:1660:GLN:N	2.27	0.49
1:C:1160:ILE:HB	1:C:1179:PHE:CG	2.48	0.49
1:D:633:LEU:HB3	1:D:1639:LEU:HD22	1.94	0.49
1:D:647:ASN:HD21	1:D:821:LEU:HA	1.77	0.49
1:D:836:GLY:O	1:D:1201:HIS:CG	2.65	0.49
1:D:869:ARG:NH2	1:D:947:GLU:OE1	2.45	0.49
1:D:2110:TYR:HB2	1:D:3695:PRO:HD2	1.93	0.49
1:B:563:VAL:HA	1:B:566:CYS:SG	2.52	0.49
1:B:1663:HIS:HD2	1:B:1707:LEU:HD21	1.77	0.49
1:B:1927:LEU:HB3	1:B:1939:MET:HE1	1.94	0.49
1:B:2212:VAL:HA	1:B:2215:LEU:HB2	1.93	0.49
1:B:4182:GLU:O	1:B:4988:TYR:OH	2.29	0.49
1:C:743:VAL:O	1:C:760:ASN:N	2.45	0.49
1:C:1653:LEU:HD12	1:C:1660:GLN:N	2.27	0.49
1:C:1715:LEU:C	1:C:1715:LEU:CD2	2.85	0.49
1:C:1941:ASN:O	1:C:1944:GLU:HG3	2.12	0.49
1:D:870:ILE:HD11	1:D:1049:TYR:HB3	1.93	0.49
1:D:2243:SER:OG	1:D:2244:ARG:N	2.45	0.49
1:D:4979:THR:HG23	2:D:5101:ATP:N1	2.27	0.49
1:A:317:ARG:O	1:A:347:PHE:N	2.44	0.49
1:A:563:VAL:HA	1:A:566:CYS:SG	2.52	0.49
1:A:894:GLY:HA3	1:A:903:LEU:HG	1.94	0.49
1:A:1434:TYR:HB2	1:A:1519:LEU:HB3	1.94	0.49
1:A:3941:ASP:O	1:A:4002:LYS:NZ	2.46	0.49
1:A:4979:THR:HG23	2:A:5101:ATP:N1	2.27	0.49
1:B:1774:PRO:HG2	1:B:1776:HIS:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:GLY:HA2	1:C:443:LEU:HG	1.94	0.49
1:C:647:ASN:HD21	1:C:821:LEU:HA	1.77	0.49
1:C:670:GLU:HG2	1:C:787:VAL:HA	1.95	0.49
1:C:1257:VAL:HG11	1:C:1597:VAL:HG13	1.88	0.49
1:C:4869:GLU:O	1:C:4870:ASP:C	2.54	0.49
1:B:1636:MET:HE2	1:B:1638:ALA:HB2	1.94	0.49
1:B:1941:ASN:O	1:B:1944:GLU:HG3	2.12	0.49
1:C:317:ARG:O	1:C:347:PHE:N	2.44	0.49
1:C:3695:PRO:HB2	1:C:3700:GLN:HG3	1.94	0.49
1:D:670:GLU:HG2	1:D:787:VAL:HA	1.95	0.49
1:D:1663:HIS:HD2	1:D:1707:LEU:HD21	1.77	0.49
1:A:1708:ARG:NH2	1:A:1712:TYR:HE1	2.09	0.49
1:A:1835:GLU:O	1:A:1839:VAL:HG23	2.11	0.49
1:A:2349:ASN:O	1:A:2353:VAL:HG23	2.13	0.49
1:B:4666:VAL:C	1:B:4668:LEU:N	2.69	0.49
1:C:1247:PRO:HA	1:C:1598:GLN:HA	1.95	0.49
1:C:1786:LEU:HG	1:C:1787:PRO:HD2	1.95	0.49
1:C:4211:LYS:NZ	1:C:4211:LYS:CB	2.73	0.49
1:D:1434:TYR:HB2	1:D:1519:LEU:HB3	1.94	0.49
1:D:4869:GLU:O	1:D:4870:ASP:C	2.54	0.49
1:A:1139:PHE:HE2	1:A:1162:PHE:HD2	1.60	0.49
1:B:43:GLY:HA2	1:B:443:LEU:HG	1.94	0.49
1:B:1247:PRO:HA	1:B:1598:GLN:HA	1.95	0.49
1:B:4211:LYS:NZ	1:B:4211:LYS:CB	2.73	0.49
1:C:1944:GLU:HA	1:C:1947:CYS:SG	2.52	0.49
1:C:2349:ASN:O	1:C:2353:VAL:HG23	2.13	0.49
1:D:2212:VAL:HA	1:D:2215:LEU:HB2	1.93	0.49
1:A:870:ILE:HD11	1:A:1049:TYR:HB3	1.93	0.49
1:A:1160:ILE:HB	1:A:1179:PHE:CG	2.48	0.49
1:A:1774:PRO:HG2	1:A:1776:HIS:CE1	2.48	0.49
1:A:3695:PRO:HB2	1:A:3700:GLN:HG3	1.94	0.49
1:A:4901:ILE:HB	1:A:4913:ARG:NH1	2.28	0.49
1:B:3695:PRO:HB3	1:B:3699:HIS:CD2	2.44	0.49
1:B:3941:ASP:O	1:B:4002:LYS:NZ	2.46	0.49
1:C:311:ALA:O	1:C:350:HIS:NE2	2.38	0.49
1:C:1774:PRO:HG2	1:C:1776:HIS:CE1	2.48	0.49
1:D:1719:HIS:CE1	1:D:1800:PRO:HG2	2.46	0.49
1:D:1743:ARG:NH2	1:D:1963:GLU:OE2	2.45	0.49
1:D:4979:THR:CG2	2:D:5101:ATP:C2	2.96	0.49
1:A:638:ILE:HD11	1:A:702:TRP:HE3	1.78	0.49
1:A:1247:PRO:HA	1:A:1598:GLN:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2447:LYS:HG3	1:B:2449:GLU:H	1.78	0.49
1:C:649:PHE:HB3	1:C:776:LEU:HD22	1.93	0.49
1:C:771:PHE:HB3	1:C:1472:VAL:HG23	1.94	0.49
1:C:1835:GLU:O	1:C:1839:VAL:HG23	2.11	0.49
1:C:2447:LYS:HG3	1:C:2449:GLU:H	1.78	0.49
1:C:4979:THR:HG23	2:C:5101:ATP:N1	2.27	0.49
1:D:1944:GLU:HA	1:D:1947:CYS:SG	2.52	0.49
1:D:3941:ASP:O	1:D:4002:LYS:NZ	2.46	0.49
1:A:1743:ARG:NH2	1:A:1963:GLU:OE2	2.45	0.49
1:A:1941:ASN:O	1:A:1944:GLU:HG3	2.12	0.49
1:B:1105:ALA:O	1:B:1189:LEU:N	2.46	0.49
1:B:3787:LYS:N	1:B:3789:GLU:OE1	2.43	0.49
1:C:717:ASP:OD1	1:C:720:HIS:ND1	2.41	0.49
1:D:1160:ILE:HB	1:D:1179:PHE:CG	2.48	0.49
1:D:1257:VAL:CG1	1:D:1597:VAL:HG11	2.31	0.49
1:D:2447:LYS:HG3	1:D:2449:GLU:H	1.78	0.49
1:A:728:ARG:CZ	1:A:1474:VAL:HG11	2.43	0.49
1:A:1257:VAL:HG11	1:A:1597:VAL:HG13	1.88	0.49
1:A:4182:GLU:O	1:A:4988:TYR:OH	2.29	0.49
1:B:670:GLU:HG2	1:B:787:VAL:HA	1.95	0.49
1:B:4855:ALA:HA	1:B:4859:PHE:HD2	1.78	0.49
1:D:1105:ALA:O	1:D:1189:LEU:N	2.46	0.49
1:D:1139:PHE:HE2	1:D:1162:PHE:HD2	1.60	0.49
1:D:4863:TYR:HB2	1:D:4876:CYS:SG	2.53	0.49
1:B:638:ILE:HD11	1:B:702:TRP:HE3	1.78	0.48
1:B:728:ARG:CZ	1:B:1474:VAL:HG11	2.43	0.48
1:B:1139:PHE:HE2	1:B:1162:PHE:HD2	1.60	0.48
1:C:745:SER:O	1:C:757:PHE:CA	2.58	0.48
1:C:1257:VAL:HG21	1:C:1597:VAL:HG11	1.95	0.48
1:C:4855:ALA:HA	1:C:4859:PHE:HD2	1.78	0.48
1:C:5035:GLN:C	1:C:5036:LEU:HD12	2.38	0.48
1:A:540:PHE:HD2	1:A:567:VAL:HG21	1.79	0.48
1:A:670:GLU:HG2	1:A:787:VAL:HA	1.95	0.48
1:A:3895:HIS:HE1	1:A:3970:GLN:HB3	1.78	0.48
1:A:4875:LYS:HB3	1:A:4875:LYS:HE3	1.57	0.48
1:B:273:HIS:CE1	1:B:337:PRO:HB3	2.48	0.48
1:B:1160:ILE:HB	1:B:1179:PHE:CG	2.48	0.48
1:B:1257:VAL:HG11	1:B:1597:VAL:HG13	1.88	0.48
1:B:4865:LYS:O	1:B:4866:SER:C	2.56	0.48
1:B:5035:GLN:C	1:B:5036:LEU:HD12	2.38	0.48
1:C:4875:LYS:HE3	1:C:4875:LYS:HB3	1.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:638:ILE:HD11	1:D:702:TRP:HE3	1.78	0.48
1:D:1247:PRO:HA	1:D:1598:GLN:HA	1.95	0.48
1:D:3895:HIS:HE1	1:D:3970:GLN:HB3	1.78	0.48
1:A:745:SER:O	1:A:757:PHE:CA	2.58	0.48
1:A:1663:HIS:HD2	1:A:1707:LEU:HD21	1.77	0.48
1:A:1715:LEU:C	1:A:1715:LEU:CD2	2.85	0.48
1:B:889:GLN:OE1	1:B:891:TRP:NE1	2.29	0.48
1:B:2349:ASN:O	1:B:2353:VAL:HG23	2.13	0.48
1:C:540:PHE:HD2	1:C:567:VAL:HG21	1.79	0.48
1:C:638:ILE:HD11	1:C:702:TRP:HE3	1.78	0.48
1:C:1139:PHE:HE2	1:C:1162:PHE:HD2	1.60	0.48
1:D:771:PHE:HB3	1:D:1472:VAL:HG23	1.94	0.48
1:D:1257:VAL:HG21	1:D:1597:VAL:HG11	1.95	0.48
1:D:4865:LYS:O	1:D:4866:SER:C	2.56	0.48
1:A:755:ILE:HG22	1:A:768:PHE:CB	2.44	0.48
1:A:976:ARG:HH21	1:A:979:PRO:HA	1.79	0.48
1:A:4243:PHE:HE2	1:A:4667:PRO:O	1.97	0.48
1:A:4863:TYR:HB2	1:A:4876:CYS:SG	2.53	0.48
1:A:5035:GLN:C	1:A:5036:LEU:HD12	2.38	0.48
1:B:894:GLY:HA3	1:B:903:LEU:HG	1.94	0.48
1:B:1257:VAL:HG21	1:B:1597:VAL:HG11	1.95	0.48
1:B:1786:LEU:HG	1:B:1787:PRO:HD2	1.95	0.48
1:B:4243:PHE:HE2	1:B:4667:PRO:O	1.97	0.48
1:C:728:ARG:CZ	1:C:1474:VAL:HG11	2.43	0.48
1:C:755:ILE:HG22	1:C:768:PHE:CB	2.44	0.48
1:C:970:LEU:HD21	1:C:1048:GLY:HA3	1.96	0.48
1:C:1636:MET:HE2	1:C:1638:ALA:HB2	1.94	0.48
1:C:1927:LEU:HD23	1:C:1927:LEU:H	1.79	0.48
1:C:3895:HIS:HE1	1:C:3970:GLN:HB3	1.78	0.48
1:C:3941:ASP:O	1:C:4002:LYS:NZ	2.46	0.48
1:C:4863:TYR:HB2	1:C:4876:CYS:SG	2.53	0.48
1:C:4973:HIS:HB3	1:C:4976:GLU:HB3	1.96	0.48
1:D:3787:LYS:N	1:D:3789:GLU:OE1	2.43	0.48
1:D:4901:ILE:HB	1:D:4913:ARG:NH1	2.28	0.48
1:A:4864:ASN:C	1:A:4866:SER:H	2.19	0.48
1:A:4973:HIS:HB3	1:A:4976:GLU:HB3	1.96	0.48
1:B:633:LEU:HB3	1:B:1639:LEU:HD22	1.94	0.48
1:B:717:ASP:OD1	1:B:720:HIS:ND1	2.41	0.48
1:B:755:ILE:HG22	1:B:768:PHE:CB	2.44	0.48
1:B:771:PHE:HB3	1:B:1472:VAL:HG23	1.94	0.48
1:B:970:LEU:HD21	1:B:1048:GLY:HA3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:976:ARG:HH21	1:B:979:PRO:HA	1.79	0.48
1:B:4863:TYR:HB2	1:B:4876:CYS:SG	2.53	0.48
1:C:633:LEU:HB3	1:C:1639:LEU:HD22	1.94	0.48
1:C:1105:ALA:O	1:C:1189:LEU:N	2.46	0.48
1:C:1434:TYR:HB2	1:C:1519:LEU:HB3	1.94	0.48
1:D:461:HIS:O	1:D:465:GLN:HG2	2.14	0.48
1:D:755:ILE:HG22	1:D:768:PHE:CB	2.44	0.48
1:D:5035:GLN:C	1:D:5036:LEU:HD12	2.38	0.48
1:A:869:ARG:NH2	1:A:947:GLU:OE1	2.45	0.48
1:A:1105:ALA:O	1:A:1189:LEU:N	2.46	0.48
1:A:4855:ALA:HA	1:A:4859:PHE:HD2	1.78	0.48
1:A:4979:THR:CG2	2:A:5101:ATP:C2	2.96	0.48
1:B:1683:HIS:ND1	1:B:1797:ARG:HB3	2.29	0.48
1:B:1927:LEU:HD23	1:B:1927:LEU:H	1.79	0.48
1:B:3895:HIS:HE1	1:B:3970:GLN:HB3	1.78	0.48
1:C:265:LEU:HD12	1:C:279:PRO:HB2	1.96	0.48
1:C:461:HIS:O	1:C:465:GLN:HG2	2.14	0.48
1:C:4979:THR:CG2	2:C:5101:ATP:C2	2.96	0.48
1:D:728:ARG:CZ	1:D:1474:VAL:HG11	2.43	0.48
1:D:1683:HIS:ND1	1:D:1797:ARG:HB3	2.29	0.48
1:D:1774:PRO:HG2	1:D:1776:HIS:CE1	2.48	0.48
1:D:2349:ASN:O	1:D:2353:VAL:HG23	2.13	0.48
1:A:745:SER:HB2	1:A:758:ARG:H	1.79	0.48
1:A:1451:GLY:HA3	1:A:1494:MET:HA	1.95	0.48
1:B:265:LEU:HD12	1:B:279:PRO:HB2	1.96	0.48
1:B:869:ARG:NH2	1:B:947:GLU:OE1	2.45	0.48
1:C:745:SER:HB2	1:C:758:ARG:H	1.79	0.48
1:C:4865:LYS:O	1:C:4866:SER:C	2.56	0.48
1:A:771:PHE:HB3	1:A:1472:VAL:HG23	1.94	0.48
1:A:1070:ASP:OD2	1:A:1071:ARG:NH1	2.47	0.48
1:B:1434:TYR:HB2	1:B:1519:LEU:HB3	1.94	0.48
1:B:4979:THR:CG2	2:B:5101:ATP:C2	2.96	0.48
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.95	0.48
1:C:1663:HIS:HD2	1:C:1707:LEU:HD21	1.77	0.48
1:D:1451:GLY:HA3	1:D:1494:MET:HA	1.95	0.48
1:D:1927:LEU:H	1:D:1927:LEU:HD23	1.79	0.48
1:D:4874:MET:C	1:D:4876:CYS:H	2.22	0.48
1:A:265:LEU:HD12	1:A:279:PRO:HB2	1.96	0.48
1:B:745:SER:HB2	1:B:758:ARG:H	1.79	0.48
1:B:1070:ASP:OD2	1:B:1071:ARG:NH1	2.47	0.48
1:B:4901:ILE:HB	1:B:4913:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4973:HIS:HB3	1:B:4976:GLU:HB3	1.96	0.48
1:D:1786:LEU:HG	1:D:1787:PRO:HD2	1.95	0.48
1:A:273:HIS:CE1	1:A:337:PRO:HB3	2.48	0.48
1:A:892:THR:HG23	1:A:903:LEU:HD12	1.96	0.48
1:A:970:LEU:HD21	1:A:1048:GLY:HA3	1.96	0.48
1:A:4874:MET:C	1:A:4876:CYS:H	2.22	0.48
1:B:540:PHE:HD2	1:B:567:VAL:HG21	1.79	0.48
1:C:273:HIS:CE1	1:C:337:PRO:HB3	2.48	0.48
1:C:892:THR:HG23	1:C:903:LEU:HD12	1.96	0.48
1:D:745:SER:HB2	1:D:758:ARG:H	1.79	0.48
1:D:1115:LEU:H	1:D:1115:LEU:HD12	1.79	0.48
1:A:1786:LEU:HG	1:A:1787:PRO:HD2	1.95	0.47
1:A:4865:LYS:O	1:A:4866:SER:C	2.56	0.47
1:B:461:HIS:O	1:B:465:GLN:HG2	2.14	0.47
1:C:1070:ASP:OD2	1:C:1071:ARG:NH1	2.47	0.47
1:C:2095:GLN:HA	1:C:2127:GLN:HE21	1.79	0.47
1:C:2258:LEU:HD23	1:C:2297:LYS:HE3	1.96	0.47
1:C:3657:TYR:HE2	1:C:3662:ILE:HG23	1.79	0.47
1:C:4243:PHE:HE2	1:C:4667:PRO:O	1.97	0.47
1:C:4979:THR:HG23	2:C:5101:ATP:C6	2.50	0.47
1:D:976:ARG:HH21	1:D:979:PRO:HA	1.79	0.47
1:D:3657:TYR:HE2	1:D:3662:ILE:HG23	1.79	0.47
1:A:292:ALA:HB2	1:A:312:THR:HG22	1.96	0.47
1:A:1257:VAL:HG21	1:A:1597:VAL:HG11	1.95	0.47
1:A:1927:LEU:HD23	1:A:1927:LEU:H	1.79	0.47
1:B:1115:LEU:H	1:B:1115:LEU:HD12	1.79	0.47
1:B:4979:THR:HG23	2:B:5101:ATP:C6	2.50	0.47
1:C:1115:LEU:H	1:C:1115:LEU:HD12	1.79	0.47
1:D:4243:PHE:HE2	1:D:4667:PRO:O	1.97	0.47
1:D:4855:ALA:HA	1:D:4859:PHE:HD2	1.78	0.47
1:D:4876:CYS:CB	1:D:4882:CYS:SG	2.94	0.47
1:D:4973:HIS:HB3	1:D:4976:GLU:HB3	1.96	0.47
1:A:2447:LYS:HG3	1:A:2449:GLU:H	1.78	0.47
1:B:292:ALA:HB2	1:B:312:THR:HG22	1.96	0.47
1:B:319:SER:OG	1:B:320:LYS:N	2.47	0.47
1:B:3722:TYR:HD2	1:B:3793:MET:HE2	1.79	0.47
1:B:4924:VAL:HA	1:B:4928:LEU:HB2	1.96	0.47
1:B:4985:LEU:HG	2:B:5101:ATP:N6	2.30	0.47
1:C:319:SER:OG	1:C:320:LYS:N	2.47	0.47
1:C:1683:HIS:ND1	1:C:1797:ARG:HB3	2.29	0.47
1:D:970:LEU:HD21	1:D:1048:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2258:LEU:HD23	1:D:2297:LYS:HE3	1.96	0.47
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.95	0.47
1:A:629:ARG:HB3	1:A:634:GLN:CD	2.40	0.47
1:A:3960:GLN:NE2	1:A:3960:GLN:O	2.48	0.47
1:C:686:TRP:CE2	1:C:746:CYS:SG	3.08	0.47
1:C:889:GLN:OE1	1:C:891:TRP:NE1	2.29	0.47
1:C:4924:VAL:HA	1:C:4928:LEU:HB2	1.96	0.47
1:D:265:LEU:HD12	1:D:279:PRO:HB2	1.96	0.47
1:D:4175:ARG:O	1:D:4177:TYR:N	2.48	0.47
1:A:461:HIS:O	1:A:465:GLN:HG2	2.14	0.47
1:A:3787:LYS:N	1:A:3789:GLU:OE1	2.43	0.47
1:B:1257:VAL:CG1	1:B:1597:VAL:HG11	2.31	0.47
1:B:4979:THR:HG23	2:B:5101:ATP:C2	2.50	0.47
1:C:4874:MET:C	1:C:4876:CYS:H	2.22	0.47
1:D:3960:GLN:O	1:D:3960:GLN:NE2	2.48	0.47
1:A:686:TRP:CE2	1:A:746:CYS:SG	3.08	0.47
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.95	0.47
1:B:1451:GLY:HA3	1:B:1494:MET:HA	1.95	0.47
1:B:4875:LYS:HE3	1:B:4875:LYS:HB3	1.57	0.47
1:C:302:VAL:HB	1:C:306:LYS:HB2	1.97	0.47
1:C:3658:LYS:HA	1:C:3661:TRP:CD2	2.50	0.47
1:C:4666:VAL:C	1:C:4668:LEU:N	2.69	0.47
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.95	0.47
1:D:273:HIS:CE1	1:D:337:PRO:HB3	2.48	0.47
1:D:889:GLN:OE1	1:D:891:TRP:NE1	2.29	0.47
1:A:319:SER:OG	1:A:320:LYS:N	2.47	0.47
1:A:717:ASP:OD1	1:A:720:HIS:ND1	2.41	0.47
1:A:1101:ARG:HB3	1:A:1123:VAL:HG21	1.96	0.47
1:A:1115:LEU:HD12	1:A:1115:LEU:H	1.79	0.47
1:A:2243:SER:HG	1:A:2246:ASN:H	1.63	0.47
1:B:686:TRP:HZ2	1:B:746:CYS:HG	1.62	0.47
1:B:3657:TYR:HE2	1:B:3662:ILE:HG23	1.79	0.47
1:B:3658:LYS:HA	1:B:3661:TRP:CD2	2.50	0.47
1:B:4874:MET:C	1:B:4876:CYS:H	2.22	0.47
1:C:629:ARG:HB3	1:C:634:GLN:CD	2.40	0.47
1:D:302:VAL:HB	1:D:306:LYS:HB2	1.97	0.47
1:D:540:PHE:HD2	1:D:567:VAL:HG21	1.79	0.47
1:D:1101:ARG:HB3	1:D:1123:VAL:HG21	1.96	0.47
1:D:2095:GLN:HA	1:D:2127:GLN:HE21	1.79	0.47
1:D:4211:LYS:HB3	1:D:4211:LYS:HZ3	1.78	0.47
1:A:2095:GLN:HA	1:A:2127:GLN:HE21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3722:TYR:HD2	1:A:3793:MET:HE2	1.79	0.47
1:A:4979:THR:HG23	2:A:5101:ATP:C2	2.50	0.47
1:B:342:GLY:HA2	1:B:389:PHE:HD2	1.80	0.47
1:B:2258:LEU:HD23	1:B:2297:LYS:HE3	1.96	0.47
1:C:24:CYS:SG	1:C:35:LEU:HB2	2.55	0.47
1:C:688:LEU:O	1:C:688:LEU:HD12	2.15	0.47
1:D:685:GLY:HA3	1:D:714:TYR:O	2.15	0.47
1:D:686:TRP:CE2	1:D:746:CYS:SG	3.08	0.47
1:D:1070:ASP:OD2	1:D:1071:ARG:NH1	2.47	0.47
1:D:3658:LYS:HA	1:D:3661:TRP:CD2	2.50	0.47
1:A:685:GLY:HA3	1:A:714:TYR:O	2.15	0.47
1:B:1708:ARG:NH2	1:B:1712:TYR:HE1	2.09	0.47
1:C:836:GLY:O	1:C:1201:HIS:CD2	2.68	0.47
1:C:1451:GLY:HA3	1:C:1494:MET:HA	1.95	0.47
1:C:4901:ILE:HB	1:C:4913:ARG:NH1	2.28	0.47
1:C:4985:LEU:HG	2:C:5101:ATP:N6	2.30	0.47
1:D:550:LYS:HG3	1:D:551:LEU:H	1.80	0.47
1:D:629:ARG:HB3	1:D:634:GLN:CD	2.40	0.47
1:D:4696:ASP:O	1:D:4699:GLY:N	2.47	0.47
1:D:4979:THR:HG23	2:D:5101:ATP:C6	2.50	0.47
1:D:4985:LEU:HG	2:D:5101:ATP:N6	2.30	0.47
1:A:4979:THR:HG23	2:A:5101:ATP:C6	2.50	0.47
1:B:24:CYS:SG	1:B:35:LEU:HB2	2.55	0.47
1:B:302:VAL:HB	1:B:306:LYS:HB2	1.97	0.47
1:B:629:ARG:HB3	1:B:634:GLN:CD	2.40	0.47
1:B:686:TRP:CE2	1:B:746:CYS:SG	3.08	0.47
1:B:892:THR:HG23	1:B:903:LEU:HD12	1.96	0.47
1:B:3994:HIS:CE1	1:B:3998:HIS:HE1	2.33	0.47
1:D:836:GLY:O	1:D:1201:HIS:CD2	2.68	0.47
1:D:892:THR:HG23	1:D:903:LEU:HD12	1.96	0.47
1:D:1257:VAL:HG11	1:D:1597:VAL:HG13	1.88	0.47
1:D:1708:ARG:NH2	1:D:1712:TYR:HE1	2.09	0.47
1:D:3994:HIS:CE1	1:D:3998:HIS:HE1	2.33	0.47
1:D:4979:THR:HG23	2:D:5101:ATP:C2	2.50	0.47
1:A:550:LYS:HG3	1:A:551:LEU:H	1.80	0.46
1:A:3657:TYR:HE2	1:A:3662:ILE:HG23	1.79	0.46
1:A:4985:LEU:HG	2:A:5101:ATP:N6	2.30	0.46
1:B:2095:GLN:HA	1:B:2127:GLN:HE21	1.79	0.46
1:B:3960:GLN:O	1:B:3960:GLN:NE2	2.48	0.46
1:B:4175:ARG:O	1:B:4177:TYR:N	2.48	0.46
1:C:548:VAL:HG21	1:C:582:HIS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:CYS:SG	1:D:35:LEU:HB2	2.55	0.46
1:D:548:VAL:HG21	1:D:582:HIS:HB3	1.97	0.46
1:A:58:VAL:HG12	1:A:305:CYS:HA	1.97	0.46
1:A:1683:HIS:ND1	1:A:1797:ARG:HB3	2.29	0.46
1:A:3994:HIS:CE1	1:A:3998:HIS:HE1	2.33	0.46
1:A:4580:TYR:CE1	1:A:4631:PHE:HB2	2.51	0.46
1:B:311:ALA:O	1:B:350:HIS:NE2	2.38	0.46
1:B:688:LEU:HD12	1:B:688:LEU:O	2.15	0.46
1:C:976:ARG:HH21	1:C:979:PRO:HA	1.79	0.46
1:C:4098:ASP:OD1	1:C:4098:ASP:N	2.48	0.46
1:D:292:ALA:HB2	1:D:312:THR:HG22	1.96	0.46
1:D:319:SER:OG	1:D:320:LYS:N	2.47	0.46
1:D:3722:TYR:HD2	1:D:3793:MET:HE2	1.79	0.46
1:B:836:GLY:O	1:B:1201:HIS:CD2	2.68	0.46
1:C:3960:GLN:NE2	1:C:3960:GLN:O	2.48	0.46
1:D:3658:LYS:O	1:D:3661:TRP:N	2.48	0.46
1:A:3658:LYS:HA	1:A:3661:TRP:CD2	2.50	0.46
1:B:494:LEU:HD12	1:B:515:TRP:CD1	2.51	0.46
1:B:3937:TYR:OH	1:B:3944:GLU:OE1	2.21	0.46
1:B:4580:TYR:CE1	1:B:4631:PHE:HB2	2.51	0.46
1:C:590:LEU:HD22	1:C:631:LEU:HD21	1.98	0.46
1:C:973:SER:HA	1:C:1044:ARG:NH2	2.31	0.46
1:C:4979:THR:HG23	2:C:5101:ATP:C2	2.50	0.46
1:D:4924:VAL:HA	1:D:4928:LEU:HB2	1.96	0.46
1:A:4175:ARG:O	1:A:4177:TYR:N	2.48	0.46
1:A:4666:VAL:C	1:A:4668:LEU:N	2.69	0.46
1:B:58:VAL:HG12	1:B:305:CYS:HA	1.97	0.46
1:B:548:VAL:HG21	1:B:582:HIS:HB3	1.97	0.46
1:B:745:SER:O	1:B:757:PHE:CA	2.58	0.46
1:B:1101:ARG:HB3	1:B:1123:VAL:HG21	1.96	0.46
1:C:292:ALA:HB2	1:C:312:THR:HG22	1.96	0.46
1:C:342:GLY:HA2	1:C:389:PHE:HD2	1.80	0.46
1:C:550:LYS:HG3	1:C:551:LEU:H	1.80	0.46
1:C:1101:ARG:HB3	1:C:1123:VAL:HG21	1.96	0.46
1:C:3722:TYR:HD2	1:C:3793:MET:HE2	1.79	0.46
1:D:342:GLY:HA2	1:D:389:PHE:HD2	1.80	0.46
1:D:534:ARG:HA	1:D:537:CYS:SG	2.56	0.46
1:D:590:LEU:HD22	1:D:631:LEU:HD21	1.98	0.46
1:D:4580:TYR:CE1	1:D:4631:PHE:HB2	2.51	0.46
1:A:2280:VAL:O	1:A:2280:VAL:HG12	2.16	0.46
1:B:1719:HIS:NE2	1:B:1802:ILE:CG1	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:THR:OG1	1:A:1693:GLN:NE2	2.40	0.46
1:A:4924:VAL:HA	1:A:4928:LEU:HB2	1.96	0.46
1:B:590:LEU:HD22	1:B:631:LEU:HD21	1.98	0.46
1:B:4069:LYS:HE2	1:B:4133:GLN:HG3	1.97	0.46
1:B:4098:ASP:OD1	1:B:4098:ASP:N	2.48	0.46
1:B:4954:MET:HE3	2:B:5101:ATP:H1'	1.98	0.46
1:C:289:ARG:HB3	1:C:302:VAL:O	2.16	0.46
1:C:3994:HIS:CE1	1:C:3998:HIS:HE1	2.33	0.46
1:A:302:VAL:HB	1:A:306:LYS:HB2	1.97	0.46
1:A:582:HIS:O	1:A:585:SER:OG	2.27	0.46
1:A:2110:TYR:HA	1:A:3700:GLN:HE22	1.74	0.46
1:B:879:HIS:CE1	1:B:913:LEU:HD21	2.51	0.46
1:C:1719:HIS:NE2	1:C:1802:ILE:CG1	2.78	0.46
1:C:4951:LYS:HE2	1:C:4951:LYS:HB2	1.86	0.46
1:D:978:THR:HG22	1:D:981:GLN:H	1.81	0.46
1:A:2258:LEU:HD23	1:A:2297:LYS:HE3	1.96	0.46
1:A:3816:MET:HE3	1:A:3816:MET:HB2	1.87	0.46
1:A:4069:LYS:HE2	1:A:4133:GLN:HG3	1.97	0.46
1:B:289:ARG:HB3	1:B:302:VAL:O	2.16	0.46
1:B:564:LEU:O	1:B:568:LEU:HG	2.16	0.46
1:C:879:HIS:CE1	1:C:913:LEU:HD21	2.51	0.46
1:C:2228:MET:HE3	1:C:2228:MET:HB3	1.84	0.46
1:C:4069:LYS:HE2	1:C:4133:GLN:HG3	1.97	0.46
1:C:4580:TYR:CE1	1:C:4631:PHE:HB2	2.51	0.46
1:D:688:LEU:HD12	1:D:688:LEU:O	2.15	0.46
1:D:879:HIS:CE1	1:D:913:LEU:HD21	2.51	0.46
1:D:2110:TYR:HA	1:D:3700:GLN:HE22	1.74	0.46
1:D:2185:ILE:O	1:D:2188:ASN:ND2	2.49	0.46
1:A:342:GLY:HA2	1:A:389:PHE:HD2	1.80	0.46
1:A:494:LEU:HD12	1:A:515:TRP:CD1	2.51	0.46
1:A:836:GLY:O	1:A:1201:HIS:CD2	2.68	0.46
1:B:973:SER:HA	1:B:1044:ARG:NH2	2.31	0.46
1:B:1293:LEU:HD22	1:B:1579:MET:SD	2.56	0.46
1:B:1929:MET:C	1:B:1931:LEU:H	2.24	0.46
1:C:22:LEU:HD12	1:C:37:LEU:HB2	1.98	0.46
1:A:544:LEU:HA	1:A:547:VAL:HG22	1.99	0.45
1:A:914:PRO:HD2	1:A:917:GLU:HG3	1.98	0.45
1:A:4098:ASP:N	1:A:4098:ASP:OD1	2.48	0.45
1:A:4954:MET:HE3	2:A:5101:ATP:H1'	1.98	0.45
1:B:685:GLY:HA3	1:B:714:TYR:O	2.15	0.45
1:B:1719:HIS:HE1	1:B:1800:PRO:HG2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2280:VAL:O	1:B:2280:VAL:HG12	2.16	0.45
1:C:58:VAL:HG12	1:C:305:CYS:HA	1.97	0.45
1:C:978:THR:HG22	1:C:981:GLN:H	1.81	0.45
1:C:4774:LYS:HE2	1:C:4774:LYS:HB3	1.75	0.45
1:A:24:CYS:SG	1:A:35:LEU:HB2	2.55	0.45
1:A:688:LEU:HD12	1:A:688:LEU:O	2.15	0.45
1:A:973:SER:HA	1:A:1044:ARG:NH2	2.31	0.45
1:A:4211:LYS:HB3	1:A:4211:LYS:HZ3	1.81	0.45
1:B:550:LYS:HG3	1:B:551:LEU:H	1.80	0.45
1:B:914:PRO:HD2	1:B:917:GLU:HG3	1.98	0.45
1:C:869:ARG:NH2	1:C:947:GLU:OE1	2.45	0.45
1:C:914:PRO:HD2	1:C:917:GLU:HG3	1.98	0.45
1:C:4175:ARG:O	1:C:4177:TYR:N	2.48	0.45
1:A:35:LEU:HB3	1:A:49:LEU:HD22	1.99	0.45
1:A:1719:HIS:NE2	1:A:1802:ILE:CG1	2.78	0.45
1:B:978:THR:HG22	1:B:981:GLN:H	1.81	0.45
1:B:1762:LEU:N	1:B:1762:LEU:CD2	2.79	0.45
1:D:22:LEU:HD12	1:D:37:LEU:HB2	1.98	0.45
1:D:35:LEU:HB3	1:D:49:LEU:HD22	1.99	0.45
1:D:58:VAL:HG12	1:D:305:CYS:HA	1.97	0.45
1:A:2207:VAL:HA	1:A:2210:VAL:HG12	1.99	0.45
1:A:4958:CYS:O	2:A:5101:ATP:C2	2.70	0.45
1:C:19:GLU:HG2	1:C:66:CYS:HB3	1.99	0.45
1:C:635:THR:OG1	1:C:1693:GLN:NE2	2.40	0.45
1:C:1293:LEU:HD22	1:C:1579:MET:SD	2.56	0.45
1:C:4863:TYR:O	1:C:4865:LYS:N	2.49	0.45
1:C:4958:CYS:O	2:C:5101:ATP:C2	2.70	0.45
1:D:564:LEU:O	1:D:568:LEU:HG	2.16	0.45
1:D:1929:MET:C	1:D:1931:LEU:H	2.24	0.45
1:A:747:CYS:O	1:A:747:CYS:SG	2.75	0.45
1:A:879:HIS:CE1	1:A:913:LEU:HD21	2.51	0.45
1:A:978:THR:HG22	1:A:981:GLN:H	1.81	0.45
1:A:1651:LEU:O	1:A:1654:SER:OG	2.35	0.45
1:A:1762:LEU:N	1:A:1762:LEU:CD2	2.79	0.45
1:A:4874:MET:O	1:A:4876:CYS:N	2.50	0.45
1:A:4984:ASN:C	1:A:4986:ALA:H	2.25	0.45
1:B:534:ARG:HA	1:B:537:CYS:SG	2.56	0.45
1:B:544:LEU:HA	1:B:547:VAL:HG22	1.99	0.45
1:B:582:HIS:O	1:B:585:SER:OG	2.27	0.45
1:B:639:ASN:HA	1:B:1635:THR:HA	1.99	0.45
1:B:2207:VAL:HA	1:B:2210:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:544:LEU:HA	1:C:547:VAL:HG22	1.99	0.45
1:C:564:LEU:O	1:C:568:LEU:HG	2.16	0.45
1:D:210:GLU:OE1	1:D:273:HIS:NE2	2.48	0.45
1:D:811:CYS:HA	1:D:815:VAL:HG21	1.98	0.45
1:D:973:SER:HA	1:D:1044:ARG:NH2	2.31	0.45
1:D:4874:MET:C	1:D:4876:CYS:N	2.75	0.45
1:D:4984:ASN:C	1:D:4986:ALA:H	2.25	0.45
1:A:548:VAL:HG21	1:A:582:HIS:HB3	1.97	0.45
1:A:564:LEU:O	1:A:568:LEU:HG	2.16	0.45
1:A:1257:VAL:CG1	1:A:1597:VAL:HG11	2.31	0.45
1:A:2185:ILE:O	1:A:2188:ASN:ND2	2.49	0.45
1:A:4696:ASP:O	1:A:4699:GLY:N	2.47	0.45
1:B:464:LYS:HB2	1:B:464:LYS:HE3	1.81	0.45
1:C:534:ARG:HA	1:C:537:CYS:SG	2.56	0.45
1:C:639:ASN:HA	1:C:1635:THR:HA	1.99	0.45
1:C:1762:LEU:N	1:C:1762:LEU:CD2	2.79	0.45
1:C:2207:VAL:HA	1:C:2210:VAL:HG12	1.99	0.45
1:C:4874:MET:O	1:C:4876:CYS:N	2.50	0.45
1:C:4954:MET:HE3	2:C:5101:ATP:H1'	1.98	0.45
1:C:5027:CYS:C	1:C:5029:ARG:H	2.25	0.45
1:D:494:LEU:HD12	1:D:515:TRP:CD1	2.51	0.45
1:D:635:THR:OG1	1:D:1693:GLN:NE2	2.40	0.45
1:A:590:LEU:HD22	1:A:631:LEU:HD21	1.98	0.45
1:A:1293:LEU:HD22	1:A:1579:MET:SD	2.56	0.45
1:A:2228:MET:HE3	1:A:2228:MET:HB3	1.84	0.45
1:A:4079:ASP:OD1	1:A:4079:ASP:N	2.49	0.45
1:B:392:ARG:NH1	1:B:393:CYS:H	2.15	0.45
1:B:3658:LYS:O	1:B:3661:TRP:N	2.48	0.45
1:C:494:LEU:HD12	1:C:515:TRP:CD1	2.51	0.45
1:C:685:GLY:HA3	1:C:714:TYR:O	2.15	0.45
1:C:2280:VAL:O	1:C:2280:VAL:HG12	2.16	0.45
1:D:289:ARG:HB3	1:D:302:VAL:O	2.16	0.45
1:D:747:CYS:O	1:D:747:CYS:SG	2.75	0.45
1:D:1651:LEU:O	1:D:1654:SER:OG	2.35	0.45
1:D:2207:VAL:HA	1:D:2210:VAL:HG12	1.99	0.45
1:D:4666:VAL:N	1:D:4667:PRO:CD	2.80	0.45
1:D:4863:TYR:O	1:D:4865:LYS:N	2.49	0.45
1:A:534:ARG:HA	1:A:537:CYS:SG	2.56	0.45
1:A:811:CYS:HA	1:A:815:VAL:HG21	1.98	0.45
1:A:1548:LEU:HD23	1:A:1548:LEU:HA	1.83	0.45
1:B:497:TYR:HA	1:B:503:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2185:ILE:O	1:B:2188:ASN:ND2	2.49	0.45
1:B:4958:CYS:O	2:B:5101:ATP:C2	2.70	0.45
1:B:4984:ASN:C	1:B:4986:ALA:H	2.25	0.45
1:B:5027:CYS:C	1:B:5029:ARG:H	2.25	0.45
1:D:4901:ILE:HG22	1:D:4902:GLU:H	1.82	0.45
1:A:100:THR:HG21	1:A:162:LYS:HE3	1.99	0.45
1:A:1180:ARG:HA	1:A:1180:ARG:HE	1.81	0.45
1:A:4666:VAL:N	1:A:4667:PRO:CD	2.80	0.45
1:B:4666:VAL:N	1:B:4667:PRO:CD	2.80	0.45
1:C:886:ARG:HH21	1:C:897:ARG:HH22	1.65	0.45
1:C:2185:ILE:O	1:C:2188:ASN:ND2	2.49	0.45
1:D:1211:LEU:HB3	1:D:1214:PHE:HB2	1.99	0.45
1:D:1749:PRO:HB2	1:D:1755:GLY:HA3	1.99	0.45
1:D:1762:LEU:N	1:D:1762:LEU:CD2	2.79	0.45
1:D:4069:LYS:HE2	1:D:4133:GLN:HG3	1.97	0.45
1:A:497:TYR:HA	1:A:503:PHE:CE2	2.52	0.45
1:B:4696:ASP:O	1:B:4699:GLY:N	2.47	0.45
1:B:4876:CYS:CB	1:B:4882:CYS:SG	2.94	0.45
1:C:1211:LEU:HB3	1:C:1214:PHE:HB2	1.99	0.45
1:C:1649:ASP:OD1	1:C:1650:ILE:N	2.49	0.45
1:D:1293:LEU:HD22	1:D:1579:MET:SD	2.56	0.45
1:D:2228:MET:HE3	1:D:2228:MET:HB3	1.84	0.45
1:D:4874:MET:O	1:D:4876:CYS:N	2.50	0.45
1:D:4958:CYS:O	2:D:5101:ATP:C2	2.70	0.45
1:A:1689:VAL:HG23	1:A:1690:ASP:H	1.83	0.44
1:B:1289:LEU:CD2	1:B:1597:VAL:HG23	2.45	0.44
1:B:3661:TRP:HB3	1:B:3663:LEU:HB2	2.00	0.44
1:B:4874:MET:C	1:B:4876:CYS:N	2.75	0.44
1:B:4874:MET:O	1:B:4876:CYS:N	2.50	0.44
1:C:1719:HIS:HE1	1:C:1800:PRO:HG2	1.82	0.44
1:C:4666:VAL:N	1:C:4667:PRO:CD	2.80	0.44
1:D:100:THR:HG21	1:D:162:LYS:HE3	1.99	0.44
1:D:544:LEU:HA	1:D:547:VAL:HG22	1.99	0.44
1:D:3661:TRP:HB3	1:D:3663:LEU:HB2	2.00	0.44
1:A:210:GLU:OE1	1:A:273:HIS:NE2	2.48	0.44
1:A:289:ARG:HB3	1:A:302:VAL:O	2.16	0.44
1:A:662:TRP:HZ3	1:A:811:CYS:H	1.65	0.44
1:A:838:HIS:CA	1:A:1201:HIS:HB3	2.46	0.44
1:A:4874:MET:C	1:A:4876:CYS:N	2.75	0.44
1:B:19:GLU:HG2	1:B:66:CYS:HB3	1.99	0.44
1:B:22:LEU:HD12	1:B:37:LEU:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:THR:HG21	1:B:162:LYS:HE3	1.99	0.44
1:B:210:GLU:OE1	1:B:273:HIS:NE2	2.48	0.44
1:B:797:HIS:HB3	1:B:1624:LEU:HA	1.99	0.44
1:B:1749:PRO:HB2	1:B:1755:GLY:HA3	1.99	0.44
1:B:4802:GLY:HA3	1:B:4809:PHE:CZ	2.52	0.44
1:B:4843:LEU:HD22	1:C:4823:LEU:HD11	2.00	0.44
1:B:4863:TYR:O	1:B:4865:LYS:N	2.49	0.44
1:C:497:TYR:HA	1:C:503:PHE:CE2	2.52	0.44
1:C:1180:ARG:HA	1:C:1180:ARG:HE	1.81	0.44
1:C:1749:PRO:HB2	1:C:1755:GLY:HA3	1.99	0.44
1:C:4176:PRO:O	1:C:4177:TYR:CG	2.70	0.44
1:D:914:PRO:HD2	1:D:917:GLU:HG3	1.98	0.44
1:D:1649:ASP:OD1	1:D:1650:ILE:N	2.49	0.44
1:D:1689:VAL:HG23	1:D:1690:ASP:H	1.83	0.44
1:D:1719:HIS:HE1	1:D:1800:PRO:HG2	1.82	0.44
1:D:3816:MET:HE3	1:D:3816:MET:HB2	1.87	0.44
1:D:4712:PRO:HG2	1:D:4718:LYS:HA	1.99	0.44
1:D:4767:TRP:O	1:D:4770:SER:OG	2.34	0.44
1:A:4802:GLY:HA3	1:A:4809:PHE:CZ	2.52	0.44
1:A:4823:LEU:HD11	1:D:4843:LEU:HD22	2.00	0.44
1:B:794:GLY:HA2	1:B:800:PHE:HE1	1.83	0.44
1:C:100:THR:HG21	1:C:162:LYS:HE3	1.99	0.44
1:C:408:ALA:HA	1:C:486:LEU:HD21	2.00	0.44
1:C:1708:ARG:NH2	1:C:1712:TYR:HE1	2.09	0.44
1:C:1929:MET:C	1:C:1931:LEU:H	2.24	0.44
1:C:4901:ILE:HG22	1:C:4902:GLU:H	1.82	0.44
1:D:484:LEU:O	1:D:488:LEU:HG	2.18	0.44
1:D:1180:ARG:HA	1:D:1180:ARG:HE	1.81	0.44
1:D:4176:PRO:O	1:D:4177:TYR:CG	2.70	0.44
1:D:4954:MET:HE3	2:D:5101:ATP:H1'	1.98	0.44
1:A:19:GLU:HG2	1:A:66:CYS:HB3	1.99	0.44
1:A:1929:MET:C	1:A:1931:LEU:H	2.24	0.44
1:B:183:SER:OG	1:B:192:ASP:OD1	2.30	0.44
1:B:747:CYS:O	1:B:747:CYS:SG	2.75	0.44
1:B:3670:GLU:OE1	1:B:3670:GLU:N	2.51	0.44
1:B:4956:THR:O	1:B:4965:SER:N	2.50	0.44
1:C:747:CYS:O	1:C:747:CYS:SG	2.75	0.44
1:C:4843:LEU:HD22	1:D:4823:LEU:HD11	2.00	0.44
1:C:4875:LYS:H	1:C:4875:LYS:HG2	1.50	0.44
1:D:2280:VAL:O	1:D:2280:VAL:HG12	2.16	0.44
1:A:639:ASN:HA	1:A:1635:THR:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1649:ASP:OD1	1:A:1650:ILE:N	2.49	0.44
1:A:3946:GLN:NE2	1:A:3949:ARG:HH22	2.16	0.44
1:A:4176:PRO:O	1:A:4177:TYR:CG	2.70	0.44
1:A:4843:LEU:HD22	1:B:4823:LEU:HD11	2.00	0.44
1:A:4876:CYS:CB	1:A:4882:CYS:SG	2.94	0.44
1:B:1211:LEU:HB3	1:B:1214:PHE:HB2	1.99	0.44
1:B:1437:VAL:HG11	1:B:1450:VAL:HG11	1.99	0.44
1:B:3946:GLN:NE2	1:B:3949:ARG:HH22	2.16	0.44
1:B:4774:LYS:HE2	1:B:4774:LYS:HB3	1.75	0.44
1:C:1047:LEU:HD11	1:C:1052:ASN:OD1	2.18	0.44
1:C:1437:VAL:HG11	1:C:1450:VAL:HG11	1.99	0.44
1:C:4767:TRP:O	1:C:4770:SER:OG	2.34	0.44
1:C:4874:MET:C	1:C:4876:CYS:N	2.75	0.44
1:C:4984:ASN:C	1:C:4986:ALA:H	2.25	0.44
1:D:594:GLY:HA2	1:D:1594:ARG:HD3	1.99	0.44
1:D:1293:LEU:HD22	1:D:1579:MET:HB3	1.98	0.44
1:A:794:GLY:HA2	1:A:800:PHE:HE1	1.83	0.44
1:A:4901:ILE:HG22	1:A:4902:GLU:H	1.82	0.44
1:B:1651:LEU:O	1:B:1654:SER:OG	2.35	0.44
1:B:4979:THR:HG21	2:B:5101:ATP:N3	2.33	0.44
1:C:811:CYS:HA	1:C:815:VAL:HG21	1.98	0.44
1:C:3661:TRP:HB3	1:C:3663:LEU:HB2	2.00	0.44
1:C:4712:PRO:HG2	1:C:4718:LYS:HA	1.99	0.44
1:C:4956:THR:O	1:C:4965:SER:N	2.50	0.44
1:D:4979:THR:HG21	2:D:5101:ATP:N3	2.33	0.44
1:D:5027:CYS:C	1:D:5029:ARG:H	2.25	0.44
1:A:484:LEU:O	1:A:488:LEU:HG	2.18	0.44
1:A:2364:PHE:HE1	1:A:2429:LEU:HD11	1.83	0.44
1:A:3842:LEU:O	1:A:3929:SER:OG	2.36	0.44
1:B:811:CYS:HA	1:B:815:VAL:HG21	1.98	0.44
1:C:35:LEU:HB3	1:C:49:LEU:HD22	1.99	0.44
1:D:794:GLY:HA2	1:D:800:PHE:HE1	1.83	0.44
1:D:3716:LEU:HD12	1:D:3716:LEU:HA	1.84	0.44
1:A:392:ARG:HD2	1:A:392:ARG:HA	1.79	0.44
1:A:797:HIS:HB3	1:A:1624:LEU:HA	1.99	0.44
1:A:1437:VAL:HG11	1:A:1450:VAL:HG11	1.99	0.44
1:A:3661:TRP:HB3	1:A:3663:LEU:HB2	2.00	0.44
1:B:662:TRP:HZ3	1:B:811:CYS:H	1.65	0.44
1:B:4175:ARG:C	1:B:4177:TYR:N	2.75	0.44
1:B:4176:PRO:O	1:B:4177:TYR:CG	2.70	0.44
1:C:797:HIS:HB3	1:C:1624:LEU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2460:LEU:HD23	1:C:2460:LEU:HA	1.85	0.44
1:C:3816:MET:HE3	1:C:3816:MET:HB2	1.87	0.44
1:C:4802:GLY:HA3	1:C:4809:PHE:CZ	2.52	0.44
1:C:4979:THR:HG21	2:C:5101:ATP:N3	2.33	0.44
1:D:615:ARG:NH2	1:D:1677:GLY:O	2.51	0.44
1:D:639:ASN:HA	1:D:1635:THR:HA	1.99	0.44
1:D:1437:VAL:HG11	1:D:1450:VAL:HG11	1.99	0.44
1:D:4774:LYS:HE2	1:D:4774:LYS:HB3	1.75	0.44
1:D:4802:GLY:HA3	1:D:4809:PHE:CZ	2.52	0.44
1:A:22:LEU:HD12	1:A:37:LEU:HB2	1.98	0.44
1:A:1211:LEU:HB3	1:A:1214:PHE:HB2	1.99	0.44
1:A:1719:HIS:HE1	1:A:1800:PRO:HG2	1.82	0.44
1:A:4712:PRO:HG2	1:A:4718:LYS:HA	1.99	0.44
1:A:5027:CYS:C	1:A:5029:ARG:H	2.25	0.44
1:B:35:LEU:HB3	1:B:49:LEU:HD22	1.99	0.44
1:B:408:ALA:HA	1:B:486:LEU:HD21	2.00	0.44
1:B:4767:TRP:O	1:B:4770:SER:OG	2.34	0.44
1:C:662:TRP:HZ3	1:C:811:CYS:H	1.65	0.44
1:C:700:GLU:HA	1:C:1646:ARG:HA	2.00	0.44
1:C:1804:LEU:HD23	1:C:1804:LEU:H	1.83	0.44
1:D:19:GLU:HG2	1:D:66:CYS:HB3	1.99	0.44
1:D:839:LEU:N	1:D:1200:GLY:O	2.51	0.44
1:D:886:ARG:HH21	1:D:897:ARG:HH22	1.65	0.44
1:D:4710:SER:O	1:D:4710:SER:OG	2.31	0.44
1:A:1047:LEU:HD11	1:A:1052:ASN:OD1	2.18	0.43
1:A:1749:PRO:HB2	1:A:1755:GLY:HA3	1.99	0.43
1:A:3670:GLU:OE1	1:A:3670:GLU:N	2.51	0.43
1:A:3891:LEU:HD13	1:A:3899:PHE:CE1	2.53	0.43
1:A:4088:ILE:HG22	1:A:4089:SER:O	2.18	0.43
1:A:4979:THR:HG21	2:A:5101:ATP:N3	2.33	0.43
1:B:1180:ARG:HA	1:B:1180:ARG:HE	1.81	0.43
1:B:2364:PHE:HE1	1:B:2429:LEU:HD11	1.83	0.43
1:B:3716:LEU:HD12	1:B:3716:LEU:HA	1.84	0.43
1:B:3722:TYR:CD2	1:B:3793:MET:HE2	2.53	0.43
1:B:4088:ILE:HG22	1:B:4089:SER:O	2.18	0.43
1:C:594:GLY:HA2	1:C:1594:ARG:HD3	1.99	0.43
1:D:1719:HIS:NE2	1:D:1802:ILE:CG1	2.78	0.43
1:D:1804:LEU:H	1:D:1804:LEU:HD23	1.83	0.43
1:D:4153:HIS:O	1:D:4155:PRO:HD3	2.18	0.43
1:D:4175:ARG:C	1:D:4177:TYR:N	2.75	0.43
1:A:615:ARG:NH2	1:A:1677:GLY:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:700:GLU:HA	1:B:1646:ARG:HA	2.00	0.43
1:B:732:SER:O	1:B:735:GLN:NE2	2.51	0.43
1:B:1689:VAL:HG23	1:B:1690:ASP:H	1.83	0.43
1:B:4901:ILE:HG22	1:B:4902:GLU:H	1.82	0.43
1:C:732:SER:O	1:C:735:GLN:NE2	2.51	0.43
1:D:793:LEU:HG	1:D:1625:GLY:HA2	2.00	0.43
1:D:2364:PHE:HE1	1:D:2429:LEU:HD11	1.83	0.43
1:D:4098:ASP:OD1	1:D:4098:ASP:N	2.48	0.43
1:A:732:SER:O	1:A:735:GLN:NE2	2.51	0.43
1:A:1689:VAL:HG23	1:A:1690:ASP:N	2.33	0.43
1:A:2110:TYR:C	1:A:2110:TYR:CD1	2.96	0.43
1:B:886:ARG:HH21	1:B:897:ARG:HH22	1.65	0.43
1:B:1649:ASP:OD1	1:B:1650:ILE:N	2.49	0.43
1:B:4153:HIS:O	1:B:4155:PRO:HD3	2.18	0.43
1:C:119:SER:OG	1:C:136:GLY:O	2.24	0.43
1:C:3722:TYR:CD2	1:C:3793:MET:HE2	2.53	0.43
1:D:497:TYR:HA	1:D:503:PHE:CE2	2.52	0.43
1:D:1679:ASN:HA	1:D:1682:ALA:HB3	2.01	0.43
1:D:2110:TYR:C	1:D:2110:TYR:CD1	2.96	0.43
1:C:1212:ARG:HA	1:C:1212:ARG:HD2	1.87	0.43
1:C:1289:LEU:CD2	1:C:1597:VAL:HG23	2.45	0.43
1:C:1452:TRP:HB3	1:C:1548:LEU:HD13	2.00	0.43
1:C:1689:VAL:HG23	1:C:1690:ASP:H	1.83	0.43
1:C:4088:ILE:HG22	1:C:4089:SER:O	2.18	0.43
1:D:1715:LEU:C	1:D:1715:LEU:CD2	2.85	0.43
1:D:3891:LEU:HD13	1:D:3899:PHE:CE1	2.53	0.43
1:D:4088:ILE:HG22	1:D:4089:SER:O	2.18	0.43
1:A:594:GLY:HA2	1:A:1594:ARG:HD3	1.99	0.43
1:A:1804:LEU:HD23	1:A:1804:LEU:H	1.83	0.43
1:A:4211:LYS:NZ	1:A:4211:LYS:CB	2.73	0.43
1:B:484:LEU:O	1:B:488:LEU:HG	2.18	0.43
1:B:487:VAL:HG23	1:B:522:LEU:HD22	2.01	0.43
1:B:594:GLY:HA2	1:B:1594:ARG:HD3	1.99	0.43
1:B:1778:SER:OG	1:B:1798:LEU:HB2	2.19	0.43
1:C:392:ARG:NH1	1:C:393:CYS:H	2.15	0.43
1:C:484:LEU:O	1:C:488:LEU:HG	2.18	0.43
1:C:794:GLY:HA2	1:C:800:PHE:HE1	1.83	0.43
1:C:4175:ARG:C	1:C:4177:TYR:N	2.75	0.43
1:C:4876:CYS:CB	1:C:4882:CYS:SG	2.94	0.43
1:D:1293:LEU:HD13	1:D:1580:PHE:CE1	2.53	0.43
1:D:3946:GLN:NE2	1:D:3949:ARG:HH22	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:VAL:HG22	1:A:616:SER:H	1.84	0.43
1:A:700:GLU:HA	1:A:1646:ARG:HA	2.00	0.43
1:A:1778:SER:OG	1:A:1798:LEU:HB2	2.19	0.43
1:B:410:LEU:HD21	1:B:441:VAL:HA	2.00	0.43
1:B:839:LEU:N	1:B:1200:GLY:O	2.51	0.43
1:B:1089:TYR:CE1	1:B:1150:GLY:HA3	2.54	0.43
1:B:1689:VAL:HG23	1:B:1690:ASP:N	2.33	0.43
1:B:4875:LYS:H	1:B:4875:LYS:HG2	1.50	0.43
1:B:4943:LEU:HD23	1:B:4943:LEU:HA	1.87	0.43
1:C:615:ARG:NH2	1:C:1677:GLY:O	2.51	0.43
1:C:1703:LEU:HD23	1:C:1703:LEU:HA	1.86	0.43
1:C:1778:SER:OG	1:C:1798:LEU:HB2	2.19	0.43
1:D:312:THR:OG1	1:D:313:SER:N	2.52	0.43
1:D:614:VAL:HG22	1:D:616:SER:H	1.84	0.43
1:D:1047:LEU:HD11	1:D:1052:ASN:OD1	2.18	0.43
1:D:1452:TRP:HB3	1:D:1548:LEU:HD13	2.00	0.43
1:A:920:TYR:O	1:A:923:GLN:HG3	2.19	0.43
1:A:1289:LEU:CD2	1:A:1597:VAL:HG23	2.45	0.43
1:A:1452:TRP:HB3	1:A:1548:LEU:HD13	2.00	0.43
1:A:1935:VAL:HG22	1:A:1936:LYS:N	2.34	0.43
1:A:3658:LYS:O	1:A:3661:TRP:N	2.48	0.43
1:B:392:ARG:NH1	1:B:393:CYS:O	2.52	0.43
1:B:392:ARG:HD2	1:B:392:ARG:HA	1.79	0.43
1:B:614:VAL:HG22	1:B:616:SER:H	1.84	0.43
1:B:615:ARG:NH2	1:B:1677:GLY:O	2.51	0.43
1:B:758:ARG:HA	1:B:764:VAL:HG23	2.01	0.43
1:B:1952:GLN:O	1:B:1956:GLU:HG2	2.19	0.43
1:B:3891:LEU:HD13	1:B:3899:PHE:CE1	2.53	0.43
1:C:614:VAL:HG22	1:C:616:SER:H	1.84	0.43
1:C:758:ARG:HA	1:C:764:VAL:HG23	2.01	0.43
1:C:1180:ARG:HA	1:C:1180:ARG:NE	2.34	0.43
1:C:1748:PHE:O	1:C:1750:PRO:HD3	2.19	0.43
1:C:4153:HIS:O	1:C:4155:PRO:HD3	2.18	0.43
1:D:410:LEU:HD21	1:D:441:VAL:HA	2.00	0.43
1:D:732:SER:O	1:D:735:GLN:NE2	2.51	0.43
1:D:1689:VAL:HG23	1:D:1690:ASP:N	2.33	0.43
1:D:4984:ASN:C	2:D:5101:ATP:HN61	2.27	0.43
1:A:410:LEU:HD21	1:A:441:VAL:HA	2.00	0.43
1:A:487:VAL:HG23	1:A:522:LEU:HD22	2.01	0.43
1:A:1293:LEU:HD22	1:A:1579:MET:HB3	1.98	0.43
1:A:1685:LEU:HD23	1:A:1688:HIS:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4175:ARG:C	1:A:4177:TYR:N	2.75	0.43
1:B:889:GLN:HB3	1:B:891:TRP:CD1	2.54	0.43
1:B:1152:MET:HB3	1:B:1223:PHE:CE2	2.54	0.43
1:B:1867:GLU:N	1:B:1868:PRO:HD2	2.34	0.43
1:B:4984:ASN:C	2:B:5101:ATP:HN61	2.27	0.43
1:C:1293:LEU:HD22	1:C:1579:MET:HB3	1.98	0.43
1:C:2364:PHE:HE1	1:C:2429:LEU:HD11	1.83	0.43
1:C:3946:GLN:NE2	1:C:3949:ARG:HH22	2.16	0.43
1:C:4984:ASN:C	2:C:5101:ATP:HN61	2.27	0.43
1:D:662:TRP:HZ3	1:D:811:CYS:H	1.65	0.43
1:D:743:VAL:N	1:D:760:ASN:HB3	2.21	0.43
1:D:797:HIS:HB3	1:D:1624:LEU:HA	1.99	0.43
1:D:3670:GLU:OE1	1:D:3670:GLU:N	2.51	0.43
1:D:3722:TYR:CD2	1:D:3793:MET:HE2	2.53	0.43
1:A:392:ARG:NH1	1:A:393:CYS:O	2.52	0.43
1:A:408:ALA:HA	1:A:486:LEU:HD21	2.00	0.43
1:A:580:GLU:HG3	1:A:620:LEU:HD22	2.01	0.43
1:A:1705:GLY:HA2	1:A:1708:ARG:HB3	2.01	0.43
1:A:1748:PHE:O	1:A:1750:PRO:HD3	2.19	0.43
1:A:4774:LYS:HE2	1:A:4774:LYS:HB3	1.75	0.43
1:B:662:TRP:HZ2	1:B:814:ALA:HB3	1.84	0.43
1:B:1748:PHE:O	1:B:1750:PRO:HD3	2.19	0.43
1:B:3842:LEU:O	1:B:3929:SER:OG	2.36	0.43
1:B:4712:PRO:HG2	1:B:4718:LYS:HA	1.99	0.43
1:C:793:LEU:HG	1:C:1625:GLY:HA2	2.00	0.43
1:C:889:GLN:HB3	1:C:891:TRP:CD1	2.54	0.43
1:C:1548:LEU:HD23	1:C:1548:LEU:HA	1.83	0.43
1:C:4211:LYS:HZ3	1:C:4211:LYS:CB	2.32	0.43
1:D:582:HIS:O	1:D:585:SER:OG	2.27	0.43
1:D:700:GLU:HA	1:D:1646:ARG:HA	2.00	0.43
1:D:1089:TYR:CE1	1:D:1150:GLY:HA3	2.54	0.43
1:D:1180:ARG:HA	1:D:1180:ARG:NE	2.34	0.43
1:D:1715:LEU:HD23	1:D:1715:LEU:O	2.19	0.43
1:D:3842:LEU:O	1:D:3929:SER:OG	2.36	0.43
1:D:4875:LYS:H	1:D:4875:LYS:HG2	1.50	0.43
1:A:660:GLY:CA	1:A:750:LEU:HD12	2.49	0.43
1:A:886:ARG:HH21	1:A:897:ARG:HH22	1.65	0.43
1:C:839:LEU:N	1:C:1200:GLY:O	2.51	0.43
1:C:1689:VAL:HG23	1:C:1690:ASP:N	2.33	0.43
1:C:1935:VAL:HG22	1:C:1936:LYS:N	2.34	0.43
1:D:408:ALA:HA	1:D:486:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:842:PRO:HD3	1:D:1073:ARG:HG3	2.01	0.43
1:D:920:TYR:O	1:D:923:GLN:HG3	2.19	0.43
1:D:1152:MET:HB3	1:D:1223:PHE:CE2	2.54	0.43
1:D:1685:LEU:HD23	1:D:1688:HIS:HB3	2.01	0.43
1:D:4175:ARG:N	1:D:4176:PRO:CD	2.77	0.43
1:A:793:LEU:HG	1:A:1625:GLY:HA2	2.00	0.42
1:A:839:LEU:N	1:A:1200:GLY:O	2.51	0.42
1:A:1089:TYR:CE1	1:A:1150:GLY:HA3	2.54	0.42
1:A:1152:MET:HB3	1:A:1223:PHE:CE2	2.54	0.42
1:A:4563:ARG:HD2	1:A:4563:ARG:HA	1.81	0.42
1:B:312:THR:OG1	1:B:313:SER:N	2.52	0.42
1:B:580:GLU:HG3	1:B:620:LEU:HD22	2.01	0.42
1:B:884:LEU:HD13	1:B:967:PRO:HG2	2.01	0.42
1:B:1452:TRP:HB3	1:B:1548:LEU:HD13	2.00	0.42
1:B:1804:LEU:HD23	1:B:1804:LEU:H	1.83	0.42
1:C:210:GLU:OE1	1:C:273:HIS:NE2	2.48	0.42
1:C:410:LEU:HD21	1:C:441:VAL:HA	2.00	0.42
1:C:662:TRP:HZ2	1:C:814:ALA:HB3	1.84	0.42
1:C:1715:LEU:HD23	1:C:1715:LEU:O	2.19	0.42
1:D:662:TRP:HZ2	1:D:814:ALA:HB3	1.84	0.42
1:A:2252:ASP:N	1:A:2252:ASP:OD1	2.52	0.42
1:B:3941:ASP:OD1	1:B:3941:ASP:N	2.53	0.42
1:C:392:ARG:NH1	1:C:393:CYS:O	2.52	0.42
1:C:487:VAL:HG23	1:C:522:LEU:HD22	2.01	0.42
1:C:1679:ASN:HA	1:C:1682:ALA:HB3	2.01	0.42
1:D:580:GLU:HG3	1:D:620:LEU:HD22	2.01	0.42
1:D:1748:PHE:O	1:D:1750:PRO:HD3	2.19	0.42
1:D:4211:LYS:NZ	1:D:4211:LYS:CB	2.73	0.42
1:D:4862:PHE:HD1	1:D:4902:GLU:HB2	1.84	0.42
1:D:4875:LYS:HE3	1:D:4875:LYS:HB3	1.57	0.42
1:A:45:ARG:HA	1:A:45:ARG:HD3	1.92	0.42
1:A:662:TRP:HZ2	1:A:814:ALA:HB3	1.84	0.42
1:A:686:TRP:CE3	1:A:777:PHE:HB3	2.55	0.42
1:A:758:ARG:HA	1:A:764:VAL:HG23	2.01	0.42
1:A:1652:GLU:O	1:A:1656:ARG:HG2	2.20	0.42
1:A:3722:TYR:CD2	1:A:3793:MET:HE2	2.53	0.42
1:A:3760:LYS:HE3	1:A:3760:LYS:HB2	1.91	0.42
1:B:793:LEU:HG	1:B:1625:GLY:HA2	2.00	0.42
1:B:1705:GLY:HA2	1:B:1708:ARG:HB3	2.01	0.42
1:B:2110:TYR:CD1	1:B:2110:TYR:C	2.96	0.42
1:B:4079:ASP:N	1:B:4079:ASP:OD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1076:ARG:NH1	1:C:1077:ALA:O	2.53	0.42
1:C:1245:PHE:CZ	1:C:1290:ARG:CB	3.03	0.42
1:C:1297:PHE:HA	1:C:1522:LEU:HD12	2.02	0.42
1:C:1651:LEU:O	1:C:1654:SER:OG	2.35	0.42
1:C:2110:TYR:CD1	1:C:2110:TYR:C	2.96	0.42
1:C:3658:LYS:O	1:C:3661:TRP:N	2.48	0.42
1:C:3670:GLU:N	1:C:3670:GLU:OE1	2.51	0.42
1:D:884:LEU:HD13	1:D:967:PRO:HG2	2.01	0.42
1:D:1074:ILE:HB	1:D:1239:SER:HB2	2.02	0.42
1:D:4711:PHE:HB3	1:D:4712:PRO:HD3	2.01	0.42
1:A:1952:GLN:O	1:A:1956:GLU:HG2	2.19	0.42
1:A:4153:HIS:O	1:A:4155:PRO:HD3	2.18	0.42
1:B:1652:GLU:O	1:B:1656:ARG:HG2	2.20	0.42
1:C:21:VAL:HG23	1:C:203:ASN:HB2	2.01	0.42
1:C:101:LEU:H	1:C:101:LEU:HD12	1.84	0.42
1:C:660:GLY:CA	1:C:750:LEU:HD12	2.49	0.42
1:C:1089:TYR:CE1	1:C:1150:GLY:HA3	2.54	0.42
1:C:1152:MET:HB3	1:C:1223:PHE:CE2	2.54	0.42
1:C:1476:MET:N	1:C:1485:SER:O	2.48	0.42
1:C:1867:GLU:N	1:C:1868:PRO:HD2	2.34	0.42
1:C:2252:ASP:OD1	1:C:2252:ASP:N	2.52	0.42
1:C:3891:LEU:HD13	1:C:3899:PHE:CE1	2.53	0.42
1:C:4862:PHE:HD1	1:C:4902:GLU:HB2	1.84	0.42
1:D:1216:ILE:HG22	1:D:1217:CYS:SG	2.60	0.42
1:A:101:LEU:HD12	1:A:101:LEU:H	1.84	0.42
1:A:1129:GLY:O	1:A:1139:PHE:N	2.45	0.42
1:A:1679:ASN:HA	1:A:1682:ALA:HB3	2.01	0.42
1:A:1715:LEU:HD23	1:A:1715:LEU:O	2.19	0.42
1:B:101:LEU:H	1:B:101:LEU:HD12	1.84	0.42
1:B:660:GLY:CA	1:B:750:LEU:HD12	2.49	0.42
1:B:686:TRP:CE3	1:B:777:PHE:HB3	2.55	0.42
1:B:920:TYR:O	1:B:923:GLN:HG3	2.19	0.42
1:B:1047:LEU:HD11	1:B:1052:ASN:OD1	2.18	0.42
1:B:3770:LEU:HD12	1:B:3770:LEU:HA	1.85	0.42
1:B:4189:ARG:HE	1:B:4189:ARG:HB2	1.58	0.42
1:C:842:PRO:HD3	1:C:1073:ARG:HG3	2.01	0.42
1:C:920:TYR:O	1:C:923:GLN:HG3	2.19	0.42
1:C:1074:ILE:HB	1:C:1239:SER:HB2	2.02	0.42
1:C:3842:LEU:HD23	1:C:3842:LEU:HA	1.93	0.42
1:C:4696:ASP:O	1:C:4699:GLY:N	2.47	0.42
1:C:4711:PHE:HB3	1:C:4712:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4943:LEU:HD23	1:C:4943:LEU:HA	1.87	0.42
1:D:392:ARG:NH1	1:D:393:CYS:O	2.52	0.42
1:D:1778:SER:OG	1:D:1798:LEU:HB2	2.19	0.42
1:A:312:THR:OG1	1:A:313:SER:N	2.52	0.42
1:A:884:LEU:HD13	1:A:967:PRO:HG2	2.01	0.42
1:A:1216:ILE:HG22	1:A:1217:CYS:SG	2.60	0.42
1:A:3937:TYR:OH	1:A:3944:GLU:OE1	2.21	0.42
1:B:1074:ILE:HB	1:B:1239:SER:HB2	2.02	0.42
1:B:1076:ARG:NH1	1:B:1077:ALA:O	2.53	0.42
1:B:1216:ILE:HG22	1:B:1217:CYS:SG	2.60	0.42
1:C:1952:GLN:O	1:C:1956:GLU:HG2	2.19	0.42
1:C:4085:ARG:HD3	1:C:4087:LEU:HD12	2.02	0.42
1:D:973:SER:HA	1:D:1044:ARG:HH21	1.85	0.42
1:D:1297:PHE:HA	1:D:1522:LEU:HD12	2.02	0.42
1:D:1867:GLU:N	1:D:1868:PRO:HD2	2.34	0.42
1:A:1076:ARG:NH1	1:A:1077:ALA:O	2.53	0.42
1:A:1839:VAL:O	1:A:1840:PRO:C	2.61	0.42
1:A:1867:GLU:N	1:A:1868:PRO:HD2	2.34	0.42
1:A:4691:GLN:NE2	1:A:4703:ARG:HH22	2.18	0.42
1:A:4857:ASN:HD21	1:B:4807:PHE:HD2	1.68	0.42
1:A:4956:THR:O	1:A:4965:SER:N	2.50	0.42
1:B:556:ALA:HA	1:B:560:ILE:HD13	2.02	0.42
1:B:4691:GLN:NE2	1:B:4703:ARG:HH22	2.18	0.42
1:C:464:LYS:HB2	1:C:464:LYS:HE3	1.81	0.42
1:C:2442:LEU:HG	1:C:2443:ILE:HG23	2.02	0.42
1:D:21:VAL:HG23	1:D:203:ASN:HB2	2.01	0.42
1:D:686:TRP:CE3	1:D:777:PHE:HB3	2.55	0.42
1:D:758:ARG:HA	1:D:764:VAL:HG23	2.01	0.42
1:D:2186:MET:HE1	1:D:2234:ARG:HG3	2.02	0.42
1:D:2466:LEU:HD23	1:D:2466:LEU:H	1.85	0.42
1:D:4037:ASN:HD21	1:D:5036:LEU:HD21	1.85	0.42
1:A:21:VAL:HG21	1:A:205:ILE:HD13	2.02	0.42
1:A:973:SER:HA	1:A:1044:ARG:HH21	1.85	0.42
1:A:2213:ASN:OD1	1:A:2214:VAL:N	2.53	0.42
1:A:3718:GLU:OE1	1:A:3720:TYR:N	2.53	0.42
1:A:4807:PHE:HD2	1:D:4857:ASN:HD21	1.68	0.42
1:A:4984:ASN:C	2:A:5101:ATP:HN61	2.27	0.42
1:B:21:VAL:HG23	1:B:203:ASN:HB2	2.01	0.42
1:B:1715:LEU:HD23	1:B:1715:LEU:O	2.19	0.42
1:B:2252:ASP:OD1	1:B:2252:ASP:N	2.52	0.42
1:C:222:LEU:HG	1:C:390:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:973:SER:HA	1:C:1044:ARG:HH21	1.85	0.42
1:C:2466:LEU:HD23	1:C:2466:LEU:H	1.85	0.42
1:C:4037:ASN:HD21	1:C:5036:LEU:HD21	1.85	0.42
1:C:4815:ASP:O	1:C:4819:GLY:N	2.52	0.42
1:D:487:VAL:HG23	1:D:522:LEU:HD22	2.01	0.42
1:D:660:GLY:CA	1:D:750:LEU:HD12	2.49	0.42
1:D:1289:LEU:CD2	1:D:1597:VAL:HG23	2.45	0.42
1:D:1705:GLY:HA2	1:D:1708:ARG:HB3	2.01	0.42
1:D:3718:GLU:OE1	1:D:3720:TYR:N	2.53	0.42
1:D:4085:ARG:HD3	1:D:4087:LEU:HD12	2.02	0.42
1:A:257:ARG:O	1:A:284:HIS:NE2	2.53	0.42
1:A:1074:ILE:HB	1:A:1239:SER:HB2	2.02	0.42
1:A:1180:ARG:HA	1:A:1180:ARG:NE	2.34	0.42
1:B:257:ARG:O	1:B:284:HIS:NE2	2.53	0.42
1:B:1679:ASN:HA	1:B:1682:ALA:HB3	2.01	0.42
1:B:1685:LEU:HD23	1:B:1688:HIS:HB3	2.01	0.42
1:B:1860:LYS:HE3	1:B:1860:LYS:HB2	1.82	0.42
1:B:3718:GLU:OE1	1:B:3720:TYR:N	2.53	0.42
1:B:3816:MET:HE3	1:B:3816:MET:HB2	1.87	0.42
1:C:580:GLU:HG3	1:C:620:LEU:HD22	2.01	0.42
1:D:889:GLN:HB3	1:D:891:TRP:CD1	2.54	0.42
1:D:1652:GLU:O	1:D:1656:ARG:HG2	2.20	0.42
1:D:4730:ASP:OD1	1:D:4730:ASP:N	2.45	0.42
1:D:4815:ASP:O	1:D:4819:GLY:N	2.52	0.42
1:A:285:VAL:HG23	1:A:286:THR:HG23	2.02	0.42
1:A:2186:MET:HE1	1:A:2234:ARG:HG3	2.02	0.42
1:C:838:HIS:CA	1:C:1201:HIS:HB3	2.46	0.42
1:C:1685:LEU:HD23	1:C:1688:HIS:HB3	2.01	0.42
1:C:2213:ASN:OD1	1:C:2214:VAL:N	2.53	0.42
1:D:1952:GLN:O	1:D:1956:GLU:HG2	2.19	0.42
1:D:2213:ASN:OD1	1:D:2214:VAL:N	2.53	0.42
1:D:4956:THR:O	1:D:4965:SER:N	2.50	0.42
1:B:21:VAL:HG21	1:B:205:ILE:HD13	2.02	0.41
1:B:973:SER:HA	1:B:1044:ARG:HH21	1.85	0.41
1:B:1245:PHE:CZ	1:B:1290:ARG:CB	3.03	0.41
1:B:1297:PHE:HA	1:B:1522:LEU:HD12	2.02	0.41
1:B:3772:THR:OG1	1:B:3815:LYS:NZ	2.52	0.41
1:B:4037:ASN:HD21	1:B:5036:LEU:HD21	1.85	0.41
1:C:312:THR:OG1	1:C:313:SER:N	2.52	0.41
1:C:1652:GLU:O	1:C:1656:ARG:HG2	2.20	0.41
1:C:4862:PHE:HB3	1:C:4901:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:VAL:HG23	1:D:286:THR:HG23	2.02	0.41
1:D:609:CYS:SG	1:D:610:ASN:N	2.93	0.41
1:D:1935:VAL:HG22	1:D:1936:LYS:N	2.34	0.41
1:D:2442:LEU:HG	1:D:2443:ILE:HG23	2.02	0.41
1:D:4127:GLU:OE2	1:D:4131:ARG:NH1	2.54	0.41
1:D:4862:PHE:HB3	1:D:4901:ILE:HG22	2.02	0.41
1:A:842:PRO:HD3	1:A:1073:ARG:HG3	2.01	0.41
1:A:4057:MET:HE2	1:A:4057:MET:HB3	1.96	0.41
1:B:842:PRO:HD3	1:B:1073:ARG:HG3	2.01	0.41
1:B:1089:TYR:HE1	1:B:1150:GLY:HA3	1.85	0.41
1:B:1839:VAL:O	1:B:1840:PRO:C	2.61	0.41
1:B:2213:ASN:OD1	1:B:2214:VAL:N	2.53	0.41
1:C:178:ARG:HA	1:C:178:ARG:HD3	1.89	0.41
1:C:686:TRP:CE3	1:C:777:PHE:HB3	2.55	0.41
1:D:101:LEU:HD12	1:D:101:LEU:H	1.84	0.41
1:D:838:HIS:CA	1:D:1201:HIS:HB3	2.46	0.41
1:D:4185:GLY:C	1:D:4187:SER:H	2.28	0.41
1:A:119:SER:OG	1:A:136:GLY:O	2.24	0.41
1:A:889:GLN:HB3	1:A:891:TRP:CD1	2.54	0.41
1:A:889:GLN:HB3	1:A:891:TRP:HD1	1.85	0.41
1:A:1089:TYR:HE1	1:A:1150:GLY:HA3	1.85	0.41
1:A:1245:PHE:CZ	1:A:1290:ARG:CB	3.03	0.41
1:A:2185:ILE:HA	1:A:2188:ASN:HD22	1.86	0.41
1:A:2460:LEU:HD23	1:A:2460:LEU:HA	1.85	0.41
1:A:3941:ASP:OD1	1:A:3941:ASP:N	2.53	0.41
1:B:755:ILE:CG2	1:B:768:PHE:CB	2.99	0.41
1:B:2255:SER:HA	1:B:2297:LYS:HZ1	1.85	0.41
1:B:3680:ALA:HB3	1:B:3697:PRO:HG2	2.02	0.41
1:B:4815:ASP:O	1:B:4819:GLY:N	2.52	0.41
1:B:4862:PHE:HD1	1:B:4902:GLU:HB2	1.84	0.41
1:C:21:VAL:HG21	1:C:205:ILE:HD13	2.02	0.41
1:C:609:CYS:SG	1:C:610:ASN:N	2.93	0.41
1:C:884:LEU:HD13	1:C:967:PRO:HG2	2.01	0.41
1:C:1216:ILE:HG22	1:C:1217:CYS:SG	2.60	0.41
1:C:1705:GLY:HA2	1:C:1708:ARG:HB3	2.01	0.41
1:C:1860:LYS:HB2	1:C:1860:LYS:HE3	1.82	0.41
1:C:4079:ASP:OD1	1:C:4079:ASP:N	2.49	0.41
1:D:110:ARG:NH1	1:D:117:TYR:OH	2.53	0.41
1:D:705:ASN:HB3	1:D:709:ASP:OD2	2.20	0.41
1:D:1245:PHE:CZ	1:D:1290:ARG:CB	3.03	0.41
1:D:1839:VAL:O	1:D:1840:PRO:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3680:ALA:HB3	1:D:3697:PRO:HG2	2.02	0.41
1:D:4951:LYS:HE2	1:D:4951:LYS:HB2	1.86	0.41
1:B:1548:LEU:HD23	1:B:1548:LEU:HA	1.83	0.41
1:B:1935:VAL:HG22	1:B:1936:LYS:N	2.34	0.41
1:B:2466:LEU:HD23	1:B:2466:LEU:H	1.85	0.41
1:B:4185:GLY:C	1:B:4187:SER:H	2.28	0.41
1:D:392:ARG:NH1	1:D:393:CYS:H	2.15	0.41
1:D:1076:ARG:NH1	1:D:1077:ALA:O	2.53	0.41
1:D:1130:GLN:HG2	1:D:1138:PRO:HA	2.03	0.41
1:D:4691:GLN:NE2	1:D:4703:ARG:HH22	2.18	0.41
1:A:21:VAL:HG23	1:A:203:ASN:HB2	2.01	0.41
1:A:342:GLY:HA2	1:A:389:PHE:CD2	2.56	0.41
1:A:1860:LYS:HE3	1:A:1860:LYS:HB2	1.82	0.41
1:A:1863:LEU:HG	1:A:1870:VAL:HG21	2.03	0.41
1:A:4037:ASN:HD21	1:A:5036:LEU:HD21	1.85	0.41
1:A:4862:PHE:HD1	1:A:4902:GLU:HB2	1.84	0.41
1:B:110:ARG:NH1	1:B:117:TYR:OH	2.53	0.41
1:B:119:SER:OG	1:B:136:GLY:O	2.24	0.41
1:B:222:LEU:HG	1:B:390:LEU:HD22	2.02	0.41
1:B:644:ILE:HG22	1:B:823:LEU:HD12	2.02	0.41
1:B:705:ASN:HB3	1:B:709:ASP:OD2	2.20	0.41
1:B:1293:LEU:HD22	1:B:1579:MET:HB3	1.98	0.41
1:B:2186:MET:HE1	1:B:2234:ARG:HG3	2.02	0.41
1:B:4085:ARG:HD3	1:B:4087:LEU:HD12	2.02	0.41
1:B:4675:LYS:O	1:B:4679:ARG:HG2	2.21	0.41
1:C:101:LEU:HB2	1:C:163:VAL:HG11	2.03	0.41
1:C:257:ARG:O	1:C:284:HIS:NE2	2.53	0.41
1:C:1089:TYR:HE1	1:C:1150:GLY:HA3	1.85	0.41
1:C:2313:LEU:HD13	1:C:2318:TYR:CE2	2.56	0.41
1:D:464:LYS:HE3	1:D:464:LYS:HB2	1.81	0.41
1:D:842:PRO:HG3	1:D:1072:VAL:HA	2.03	0.41
1:D:1926:LEU:HA	1:D:1929:MET:HE2	2.03	0.41
1:D:3715:LYS:HB3	1:D:3715:LYS:HE3	1.87	0.41
1:A:134:ASP:OD1	1:A:134:ASP:N	2.54	0.41
1:A:4767:TRP:O	1:A:4770:SER:OG	2.34	0.41
1:A:4836:GLN:H	1:A:4836:GLN:HG2	1.77	0.41
1:A:4951:LYS:HE2	1:A:4951:LYS:HB2	1.86	0.41
1:B:43:GLY:N	1:B:447:ASP:OD2	2.54	0.41
1:B:1476:MET:N	1:B:1485:SER:O	2.48	0.41
1:B:4857:ASN:HD21	1:C:4807:PHE:HD2	1.68	0.41
1:C:755:ILE:CG2	1:C:768:PHE:CB	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1839:VAL:O	1:C:1840:PRO:C	2.61	0.41
1:C:1926:LEU:HA	1:C:1929:MET:HE2	2.03	0.41
1:C:2185:ILE:HA	1:C:2188:ASN:HD22	1.86	0.41
1:C:4060:LYS:HG3	1:C:4064:MET:HE3	2.03	0.41
1:C:4904:PRO:HB3	1:C:4913:ARG:HH21	1.86	0.41
1:D:34:LYS:HD3	1:D:34:LYS:HA	1.86	0.41
1:D:496:VAL:O	1:D:496:VAL:HG23	2.21	0.41
1:D:889:GLN:HB3	1:D:891:TRP:HD1	1.85	0.41
1:D:1089:TYR:HE1	1:D:1150:GLY:HA3	1.85	0.41
1:D:4904:PRO:HB3	1:D:4913:ARG:HH21	1.86	0.41
1:A:34:LYS:HD3	1:A:34:LYS:HA	1.86	0.41
1:A:222:LEU:HG	1:A:390:LEU:HD22	2.02	0.41
1:A:496:VAL:HG23	1:A:496:VAL:O	2.21	0.41
1:A:523:TYR:CE2	1:A:560:ILE:HD11	2.56	0.41
1:A:1130:GLN:HG2	1:A:1138:PRO:HA	2.03	0.41
1:A:1297:PHE:HA	1:A:1522:LEU:HD12	2.02	0.41
1:A:2466:LEU:HD23	1:A:2466:LEU:H	1.85	0.41
1:A:4815:ASP:O	1:A:4819:GLY:N	2.52	0.41
1:B:744:VAL:HG12	1:B:745:SER:N	2.36	0.41
1:B:1130:GLN:HG2	1:B:1138:PRO:HA	2.03	0.41
1:B:1131:ARG:HG2	1:B:1139:PHE:HB3	2.03	0.41
1:B:1162:PHE:CE2	1:B:1179:PHE:CE2	3.09	0.41
1:B:1703:LEU:HD23	1:B:1703:LEU:HA	1.86	0.41
1:B:1762:LEU:HD23	1:B:1762:LEU:H	1.85	0.41
1:B:3715:LYS:HE3	1:B:3715:LYS:HB3	1.87	0.41
1:B:3778:MET:HA	1:B:3781:GLN:HE21	1.86	0.41
1:B:4060:LYS:HG3	1:B:4064:MET:HE3	2.03	0.41
1:C:34:LYS:HD3	1:C:34:LYS:HA	1.86	0.41
1:C:43:GLY:N	1:C:447:ASP:OD2	2.54	0.41
1:C:110:ARG:NH1	1:C:117:TYR:OH	2.53	0.41
1:C:556:ALA:HA	1:C:560:ILE:HD13	2.02	0.41
1:C:705:ASN:HB3	1:C:709:ASP:OD2	2.20	0.41
1:C:833:GLY:H	1:C:837:PRO:HB3	1.86	0.41
1:C:3891:LEU:HD23	1:C:3891:LEU:HA	1.88	0.41
1:C:4877:ASP:OD1	1:C:4878:ASP:N	2.54	0.41
1:D:644:ILE:HG22	1:D:823:LEU:HD12	2.02	0.41
1:D:1293:LEU:CD1	1:D:1580:PHE:HE1	2.30	0.41
1:D:3760:LYS:HE3	1:D:3760:LYS:HB2	1.91	0.41
1:D:3772:THR:OG1	1:D:3815:LYS:NZ	2.52	0.41
1:D:3778:MET:HA	1:D:3781:GLN:HE21	1.86	0.41
1:A:3891:LEU:HD23	1:A:3891:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4085:ARG:HD3	1:A:4087:LEU:HD12	2.02	0.41
1:A:4127:GLU:OE2	1:A:4131:ARG:NH1	2.54	0.41
1:A:4863:TYR:O	1:A:4865:LYS:N	2.49	0.41
1:B:285:VAL:HG23	1:B:286:THR:HG23	2.02	0.41
1:B:755:ILE:O	1:B:767:VAL:HG23	2.21	0.41
1:B:2185:ILE:HA	1:B:2188:ASN:HD22	1.86	0.41
1:B:2313:LEU:HD13	1:B:2318:TYR:CE2	2.56	0.41
1:B:4979:THR:HG21	2:B:5101:ATP:C2	2.56	0.41
1:C:496:VAL:HG23	1:C:496:VAL:O	2.21	0.41
1:C:744:VAL:HG12	1:C:745:SER:N	2.36	0.41
1:C:1130:GLN:HG2	1:C:1138:PRO:HA	2.03	0.41
1:C:4127:GLU:OE2	1:C:4131:ARG:NH1	2.54	0.41
1:C:4185:GLY:C	1:C:4187:SER:H	2.28	0.41
1:C:4691:GLN:NE2	1:C:4703:ARG:HH22	2.18	0.41
1:C:5029:ARG:HE	1:C:5029:ARG:HB3	1.69	0.41
1:D:21:VAL:HG21	1:D:205:ILE:HD13	2.02	0.41
1:D:178:ARG:HA	1:D:178:ARG:HD3	1.89	0.41
1:D:285:VAL:HG23	1:D:286:THR:H	1.86	0.41
1:D:652:ARG:CZ	1:D:750:LEU:O	2.69	0.41
1:D:4666:VAL:C	1:D:4668:LEU:N	2.69	0.41
1:D:4979:THR:HG21	2:D:5101:ATP:C2	2.56	0.41
1:A:609:CYS:SG	1:A:610:ASN:N	2.93	0.41
1:A:755:ILE:CG2	1:A:768:PHE:CB	2.99	0.41
1:A:842:PRO:HG3	1:A:1072:VAL:HA	2.03	0.41
1:A:1530:THR:HA	1:A:1535:GLU:HA	2.03	0.41
1:A:2149:VAL:O	1:A:2153:MET:HG2	2.21	0.41
1:A:2442:LEU:HG	1:A:2443:ILE:HG23	2.02	0.41
1:A:4048:LEU:HD23	1:A:4048:LEU:HA	1.95	0.41
1:A:4711:PHE:HB3	1:A:4712:PRO:HD3	2.01	0.41
1:A:4979:THR:HG21	2:A:5101:ATP:C2	2.56	0.41
1:B:842:PRO:HG3	1:B:1072:VAL:HA	2.03	0.41
1:B:889:GLN:HB3	1:B:891:TRP:HD1	1.85	0.41
1:B:978:THR:OG1	1:B:1054:GLU:OE2	2.39	0.41
1:B:1180:ARG:HA	1:B:1180:ARG:NE	2.34	0.41
1:B:1293:LEU:CD1	1:B:1580:PHE:HE1	2.30	0.41
1:B:1717:SER:CA	1:B:1720:LEU:HD23	2.47	0.41
1:B:1863:LEU:HG	1:B:1870:VAL:HG21	2.03	0.41
1:B:4127:GLU:OE2	1:B:4131:ARG:NH1	2.54	0.41
1:C:285:VAL:HG23	1:C:286:THR:HG23	2.02	0.41
1:C:350:HIS:HE1	1:C:352:ALA:HB3	1.86	0.41
1:C:497:TYR:CE1	1:C:504:ALA:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:644:ILE:HG22	1:C:823:LEU:HD12	2.02	0.41
1:C:652:ARG:CZ	1:C:750:LEU:O	2.69	0.41
1:C:842:PRO:HG3	1:C:1072:VAL:HA	2.03	0.41
1:C:2186:MET:HE1	1:C:2234:ARG:HG3	2.02	0.41
1:C:3781:GLN:H	1:C:3781:GLN:HG2	1.72	0.41
1:C:4857:ASN:HD21	1:D:4807:PHE:HD2	1.68	0.41
1:C:4958:CYS:O	2:C:5101:ATP:N1	2.54	0.41
1:D:497:TYR:CE1	1:D:504:ALA:HA	2.56	0.41
1:D:1162:PHE:CE2	1:D:1179:PHE:CE2	3.09	0.41
1:D:1863:LEU:HG	1:D:1870:VAL:HG21	2.03	0.41
1:D:2182:ILE:HG22	1:D:2186:MET:HE3	2.03	0.41
1:D:2358:ILE:HD12	1:D:2358:ILE:HA	1.91	0.41
1:D:4675:LYS:O	1:D:4679:ARG:HG2	2.21	0.41
1:A:110:ARG:NH1	1:A:117:TYR:OH	2.53	0.41
1:A:1147:ASP:N	1:A:1147:ASP:OD1	2.54	0.41
1:A:1293:LEU:HD13	1:A:1580:PHE:CE1	2.53	0.41
1:A:4958:CYS:O	2:A:5101:ATP:N1	2.54	0.41
1:A:4959:PHE:CD2	1:A:4985:LEU:HD11	2.56	0.41
1:B:833:GLY:H	1:B:837:PRO:HB3	1.86	0.41
1:B:2149:VAL:O	1:B:2153:MET:HG2	2.21	0.41
1:C:582:HIS:O	1:C:585:SER:OG	2.27	0.41
1:C:1084:GLN:NE2	1:C:1185:GLY:O	2.54	0.41
1:C:1124:PHE:HB2	1:C:1162:PHE:CE2	2.56	0.41
1:C:1131:ARG:HG2	1:C:1139:PHE:HB3	2.03	0.41
1:C:1530:THR:HA	1:C:1535:GLU:HA	2.03	0.41
1:C:2155:LEU:HD21	1:C:2188:ASN:CG	2.47	0.41
1:C:2182:ILE:HG22	1:C:2186:MET:HE3	2.03	0.41
1:C:3715:LYS:HE3	1:C:3715:LYS:HB3	1.87	0.41
1:C:3718:GLU:OE1	1:C:3720:TYR:N	2.53	0.41
1:D:257:ARG:O	1:D:284:HIS:NE2	2.53	0.41
1:D:556:ALA:HA	1:D:560:ILE:HD13	2.02	0.41
1:D:2313:LEU:HD13	1:D:2318:TYR:CE2	2.56	0.41
1:A:43:GLY:N	1:A:447:ASP:OD2	2.54	0.40
1:A:183:SER:OG	1:A:192:ASP:OD1	2.30	0.40
1:A:285:VAL:HG23	1:A:286:THR:H	1.86	0.40
1:A:392:ARG:NH1	1:A:393:CYS:H	2.15	0.40
1:A:644:ILE:HG22	1:A:823:LEU:HD12	2.02	0.40
1:A:705:ASN:HB3	1:A:709:ASP:OD2	2.20	0.40
1:A:744:VAL:HG12	1:A:745:SER:N	2.36	0.40
1:A:2182:ILE:HG22	1:A:2186:MET:HE3	2.03	0.40
1:A:4820:VAL:HB	1:A:4823:LEU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4904:PRO:HB3	1:A:4913:ARG:HH21	1.86	0.40
1:B:2176:ASN:OD1	1:B:2176:ASN:N	2.54	0.40
1:B:4711:PHE:HB3	1:B:4712:PRO:HD3	2.01	0.40
1:C:889:GLN:HB3	1:C:891:TRP:HD1	1.85	0.40
1:C:897:ARG:HA	1:C:903:LEU:O	2.21	0.40
1:C:1780:PRO:HD3	1:C:1801:ALA:H	1.86	0.40
1:C:2176:ASN:OD1	1:C:2176:ASN:N	2.54	0.40
1:C:3778:MET:HA	1:C:3781:GLN:HE21	1.86	0.40
1:C:3842:LEU:O	1:C:3929:SER:OG	2.36	0.40
1:D:43:GLY:N	1:D:447:ASP:OD2	2.54	0.40
1:D:183:SER:OG	1:D:192:ASP:OD1	2.30	0.40
1:D:400:ALA:HB1	1:D:478:PHE:HE1	1.86	0.40
1:D:755:ILE:CG2	1:D:768:PHE:CB	2.99	0.40
1:D:978:THR:OG1	1:D:1054:GLU:OE2	2.39	0.40
1:D:2223:ILE:HD12	1:D:2223:ILE:HA	1.95	0.40
1:D:3842:LEU:HD23	1:D:3842:LEU:HA	1.93	0.40
1:D:4060:LYS:HG3	1:D:4064:MET:HE3	2.03	0.40
1:D:4848:VAL:HG21	1:D:4887:MET:SD	2.61	0.40
1:D:4958:CYS:O	2:D:5101:ATP:N1	2.54	0.40
1:A:119:SER:HA	1:A:146:CYS:HA	2.03	0.40
1:A:652:ARG:CZ	1:A:750:LEU:O	2.69	0.40
1:A:1124:PHE:HB2	1:A:1162:PHE:CE2	2.56	0.40
1:A:3716:LEU:HD12	1:A:3716:LEU:HA	1.84	0.40
1:A:3946:GLN:HE22	1:A:3949:ARG:HH22	1.69	0.40
1:A:4848:VAL:HG21	1:A:4887:MET:SD	2.61	0.40
1:B:488:LEU:HD22	1:B:546:TRP:CH2	2.57	0.40
1:B:496:VAL:HG23	1:B:496:VAL:O	2.21	0.40
1:B:497:TYR:CE1	1:B:504:ALA:HA	2.56	0.40
1:B:2442:LEU:HG	1:B:2443:ILE:HG23	2.02	0.40
1:B:4877:ASP:OD1	1:B:4878:ASP:N	2.54	0.40
1:B:4904:PRO:HB3	1:B:4913:ARG:HH21	1.86	0.40
1:B:4959:PHE:CD2	1:B:4985:LEU:HD11	2.56	0.40
1:C:110:ARG:HH21	1:C:115:ARG:HB3	1.87	0.40
1:C:2149:VAL:O	1:C:2153:MET:HG2	2.21	0.40
1:C:2359:ARG:HD2	1:C:2359:ARG:HA	1.89	0.40
1:D:375:LYS:NZ	1:D:376:ALA:O	2.46	0.40
1:D:523:TYR:CE2	1:D:560:ILE:HD11	2.56	0.40
1:D:833:GLY:H	1:D:837:PRO:HB3	1.86	0.40
1:D:1131:ARG:HG2	1:D:1139:PHE:HB3	2.03	0.40
1:D:2225:PHE:N	1:D:2226:PRO:HD3	2.37	0.40
1:D:2295:LEU:HA	1:D:2298:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LEU:HB2	1:A:163:VAL:HG11	2.03	0.40
1:A:621:ILE:HD13	1:A:621:ILE:HA	1.93	0.40
1:A:755:ILE:O	1:A:767:VAL:HG23	2.21	0.40
1:A:2155:LEU:HD21	1:A:2188:ASN:CG	2.47	0.40
1:A:2185:ILE:HA	1:A:2185:ILE:HD13	1.94	0.40
1:A:3781:GLN:H	1:A:3781:GLN:HG2	1.72	0.40
1:A:4185:GLY:C	1:A:4187:SER:H	2.28	0.40
1:A:4730:ASP:N	1:A:4730:ASP:OD1	2.45	0.40
1:A:4862:PHE:HB3	1:A:4901:ILE:HG22	2.02	0.40
1:B:101:LEU:HB2	1:B:163:VAL:HG11	2.03	0.40
1:B:119:SER:HA	1:B:146:CYS:HA	2.03	0.40
1:B:609:CYS:SG	1:B:610:ASN:N	2.93	0.40
1:B:3786:CYS:C	1:B:3787:LYS:HD3	2.46	0.40
1:B:4211:LYS:HZ3	1:B:4211:LYS:CB	2.34	0.40
1:B:4242:ILE:HD12	1:B:4993:MET:HG2	2.04	0.40
1:C:488:LEU:HD22	1:C:546:TRP:CH2	2.57	0.40
1:C:1162:PHE:CE2	1:C:1179:PHE:CE2	3.09	0.40
1:D:222:LEU:HG	1:D:390:LEU:HD22	2.02	0.40
1:D:4578:LEU:HD23	1:D:4578:LEU:HA	1.93	0.40
1:A:488:LEU:HD22	1:A:546:TRP:CH2	2.57	0.40
1:A:977:LEU:HG	1:A:1044:ARG:HH12	1.85	0.40
1:A:978:THR:OG1	1:A:1054:GLU:OE2	2.39	0.40
1:A:3786:CYS:C	1:A:3787:LYS:HD3	2.46	0.40
1:A:3932:ASP:OD1	1:A:3933:PHE:N	2.55	0.40
1:A:4060:LYS:HG3	1:A:4064:MET:HE3	2.03	0.40
1:A:4092:ASP:O	1:A:4096:ALA:N	2.48	0.40
1:A:4675:LYS:O	1:A:4679:ARG:HG2	2.21	0.40
1:B:1124:PHE:HB2	1:B:1162:PHE:CE2	2.56	0.40
1:B:1780:PRO:HD3	1:B:1801:ALA:H	1.86	0.40
1:B:2155:LEU:HD21	1:B:2188:ASN:CG	2.47	0.40
1:B:2228:MET:HE3	1:B:2228:MET:HB3	1.84	0.40
1:B:2280:VAL:HG21	1:B:2334:PHE:HE1	1.87	0.40
1:B:4820:VAL:HB	1:B:4823:LEU:HB3	2.03	0.40
1:C:245:VAL:HG21	1:C:299:LEU:HD12	2.03	0.40
1:C:1147:ASP:OD1	1:C:1147:ASP:N	2.54	0.40
1:C:3786:CYS:C	1:C:3787:LYS:HD3	2.46	0.40
1:C:4675:LYS:O	1:C:4679:ARG:HG2	2.21	0.40
1:D:294:THR:HG23	1:D:295:GLU:N	2.34	0.40
1:D:977:LEU:HG	1:D:1044:ARG:HH12	1.85	0.40
1:D:1147:ASP:OD1	1:D:1147:ASP:N	2.54	0.40
1:D:2252:ASP:OD1	1:D:2252:ASP:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:ALA:HA	1:A:560:ILE:HD13	2.02	0.40
1:A:596:ASN:HD21	1:A:598:LYS:HB2	1.87	0.40
1:A:897:ARG:HA	1:A:903:LEU:O	2.21	0.40
1:A:4242:ILE:HD12	1:A:4993:MET:HG2	2.04	0.40
1:B:342:GLY:HA2	1:B:389:PHE:CD2	2.56	0.40
1:B:523:TYR:CE2	1:B:560:ILE:HD11	2.56	0.40
1:B:621:ILE:HD13	1:B:621:ILE:HA	1.93	0.40
1:B:1108:GLU:N	1:B:1108:GLU:OE1	2.55	0.40
1:B:1926:LEU:HA	1:B:1929:MET:HE2	2.03	0.40
1:B:2182:ILE:HG22	1:B:2186:MET:HE3	2.03	0.40
1:B:4958:CYS:O	2:B:5101:ATP:N1	2.54	0.40
1:B:4985:LEU:HA	1:B:4985:LEU:HD23	1.86	0.40
1:C:45:ARG:HD3	1:C:45:ARG:HA	1.92	0.40
1:C:134:ASP:OD1	1:C:134:ASP:N	2.54	0.40
1:C:977:LEU:HG	1:C:1044:ARG:HH12	1.85	0.40
1:C:3680:ALA:HB3	1:C:3697:PRO:HG2	2.02	0.40
1:D:1639:LEU:HD12	1:D:1653:LEU:HD21	2.04	0.40
1:D:4103:PHE:HD1	1:D:4103:PHE:HA	1.78	0.40
1:D:4563:ARG:HD2	1:D:4563:ARG:HA	1.81	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	3101/5037 (62%)	2823 (91%)	274 (9%)	4 (0%)	48	79
1	B	3101/5037 (62%)	2823 (91%)	274 (9%)	4 (0%)	48	79
1	C	3101/5037 (62%)	2823 (91%)	274 (9%)	4 (0%)	48	79
1	D	3101/5037 (62%)	2823 (91%)	274 (9%)	4 (0%)	48	79
All	All	12404/20148 (62%)	11292 (91%)	1096 (9%)	16 (0%)	49	79

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4867	GLU
1	B	4867	GLU
1	C	4867	GLU
1	D	4867	GLU
1	A	4875	LYS
1	B	4875	LYS
1	C	4875	LYS
1	D	4875	LYS
1	A	1837	GLN
1	A	4175	ARG
1	B	1837	GLN
1	B	4175	ARG
1	C	1837	GLN
1	C	4175	ARG
1	D	1837	GLN
1	D	4175	ARG

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	2350/4276 (55%)	2337 (99%)	13 (1%)	78	79
1	B	2350/4276 (55%)	2337 (99%)	13 (1%)	78	79
1	C	2350/4276 (55%)	2337 (99%)	13 (1%)	78	79
1	D	2350/4276 (55%)	2337 (99%)	13 (1%)	78	79
All	All	9400/17104 (55%)	9348 (99%)	52 (1%)	76	79

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1454	THR
1	A	1549	PHE
1	A	1722	SER
1	A	1838	PHE

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Mol	Chain	Res	Type
1	A	1841	VAL
1	A	1929	MET
1	A	1931	LEU
1	A	1935	VAL
1	A	1936	LYS
1	A	4175	ARG
1	A	4211	LYS
1	A	4865	LYS
1	A	4875	LYS
1	B	1454	THR
1	B	1549	PHE
1	B	1722	SER
1	B	1838	PHE
1	B	1841	VAL
1	B	1929	MET
1	B	1931	LEU
1	B	1935	VAL
1	B	1936	LYS
1	B	4175	ARG
1	B	4211	LYS
1	B	4865	LYS
1	B	4875	LYS
1	C	1454	THR
1	C	1549	PHE
1	C	1722	SER
1	C	1838	PHE
1	C	1841	VAL
1	C	1929	MET
1	C	1931	LEU
1	C	1935	VAL
1	C	1936	LYS
1	C	4175	ARG
1	C	4211	LYS
1	C	4865	LYS
1	C	4875	LYS
1	D	1454	THR
1	D	1549	PHE
1	D	1722	SER
1	D	1838	PHE
1	D	1841	VAL
1	D	1929	MET
1	D	1931	LEU

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Mol	Chain	Res	Type
1	D	1935	VAL
1	D	1936	LYS
1	D	4175	ARG
1	D	4211	LYS
1	D	4865	LYS
1	D	4875	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (207) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	111	HIS
1	A	113	HIS
1	A	203	ASN
1	A	379	HIS
1	A	520	ASN
1	A	597	HIS
1	A	735	GLN
1	A	736	HIS
1	A	838	HIS
1	A	877	ASN
1	A	1041	GLN
1	A	1084	GLN
1	A	1144	GLN
1	A	1158	ASN
1	A	1254	HIS
1	A	1491	ASN
1	A	1545	ASN
1	A	1660	GLN
1	A	1663	HIS
1	A	1693	GLN
1	A	1696	HIS
1	A	1861	GLN
1	A	1949	GLN
1	A	1952	GLN
1	A	2007	ASN
1	A	2127	GLN
1	A	2184	ASN
1	A	2194	HIS
1	A	2260	ASN
1	A	3700	GLN
1	A	3761	GLN

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Mol	Chain	Res	Type
1	A	3771	HIS
1	A	3781	GLN
1	A	3814	GLN
1	A	3895	HIS
1	A	3976	ASN
1	A	3978	GLN
1	A	3994	HIS
1	A	3998	HIS
1	A	4009	GLN
1	A	4109	GLN
1	A	4133	GLN
1	A	4153	HIS
1	A	4201	ASN
1	A	4553	ASN
1	A	4691	GLN
1	A	4776	GLN
1	A	4832	HIS
1	A	4946	GLN
1	A	4947	GLN
1	A	4949	GLN
1	A	4987	ASN
1	B	71	GLN
1	B	111	HIS
1	B	113	HIS
1	B	203	ASN
1	B	379	HIS
1	B	520	ASN
1	B	597	HIS
1	B	735	GLN
1	B	838	HIS
1	B	877	ASN
1	B	1084	GLN
1	B	1144	GLN
1	B	1158	ASN
1	B	1254	HIS
1	B	1491	ASN
1	B	1545	ASN
1	B	1660	GLN
1	B	1663	HIS
1	B	1693	GLN
1	B	1696	HIS
1	B	1861	GLN

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Mol	Chain	Res	Type
1	B	1949	GLN
1	B	1952	GLN
1	B	2007	ASN
1	B	2127	GLN
1	B	2184	ASN
1	B	2194	HIS
1	B	2260	ASN
1	B	3700	GLN
1	B	3761	GLN
1	B	3771	HIS
1	B	3781	GLN
1	B	3814	GLN
1	B	3895	HIS
1	B	3976	ASN
1	B	3978	GLN
1	B	3994	HIS
1	B	3998	HIS
1	B	4009	GLN
1	B	4109	GLN
1	B	4133	GLN
1	B	4153	HIS
1	B	4201	ASN
1	B	4553	ASN
1	B	4691	GLN
1	B	4776	GLN
1	B	4947	GLN
1	B	4949	GLN
1	B	4987	ASN
1	C	71	GLN
1	C	111	HIS
1	C	113	HIS
1	C	203	ASN
1	C	224	HIS
1	C	379	HIS
1	C	520	ASN
1	C	597	HIS
1	C	735	GLN
1	C	736	HIS
1	C	838	HIS
1	C	877	ASN
1	C	1084	GLN
1	C	1144	GLN

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Mol	Chain	Res	Type
1	C	1158	ASN
1	C	1254	HIS
1	C	1491	ASN
1	C	1545	ASN
1	C	1660	GLN
1	C	1663	HIS
1	C	1693	GLN
1	C	1696	HIS
1	C	1861	GLN
1	C	1949	GLN
1	C	1952	GLN
1	C	2007	ASN
1	C	2127	GLN
1	C	2161	GLN
1	C	2184	ASN
1	C	2194	HIS
1	C	2260	ASN
1	C	3700	GLN
1	C	3761	GLN
1	C	3771	HIS
1	C	3781	GLN
1	C	3814	GLN
1	C	3895	HIS
1	C	3976	ASN
1	C	3978	GLN
1	C	3994	HIS
1	C	3998	HIS
1	C	4009	GLN
1	C	4100	GLN
1	C	4109	GLN
1	C	4133	GLN
1	C	4153	HIS
1	C	4201	ASN
1	C	4553	ASN
1	C	4691	GLN
1	C	4776	GLN
1	C	4947	GLN
1	C	4949	GLN
1	C	4987	ASN
1	D	71	GLN
1	D	111	HIS
1	D	113	HIS

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Mol	Chain	Res	Type
1	D	203	ASN
1	D	224	HIS
1	D	379	HIS
1	D	520	ASN
1	D	597	HIS
1	D	735	GLN
1	D	838	HIS
1	D	877	ASN
1	D	1084	GLN
1	D	1144	GLN
1	D	1158	ASN
1	D	1254	HIS
1	D	1491	ASN
1	D	1660	GLN
1	D	1663	HIS
1	D	1693	GLN
1	D	1696	HIS
1	D	1861	GLN
1	D	1949	GLN
1	D	1952	GLN
1	D	2007	ASN
1	D	2127	GLN
1	D	2161	GLN
1	D	2184	ASN
1	D	2194	HIS
1	D	2260	ASN
1	D	3700	GLN
1	D	3761	GLN
1	D	3771	HIS
1	D	3781	GLN
1	D	3814	GLN
1	D	3895	HIS
1	D	3909	ASN
1	D	3960	GLN
1	D	3976	ASN
1	D	3978	GLN
1	D	3994	HIS
1	D	3998	HIS
1	D	4009	GLN
1	D	4109	GLN
1	D	4133	GLN
1	D	4153	HIS

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Mol	Chain	Res	Type
1	D	4201	ASN
1	D	4553	ASN
1	D	4691	GLN
1	D	4776	GLN
1	D	4947	GLN
1	D	4949	GLN
1	D	4987	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ATP	D	5101	-	32,33,33	1.30	5 (15%)	48,52,52	1.80	14 (29%)
2	ATP	A	5101	-	32,33,33	1.30	5 (15%)	48,52,52	1.80	14 (29%)
2	ATP	C	5101	-	32,33,33	1.30	5 (15%)	48,52,52	1.80	14 (29%)
2	ATP	B	5101	-	32,33,33	1.30	5 (15%)	48,52,52	1.80	14 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	D	5101	-	-	6/22/38/38	0/3/3/3
2	ATP	A	5101	-	-	6/22/38/38	0/3/3/3
2	ATP	C	5101	-	-	6/22/38/38	0/3/3/3
2	ATP	B	5101	-	-	6/22/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5101	ATP	C5-C4	4.07	1.46	1.39
2	B	5101	ATP	C5-C4	4.07	1.46	1.39
2	C	5101	ATP	C5-C4	4.07	1.46	1.39
2	D	5101	ATP	C5-C4	4.07	1.46	1.39
2	A	5101	ATP	C4-N9	-2.81	1.31	1.37
2	B	5101	ATP	C4-N9	-2.81	1.31	1.37
2	C	5101	ATP	C4-N9	-2.81	1.31	1.37
2	D	5101	ATP	C4-N9	-2.81	1.31	1.37
2	A	5101	ATP	C5-N7	-2.41	1.34	1.39
2	B	5101	ATP	C5-N7	-2.41	1.34	1.39
2	C	5101	ATP	C5-N7	-2.41	1.34	1.39
2	D	5101	ATP	C5-N7	-2.41	1.34	1.39
2	A	5101	ATP	C8-N7	2.25	1.36	1.31
2	B	5101	ATP	C8-N7	2.25	1.36	1.31
2	C	5101	ATP	C8-N7	2.25	1.36	1.31
2	D	5101	ATP	C8-N7	2.25	1.36	1.31
2	A	5101	ATP	C5-C6	2.25	1.47	1.41
2	B	5101	ATP	C5-C6	2.25	1.47	1.41
2	C	5101	ATP	C5-C6	2.25	1.47	1.41
2	D	5101	ATP	C5-C6	2.25	1.47	1.41

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5101	ATP	C5-C4-N3	-4.36	120.71	126.72
2	B	5101	ATP	C5-C4-N3	-4.36	120.71	126.72
2	C	5101	ATP	C5-C4-N3	-4.36	120.71	126.72
2	D	5101	ATP	C5-C4-N3	-4.36	120.71	126.72
2	A	5101	ATP	C2'-C1'-N9	-3.71	104.08	113.30
2	B	5101	ATP	C2'-C1'-N9	-3.71	104.08	113.30
2	C	5101	ATP	C2'-C1'-N9	-3.71	104.08	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5101	ATP	C2'-C1'-N9	-3.71	104.08	113.30
2	A	5101	ATP	N3-C2-N1	-3.55	123.20	128.58
2	B	5101	ATP	N3-C2-N1	-3.55	123.20	128.58
2	C	5101	ATP	N3-C2-N1	-3.55	123.20	128.58
2	D	5101	ATP	N3-C2-N1	-3.55	123.20	128.58
2	A	5101	ATP	N3-C4-N9	3.42	132.98	127.17
2	B	5101	ATP	N3-C4-N9	3.42	132.98	127.17
2	C	5101	ATP	N3-C4-N9	3.42	132.98	127.17
2	D	5101	ATP	N3-C4-N9	3.42	132.98	127.17
2	A	5101	ATP	C4-N9-C8	3.41	109.31	105.74
2	B	5101	ATP	C4-N9-C8	3.41	109.31	105.74
2	C	5101	ATP	C4-N9-C8	3.41	109.31	105.74
2	D	5101	ATP	C4-N9-C8	3.41	109.31	105.74
2	A	5101	ATP	C4-C5-N7	-3.31	106.79	110.58
2	B	5101	ATP	C4-C5-N7	-3.31	106.79	110.58
2	C	5101	ATP	C4-C5-N7	-3.31	106.79	110.58
2	D	5101	ATP	C4-C5-N7	-3.31	106.79	110.58
2	A	5101	ATP	C2-N3-C4	3.23	119.73	111.83
2	B	5101	ATP	C2-N3-C4	3.23	119.73	111.83
2	C	5101	ATP	C2-N3-C4	3.23	119.73	111.83
2	D	5101	ATP	C2-N3-C4	3.23	119.73	111.83
2	A	5101	ATP	C6-C5-N7	2.59	137.08	132.09
2	B	5101	ATP	C6-C5-N7	2.59	137.08	132.09
2	C	5101	ATP	C6-C5-N7	2.59	137.08	132.09
2	D	5101	ATP	C6-C5-N7	2.59	137.08	132.09
2	A	5101	ATP	N9-C8-N7	-2.53	110.34	113.94
2	B	5101	ATP	N9-C8-N7	-2.53	110.34	113.94
2	C	5101	ATP	N9-C8-N7	-2.53	110.34	113.94
2	D	5101	ATP	N9-C8-N7	-2.53	110.34	113.94
2	A	5101	ATP	C2-N1-C6	2.51	122.85	118.73
2	B	5101	ATP	C2-N1-C6	2.51	122.85	118.73
2	C	5101	ATP	C2-N1-C6	2.51	122.85	118.73
2	D	5101	ATP	C2-N1-C6	2.51	122.85	118.73
2	A	5101	ATP	C5-N7-C8	2.41	107.24	103.45
2	B	5101	ATP	C5-N7-C8	2.41	107.24	103.45
2	C	5101	ATP	C5-N7-C8	2.41	107.24	103.45
2	D	5101	ATP	C5-N7-C8	2.41	107.24	103.45
2	A	5101	ATP	C4-N9-C1'	-2.26	121.36	126.63
2	B	5101	ATP	C4-N9-C1'	-2.26	121.36	126.63
2	C	5101	ATP	C4-N9-C1'	-2.26	121.36	126.63
2	D	5101	ATP	C4-N9-C1'	-2.26	121.36	126.63
2	A	5101	ATP	C3'-C2'-C1'	2.24	105.71	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5101	ATP	C3'-C2'-C1'	2.24	105.71	101.46
2	C	5101	ATP	C3'-C2'-C1'	2.24	105.71	101.46
2	D	5101	ATP	C3'-C2'-C1'	2.24	105.71	101.46
2	A	5101	ATP	O4'-C1'-N9	2.20	112.31	108.09
2	B	5101	ATP	O4'-C1'-N9	2.20	112.31	108.09
2	C	5101	ATP	O4'-C1'-N9	2.20	112.31	108.09
2	D	5101	ATP	O4'-C1'-N9	2.20	112.31	108.09

There are no chirality outliers.

All (24) torsion outliers are listed below:

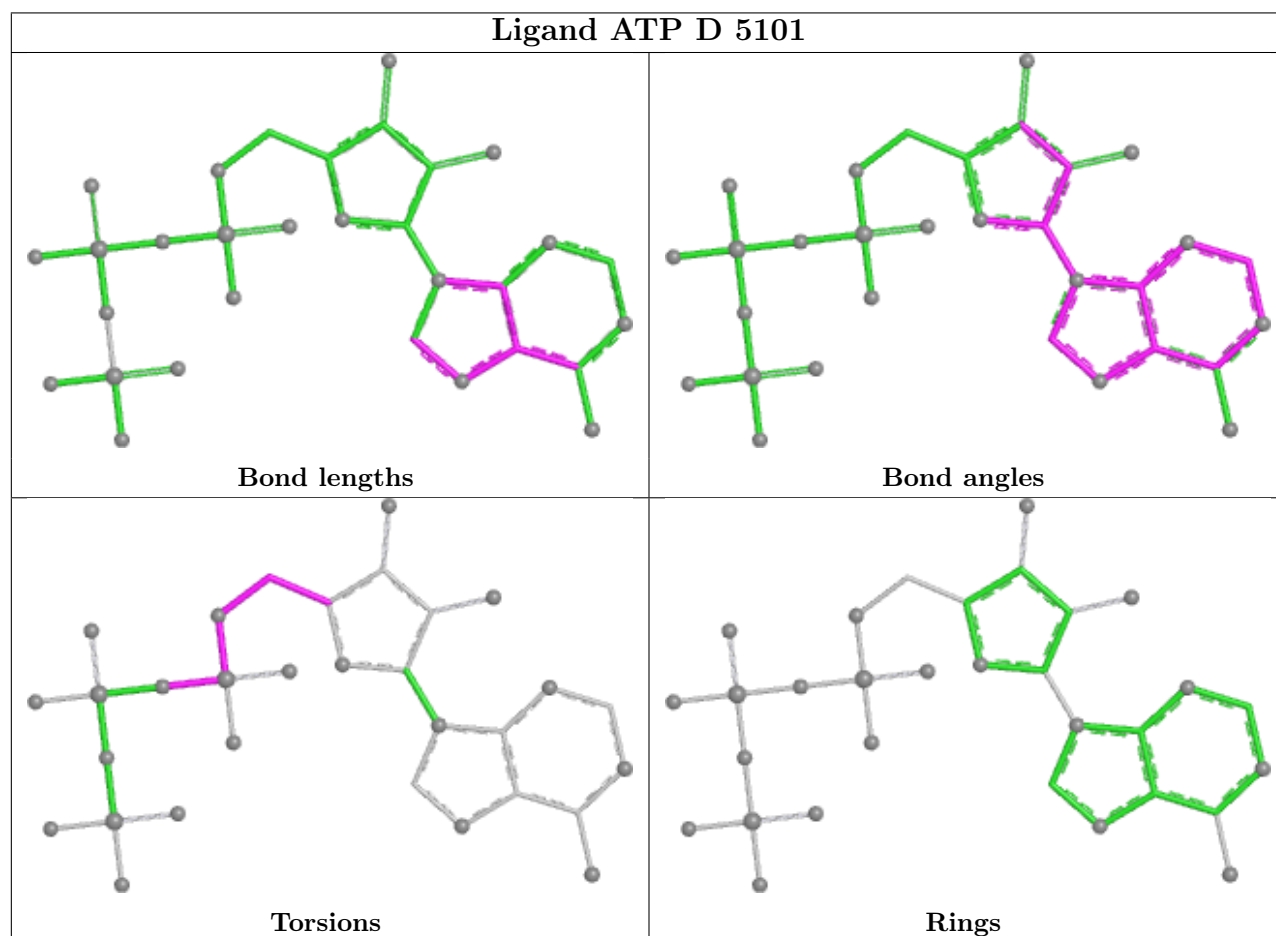
Mol	Chain	Res	Type	Atoms
2	A	5101	ATP	C5'-O5'-PA-O3A
2	A	5101	ATP	C4'-C5'-O5'-PA
2	B	5101	ATP	C5'-O5'-PA-O3A
2	B	5101	ATP	C4'-C5'-O5'-PA
2	C	5101	ATP	C5'-O5'-PA-O3A
2	C	5101	ATP	C4'-C5'-O5'-PA
2	D	5101	ATP	C5'-O5'-PA-O3A
2	D	5101	ATP	C4'-C5'-O5'-PA
2	A	5101	ATP	O4'-C4'-C5'-O5'
2	B	5101	ATP	O4'-C4'-C5'-O5'
2	C	5101	ATP	O4'-C4'-C5'-O5'
2	D	5101	ATP	O4'-C4'-C5'-O5'
2	A	5101	ATP	C3'-C4'-C5'-O5'
2	B	5101	ATP	C3'-C4'-C5'-O5'
2	C	5101	ATP	C3'-C4'-C5'-O5'
2	D	5101	ATP	C3'-C4'-C5'-O5'
2	A	5101	ATP	PB-O3A-PA-O5'
2	B	5101	ATP	PB-O3A-PA-O5'
2	C	5101	ATP	PB-O3A-PA-O5'
2	D	5101	ATP	PB-O3A-PA-O5'
2	A	5101	ATP	C5'-O5'-PA-O1A
2	B	5101	ATP	C5'-O5'-PA-O1A
2	C	5101	ATP	C5'-O5'-PA-O1A
2	D	5101	ATP	C5'-O5'-PA-O1A

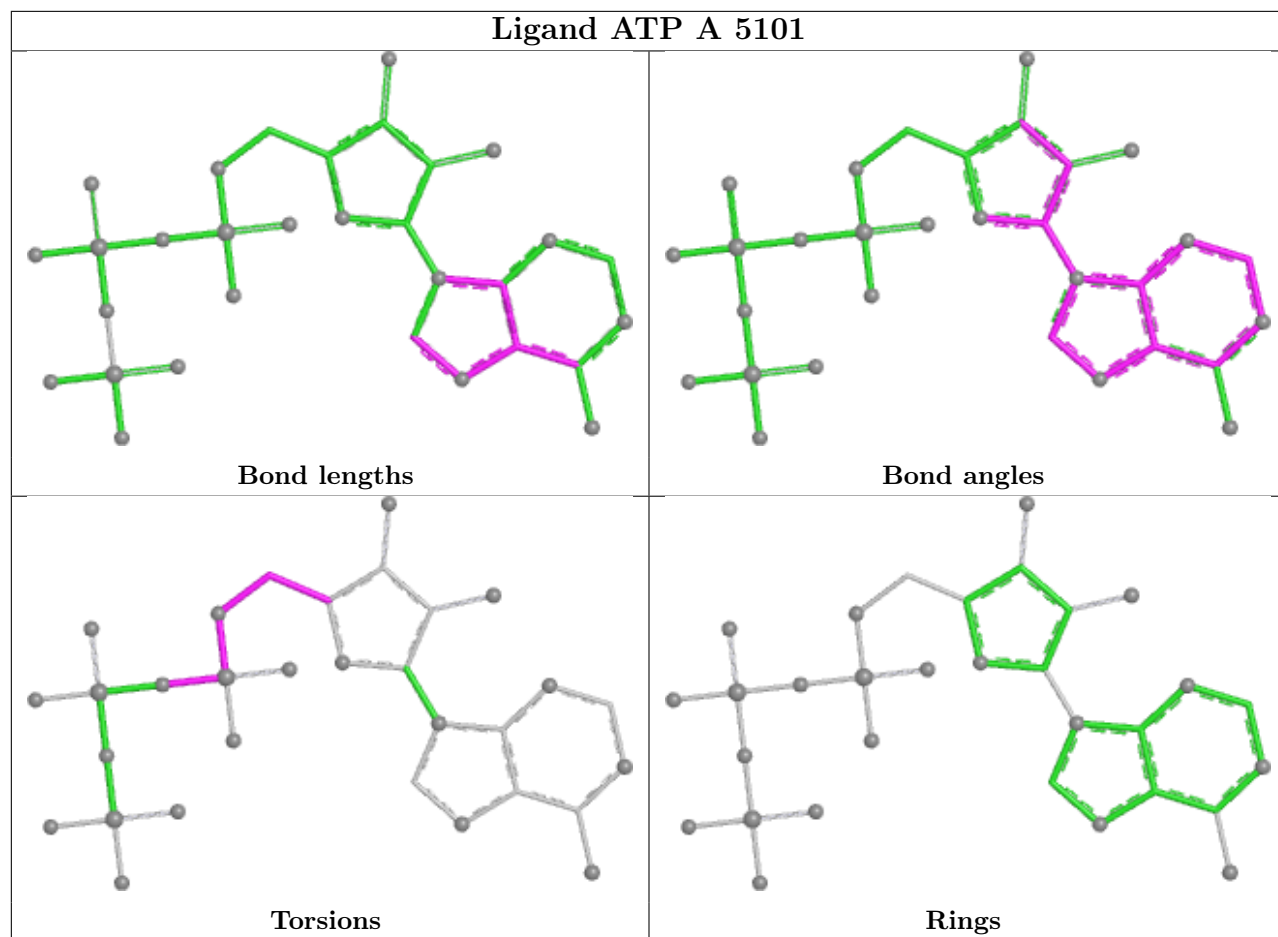
There are no ring outliers.

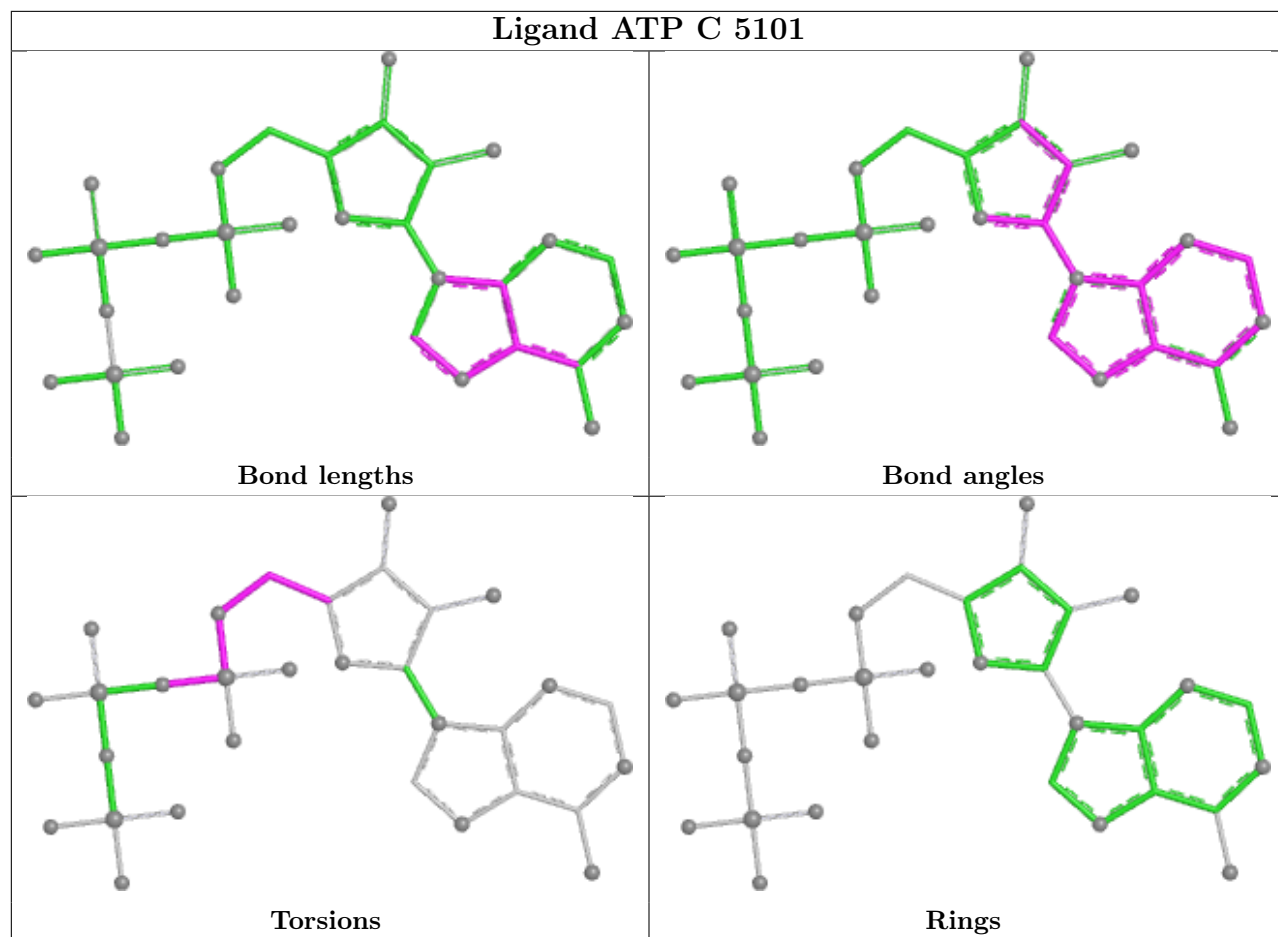
4 monomers are involved in 43 short contacts:

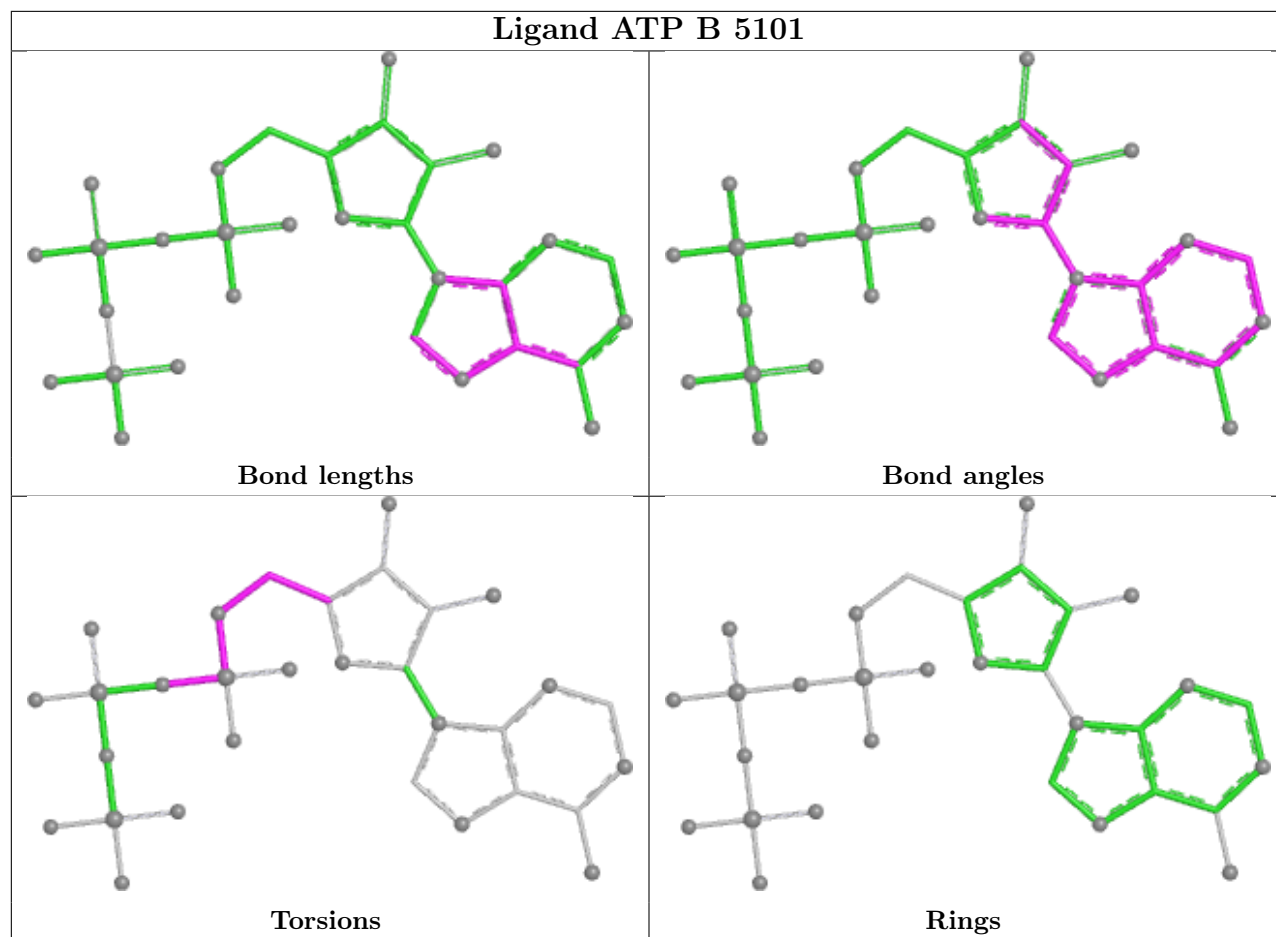
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	5101	ATP	11	0
2	A	5101	ATP	11	0
2	C	5101	ATP	10	0
2	B	5101	ATP	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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.

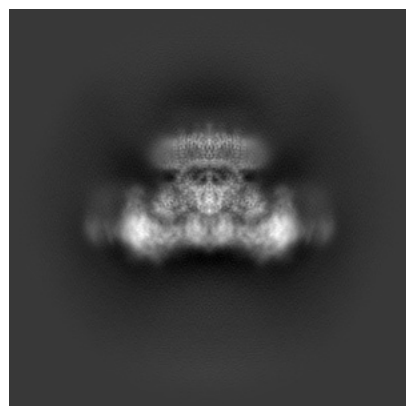
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38046. These allow visual inspection of the internal detail of the map and identification of artifacts.

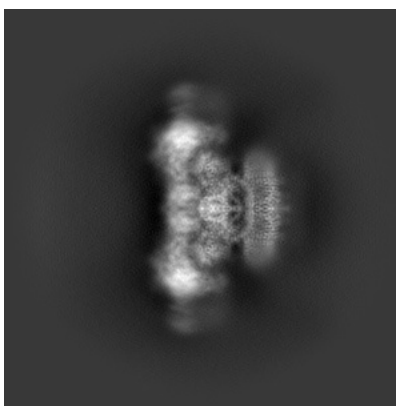
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

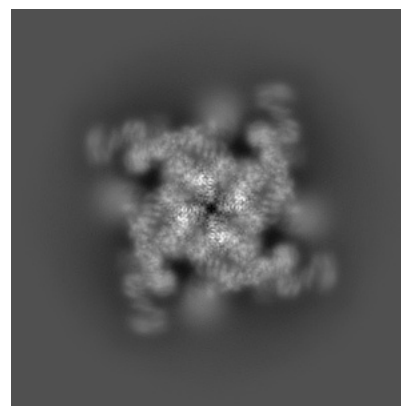
6.1.1 Primary map



X

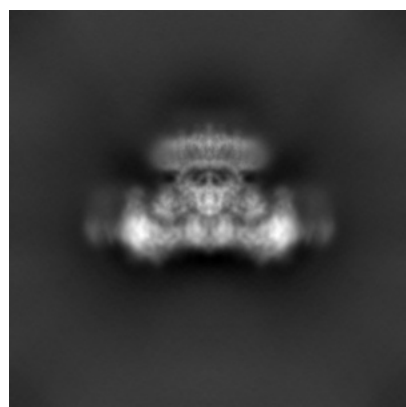


Y

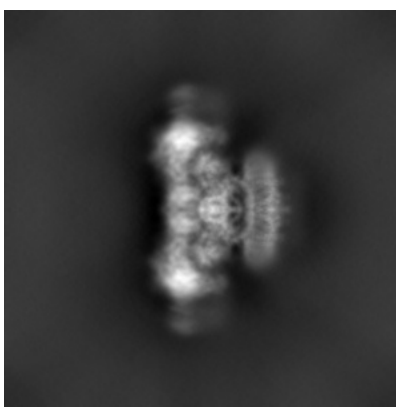


Z

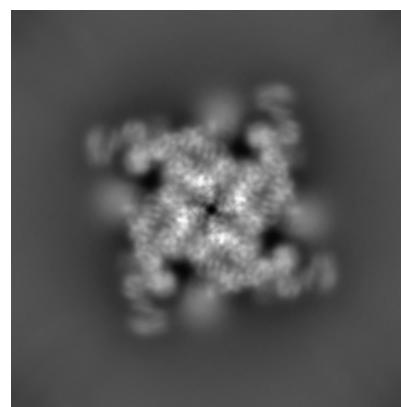
6.1.2 Raw map



X



Y

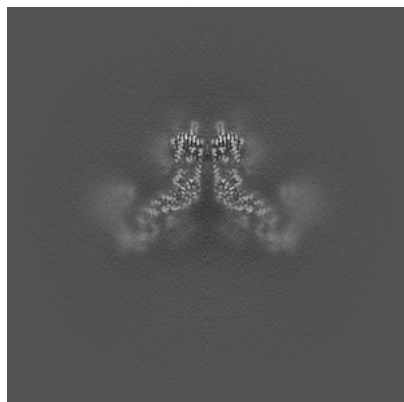


Z

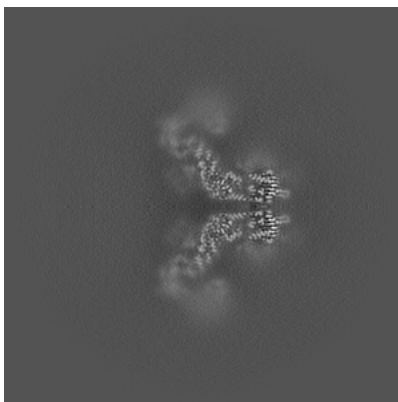
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

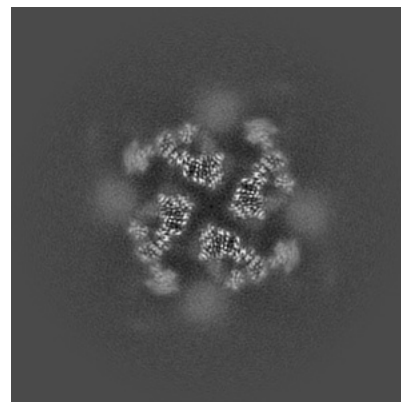
6.2.1 Primary map



X Index: 240

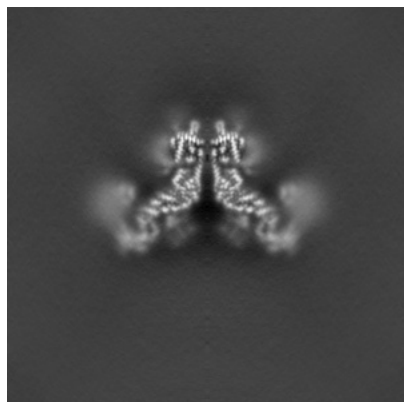


Y Index: 240

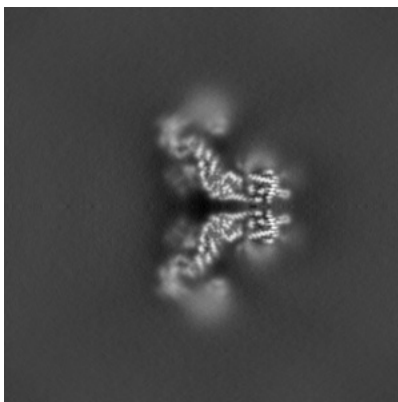


Z Index: 240

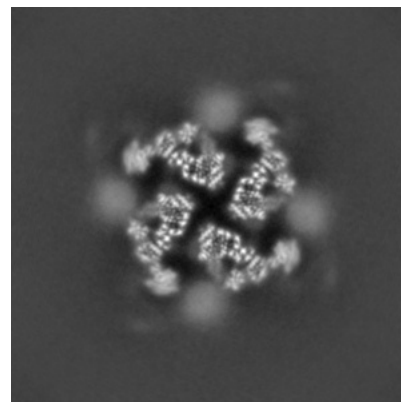
6.2.2 Raw map



X Index: 240



Y Index: 240

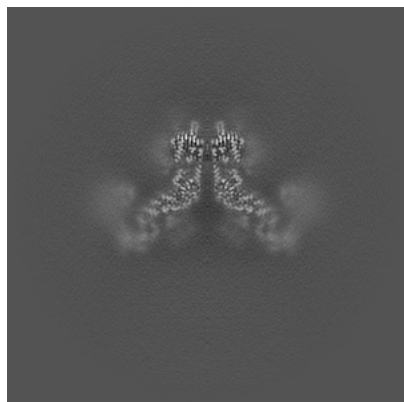


Z Index: 240

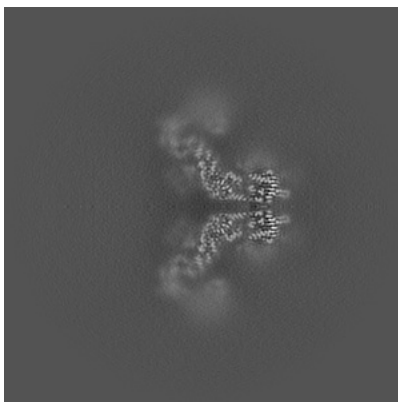
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

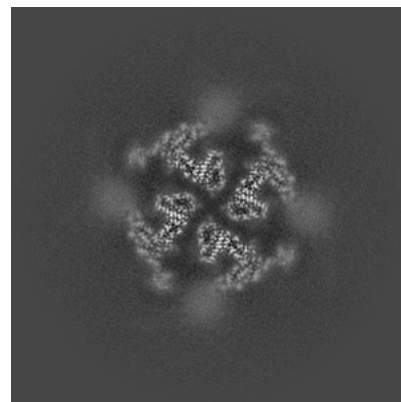
6.3.1 Primary map



X Index: 240

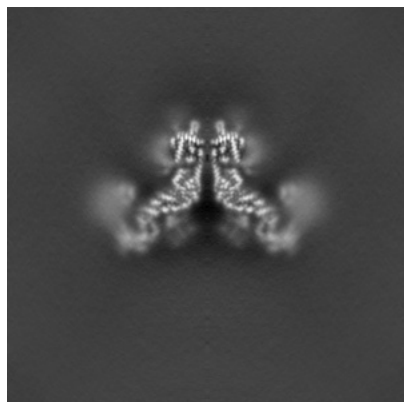


Y Index: 240

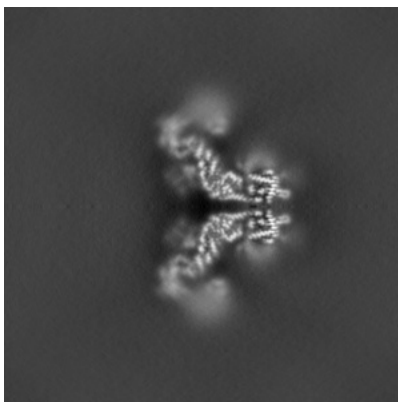


Z Index: 246

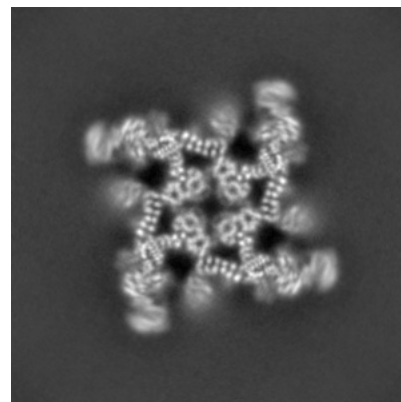
6.3.2 Raw map



X Index: 240



Y Index: 240

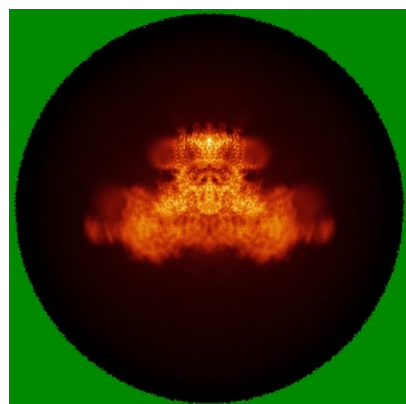


Z Index: 216

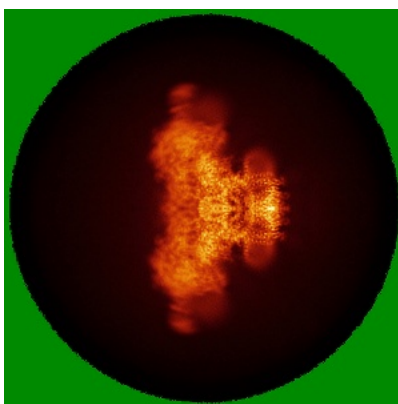
The images above show the largest variance slices of the map in three orthogonal directions.

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

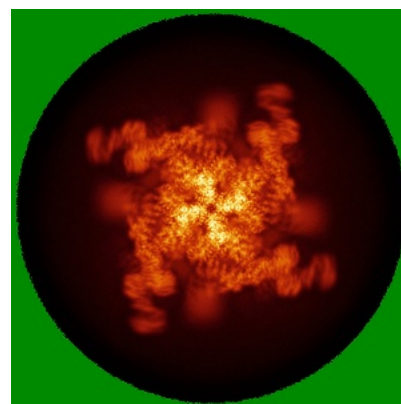
6.4.1 Primary map



X

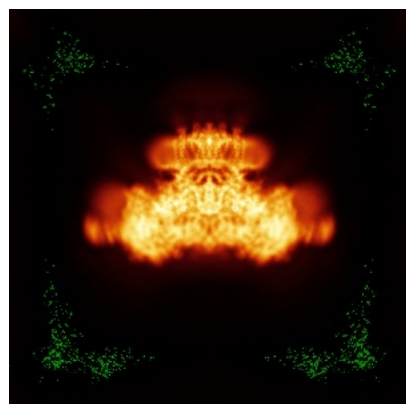


Y

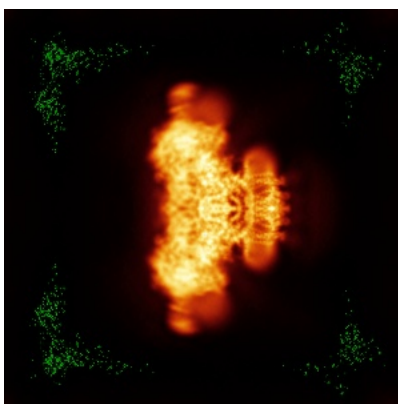


Z

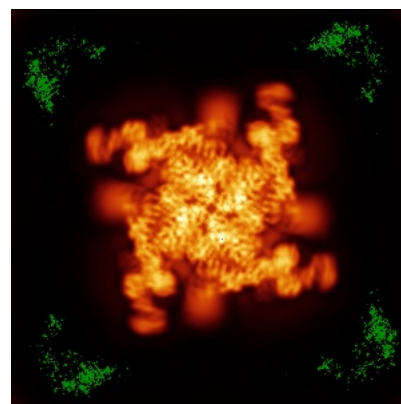
6.4.2 Raw map



X



Y

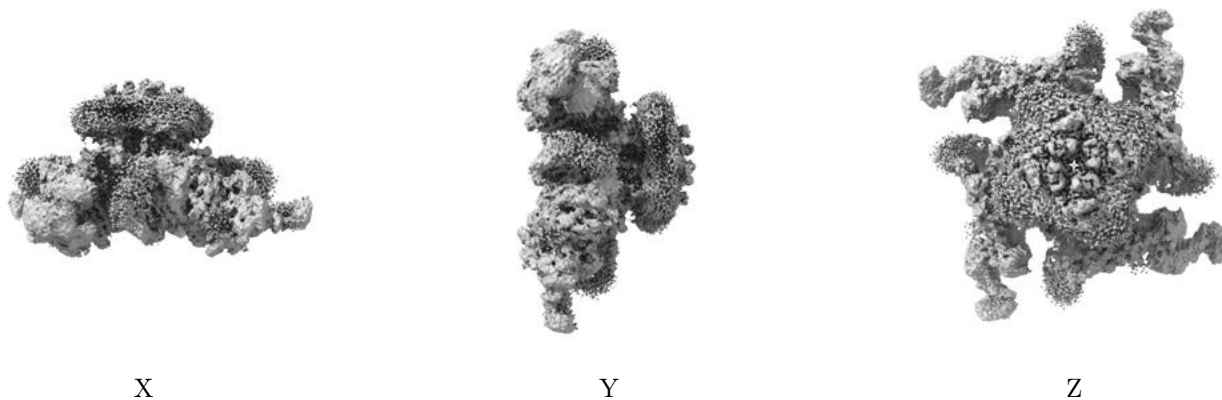


Z

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

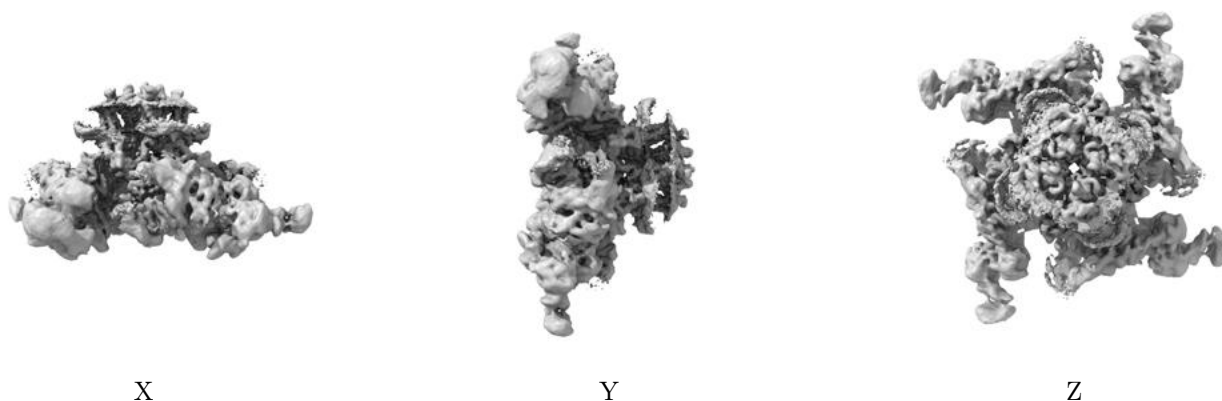
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.591. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

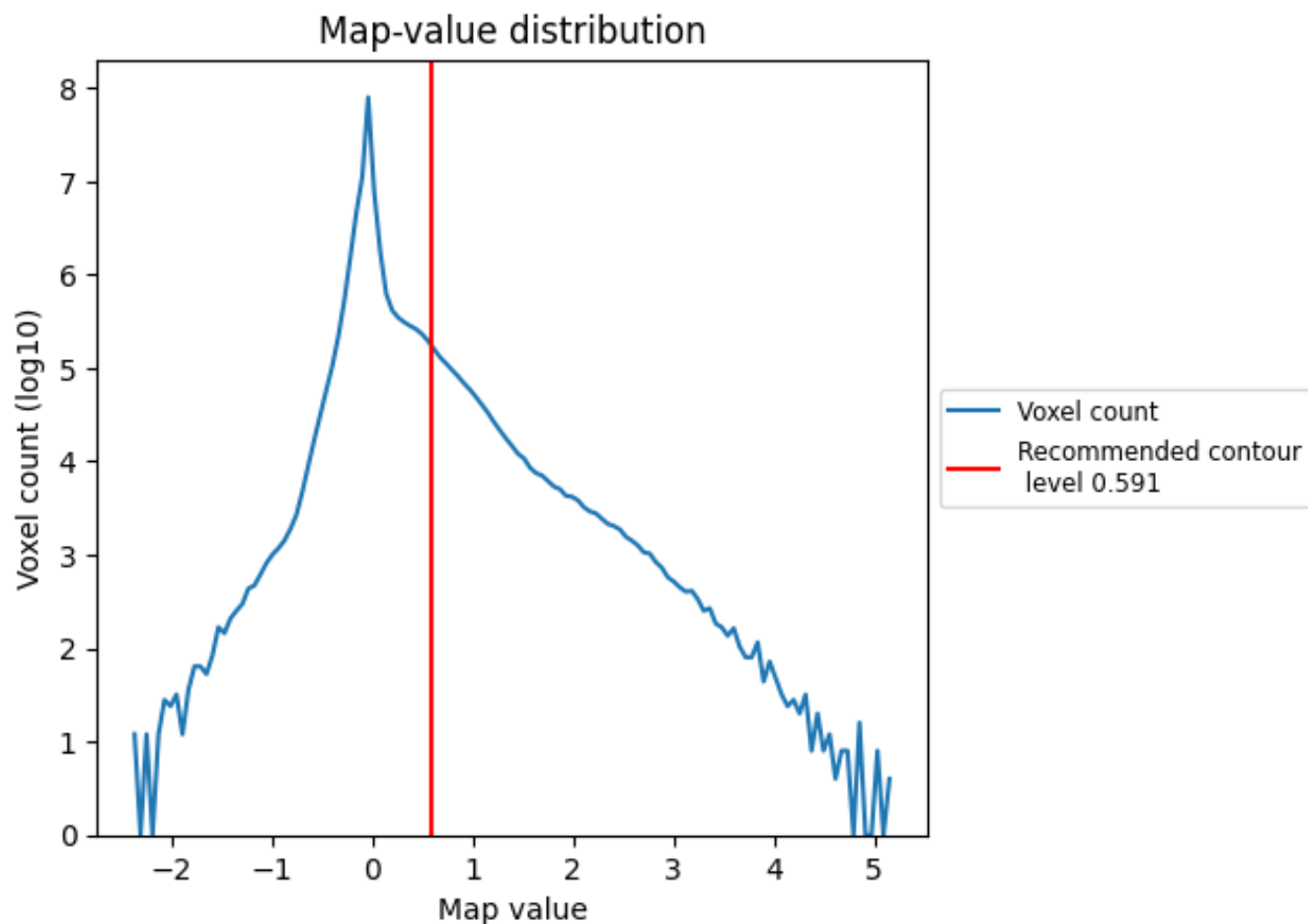
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

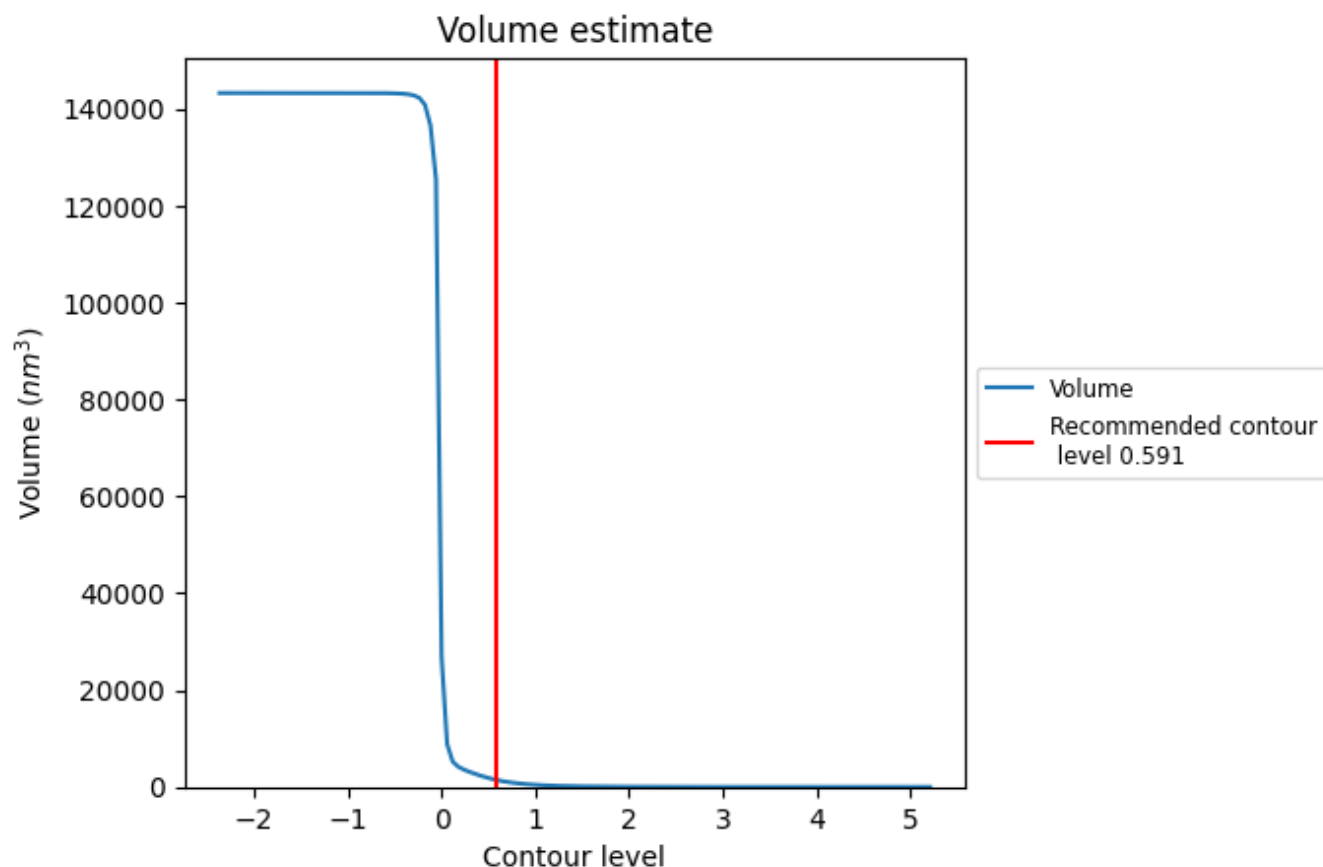
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

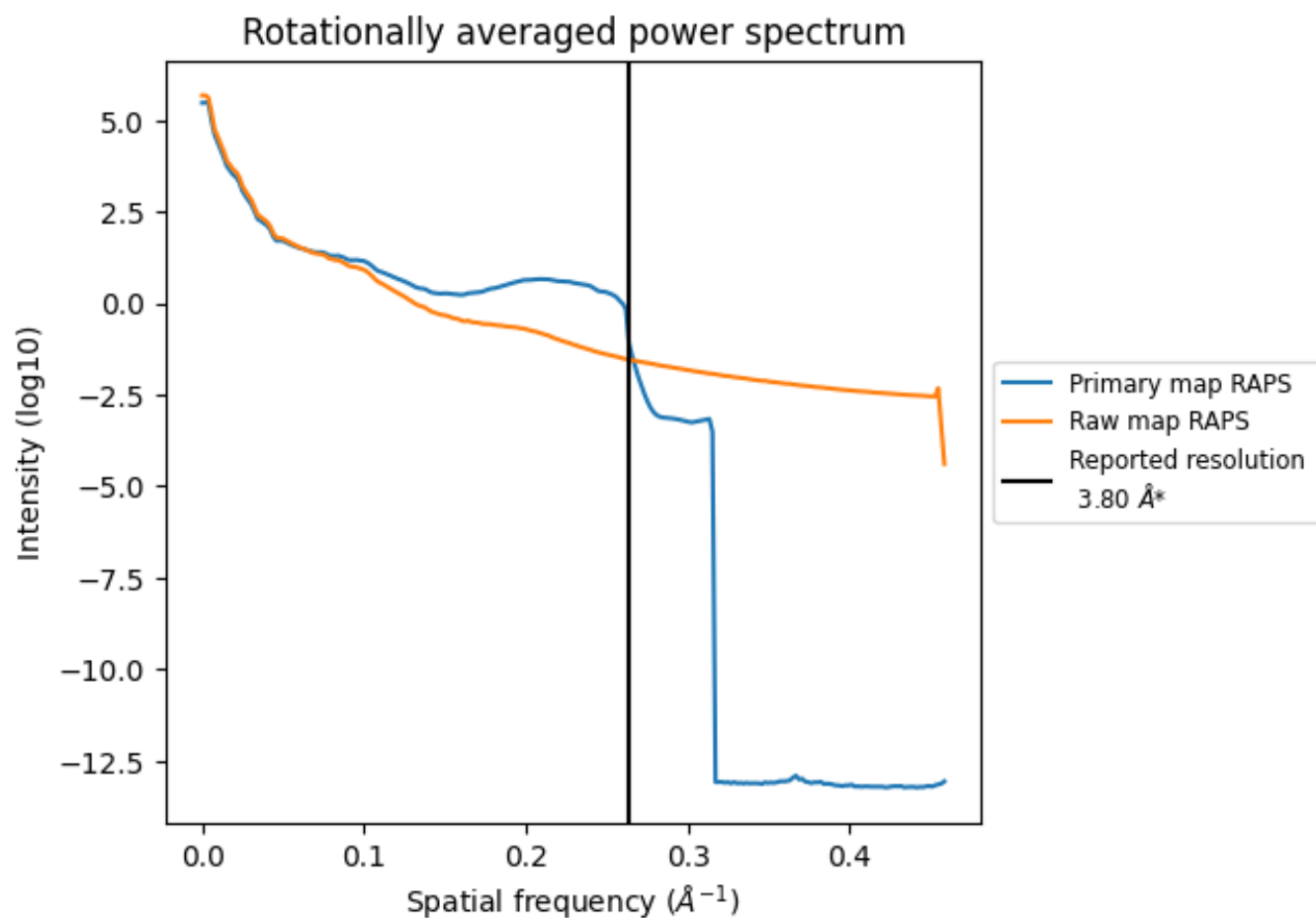
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1424 nm^3 ; this corresponds to an approximate mass of 1286 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 ⓘ

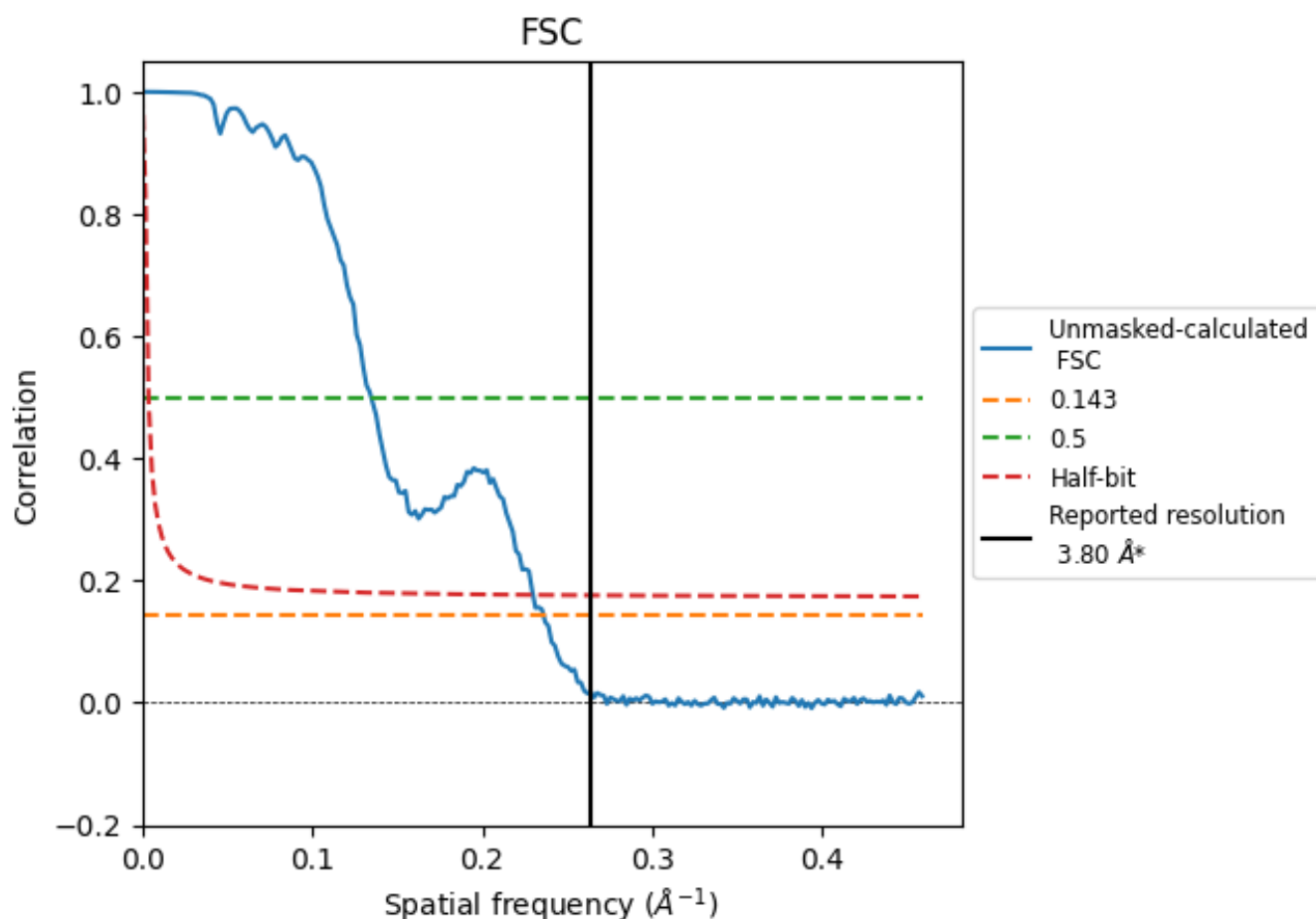


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

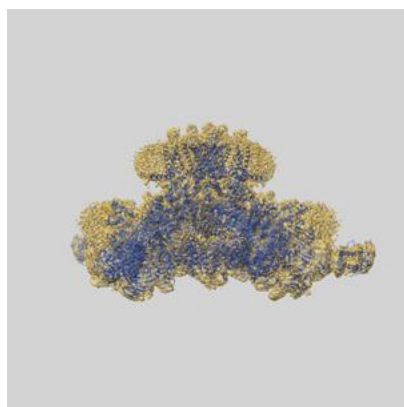
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	7.43	4.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 3.8 by more than 10 %

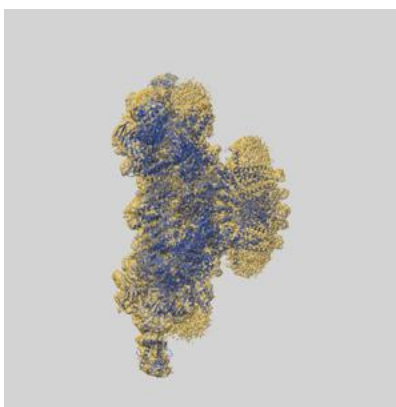
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38046 and PDB model 8X4C. Per-residue inclusion information can be found in section [3](#) on page [6](#).

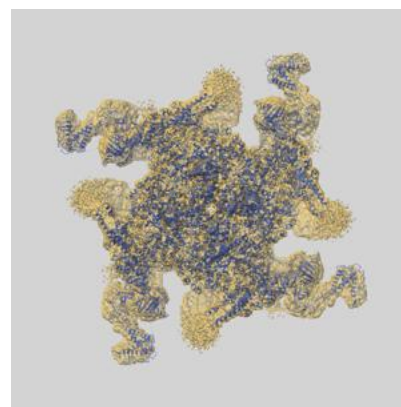
9.1 Map-model overlay [i](#)



X



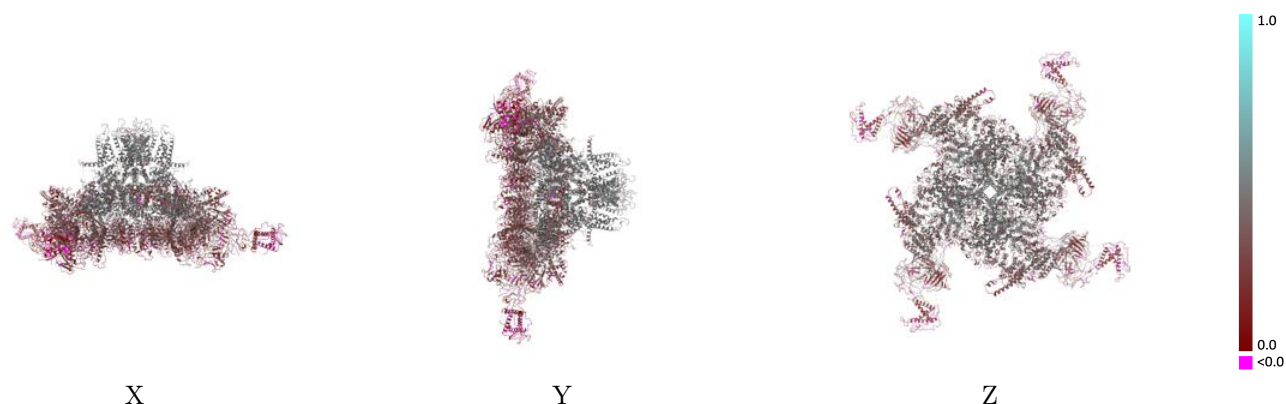
Y



Z

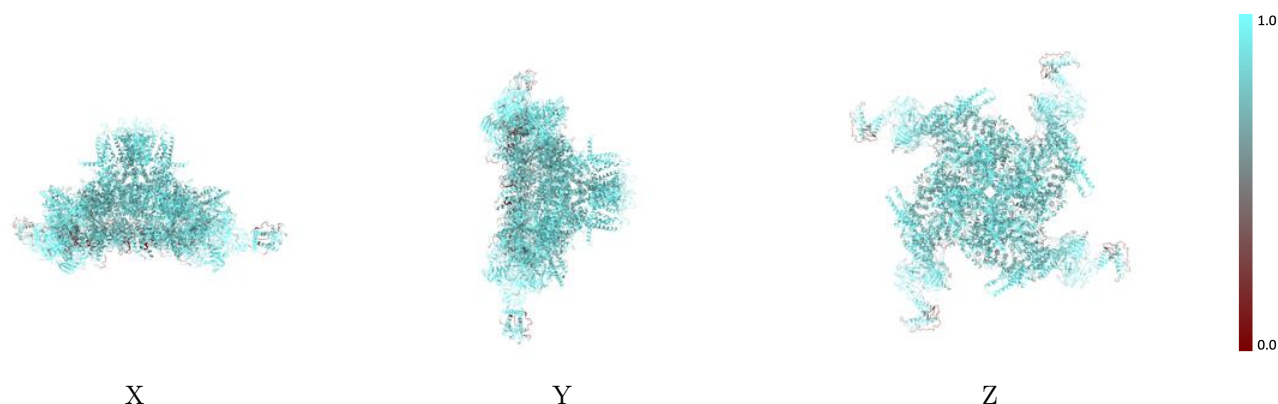
The images above show the 3D surface view of the map at the recommended contour level 0.591 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



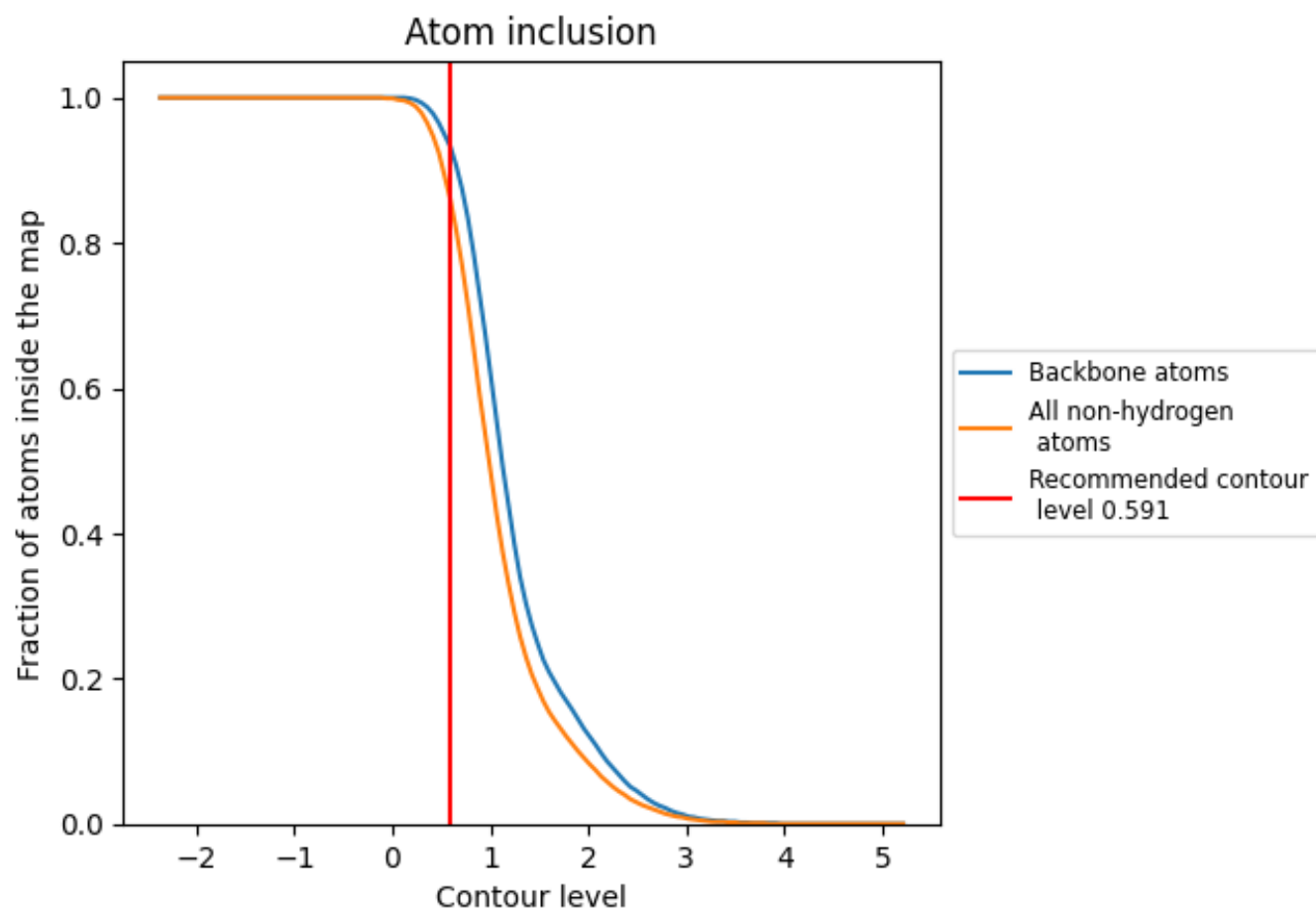
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.591).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 86% 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 (0.591) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8610	0.3270
A	0.8610	0.3270
B	0.8610	0.3270
C	0.8610	0.3270
D	0.8610	0.3270

