



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 06:39 AM EST

PDB ID : 7K0S
EMDB ID : EMD-22615
Title : Cryo-EM structure of rabbit RyR1 in the presence of Mg²⁺ and AMP-PCP in nanodisc
Authors : Nayak, A.R.; Samso, M.
Deposited on : 2020-09-05
Resolution : 4.50 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

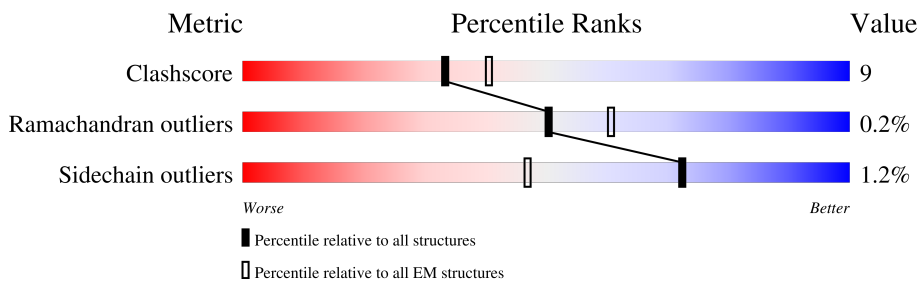
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	

2 Entry composition [i](#)

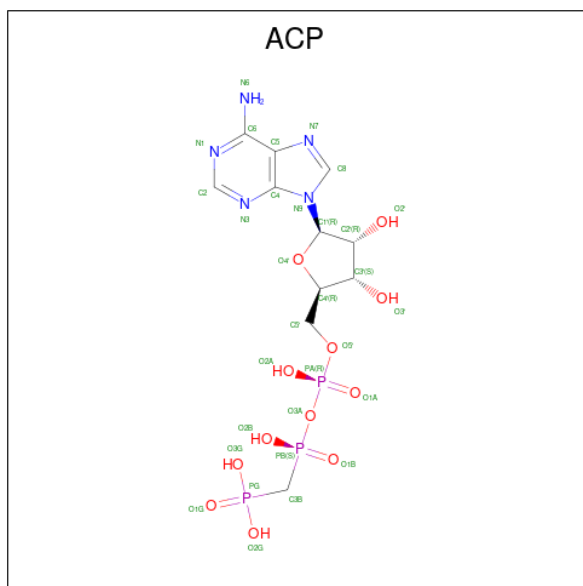
There are 4 unique types of molecules in this entry. The entry contains 115935 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RyR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4110	Total	C	N	O	S	0	0
			28941	18335	5131	5318	157		
1	B	4110	Total	C	N	O	S	0	0
			28940	18334	5135	5315	156		
1	D	4110	Total	C	N	O	S	0	0
			28963	18348	5134	5324	157		
1	C	4110	Total	C	N	O	S	0	0
			28958	18354	5132	5317	155		

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	11	5	12	3	
2	B	1	Total	C	N	O	P	0
			31	11	5	12	3	

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Mol	Chain	Residues	Atoms					AltConf
2	D	1	Total	C	N	O	P	0
			31	11	5	12	3	
2	C	1	Total	C	N	O	P	0
			31	11	5	12	3	

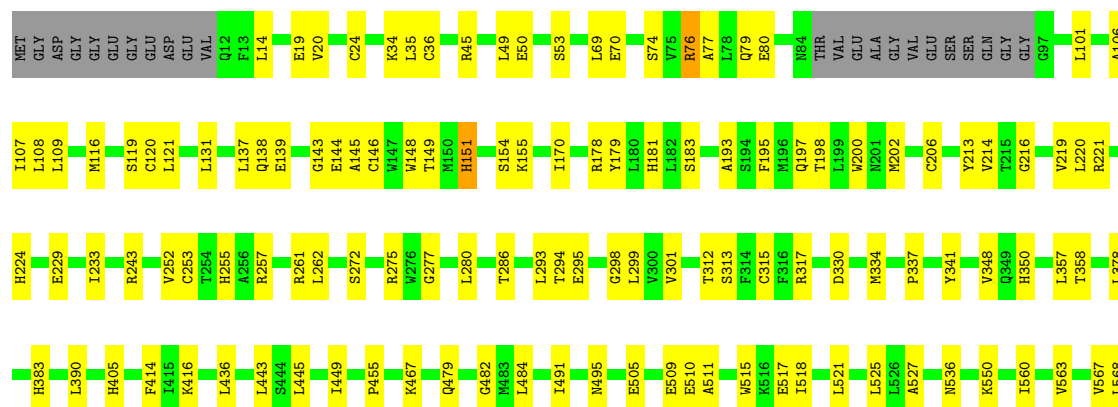
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

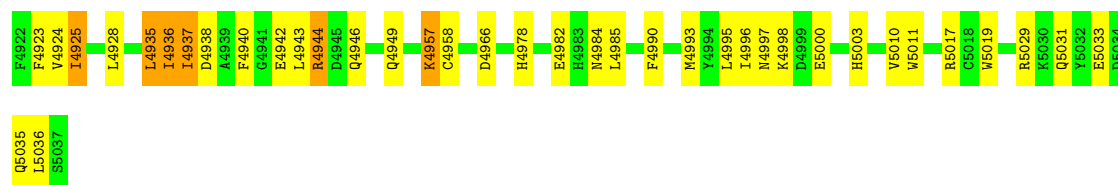
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	2	Total	Mg	0
			2	2	
4	D	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	





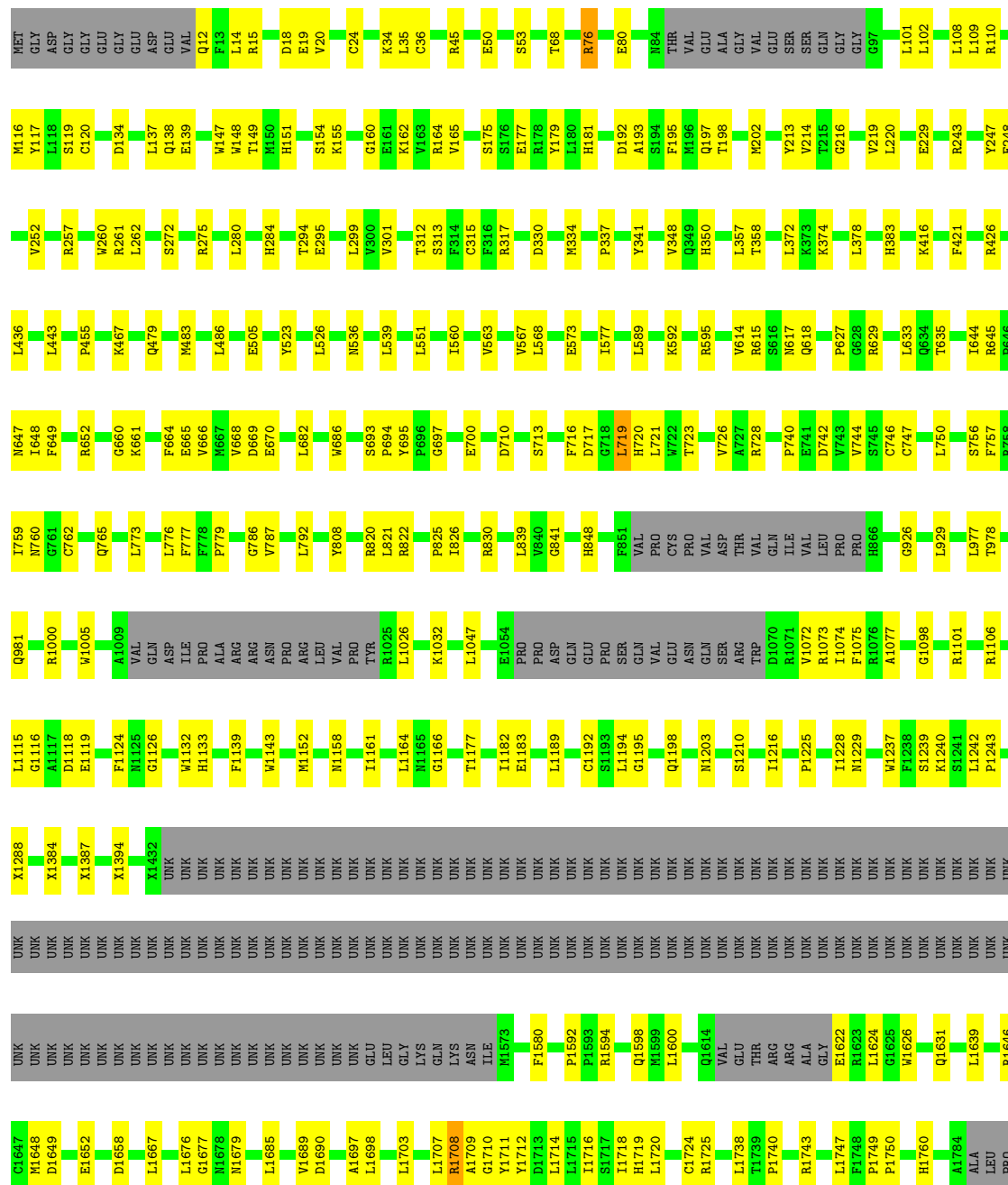






• Molecule 1: RyR1

Chain D: 69% 13% 18%







S5037	F4921	I4783	GLY	PRO	THR	GLY	GLY	VAL	M4097	L3965	Q3830	M3729	VAL	UNK
F4922	F4784	F4785	TRP	LYS	THR	TRP	GLY	ALA	K4101	Y3968	Q3833	H3732	TRP	UNK
F4923	V4924	T4785	GLY	LYS	PRO	GLY	ASP	ARG	Q4102	Y3968	Q3833	S3732	HIS	UNK
I4925	I4925	M4798	GLY	PRO	PRO	GLY	GLY	ALA	F4103	N3976	L3835	C3733	LYS	UNK
L4928	L4928	H4812	ALA	SER	PRO	ALA	ALA	ALA	T4104	R3984	S3840	E3737	LEU	UNK
L4929	L4929	H4812	GLY	PRO	THR	GLY	GLY	GLY	E4107	L3985	V3841	E3737	SER	UNK
L4930	L4930	I4816	GLY	PRO	PRO	GLY	GLY	THR	F3986	L3986	L3842	N3741	LYS	UNK
L4931	L4931	I4816	ALA	ALA	PRO	GLY	GLY	ALA	F4132	D3987	L3843	GLY	GLN	UNK
L4932	L4932	V4820	GLY	LYS	GLY	GLY	GLY	ALA	A3988	L3844	L3844	ARG	ARG	UNK
Q4933	Q4933	V4820	SER	LYS	SER	ALA	ALA	ALA	V3989	N3845	N3845	ARG	ARG	UNK
Q4934	Q4934	L4823	GLY	GLY	PRO	GLY	GLY	ALA	P4158	V3989	A3846	ALA	ALA	UNK
L4935	L4935	L4823	GLY	GLY	ILE	GLY	GLY	GLY	R4161	F3996	R3849	GLY	VAL	UNK
L4936	L4936	V4838	ASP	ALA	LEU	THR	ASP	ALA	Y4173	M3999	A3853	E3747	VAL	UNK
L4937	L4937	M4839	GLY	GLY	LYS	ALA	ALA	LEU	R4180	K4002	A3853	V3751	ALA	UNK
D4938	D4938	T4840	GLY	ALA	ARG	ALA	ALA	ARG	F4180	L4003	V3865	E3755	CYS	UNK
A4939	A4939	V4841	GLY	ALA	LYS	LEU	GLY	LEU	M4184	L4003	I3866	E3755	ARG	UNK
F4940	F4940	L4844	GLY	MET	GLY	TRP	ASP	ALA	I4190	L4010	D3877	E3757	ARG	UNK
R4944	R4944	L4844	GLY	GLY	VAL	GLY	GLY	ALA	I4197	L4010	R3886	K3760	MET	UNK
D4945	D4945	Y4851	GLY	GLY	ASP	GLY	GLY	GLY	E4011	E4011	F3887	Q3761	UNK	UNK
Q4946	Q4946	V4666	GLY	GLY	GLY	GLY	GLY	ALA	L4012	L4012	L3888	R3762	UNK	UNK
Q4949	Q4949	P4667	GLY	GLY	GLY	GLY	VAL	ALA	L4013	L4013	Q3889	L3763	UNK	UNK
C4958	C4958	F4671	GLY	GLY	GLY	GLY	GLY	GLY	L4017	L4017	L3888	L3763	UNK	UNK
F4959	F4959	F4672	GLY	GLY	LEU	GLY	GLY	GLY	D4018	D4018	Q3889	L3764	UNK	UNK
F4963	F4963	R4673	GLY	VAL	VAL	GLY	GLY	VAL	L4019	L4019	L3891	Y3765	UNK	UNK
D4966	D4966	N4864	PRO	PRO	PRO	ALA	ALA	SER	Q4020	Q4020	L3891	Q3766	UNK	UNK
K4865	K4865	T4689	GLY	GLY	GLY	GLY	GLY	TYR	D4022	D4022	N3896	Q3767	UNK	UNK
S4866	S4866	E4690	PRO	PRO	PRO	PRO	PRO	ALA	Y4025	Y4025	F3899	S3768	UNK	UNK
E4867	E4867	Q4691	GLY	GLY	GLY	GLY	GLY	LYS	M4026	M4026	Q3900	R3769	UNK	UNK
D4868	D4868	K4698	GLY	GLY	GLY	GLY	GLY	LEU	L4027	L4027	N3901	H3771	UNK	UNK
E4869	E4869	K4698	GLY	GLY	GLY	GLY	GLY	ALA	E4253	E4253	Y3902	T3772	UNK	UNK
D4870	D4870	O4700	GLY	GLY	GLY	GLY	GLY	THR	PRO	PRO	L3903	R3773	UNK	UNK
M4874	M4874	K4875	GLY	GLY	PRO	VAL	VAL	ARG	GLY	GLY	E3904	G3774	UNK	UNK
C4876	C4876	D4702	VAL	GLY	GLY	VAL	VAL	THR	GLY	GLY	I3913	A3775	UNK	UNK
Y4888	Y4888	L4704	VAL	ASP	GLY	VAL	VAL	ARG	PRO	PRO	Q3906	M3778	UNK	UNK
Y4888	Y4888	V4705	VAL	ASP	GLY	VAL	VAL	ARG	GLY	GLY	I3913	V3779	UNK	UNK
V4891	V4891	F4711	GLY	MET	ASP	GLY	GLY	GLY	ASP	ASP	L3824	L3780	UNK	UNK
R4892	R4892	F4711	GLY	GLY	GLY	GLY	GLY	THR	ASP	ASP	Q3927	Q3781	X3102	X3102
G4895	G4895	V4716	SER	GLY	GLY	GLY	GLY	PRO	GLY	GLY	Q3927	K3787	X3106	X3106
G4896	G4896	F4719	ALA	ALA	ASN	PHE	PHE	ARG	GLY	GLY	E3928	M3793	X3406	X3406
I4897	I4897	G4898	ALA	GLY	GLY	THR	THR	ARG	MET	MET	G3681	V3794	X3410	X3410
G4898	G4898	K4723	ASP	ASP	LYS	PRO	PRO	ALA	GLY	GLY	S3931	V3794	X3535	X3535
P4904	P4904	I4731	LEU	LEU	GLY	GLY	GLY	THR	ALA	ALA	D3941	T3797	X3536	X3536
C5018	C5018	F4732	ALA	ALA	GLY	VAL	VAL	VAL	F4065	F4065	E3944	G3801	X3537	X3537
Y5019	Y5019	I4750	ALA	ALA	PRO	GLY	GLY	GLY	K4067	K4067	E3944	L3802	P3697	P3697
R4913	R4913	I4750	GLY	GLY	GLY	GLY	GLY	LEU	I4071	I4071	G3947	S3803	X3613	X3613
D4917	D4917	K4774	SER	SER	ALA	ALA	ALA	ALA	GLY	GLY	L3804	T3804	E3712	LYS
I4918	I4918	F4779	GLY	GLY	PRO	PRO	PRO	LEU	F4093	F4093	A3954	L3805	SER	SER
E5033	E5033	W4778	GLY	GLY	PRO	PRO	PRO	ALA	Q4094	Q4094	M3955	M3723	LYS	LYS
F4920	F4920	K4779	ASP	SER	PRO	PRO	PRO	PRO	A4096	A4096	S3964	X3725	ALA	ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	68155	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.200	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	478.72, 478.72, 478.72	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.26	0/25057	0.50	1/34021 (0.0%)
1	B	0.27	0/25055	0.50	3/34016 (0.0%)
1	C	0.26	0/25076	0.50	2/34047 (0.0%)
1	D	0.26	0/25078	0.50	2/34045 (0.0%)
All	All	0.26	0/100266	0.50	8/136129 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3751	VAL	C-N-CA	-5.77	107.27	121.70
1	B	719	LEU	CA-CB-CG	5.62	128.23	115.30
1	D	3751	VAL	C-N-CA	-5.62	107.66	121.70
1	D	719	LEU	CA-CB-CG	5.56	128.08	115.30
1	C	4891	VAL	O-C-N	5.30	131.18	122.70
1	C	4862	PHE	O-C-N	5.27	131.13	122.70
1	B	4872	PRO	CA-N-CD	-5.26	104.13	111.50
1	A	3753	PHE	CB-CA-C	-5.21	99.97	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	4892	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	28941	0	24397	483	0
1	B	28940	0	24404	519	0
1	C	28958	0	24429	510	0
1	D	28963	0	24439	493	0
2	A	31	0	14	7	0
2	B	31	0	14	4	0
2	C	31	0	14	3	0
2	D	31	0	14	8	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
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	115935	0	97725	1937	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 9.

All (1937) 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:3773:ARG:CB	1:A:3815:LYS:HE3	1.46	1.45
1:C:3765:TYR:CE1	1:C:4750:ILE:HG23	1.52	1.40
1:A:4921:PHE:O	1:A:4925:ILE:HG22	1.27	1.30
1:A:3767:GLN:O	1:A:3772:THR:HB	1.29	1.28
1:D:3674:ILE:HG12	1:D:3769:ARG:CD	1.64	1.28
1:B:3765:TYR:CE1	1:B:4750:ILE:CG2	2.20	1.24
1:C:3757:GLU:O	1:C:3760:LYS:HG3	1.40	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3674:ILE:CG1	1:D:3769:ARG:HD2	1.71	1.20
1:A:3702:VAL:HG11	1:A:3775:ALA:HB1	1.28	1.15
1:B:4935:LEU:HD23	1:C:4940:PHE:HE2	1.03	1.15
1:B:4573:ILE:HD13	1:B:4809:PHE:CE2	1.83	1.13
1:A:4904:PRO:HG3	1:A:4913:ARG:NH1	1.65	1.11
1:D:3674:ILE:O	1:D:3769:ARG:HD3	1.52	1.09
1:B:3765:TYR:CE1	1:B:4750:ILE:HG23	1.87	1.08
1:B:4573:ILE:CD1	1:B:4809:PHE:HE2	1.67	1.08
1:A:3773:ARG:CB	1:A:3815:LYS:CE	2.33	1.07
1:B:4577:LEU:HD21	1:B:4807:PHE:CE1	1.90	1.07
1:D:4985:LEU:HG	2:D:5101:ACP:HN61	1.12	1.07
1:C:3765:TYR:CE1	1:C:4750:ILE:CG2	2.38	1.06
1:B:4935:LEU:HD23	1:C:4940:PHE:CE2	1.90	1.06
1:A:4985:LEU:HD23	2:A:5101:ACP:HN61	1.19	1.05
1:B:4865:LYS:HA	1:B:4865:LYS:HE3	1.37	1.02
1:A:3702:VAL:HG11	1:A:3775:ALA:CB	1.88	1.01
1:B:4866:SER:O	1:B:4867:GLU:CG	2.07	1.01
1:D:4985:LEU:CG	2:D:5101:ACP:HN61	1.71	1.01
1:C:100:THR:HG21	1:C:162:LYS:HE3	1.42	1.00
1:B:4577:LEU:HD21	1:B:4807:PHE:CD1	1.97	0.99
1:A:3201:UNK:CB	1:A:3249:UNK:CB	2.41	0.98
1:C:3765:TYR:CZ	1:C:4750:ILE:HG23	1.98	0.97
1:D:3674:ILE:HG12	1:D:3769:ARG:HD2	0.98	0.97
1:B:4801:LEU:HD23	1:B:4808:PHE:CE2	2.01	0.96
1:C:3765:TYR:HE1	1:C:4750:ILE:HG23	1.18	0.95
1:B:3765:TYR:HE1	1:B:4750:ILE:HG21	1.31	0.95
1:B:4573:ILE:HD13	1:B:4809:PHE:HE2	1.14	0.95
1:B:3765:TYR:CE1	1:B:4750:ILE:HG21	2.01	0.94
1:B:3674:ILE:CG2	1:B:3769:ARG:HD2	1.97	0.94
1:B:4574:ASN:HD22	1:B:4813:LEU:HD22	1.31	0.94
1:C:162:LYS:HB2	1:C:164:ARG:HH11	1.33	0.94
1:B:3674:ILE:HG22	1:B:3769:ARG:CD	1.98	0.93
1:B:4866:SER:O	1:B:4867:GLU:HG3	1.67	0.93
1:B:4801:LEU:CD2	1:B:4808:PHE:HE2	1.81	0.92
1:D:4820:VAL:HG11	1:D:4823:LEU:HD23	1.51	0.91
1:B:4865:LYS:HB3	1:B:4875:LYS:HG2	1.49	0.91
1:A:4860:ARG:HH11	1:A:4860:ARG:HG3	1.35	0.91
1:A:3702:VAL:CG1	1:A:3775:ALA:HB1	2.00	0.90
1:A:4932:ILE:O	1:A:4936:ILE:HD13	1.71	0.90
1:A:3549:UNK:O	1:A:3550:UNK:C	2.18	0.90
1:D:3767:GLN:HE22	1:D:3804:ILE:HA	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:LEU:HD12	1:C:163:VAL:O	1.72	0.89
1:C:3765:TYR:HE2	1:C:3769:ARG:NH2	1.71	0.89
1:D:4940:PHE:CE2	1:C:4935:LEU:CD2	2.54	0.89
1:D:5029:ARG:O	1:D:5033:GLU:HB3	1.72	0.89
1:B:4921:PHE:O	1:B:4925:ILE:HG22	1.71	0.88
1:D:4961:CYS:SG	1:D:4983:HIS:CE1	2.67	0.88
1:B:3765:TYR:CD1	1:B:4750:ILE:HG23	2.08	0.88
1:B:4573:ILE:CD1	1:B:4809:PHE:CE2	2.51	0.88
1:A:4921:PHE:O	1:A:4925:ILE:CG2	2.20	0.88
1:B:4016:LEU:HD23	1:B:4020:GLN:HE22	1.38	0.87
1:D:4662:ASN:HA	1:D:4666:VAL:HG21	1.55	0.86
1:B:4801:LEU:HD23	1:B:4808:PHE:HE2	1.36	0.85
1:A:759:ILE:HG22	1:A:762:CYS:HB2	1.57	0.85
1:A:4666:VAL:N	1:A:4667:PRO:HD2	1.91	0.85
1:C:3765:TYR:OH	1:C:4750:ILE:CG2	2.24	0.85
1:C:5029:ARG:O	1:C:5033:GLU:HB3	1.77	0.85
1:A:3760:LYS:HA	1:A:3760:LYS:HZ2	1.42	0.84
1:C:3765:TYR:CZ	1:C:4750:ILE:CG2	2.58	0.84
1:C:2107:GLN:HE22	1:C:3681:GLY:HA2	1.40	0.84
1:B:4921:PHE:O	1:B:4925:ILE:CG2	2.24	0.84
1:C:74:SER:H	1:C:77:ALA:HB3	1.41	0.84
1:D:4985:LEU:HG	2:D:5101:ACP:N6	1.91	0.84
1:C:4944:ARG:HG3	1:C:4944:ARG:HH11	1.40	0.84
1:C:3964:SER:O	1:C:3968:TYR:CE1	2.30	0.84
1:D:4985:LEU:CD2	2:D:5101:ACP:HN61	1.91	0.84
1:B:5029:ARG:O	1:B:5033:GLU:HB3	1.78	0.84
1:A:4940:PHE:CE2	1:D:4935:LEU:CD2	2.61	0.83
1:B:4862:PHE:CE2	1:B:4913:ARG:HD2	2.11	0.83
1:C:4662:ASN:HA	1:C:4666:VAL:HG21	1.59	0.83
1:B:4818:MET:HA	1:B:4823:LEU:HG	1.60	0.83
1:C:162:LYS:HB2	1:C:164:ARG:NH1	1.93	0.83
1:B:4574:ASN:HD22	1:B:4813:LEU:CD2	1.89	0.83
1:C:3765:TYR:HE1	1:C:4750:ILE:CG2	1.85	0.83
1:A:3760:LYS:O	1:A:3760:LYS:HD3	1.79	0.82
1:A:5029:ARG:O	1:A:5033:GLU:HB3	1.79	0.82
1:B:4574:ASN:ND2	1:B:4813:LEU:HD22	1.93	0.82
1:A:4985:LEU:CD2	2:A:5101:ACP:HN61	1.92	0.82
1:B:4812:HIS:ND1	1:B:4812:HIS:O	2.13	0.82
1:B:3674:ILE:HG21	1:B:3769:ARG:HD2	1.60	0.81
1:A:4904:PRO:HG3	1:A:4913:ARG:HH11	1.45	0.81
1:B:4795:TYR:C	1:B:4795:TYR:HD1	1.82	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3965:LEU:HD12	1:C:3965:LEU:O	1.78	0.81
1:B:3674:ILE:CG2	1:B:3769:ARG:CD	2.57	0.81
1:B:4944:ARG:HH11	1:B:4944:ARG:HG3	1.44	0.81
1:D:4865:LYS:HA	1:D:4865:LYS:HZ2	1.46	0.80
1:B:4866:SER:C	1:B:4867:GLU:HG3	2.02	0.80
1:A:4985:LEU:HD23	2:A:5101:ACP:N6	1.97	0.80
1:B:759:ILE:HG22	1:B:762:CYS:HB2	1.62	0.80
1:A:4892:ARG:NH2	1:D:4898:GLY:H	1.79	0.80
1:C:759:ILE:HG22	1:C:762:CYS:HB2	1.63	0.79
1:B:4795:TYR:C	1:B:4795:TYR:CD1	2.54	0.79
1:C:2107:GLN:NE2	1:C:3681:GLY:HA2	1.97	0.79
1:D:4985:LEU:CD2	2:D:5101:ACP:N6	2.45	0.79
1:A:4925:ILE:HD12	1:A:4925:ILE:O	1.83	0.79
1:B:4791:TYR:OH	1:B:4816:ILE:HD13	1.81	0.79
1:A:3544:UNK:CB	1:A:3554:UNK:CB	2.62	0.78
1:A:4823:LEU:HD22	1:D:4839:MET:HE3	1.63	0.78
1:C:742:ASP:HB3	1:C:759:ILE:HD11	1.65	0.78
1:A:4892:ARG:HH22	1:D:4898:GLY:H	1.26	0.78
1:C:2447:LYS:HE2	1:C:2449:GLU:HB2	1.65	0.78
1:A:121:LEU:HD11	1:A:138:GLN:HE22	1.47	0.78
1:A:3729:MET:HG3	1:A:3770:LEU:HD11	1.65	0.78
1:D:4662:ASN:HA	1:D:4666:VAL:CG2	2.13	0.78
1:B:4574:ASN:ND2	1:B:4813:LEU:CD2	2.47	0.77
1:A:4820:VAL:HB	1:A:4823:LEU:HD23	1.66	0.77
1:B:4820:VAL:HB	1:B:4823:LEU:HD23	1.64	0.77
1:B:4866:SER:O	1:B:4867:GLU:HG2	1.83	0.77
1:A:4860:ARG:NH1	1:B:4582:VAL:HG11	1.99	0.77
1:A:2641:UNK:O	1:A:2642:UNK:CB	2.32	0.77
1:A:3490:UNK:CB	1:A:3601:UNK:CB	2.63	0.77
1:C:4919:THR:O	1:C:4923:PHE:HB2	1.85	0.76
1:D:4937:ILE:CD1	1:C:4934:GLY:HA2	2.16	0.76
1:C:4666:VAL:N	1:C:4667:PRO:CD	2.49	0.76
1:A:4240:ASP:OD1	1:A:4668:LEU:HD21	1.86	0.76
1:B:3674:ILE:HG22	1:B:3769:ARG:HD3	1.68	0.76
1:D:3787:LYS:HG3	1:D:3831:SER:HA	1.66	0.75
1:C:4662:ASN:HA	1:C:4666:VAL:CG2	2.15	0.75
1:A:74:SER:H	1:A:77:ALA:HB3	1.52	0.75
1:D:3761:GLN:NE2	1:D:3761:GLN:HA	2.01	0.75
1:D:4871:GLU:HG2	1:D:4871:GLU:O	1.86	0.75
1:B:4865:LYS:HE3	1:B:4865:LYS:CA	2.16	0.75
1:A:4904:PRO:CG	1:A:4913:ARG:NH1	2.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3674:ILE:HG21	1:D:3766:GLN:OE1	1.87	0.75
1:D:3767:GLN:NE2	1:D:3804:ILE:HG23	2.01	0.75
1:A:4666:VAL:N	1:A:4667:PRO:CD	2.49	0.74
1:B:3787:LYS:HG3	1:B:3831:SER:HA	1.67	0.74
1:D:4666:VAL:N	1:D:4667:PRO:CD	2.50	0.74
1:B:4865:LYS:CB	1:B:4875:LYS:HG2	2.17	0.74
1:A:4898:GLY:H	1:B:4892:ARG:HH22	1.36	0.74
1:A:76:ARG:NH1	1:B:3935:TRP:O	2.21	0.74
1:C:1152:MET:HB3	1:C:1161:ILE:HB	1.70	0.74
1:A:2452:ARG:NH2	1:D:177:GLU:OE1	2.21	0.74
1:A:1707:LEU:HG	1:A:1708:ARG:H	1.53	0.74
1:A:3761:GLN:OE1	1:A:3761:GLN:HA	1.87	0.74
1:D:1707:LEU:HG	1:D:1708:ARG:H	1.53	0.74
1:C:121:LEU:HD11	1:C:138:GLN:HE22	1.53	0.73
1:D:3674:ILE:HG12	1:D:3769:ARG:CG	2.18	0.73
1:A:1152:MET:HB3	1:A:1161:ILE:HB	1.71	0.73
1:C:645:ARG:HD3	1:C:826:ILE:HG22	1.70	0.73
1:C:1707:LEU:HG	1:C:1708:ARG:H	1.54	0.73
1:B:121:LEU:HD11	1:B:138:GLN:HE22	1.54	0.73
1:B:1152:MET:HB3	1:B:1161:ILE:HB	1.70	0.72
1:A:3773:ARG:CA	1:A:3815:LYS:HE3	2.18	0.72
1:D:759:ILE:HG22	1:D:762:CYS:HB2	1.69	0.72
1:A:3760:LYS:HA	1:A:3760:LYS:NZ	2.04	0.72
1:A:4860:ARG:HG3	1:A:4860:ARG:NH1	2.05	0.72
1:C:103:TYR:CE1	1:C:163:VAL:HG13	2.25	0.72
1:A:3544:UNK:C	1:A:3551:UNK:CB	2.67	0.72
1:A:4860:ARG:HH12	1:B:4582:VAL:HG11	1.51	0.72
1:B:4984:ASN:HA	2:B:5101:ACP:N6	2.04	0.72
1:C:151:HIS:HB2	1:C:170:ILE:HB	1.71	0.72
1:C:162:LYS:CB	1:C:164:ARG:HH11	2.02	0.72
1:C:4223:ASN:HD21	1:C:4946:GLN:HE22	1.38	0.72
1:D:4034:ASN:OD1	1:D:4035:VAL:N	2.23	0.72
1:D:4865:LYS:HA	1:D:4865:LYS:NZ	2.03	0.72
1:C:977:LEU:HB3	1:C:1047:LEU:HD11	1.72	0.72
1:D:1152:MET:HB3	1:D:1161:ILE:HB	1.72	0.72
1:B:977:LEU:HB3	1:B:1047:LEU:HD11	1.72	0.72
2:C:5101:ACP:O2G	2:C:5101:ACP:O2B	2.07	0.72
1:A:3935:TRP:HD1	1:D:76:ARG:HH12	1.38	0.71
1:B:3666:ASP:OD1	1:B:3666:ASP:N	2.20	0.71
1:C:3755:GLU:OE1	1:C:3755:GLU:HA	1.90	0.71
1:D:977:LEU:HB3	1:D:1047:LEU:HD11	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:ASP:HB3	1:B:759:ILE:HD11	1.71	0.71
1:D:4892:ARG:NH2	1:C:4917:ASP:OD1	2.23	0.71
1:C:4197:ILE:HG13	1:C:4198:SER:H	1.56	0.71
1:D:645:ARG:HD3	1:D:826:ILE:HG22	1.72	0.71
1:A:977:LEU:HB3	1:A:1047:LEU:HD11	1.71	0.70
1:D:3773:ARG:HA	1:D:3815:LYS:HE3	1.72	0.70
1:C:3765:TYR:CE1	1:C:4750:ILE:HD12	2.26	0.70
1:B:2095:GLN:NE2	1:B:2127:GLN:O	2.25	0.70
1:B:1707:LEU:HG	1:B:1708:ARG:H	1.55	0.70
1:B:479:GLN:OE1	1:B:536:ASN:ND2	2.25	0.70
1:B:4995:LEU:HD21	1:B:5011:TRP:HB2	1.73	0.69
1:D:479:GLN:OE1	1:D:536:ASN:ND2	2.25	0.69
1:D:4197:ILE:HG21	1:D:4990:PHE:HB3	1.73	0.69
1:D:4913:ARG:NH2	1:D:4917:ASP:OD2	2.24	0.69
1:B:3969:ILE:HD11	1:B:3980:LEU:HD12	1.74	0.69
1:B:4577:LEU:CD2	1:B:4807:PHE:CE1	2.72	0.69
1:D:3767:GLN:HE22	1:D:3804:ILE:CA	2.05	0.68
1:C:158:SER:N	1:C:161:GLU:OE1	2.24	0.68
1:C:4936:ILE:HD13	1:C:4936:ILE:N	2.08	0.68
1:D:3751:VAL:O	1:D:3752:SER:C	2.29	0.68
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.74	0.68
1:C:2095:GLN:NE2	1:C:2127:GLN:O	2.27	0.68
1:D:4574:ASN:HD22	1:D:4813:LEU:HD13	1.59	0.68
1:C:4995:LEU:HD21	1:C:5011:TRP:HB2	1.76	0.68
1:A:4197:ILE:HG13	1:A:4198:SER:H	1.57	0.68
1:C:2107:GLN:HE22	1:C:3681:GLY:CA	2.07	0.68
1:D:179:TYR:HB3	1:D:197:GLN:HB2	1.76	0.68
1:B:4182:GLU:OE2	1:B:4192:ARG:NH2	2.25	0.67
1:C:220:LEU:HD22	1:C:262:LEU:HD23	1.76	0.67
1:C:670:GLU:HG3	1:C:788:LYS:H	1.59	0.67
1:A:4244:GLU:CG	1:A:4668:LEU:HD11	2.25	0.67
1:A:4936:ILE:N	1:A:4936:ILE:HD12	2.09	0.67
1:C:4034:ASN:OD1	1:C:4035:VAL:N	2.27	0.67
1:D:2095:GLN:NE2	1:D:2127:GLN:O	2.27	0.67
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.77	0.67
1:D:742:ASP:HB3	1:D:759:ILE:HD11	1.76	0.67
1:A:4839:MET:HE3	1:B:4823:LEU:HD22	1.76	0.67
1:A:4865:LYS:HA	1:A:4865:LYS:HE3	1.77	0.67
1:C:3964:SER:O	1:C:3968:TYR:HE1	1.77	0.67
1:B:664:PHE:HB2	1:B:746:CYS:HB2	1.77	0.66
1:D:4985:LEU:CG	2:D:5101:ACP:N6	2.53	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4820:VAL:CG1	1:D:4823:LEU:HD23	2.24	0.66
1:C:4888:TYR:CE2	1:C:4892:ARG:NH1	2.58	0.66
1:B:131:LEU:HD22	1:B:178:ARG:HH22	1.61	0.66
1:B:4935:LEU:CD2	1:C:4940:PHE:HE2	1.94	0.66
1:A:3767:GLN:HG3	1:A:3809:ASN:HD21	1.61	0.66
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.77	0.66
1:C:3757:GLU:O	1:C:3760:LYS:CG	2.31	0.66
1:B:4020:GLN:HA	1:B:4023:MET:SD	2.34	0.66
1:D:2176:ASN:O	1:D:2180:GLN:NE2	2.29	0.66
1:C:158:SER:H	1:C:161:GLU:CD	1.99	0.66
1:C:3765:TYR:OH	1:C:4750:ILE:HG22	1.96	0.66
1:A:3969:ILE:HD11	1:A:3980:LEU:HD12	1.78	0.66
1:A:4665:LYS:C	1:A:4667:PRO:HD2	2.16	0.65
1:B:3668:SER:O	1:B:3672:ARG:NH2	2.28	0.65
1:D:4892:ARG:HH22	1:C:4898:GLY:H	1.42	0.65
1:C:1243:PRO:HB2	1:C:1600:LEU:HD12	1.78	0.65
1:C:3658:LYS:HA	1:C:3661:TRP:HZ3	1.62	0.65
1:B:719:LEU:O	1:B:720:HIS:ND1	2.30	0.65
1:B:4197:ILE:HG13	1:B:4198:SER:H	1.61	0.65
1:A:2095:GLN:NE2	1:A:2127:GLN:O	2.29	0.65
1:C:4892:ARG:O	1:C:4892:ARG:HG2	1.96	0.65
1:A:4839:MET:HE1	1:B:4826:ILE:HD13	1.78	0.65
1:C:4944:ARG:HG3	1:C:4944:ARG:NH1	2.09	0.65
1:A:3493:UNK:O	1:A:3494:UNK:CB	2.41	0.65
1:C:3674:ILE:HD12	1:C:3769:ARG:HD2	1.79	0.65
1:A:1679:ASN:ND2	1:A:1797:ARG:O	2.30	0.64
1:B:14:LEU:HB3	1:B:101:LEU:HD12	1.78	0.64
1:C:4223:ASN:HD21	1:C:4946:GLN:NE2	1.95	0.64
1:B:4944:ARG:HG3	1:B:4944:ARG:NH1	2.11	0.64
1:A:1229:ASN:HB3	1:A:1826:ALA:HB1	1.79	0.64
1:B:4573:ILE:HD11	1:B:4809:PHE:HE2	1.60	0.64
1:B:4832:HIS:CD2	1:B:4942:GLU:OE1	2.49	0.64
1:A:4240:ASP:CG	1:A:4668:LEU:HD21	2.18	0.64
1:D:4892:ARG:CZ	1:C:4896:GLY:HA3	2.27	0.64
1:C:4937:ILE:HD13	1:C:4937:ILE:N	2.12	0.64
1:D:216:GLY:HA2	1:D:262:LEU:HD11	1.80	0.64
1:A:3729:MET:CG	1:A:3770:LEU:HD11	2.26	0.64
1:D:3986:TRP:NE1	1:D:4043:GLN:OE1	2.29	0.64
1:D:4865:LYS:HZ3	1:D:4865:LYS:HB2	1.62	0.64
1:B:179:TYR:HB3	1:B:197:GLN:HB2	1.80	0.64
1:B:3767:GLN:OE1	1:B:3804:ILE:HA	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3674:ILE:CG2	1:D:3769:ARG:HD2	2.28	0.64
1:A:4844:LEU:HD12	1:A:4928:LEU:HD12	1.79	0.64
1:D:1679:ASN:ND2	1:D:1797:ARG:O	2.31	0.64
1:D:1931:LEU:HB3	1:D:1935:VAL:HB	1.80	0.64
1:A:3763:LEU:C	1:A:3763:LEU:HD13	2.18	0.64
1:A:4197:ILE:HG13	1:A:4198:SER:N	2.13	0.64
1:B:3927:GLN:NE2	1:B:3931:SER:OG	2.31	0.64
1:D:45:ARG:HG2	1:D:443:LEU:HD21	1.78	0.64
1:D:1074:ILE:HG22	1:D:1239:SER:HB2	1.80	0.64
1:D:4885:PHE:O	1:D:4889:VAL:HG12	1.98	0.64
1:C:150:MET:CE	1:C:163:VAL:HG11	2.28	0.64
1:A:4869:GLU:OE1	1:A:4869:GLU:HA	1.98	0.63
1:B:627:PRO:O	1:B:629:ARG:NH1	2.31	0.63
1:D:4959:PHE:CD2	1:D:4985:LEU:CD1	2.82	0.63
1:C:12:GLN:HG2	1:C:165:VAL:HG12	1.80	0.63
1:C:4869:GLU:O	1:C:4870:ASP:O	2.16	0.63
1:D:1724:CYS:SG	1:D:1725:ARG:N	2.70	0.63
1:C:3763:LEU:HD13	1:C:3763:LEU:C	2.19	0.63
1:A:1243:PRO:HB2	1:A:1600:LEU:HD12	1.79	0.63
1:B:34:LYS:HE2	1:B:53:SER:HA	1.79	0.63
1:C:3763:LEU:HD13	1:C:3763:LEU:O	1.97	0.63
1:D:3765:TYR:CD1	1:D:4750:ILE:HG23	2.34	0.63
1:C:3794:VAL:HG11	1:C:3835:LEU:HD21	1.79	0.63
1:C:4869:GLU:HA	1:C:4869:GLU:OE1	1.97	0.63
1:A:647:ASN:HD21	1:A:821:LEU:HA	1.63	0.63
1:B:4865:LYS:HG3	1:B:4875:LYS:CG	2.29	0.63
1:C:1708:ARG:HA	1:C:1711:TYR:HB2	1.79	0.63
1:A:4662:ASN:O	1:A:4666:VAL:HG12	1.98	0.63
1:B:567:VAL:HG13	1:B:568:LEU:HD12	1.81	0.63
1:D:1243:PRO:HB2	1:D:1600:LEU:HD12	1.80	0.63
1:C:4197:ILE:HG13	1:C:4198:SER:N	2.14	0.63
1:D:2185:ILE:O	1:D:2188:ASN:ND2	2.32	0.62
1:D:4892:ARG:HG2	1:C:4895:GLY:O	1.99	0.62
1:C:34:LYS:HE2	1:C:53:SER:HA	1.80	0.62
1:C:4958:CYS:SG	1:C:4978:HIS:CD2	2.91	0.62
1:A:3986:TRP:NE1	1:A:4043:GLN:OE1	2.32	0.62
1:A:4954:MET:HG3	2:A:5101:ACP:HI'	1.81	0.62
1:D:3830:GLN:HA	1:D:3833:GLN:HG2	1.80	0.62
1:A:4020:GLN:HA	1:A:4023:MET:HG2	1.81	0.62
1:B:221:ARG:HH22	1:B:253:CYS:HA	1.64	0.62
1:B:1679:ASN:ND2	1:B:1797:ARG:O	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1724:CYS:SG	1:B:1725:ARG:N	2.72	0.62
1:B:4034:ASN:OD1	1:B:4035:VAL:N	2.32	0.62
1:C:348:VAL:HB	1:C:357:LEU:HD22	1.81	0.62
1:A:647:ASN:ND2	1:A:820:ARG:O	2.33	0.62
1:D:4940:PHE:HE2	1:C:4935:LEU:CD2	2.10	0.62
1:A:4940:PHE:CE2	1:D:4935:LEU:HD23	2.33	0.62
1:B:647:ASN:ND2	1:B:820:ARG:O	2.32	0.62
1:D:3674:ILE:O	1:D:3769:ARG:CD	2.39	0.62
1:D:4940:PHE:CZ	1:C:4935:LEU:HD21	2.34	0.62
1:A:243:ARG:NH1	1:A:301:VAL:O	2.32	0.62
1:B:4865:LYS:HD3	1:B:4865:LYS:C	2.20	0.62
1:D:4027:LEU:HD13	1:D:4030:LEU:HD12	1.82	0.62
1:D:4832:HIS:NE2	1:D:4942:GLU:OE2	2.32	0.62
1:C:719:LEU:O	1:C:720:HIS:ND1	2.32	0.62
1:A:3767:GLN:O	1:A:3772:THR:CB	2.25	0.62
1:B:4860:ARG:HE	1:C:4582:VAL:HG11	1.64	0.62
1:D:4020:GLN:HG3	1:D:4023:MET:HE3	1.81	0.62
1:A:4779:LYS:HE2	1:A:4783:ILE:HD11	1.80	0.62
1:B:4197:ILE:HG13	1:B:4198:SER:N	2.14	0.62
1:D:660:GLY:HA3	1:D:750:LEU:HD13	1.82	0.62
1:D:4183:ILE:HD12	1:D:4193:ILE:HD12	1.82	0.61
1:D:4985:LEU:HD21	2:D:5101:ACP:N6	2.15	0.61
1:C:3986:TRP:NE1	1:C:4043:GLN:OE1	2.32	0.61
1:A:1708:ARG:HA	1:A:1711:TYR:HB2	1.82	0.61
1:D:647:ASN:HD21	1:D:821:LEU:HA	1.65	0.61
1:D:716:PHE:HE1	1:D:720:HIS:H	1.48	0.61
1:C:3766:GLN:OE1	1:C:3766:GLN:HA	2.00	0.61
1:B:3891:LEU:HB3	1:B:3899:PHE:HE2	1.65	0.61
1:D:1240:LYS:NZ	1:D:1242:LEU:O	2.31	0.61
1:A:2688:UNK:CB	1:A:2691:UNK:O	2.48	0.61
1:C:131:LEU:HD22	1:C:178:ARG:HH22	1.64	0.61
1:C:3765:TYR:CE2	1:C:3769:ARG:NH2	2.62	0.61
1:C:4067:LYS:HD2	1:C:4102:GLN:HG3	1.83	0.61
1:A:3941:ASP:HA	1:A:4002:LYS:HE3	1.82	0.61
1:D:3658:LYS:HA	1:D:3661:TRP:HZ3	1.65	0.61
1:A:348:VAL:HB	1:A:357:LEU:HD22	1.82	0.61
1:D:110:ARG:HA	1:D:117:TYR:HA	1.82	0.61
1:C:3941:ASP:HA	1:C:4002:LYS:HE3	1.83	0.61
1:A:3760:LYS:HB2	1:A:3760:LYS:HZ3	1.64	0.61
1:D:2248:ARG:HH21	1:D:3866:ILE:HA	1.65	0.61
1:D:3924:LEU:HD22	1:D:3984:ARG:HE	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4871:GLU:O	1:D:4871:GLU:CG	2.49	0.61
1:C:286:THR:HA	1:C:405:HIS:HB2	1.82	0.61
1:A:1074:ILE:HG22	1:A:1239:SER:HB2	1.82	0.61
1:A:4946:GLN:OE1	1:A:4946:GLN:HA	2.00	0.61
1:A:4995:LEU:HD21	1:A:5011:TRP:HB2	1.82	0.61
1:B:1708:ARG:HA	1:B:1711:TYR:HB2	1.83	0.61
1:C:3684:GLU:C	1:C:3686:GLU:H	2.04	0.61
1:A:4240:ASP:OD1	1:A:4668:LEU:CD2	2.48	0.61
1:B:4719:PHE:O	1:B:4723:LYS:NZ	2.34	0.61
1:A:3658:LYS:HA	1:A:3661:TRP:HZ3	1.64	0.61
1:A:4904:PRO:CG	1:A:4913:ARG:HH11	2.11	0.61
2:A:5101:ACP:H3B1	2:A:5101:ACP:O1A	2.00	0.61
1:B:181:HIS:H	1:B:193:ALA:HA	1.66	0.61
1:D:1708:ARG:HA	1:D:1711:TYR:HB2	1.81	0.61
1:C:1724:CYS:SG	1:C:1725:ARG:N	2.74	0.61
1:A:2196:ASN:OD1	1:A:2199:ARG:NH1	2.34	0.60
1:C:1387:UNK:HA	1:C:1394:UNK:HA	1.82	0.60
1:C:3737:GLU:HA	1:C:3763:LEU:HD23	1.82	0.60
1:C:4666:VAL:N	1:C:4667:PRO:HD3	2.16	0.60
1:A:4901:ILE:CB	1:A:4913:ARG:NH2	2.64	0.60
1:A:4985:LEU:CD2	2:A:5101:ACP:N6	2.62	0.60
1:A:649:PHE:HB3	1:A:776:LEU:HD13	1.83	0.60
1:A:1387:UNK:HA	1:A:1394:UNK:HA	1.84	0.60
1:C:647:ASN:ND2	1:C:820:ARG:O	2.34	0.60
1:C:4958:CYS:HA	2:C:5101:ACP:H2	1.83	0.60
1:B:2291:GLN:OE1	1:B:2294:ASP:N	2.35	0.60
1:B:3986:TRP:NE1	1:B:4043:GLN:OE1	2.35	0.60
1:B:4184:MET:HB2	1:B:4190:ILE:HG22	1.82	0.60
1:B:4801:LEU:HD21	1:B:4808:PHE:HE2	1.63	0.60
1:D:3969:ILE:HD11	1:D:3980:LEU:HD12	1.81	0.60
1:A:4034:ASN:OD1	1:A:4035:VAL:N	2.34	0.60
1:A:4832:HIS:NE2	1:A:4942:GLU:OE1	2.35	0.60
1:A:4865:LYS:HG2	1:A:4875:LYS:HG2	1.83	0.60
1:B:272:SER:HA	1:B:334:MET:HG2	1.82	0.60
1:C:1867:GLU:HA	1:C:1870:VAL:HB	1.84	0.60
1:B:2288:LEU:O	1:B:3849:ARG:NH1	2.34	0.60
1:A:567:VAL:HG13	1:A:568:LEU:HD12	1.84	0.60
1:B:348:VAL:HB	1:B:357:LEU:HD22	1.82	0.60
1:D:4940:PHE:CE2	1:C:4935:LEU:HD21	2.36	0.60
1:D:1387:UNK:HA	1:D:1394:UNK:HA	1.84	0.59
1:A:719:LEU:O	1:A:720:HIS:ND1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:644:ILE:HA	1:D:825:PRO:HA	1.84	0.59
1:C:243:ARG:NH1	1:C:301:VAL:O	2.35	0.59
1:C:647:ASN:HD21	1:C:821:LEU:HA	1.67	0.59
1:C:1679:ASN:ND2	1:C:1797:ARG:O	2.34	0.59
1:B:2248:ARG:HH21	1:B:3866:ILE:HA	1.67	0.59
1:D:647:ASN:ND2	1:D:820:ARG:O	2.36	0.59
1:C:4820:VAL:HB	1:C:4823:LEU:HD23	1.84	0.59
1:B:4801:LEU:CD2	1:B:4808:PHE:CE2	2.66	0.59
1:A:2207:VAL:HG21	1:A:2236:LEU:HD21	1.84	0.59
1:D:3767:GLN:HE21	1:D:3804:ILE:HG23	1.67	0.59
1:D:4892:ARG:NH2	1:C:4898:GLY:H	2.01	0.59
1:C:3758:MET:HE1	1:C:3762:ARG:HH21	1.68	0.59
1:A:3760:LYS:HD3	1:A:3760:LYS:C	2.22	0.59
1:D:567:VAL:HG13	1:D:568:LEU:HD12	1.85	0.59
1:D:765:GLN:O	1:D:1387:UNK:N	2.36	0.59
1:D:3674:ILE:CB	1:D:3769:ARG:HD2	2.32	0.59
1:A:3756:LYS:O	1:A:3760:LYS:N	2.31	0.59
1:B:74:SER:H	1:B:77:ALA:HB3	1.67	0.59
1:C:776:LEU:HG	1:C:848:HIS:HA	1.85	0.59
1:A:3702:VAL:HG21	1:A:3775:ALA:CB	2.33	0.58
1:A:4704:LEU:HB2	1:A:4774:LYS:HE3	1.85	0.58
1:B:1387:UNK:HA	1:B:1394:UNK:HA	1.86	0.58
1:B:3755:GLU:HA	1:B:3755:GLU:OE1	2.02	0.58
1:B:3804:ILE:O	1:B:3809:ASN:ND2	2.36	0.58
1:D:1143:TRP:HD1	1:D:1164:LEU:HD13	1.68	0.58
1:C:2248:ARG:HH21	1:C:3866:ILE:HA	1.67	0.58
1:A:4924:VAL:O	1:A:4924:VAL:HG13	2.03	0.58
1:B:286:THR:HA	1:B:405:HIS:HB2	1.85	0.58
1:D:776:LEU:HG	1:D:848:HIS:HA	1.83	0.58
1:D:4779:LYS:HE2	1:D:4783:ILE:HD11	1.84	0.58
1:D:4959:PHE:CD2	1:D:4985:LEU:HD11	2.38	0.58
1:A:645:ARG:HD3	1:A:826:ILE:HG22	1.84	0.58
1:A:3891:LEU:HB3	1:A:3899:PHE:HE2	1.68	0.58
1:B:3886:ARG:NH1	1:B:3889:GLN:OE1	2.36	0.58
1:D:4719:PHE:O	1:D:4723:LYS:NZ	2.36	0.58
1:C:315:CYS:SG	1:C:317:ARG:NH1	2.76	0.58
1:C:1931:LEU:HB3	1:C:1935:VAL:HB	1.85	0.58
1:C:4704:LEU:HB2	1:C:4774:LYS:HE3	1.86	0.58
1:D:1738:LEU:HB2	1:D:2146:PRO:HD3	1.86	0.58
1:C:2196:ASN:OD1	1:C:2199:ARG:NH1	2.35	0.58
1:A:4852:THR:HG21	1:A:4883:TYR:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4932:ILE:O	1:A:4936:ILE:CD1	2.49	0.58
1:B:315:CYS:SG	1:B:317:ARG:NH1	2.76	0.58
1:D:3667:HIS:NE2	1:D:3671:ASP:OD2	2.36	0.58
1:C:1074:ILE:HG22	1:C:1239:SER:HB2	1.85	0.58
1:C:2257:LEU:HD11	1:C:2276:ALA:HB2	1.86	0.58
1:A:1931:LEU:HB3	1:A:1935:VAL:HB	1.84	0.58
1:D:4666:VAL:N	1:D:4667:PRO:HD3	2.18	0.58
1:C:73:LEU:HD12	1:C:77:ALA:HB1	1.86	0.58
1:C:4665:LYS:C	1:C:4667:PRO:HD2	2.24	0.58
1:A:1724:CYS:SG	1:A:1725:ARG:N	2.76	0.58
1:A:2248:ARG:HH21	1:A:3866:ILE:HA	1.68	0.58
1:B:149:THR:HG23	1:B:151:HIS:HE1	1.68	0.58
1:B:3662:ILE:O	1:B:3662:ILE:HG23	2.03	0.58
1:B:4978:HIS:ND1	1:B:4982:GLU:OE1	2.37	0.58
1:D:315:CYS:SG	1:D:317:ARG:NH1	2.76	0.58
1:D:4820:VAL:HG12	1:D:4823:LEU:HB2	1.85	0.58
1:A:3763:LEU:HD13	1:A:3763:LEU:O	2.04	0.58
1:D:4665:LYS:C	1:D:4667:PRO:HD2	2.24	0.58
1:A:272:SER:HB2	1:A:334:MET:HA	1.84	0.58
1:A:644:ILE:HA	1:A:825:PRO:HA	1.86	0.58
1:D:34:LYS:HE2	1:D:53:SER:HA	1.85	0.58
1:D:294:THR:HG23	1:D:295:GLU:H	1.68	0.58
1:C:4673:ARG:NH1	1:C:4702:ASP:OD2	2.37	0.58
1:B:262:LEU:HB2	1:B:280:LEU:HD23	1.86	0.58
1:D:3941:ASP:HA	1:D:4002:LYS:HE3	1.86	0.58
1:A:315:CYS:SG	1:A:317:ARG:NH1	2.77	0.57
1:A:2358:ILE:HA	1:A:2364:PHE:HZ	1.68	0.57
1:D:12:GLN:HG2	1:D:165:VAL:HG12	1.85	0.57
1:D:2810:LYS:HG2	1:D:2814:LYS:HE3	1.86	0.57
1:B:1738:LEU:HB2	1:B:2146:PRO:HD3	1.84	0.57
1:B:3955:MET:HG3	1:B:4019:LEU:HD22	1.86	0.57
1:C:3891:LEU:HB3	1:C:3899:PHE:HE2	1.67	0.57
1:C:4719:PHE:O	1:C:4723:LYS:NZ	2.37	0.57
1:A:34:LYS:HE2	1:A:53:SER:HA	1.85	0.57
1:B:4872:PRO:HD2	1:B:4873:ASP:N	2.19	0.57
1:C:765:GLN:O	1:C:1387:UNK:N	2.38	0.57
1:C:2185:ILE:O	1:C:2188:ASN:ND2	2.37	0.57
1:A:1238:PHE:HE1	1:A:1608:MET:HB3	1.68	0.57
1:A:3955:MET:HG3	1:A:4019:LEU:HD22	1.86	0.57
1:B:45:ARG:HG2	1:B:443:LEU:HD21	1.84	0.57
1:C:109:LEU:HD23	1:C:148:TRP:HD1	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:MET:HE2	1:C:163:VAL:HG11	1.85	0.57
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.85	0.57
1:A:509:GLU:O	1:A:510:GLU:HG3	2.05	0.57
1:B:2869:ARG:NH1	1:B:3106:UNK:O	2.37	0.57
1:B:4690:GLU:HG2	1:B:4691:GLN:N	2.20	0.57
1:C:3765:TYR:HE1	1:C:4750:ILE:HD12	1.66	0.57
1:A:1143:TRP:HD1	1:A:1164:LEU:HD13	1.68	0.57
1:C:116:MET:HG3	1:C:137:LEU:HD12	1.87	0.57
1:C:272:SER:HA	1:C:334:MET:HG2	1.86	0.57
1:A:2773:ASN:O	1:A:2773:ASN:ND2	2.37	0.57
1:A:3770:LEU:HD23	1:A:3770:LEU:O	2.05	0.57
1:A:4940:PHE:CE2	1:D:4935:LEU:HD21	2.40	0.57
1:B:243:ARG:NH1	1:B:301:VAL:O	2.38	0.57
1:B:4795:TYR:HD1	1:B:4795:TYR:O	1.88	0.57
1:D:3828:PHE:CZ	1:D:3832:ILE:HD11	2.39	0.57
1:B:2257:LEU:HD11	1:B:2276:ALA:HB2	1.87	0.57
1:B:4016:LEU:HD23	1:B:4020:GLN:NE2	2.13	0.57
1:B:4673:ARG:NH1	1:B:4702:ASP:OD2	2.38	0.57
1:C:45:ARG:HG2	1:C:443:LEU:HD21	1.86	0.57
1:C:1101:ARG:HE	1:C:1115:LEU:HD12	1.69	0.57
1:A:4719:PHE:O	1:A:4723:LYS:NZ	2.37	0.57
1:D:3765:TYR:CE1	1:D:4750:ILE:CG2	2.87	0.57
1:D:3891:LEU:HB3	1:D:3899:PHE:HE2	1.69	0.57
1:A:3924:LEU:O	1:A:3927:GLN:HG3	2.04	0.57
1:A:4633:GLU:HA	1:A:4639:MET:HG3	1.87	0.57
1:B:788:LYS:HD3	1:B:1629:GLN:HA	1.85	0.56
1:B:1229:ASN:HD21	1:B:1827:ARG:HD3	1.69	0.56
1:B:4037:ASN:HD22	1:B:5035:GLN:HE21	1.51	0.56
1:D:4940:PHE:CE2	1:C:4935:LEU:HD23	2.40	0.56
1:C:3984:ARG:HG2	1:C:3987:ASP:HB2	1.86	0.56
1:A:4993:MET:SD	1:A:4997:ASN:ND2	2.77	0.56
1:B:670:GLU:HG3	1:B:788:LYS:H	1.70	0.56
1:B:2291:GLN:HG3	1:B:2292:GLU:H	1.70	0.56
1:D:4197:ILE:HG13	1:D:4198:SER:H	1.70	0.56
1:A:78:LEU:HD21	1:A:147:TRP:CE2	2.40	0.56
1:A:2288:LEU:O	1:A:3849:ARG:NH1	2.34	0.56
1:A:4244:GLU:HG2	1:A:4668:LEU:HD11	1.87	0.56
1:A:4690:GLU:HG2	1:A:4691:GLN:N	2.20	0.56
1:B:666:VAL:HB	1:B:744:VAL:HB	1.87	0.56
1:B:1243:PRO:HB2	1:B:1600:LEU:HD12	1.87	0.56
1:B:4047:MET:SD	1:B:4048:LEU:HD22	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:MET:HG2	1:D:137:LEU:HD13	1.85	0.56
1:C:262:LEU:HB2	1:C:280:LEU:HD23	1.87	0.56
1:C:1735:ILE:HG22	1:C:2142:TYR:HB3	1.86	0.56
1:C:2869:ARG:NH1	1:C:3106:UNK:O	2.36	0.56
1:C:3804:ILE:HG23	1:C:3805:LEU:HD12	1.87	0.56
1:B:4016:LEU:O	1:B:4020:GLN:NE2	2.37	0.56
1:B:4866:SER:C	1:B:4867:GLU:CG	2.64	0.56
1:D:1124:PHE:HE1	1:D:1139:PHE:HB3	1.70	0.56
1:A:627:PRO:O	1:A:629:ARG:NH1	2.39	0.56
1:A:4940:PHE:CZ	1:D:4935:LEU:HD21	2.41	0.56
1:D:220:LEU:HD22	1:D:262:LEU:HD23	1.87	0.56
1:D:3674:ILE:HG23	1:D:3769:ARG:HD2	1.88	0.56
1:C:179:TYR:HB3	1:C:197:GLN:HB2	1.87	0.56
1:C:1240:LYS:NZ	1:C:1242:LEU:O	2.31	0.56
1:B:3751:VAL:O	1:B:3752:SER:C	2.41	0.56
1:D:1101:ARG:HE	1:D:1115:LEU:HD12	1.71	0.56
1:D:4690:GLU:HG2	1:D:4691:GLN:N	2.21	0.56
1:D:4704:LEU:HB2	1:D:4774:LYS:HE3	1.88	0.56
1:C:1866:ILE:HG22	1:C:1870:VAL:HG23	1.88	0.56
1:D:1106:ARG:NH2	1:D:1183:GLU:OE2	2.38	0.56
1:C:103:TYR:OH	1:C:157:ARG:HG2	2.06	0.56
1:C:2763:HIS:NE2	1:C:2792:ARG:O	2.34	0.56
1:C:4690:GLU:HG2	1:C:4691:GLN:N	2.20	0.56
1:A:1580:PHE:HE2	1:A:1592:PRO:HG2	1.71	0.56
1:A:2257:LEU:HD11	1:A:2276:ALA:HB2	1.87	0.56
1:D:4959:PHE:CD2	1:D:4985:LEU:HD13	2.41	0.56
1:C:216:GLY:HA2	1:C:262:LEU:HD11	1.87	0.56
1:C:1703:LEU:HB2	1:C:1707:LEU:HB3	1.88	0.56
1:D:4219:PHE:O	1:D:4223:ASN:ND2	2.38	0.56
1:C:841:GLY:HA2	1:C:1073:ARG:HD2	1.88	0.56
1:C:4223:ASN:ND2	1:C:4946:GLN:OE1	2.39	0.56
1:A:116:MET:HG3	1:A:137:LEU:HD12	1.88	0.55
1:D:4979:THR:HG21	2:D:5101:ACP:H2'	1.88	0.55
1:C:1238:PHE:HE1	1:C:1608:MET:HB3	1.72	0.55
1:C:4067:LYS:O	1:C:4071:ILE:HG12	2.06	0.55
1:A:294:THR:HG23	1:A:295:GLU:H	1.71	0.55
1:A:682:LEU:HD13	1:A:787:VAL:HG11	1.88	0.55
1:A:742:ASP:HB3	1:A:759:ILE:HD11	1.89	0.55
1:B:647:ASN:HD21	1:B:821:LEU:HA	1.70	0.55
1:C:4017:LEU:HD13	1:C:4020:GLN:NE2	2.21	0.55
1:A:131:LEU:HD22	1:A:178:ARG:HH22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4795:TYR:CD1	1:B:4795:TYR:O	2.59	0.55
1:C:3955:MET:HG3	1:C:4019:LEU:HD22	1.88	0.55
1:B:1676:LEU:HD13	1:B:2168:VAL:HG22	1.88	0.55
1:B:3828:PHE:CZ	1:B:3832:ILE:HD11	2.42	0.55
1:D:728:ARG:NH1	1:D:1384:UNK:O	2.39	0.55
1:A:1735:ILE:HG22	1:A:2142:TYR:HB3	1.88	0.55
1:B:4872:PRO:HD2	1:B:4873:ASP:H	1.72	0.55
1:D:665:GLU:HB3	1:D:792:LEU:HD12	1.88	0.55
1:D:1851:MET:HB2	1:D:1853:ILE:HG12	1.89	0.55
1:C:627:PRO:O	1:C:629:ARG:NH1	2.40	0.55
1:C:4666:VAL:O	1:C:4666:VAL:HG12	2.07	0.55
1:A:445:LEU:HD13	1:A:521:LEU:HB3	1.88	0.55
1:A:765:GLN:O	1:A:1387:UNK:N	2.40	0.55
1:B:195:PHE:O	1:C:2359:ARG:NH1	2.37	0.55
1:B:294:THR:HG23	1:B:295:GLU:H	1.72	0.55
1:D:4936:ILE:HD13	1:D:4936:ILE:N	2.20	0.55
1:A:728:ARG:NH1	1:A:1384:UNK:O	2.40	0.55
1:A:3776:ALA:O	1:A:3778:MET:N	2.40	0.55
1:A:4895:GLY:O	1:B:4892:ARG:NE	2.39	0.55
1:B:4849:TYR:HB2	1:B:4883:TYR:HE1	1.71	0.55
1:D:262:LEU:HB2	1:D:280:LEU:HD23	1.88	0.55
1:D:4673:ARG:NH1	1:D:4702:ASP:OD2	2.38	0.55
1:B:3813:GLN:OE1	1:B:3896:ASN:ND2	2.40	0.55
1:D:1992:ALA:O	1:D:1996:ARG:NH1	2.39	0.55
1:D:2423:MET:HE1	1:D:2494:UNK:HA	1.88	0.55
1:C:1143:TRP:HD1	1:C:1164:LEU:HD13	1.72	0.55
1:C:1950:GLU:OE2	1:C:2041:HIS:NE2	2.40	0.55
1:A:2869:ARG:NH1	1:A:3106:UNK:O	2.35	0.54
1:A:3544:UNK:O	1:A:3551:UNK:CB	2.55	0.54
1:B:4197:ILE:HG21	1:B:4990:PHE:HB3	1.87	0.54
1:D:2763:HIS:NE2	1:D:2792:ARG:O	2.33	0.54
1:C:615:ARG:NH1	1:C:1677:GLY:O	2.38	0.54
1:C:666:VAL:HB	1:C:744:VAL:HG23	1.89	0.54
1:C:3758:MET:CE	1:C:3762:ARG:HH21	2.21	0.54
1:A:73:LEU:HD12	1:A:77:ALA:HB1	1.89	0.54
1:A:3804:ILE:O	1:A:3809:ASN:OD1	2.25	0.54
1:B:841:GLY:HA2	1:B:1073:ARG:HD2	1.89	0.54
1:C:100:THR:CG2	1:C:162:LYS:HE3	2.26	0.54
1:A:4936:ILE:HD12	1:A:4936:ILE:H	1.72	0.54
1:D:670:GLU:HG3	1:D:787:VAL:HA	1.89	0.54
1:D:1950:GLU:OE2	1:D:2041:HIS:NE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3886:ARG:NH1	1:C:3889:GLN:OE1	2.40	0.54
1:A:286:THR:HA	1:A:405:HIS:HB2	1.89	0.54
1:B:4864:ASN:HA	1:B:4874:MET:CE	2.37	0.54
1:D:4066:LEU:HD21	1:D:4173:TYR:CZ	2.43	0.54
1:B:151:HIS:HB2	1:B:170:ILE:HB	1.89	0.54
1:D:4182:GLU:OE2	1:D:4192:ARG:NE	2.31	0.54
1:C:294:THR:HG23	1:C:295:GLU:H	1.73	0.54
1:A:3758:MET:HG3	1:A:3759:GLU:N	2.22	0.54
1:A:4859:PHE:N	1:A:4859:PHE:CD1	2.73	0.54
1:B:4067:LYS:HD2	1:B:4102:GLN:HG3	1.89	0.54
1:C:4851:TYR:HD2	1:C:4920:PHE:HD1	1.56	0.54
1:B:759:ILE:HG13	1:B:760:ASN:H	1.73	0.54
1:C:232:THR:HG21	1:C:252:VAL:HG11	1.88	0.54
1:C:644:ILE:HA	1:C:825:PRO:HA	1.90	0.54
1:A:4673:ARG:NH1	1:A:4702:ASP:OD2	2.39	0.54
1:D:3674:ILE:HG23	1:D:3769:ARG:CD	2.37	0.54
1:D:4940:PHE:CZ	1:C:4935:LEU:CD2	2.90	0.54
1:B:4924:VAL:HA	1:B:4928:LEU:HD23	1.90	0.54
1:D:668:VAL:HG23	1:D:740:PRO:HA	1.90	0.54
1:D:786:GLY:HA2	1:D:1631:GLN:HA	1.89	0.54
1:B:2904:LEU:HD21	1:B:2912:THR:HG23	1.90	0.54
1:D:2904:LEU:HD21	1:D:2912:THR:HG23	1.90	0.54
1:C:445:LEU:HD13	1:C:521:LEU:HB3	1.89	0.54
1:C:546:TRP:O	1:C:550:LYS:NZ	2.41	0.54
1:C:4779:LYS:HE2	1:C:4783:ILE:HD11	1.90	0.54
1:A:2185:ILE:O	1:A:2188:ASN:ND2	2.41	0.53
1:A:4898:GLY:N	1:B:4892:ARG:HH22	2.04	0.53
1:D:14:LEU:HB3	1:D:101:LEU:HD12	1.90	0.53
1:C:1676:LEU:HD13	1:C:2168:VAL:HG22	1.90	0.53
1:B:665:GLU:HB2	1:B:792:LEU:HB2	1.90	0.53
1:B:786:GLY:HA2	1:B:1631:GLN:HA	1.91	0.53
1:D:109:LEU:HD23	1:D:148:TRP:HD1	1.73	0.53
1:C:786:GLY:HA2	1:C:1631:GLN:HA	1.90	0.53
1:B:3773:ARG:HA	1:B:3815:LYS:HE3	1.90	0.53
1:B:4180:ARG:HG3	1:B:4194:TYR:CE1	2.42	0.53
1:A:14:LEU:HB3	1:A:101:LEU:HD12	1.89	0.53
1:A:4940:PHE:CZ	1:D:4935:LEU:CD2	2.92	0.53
1:B:509:GLU:O	1:B:510:GLU:HG3	2.09	0.53
1:B:3963:ASN:O	1:B:3966:THR:OG1	2.26	0.53
1:D:120:CYS:SG	1:D:175:SER:OG	2.66	0.53
1:D:1697:ALA:HB1	1:D:1708:ARG:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:ARG:HH21	1:C:208:CYS:HB3	1.73	0.53
1:A:3779:VAL:HG23	1:A:3797:THR:HG22	1.90	0.53
1:B:2199:ARG:NE	1:B:2246:ASN:OD1	2.40	0.53
1:B:3794:VAL:HG21	1:B:3835:LEU:HD11	1.90	0.53
1:B:4577:LEU:CD2	1:B:4807:PHE:HE1	2.19	0.53
1:D:4666:VAL:O	1:D:4666:VAL:HG12	2.07	0.53
1:D:4865:LYS:O	1:D:4865:LYS:HG3	2.07	0.53
1:D:4895:GLY:HA2	1:D:4921:PHE:CE1	2.43	0.53
1:A:3840:SER:OG	1:A:3877:ASP:OD2	2.26	0.53
1:B:4869:GLU:OE2	1:B:4870:ASP:N	2.41	0.53
1:B:4913:ARG:NH1	1:C:4888:TYR:OH	2.42	0.53
1:D:1240:LYS:NZ	1:D:1242:LEU:HB3	2.23	0.53
1:C:1738:LEU:HB2	1:C:2146:PRO:HD3	1.89	0.53
1:C:4874:MET:O	1:C:4876:CYS:N	2.42	0.53
1:C:4958:CYS:O	2:C:5101:ACP:N1	2.42	0.53
1:A:2904:LEU:HD21	1:A:2912:THR:HG23	1.91	0.53
1:B:36:CYS:HB3	1:B:50:GLU:HB3	1.90	0.53
1:B:2185:ILE:O	1:B:2188:ASN:ND2	2.41	0.53
1:C:1106:ARG:NH2	1:C:1183:GLU:OE2	2.41	0.53
1:C:2368:LEU:HD22	1:C:2376:LEU:HD21	1.91	0.53
1:C:665:GLU:HB3	1:C:792:LEU:HD12	1.91	0.53
1:C:788:LYS:HD3	1:C:1629:GLN:HA	1.91	0.53
1:C:3684:GLU:C	1:C:3686:GLU:N	2.63	0.53
1:A:4936:ILE:CD1	1:A:4936:ILE:H	2.21	0.53
1:B:1992:ALA:O	1:B:1996:ARG:NH1	2.42	0.53
1:D:4892:ARG:NH2	1:C:4896:GLY:HA3	2.24	0.53
1:D:4940:PHE:HE2	1:C:4935:LEU:HD22	1.74	0.53
1:C:617:ASN:OD1	1:C:618:GLN:N	2.42	0.53
1:C:1124:PHE:HE1	1:C:1139:PHE:HB3	1.73	0.53
1:C:2288:LEU:HD12	1:C:3853:ALA:HB2	1.91	0.53
1:A:3760:LYS:O	1:A:3763:LEU:HB3	2.09	0.53
1:A:4063:ASP:OD2	1:A:4067:LYS:NZ	2.39	0.53
1:B:2809:ILE:HD11	1:B:2926:LEU:HD13	1.91	0.53
1:B:3663:LEU:N	1:B:3663:LEU:CD1	2.72	0.53
1:D:2156:LEU:HD12	1:D:2159:LEU:HD11	1.91	0.53
1:D:4639:MET:SD	1:D:4639:MET:N	2.80	0.53
1:B:220:LEU:HD12	1:B:390:LEU:HB3	1.91	0.52
1:B:560:ILE:HA	1:B:563:VAL:HG12	1.90	0.52
1:B:765:GLN:O	1:B:1387:UNK:N	2.42	0.52
1:B:1867:GLU:HA	1:B:1870:VAL:HB	1.90	0.52
1:B:2288:LEU:HD12	1:B:3853:ALA:HB2	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1950:GLU:OE2	1:A:2041:HIS:NE2	2.42	0.52
1:A:2785:LEU:HB3	1:A:2787:THR:HG22	1.92	0.52
1:D:4928:LEU:CD2	1:D:4928:LEU:N	2.72	0.52
1:A:4731:ILE:HA	1:B:4101:LYS:HG3	1.91	0.52
1:D:627:PRO:O	1:D:629:ARG:NH1	2.43	0.52
1:D:4865:LYS:NZ	1:D:4865:LYS:CB	2.72	0.52
1:C:157:ARG:HA	1:C:161:GLU:OE1	2.08	0.52
1:D:1143:TRP:CD1	1:D:1164:LEU:HD13	2.44	0.52
1:C:479:GLN:HE22	1:C:536:ASN:HA	1.74	0.52
1:C:670:GLU:OE2	1:C:788:LYS:HB2	2.10	0.52
1:C:1867:GLU:O	1:C:1871:PHE:N	2.34	0.52
1:A:1738:LEU:HB2	1:A:2146:PRO:HD3	1.91	0.52
1:A:4662:ASN:O	1:A:4666:VAL:CG1	2.57	0.52
1:B:1697:ALA:HB1	1:B:1708:ARG:HD3	1.90	0.52
1:B:4238:CYS:O	1:B:4242:ILE:HG12	2.09	0.52
1:D:2288:LEU:HD12	1:D:3853:ALA:HB2	1.91	0.52
1:C:103:TYR:CZ	1:C:163:VAL:HG13	2.44	0.52
1:C:181:HIS:H	1:C:193:ALA:HA	1.74	0.52
1:C:652:ARG:HD2	1:C:750:LEU:HB3	1.92	0.52
1:B:4731:ILE:HA	1:C:4101:LYS:HG3	1.92	0.52
1:D:682:LEU:HD13	1:D:787:VAL:HG11	1.92	0.52
1:D:1676:LEU:HD13	1:D:2168:VAL:HG22	1.92	0.52
1:D:1697:ALA:HB1	1:D:1708:ARG:HH11	1.74	0.52
1:C:2904:LEU:HD21	1:C:2912:THR:HG23	1.91	0.52
1:A:3760:LYS:NZ	1:A:3760:LYS:CB	2.72	0.52
1:A:4066:LEU:HD21	1:A:4173:TYR:CZ	2.45	0.52
1:A:4933:GLN:O	1:A:4937:ILE:HG12	2.09	0.52
1:A:4940:PHE:HE2	1:D:4935:LEU:CD2	2.17	0.52
1:B:1950:GLU:OE2	1:B:2041:HIS:NE2	2.42	0.52
1:B:4985:LEU:HB2	2:B:5101:ACP:N1	2.25	0.52
1:C:3684:GLU:O	1:C:3686:GLU:N	2.43	0.52
1:C:4937:ILE:N	1:C:4937:ILE:CD1	2.73	0.52
1:A:1101:ARG:HE	1:A:1115:LEU:HD12	1.75	0.52
1:B:449:ILE:HG13	1:B:525:LEU:HD12	1.91	0.52
1:B:2785:LEU:HB3	1:B:2787:THR:HG22	1.92	0.52
1:D:181:HIS:H	1:D:193:ALA:HA	1.75	0.52
1:D:4920:PHE:O	1:D:4924:VAL:HG12	2.10	0.52
1:B:445:LEU:HD13	1:B:521:LEU:HB3	1.92	0.52
1:D:4063:ASP:OD2	1:D:4067:LYS:NZ	2.41	0.52
1:C:728:ARG:NH1	1:C:1384:UNK:O	2.43	0.52
1:C:1237:TRP:HH2	1:C:1652:GLU:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2785:LEU:HB3	1:C:2787:THR:HG22	1.92	0.52
1:A:617:ASN:OD1	1:A:618:GLN:N	2.43	0.52
1:A:3760:LYS:NZ	1:A:3760:LYS:CA	2.71	0.52
1:A:4933:GLN:NE2	1:D:4930:ALA:HA	2.25	0.52
1:B:617:ASN:OD1	1:B:618:GLN:N	2.43	0.52
1:D:3754:GLU:HA	1:D:3754:GLU:OE2	2.10	0.52
1:D:4864:ASN:OD1	1:D:4871:GLU:OE1	2.28	0.52
1:C:3667:HIS:NE2	1:C:3671:ASP:OD2	2.43	0.52
1:A:45:ARG:HG2	1:A:443:LEU:HD21	1.92	0.51
1:A:1697:ALA:HB1	1:A:1708:ARG:HD3	1.92	0.51
1:B:220:LEU:HD22	1:B:262:LEU:HD23	1.92	0.51
1:B:1927:LEU:HD13	1:B:2101:MET:HG3	1.91	0.51
1:B:4003:LEU:HD11	1:B:4009:GLN:HG2	1.92	0.51
1:C:2337:PHE:HA	1:C:2340:PHE:HB2	1.91	0.51
1:C:4207:MET:HE3	1:C:4210:VAL:HG23	1.91	0.51
1:B:1839:VAL:HG13	1:B:1841:VAL:HG22	1.93	0.51
1:D:197:GLN:NE2	1:D:198:THR:O	2.43	0.51
1:D:666:VAL:HB	1:D:744:VAL:HB	1.91	0.51
1:D:2881:ASN:HA	1:D:2884:ASN:HD21	1.75	0.51
1:C:509:GLU:O	1:C:510:GLU:HG3	2.10	0.51
1:C:3758:MET:HE3	1:C:3762:ARG:NH2	2.24	0.51
1:B:3716:LEU:HD23	1:B:3793:MET:HG3	1.92	0.51
1:B:3770:LEU:HD13	1:B:3804:ILE:HD11	1.91	0.51
1:C:4698:LYS:HE3	1:C:4785:THR:HB	1.93	0.51
1:C:4936:ILE:N	1:C:4936:ILE:CD1	2.73	0.51
1:A:2763:HIS:NE2	1:A:2792:ARG:O	2.34	0.51
1:B:1101:ARG:HE	1:B:1115:LEU:HD12	1.76	0.51
1:B:4801:LEU:HD23	1:B:4808:PHE:CD2	2.43	0.51
1:D:617:ASN:OD1	1:D:618:GLN:N	2.43	0.51
1:D:1126:GLY:HA3	1:D:1143:TRP:CZ3	2.45	0.51
1:D:3906:GLN:HE22	1:D:3913:ILE:HB	1.75	0.51
1:C:24:CYS:HB3	1:C:200:TRP:CE3	2.46	0.51
1:C:1240:LYS:NZ	1:C:1242:LEU:HB3	2.26	0.51
1:C:3787:LYS:N	1:C:3787:LYS:HD2	2.25	0.51
1:B:4689:THR:HA	1:B:4732:PHE:HE2	1.75	0.51
1:D:1960:ALA:O	1:D:1963:GLU:HG3	2.10	0.51
1:D:2785:LEU:HB3	1:D:2787:THR:HG22	1.92	0.51
1:C:1126:GLY:HA3	1:C:1143:TRP:CZ3	2.46	0.51
1:A:841:GLY:HA2	1:A:1073:ARG:HD2	1.93	0.51
1:A:2368:LEU:HD22	1:A:2376:LEU:HD21	1.92	0.51
1:B:4865:LYS:HG3	1:B:4875:LYS:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4639:MET:HB2	1:D:4642:ALA:HB3	1.91	0.51
1:C:102:LEU:HD13	1:C:160:GLY:HA2	1.93	0.51
1:C:157:ARG:NH2	1:C:164:ARG:NH2	2.59	0.51
1:A:4860:ARG:NH1	1:A:4860:ARG:CG	2.73	0.51
1:A:4921:PHE:CD2	1:B:4892:ARG:HD2	2.46	0.51
1:B:682:LEU:HD13	1:B:787:VAL:HG11	1.93	0.51
1:D:348:VAL:HB	1:D:357:LEU:HD22	1.91	0.51
1:D:4865:LYS:HG2	1:D:4875:LYS:HG2	1.92	0.51
1:C:102:LEU:HB2	1:C:161:GLU:O	2.11	0.51
1:A:2022:PRO:HB2	1:A:2024:PRO:HD2	1.93	0.51
1:A:2359:ARG:NH1	1:D:195:PHE:O	2.37	0.51
1:A:3753:PHE:C	1:A:3753:PHE:CD2	2.84	0.51
1:A:4584:ASP:HA	1:A:4627:MET:HA	1.93	0.51
1:A:4936:ILE:N	1:A:4936:ILE:CD1	2.73	0.51
1:B:1685:LEU:HD23	1:B:1718:ILE:HD12	1.91	0.51
1:B:4573:ILE:HD11	1:B:4809:PHE:CE2	2.40	0.51
1:C:36:CYS:HB3	1:C:50:GLU:HB3	1.91	0.51
1:C:1076:ARG:HD3	1:C:1109:LEU:HD12	1.92	0.51
1:A:776:LEU:HG	1:A:848:HIS:HA	1.93	0.51
1:A:2688:UNK:O	1:A:2691:UNK:C	2.58	0.51
1:A:2881:ASN:HA	1:A:2884:ASN:HD21	1.76	0.51
1:A:4689:THR:HA	1:A:4732:PHE:HE2	1.75	0.51
1:B:2881:ASN:HA	1:B:2884:ASN:HD21	1.76	0.51
1:D:3751:VAL:O	1:D:3751:VAL:HG23	2.10	0.51
1:D:4865:LYS:NZ	1:D:4865:LYS:CA	2.72	0.51
1:C:682:LEU:HD13	1:C:787:VAL:HG11	1.93	0.51
1:A:414:PHE:HE1	1:A:436:LEU:HD12	1.75	0.50
1:B:69:LEU:HB3	1:B:107:ILE:HD11	1.92	0.50
1:B:76:ARG:O	1:B:79:GLN:HG2	2.11	0.50
1:B:1947:CYS:SG	1:B:2126:ARG:NH2	2.77	0.50
1:B:3984:ARG:HG2	1:B:3987:ASP:HB2	1.91	0.50
1:B:4935:LEU:CD2	1:C:4940:PHE:CE2	2.79	0.50
1:D:3769:ARG:O	1:D:3771:HIS:ND1	2.45	0.50
1:C:2358:ILE:HA	1:C:2364:PHE:HZ	1.75	0.50
1:C:2871:LEU:HD12	1:C:2927:LEU:HD21	1.93	0.50
1:C:3758:MET:CE	1:C:3762:ARG:NH2	2.74	0.50
1:A:455:PRO:HG3	1:A:467:LYS:HB3	1.92	0.50
1:A:687:ALA:HB3	1:A:778:PHE:HB2	1.94	0.50
1:A:1075:PHE:HB2	1:A:1192:CYS:SG	2.51	0.50
1:A:2288:LEU:HD12	1:A:3853:ALA:HB2	1.93	0.50
1:B:710:ASP:OD1	1:B:713:SER:OG	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4141:PHE:CZ	1:B:4196:GLU:HB3	2.46	0.50
1:D:1703:LEU:HB2	1:D:1707:LEU:HB3	1.92	0.50
1:D:2924:GLN:O	1:D:2928:LYS:HG2	2.10	0.50
1:D:4181:ILE:HG12	1:D:4195:PHE:HE1	1.77	0.50
1:A:149:THR:HG23	1:A:151:HIS:CE1	2.46	0.50
1:A:4001:MET:O	1:A:4005:GLN:NE2	2.44	0.50
1:B:1840:PRO:HB3	1:B:1843:LYS:HD3	1.93	0.50
1:D:1698:LEU:HD23	1:D:1810:LYS:HD2	1.93	0.50
1:D:4026:MET:O	1:D:4030:LEU:HG	2.11	0.50
1:D:4661:TYR:O	1:D:4666:VAL:HG23	2.11	0.50
1:D:4888:TYR:OH	1:C:4913:ARG:NH1	2.43	0.50
1:C:1574:PRO:HD2	1:C:1577:ALA:HB2	1.94	0.50
1:C:3965:LEU:O	1:C:3968:TYR:HD1	1.94	0.50
1:B:2810:LYS:HG2	1:B:2814:LYS:HE3	1.93	0.50
1:D:102:LEU:HD13	1:D:160:GLY:HA2	1.93	0.50
1:D:4640:GLU:HB2	1:D:4641:PRO:HD3	1.92	0.50
1:D:4690:GLU:HG2	1:D:4691:GLN:H	1.77	0.50
1:C:3751:VAL:CG2	1:C:3755:GLU:HB3	2.40	0.50
1:C:3773:ARG:HA	1:C:3815:LYS:HE3	1.92	0.50
1:C:3999:MET:HB2	1:C:4003:LEU:HD13	1.94	0.50
1:A:4921:PHE:CD1	1:A:4921:PHE:C	2.85	0.50
1:B:1960:ALA:O	1:B:1963:GLU:HG3	2.12	0.50
1:C:2881:ASN:HA	1:C:2884:ASN:HD21	1.76	0.50
1:C:3889:GLN:HB2	1:C:3964:SER:HA	1.94	0.50
1:C:3927:GLN:NE2	1:C:3931:SER:OG	2.44	0.50
1:A:1851:MET:HB2	1:A:1853:ILE:HG12	1.94	0.50
1:A:4582:VAL:HG11	1:D:4860:ARG:HE	1.76	0.50
1:B:776:LEU:HG	1:B:848:HIS:HA	1.93	0.50
1:B:2022:PRO:HB2	1:B:2024:PRO:HD2	1.94	0.50
1:B:3760:LYS:HD2	1:B:3760:LYS:C	2.31	0.50
1:B:4985:LEU:HD23	1:B:4985:LEU:O	2.12	0.50
1:D:4823:LEU:HD22	1:C:4839:MET:HE3	1.93	0.50
1:D:4865:LYS:C	1:D:4865:LYS:HD3	2.32	0.50
1:C:2113:SER:O	1:C:2113:SER:OG	2.29	0.50
1:B:2165:LEU:HD13	1:B:2178:MET:HB3	1.94	0.50
1:D:560:ILE:HA	1:D:563:VAL:HG12	1.93	0.50
1:D:3840:SER:OG	1:D:3877:ASP:OD2	2.30	0.50
1:D:3888:LEU:HD13	1:D:3891:LEU:HD12	1.94	0.50
1:D:4698:LYS:HE3	1:D:4785:THR:HB	1.93	0.50
1:C:2107:GLN:NE2	1:C:3681:GLY:CA	2.69	0.50
1:C:2812:SER:HB2	1:C:2926:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:710:ASP:OD1	1:D:713:SER:OG	2.26	0.50
1:A:1676:LEU:HD22	1:A:2167:ILE:HG22	1.94	0.50
1:A:1698:LEU:HD23	1:A:1810:LYS:HD2	1.94	0.50
1:A:3702:VAL:HG11	1:A:3775:ALA:HB2	1.89	0.50
1:A:4011:GLU:HG2	1:A:4012:LEU:HD12	1.92	0.50
1:A:4240:ASP:OD2	1:A:4668:LEU:HD21	2.12	0.50
1:B:1075:PHE:HB2	1:B:1192:CYS:SG	2.52	0.50
1:B:3804:ILE:HG22	1:B:3805:LEU:HD12	1.94	0.50
1:D:686:TRP:CZ3	1:D:777:PHE:HB3	2.47	0.50
1:D:1867:GLU:HA	1:D:1870:VAL:HB	1.92	0.50
1:A:1106:ARG:NH2	1:A:1183:GLU:OE2	2.44	0.49
1:A:1676:LEU:HD13	1:A:2168:VAL:HG22	1.94	0.49
1:B:299:LEU:HG	1:B:378:LEU:HG	1.94	0.49
1:B:2248:ARG:NH2	1:B:3865:VAL:O	2.45	0.49
1:B:2871:LEU:HD12	1:B:2927:LEU:HD21	1.94	0.49
1:D:1166:GLY:HA3	1:D:1216:ILE:HD13	1.93	0.49
1:D:4223:ASN:OD1	1:D:4946:GLN:NE2	2.42	0.49
1:A:109:LEU:HD23	1:A:148:TRP:HD1	1.76	0.49
1:A:197:GLN:NE2	1:A:198:THR:O	2.44	0.49
1:B:3787:LYS:NZ	1:B:3830:GLN:HG3	2.27	0.49
1:B:4865:LYS:CB	1:B:4875:LYS:CG	2.88	0.49
1:D:214:VAL:HG22	1:D:341:TYR:HE1	1.77	0.49
1:D:1667:LEU:HD21	1:D:1710:GLY:HA3	1.93	0.49
1:D:3761:GLN:HA	1:D:3761:GLN:HE21	1.72	0.49
1:C:1143:TRP:CD1	1:C:1164:LEU:HD13	2.47	0.49
1:C:4892:ARG:O	1:C:4892:ARG:CG	2.60	0.49
1:A:4574:ASN:HD22	1:A:4813:LEU:HD13	1.77	0.49
1:A:4927:ILE:N	1:A:4927:ILE:CD1	2.75	0.49
1:B:2192:TYR:HD1	1:B:2242:ILE:HD13	1.77	0.49
1:B:4849:TYR:OH	1:C:4574:ASN:ND2	2.46	0.49
1:D:719:LEU:HD12	1:D:719:LEU:O	2.13	0.49
1:D:841:GLY:HA2	1:D:1073:ARG:HD2	1.93	0.49
1:D:3767:GLN:NE2	1:D:3804:ILE:HD12	2.27	0.49
1:D:3927:GLN:NE2	1:D:3931:SER:OG	2.44	0.49
1:C:4690:GLU:HG2	1:C:4691:GLN:H	1.78	0.49
1:A:2248:ARG:NH2	1:A:3865:VAL:O	2.46	0.49
1:A:2812:SER:HB2	1:A:2926:LEU:HD22	1.93	0.49
1:B:1229:ASN:HB2	1:B:1826:ALA:HB1	1.95	0.49
1:B:1747:LEU:HB3	1:B:1760:HIS:HB3	1.93	0.49
1:B:3669:PHE:O	1:B:3673:MET:HG2	2.12	0.49
1:B:4812:HIS:HD1	1:B:4812:HIS:C	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4985:LEU:HD13	2:B:5101:ACP:H2	1.92	0.49
1:D:483:MET:HA	1:D:486:LEU:HD13	1.93	0.49
1:C:759:ILE:HG13	1:C:760:ASN:H	1.76	0.49
1:A:648:ILE:HD13	1:A:779:PRO:HG2	1.93	0.49
1:A:1867:GLU:HA	1:A:1870:VAL:HB	1.94	0.49
1:B:3924:LEU:HD22	1:B:3984:ARG:HD2	1.95	0.49
1:D:717:ASP:OD1	1:D:717:ASP:N	2.45	0.49
1:D:2477:PRO:HB2	1:D:2488:UNK:HA	1.93	0.49
1:D:3887:PHE:O	1:D:3891:LEU:HG	2.12	0.49
1:C:669:ASP:OD1	1:C:669:ASP:N	2.44	0.49
1:C:790:ARG:HD3	1:C:1627:ALA:HB2	1.94	0.49
1:C:1859:VAL:HA	1:C:1862:ILE:HG22	1.93	0.49
1:C:2477:PRO:HB2	1:C:2488:UNK:HA	1.95	0.49
1:A:4850:LEU:HD13	1:B:4814:LEU:HD22	1.94	0.49
1:B:2477:PRO:HB2	1:B:2488:UNK:HA	1.95	0.49
1:B:4066:LEU:HD21	1:B:4173:TYR:CZ	2.48	0.49
1:D:1840:PRO:HB3	1:D:1843:LYS:HD3	1.95	0.49
1:D:2812:SER:HB2	1:D:2926:LEU:HD22	1.94	0.49
1:D:3779:VAL:HG23	1:D:3797:THR:HG22	1.94	0.49
1:C:214:VAL:HG22	1:C:341:TYR:HE1	1.77	0.49
1:C:3737:GLU:CA	1:C:3763:LEU:HD23	2.42	0.49
1:A:1929:MET:N	1:A:1929:MET:SD	2.86	0.49
1:A:3886:ARG:NH1	1:A:3889:GLN:OE1	2.45	0.49
1:A:3987:ASP:OD1	1:D:162:LYS:NZ	2.46	0.49
1:B:719:LEU:O	1:B:719:LEU:HD12	2.11	0.49
1:B:5017:ARG:HH21	1:B:5019:TRP:HE1	1.60	0.49
1:D:36:CYS:HB3	1:D:50:GLU:HB3	1.94	0.49
1:D:2809:ILE:HD11	1:D:2926:LEU:HD13	1.94	0.49
1:D:3767:GLN:NE2	1:D:3804:ILE:CD1	2.75	0.49
1:C:652:ARG:HD3	1:C:773:LEU:HD12	1.94	0.49
1:C:1075:PHE:HB2	1:C:1192:CYS:SG	2.53	0.49
1:C:3840:SER:OG	1:C:3877:ASP:OD2	2.30	0.49
1:A:154:SER:OG	1:A:155:LYS:N	2.46	0.49
1:A:1143:TRP:CD1	1:A:1164:LEU:HD13	2.48	0.49
1:A:3561:UNK:O	1:A:3562:UNK:CB	2.61	0.49
1:A:4550:LYS:HA	1:A:4553:ASN:ND2	2.27	0.49
1:B:667:MET:HB2	1:B:790:ARG:HB2	1.95	0.49
1:B:728:ARG:NH1	1:B:1384:UNK:O	2.46	0.49
1:B:2337:PHE:HA	1:B:2340:PHE:HB2	1.94	0.49
1:B:2763:HIS:NE2	1:B:2792:ARG:O	2.34	0.49
1:B:4066:LEU:HD21	1:B:4173:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1228:ILE:HG23	1:D:1229:ASN:H	1.77	0.49
1:D:1740:PRO:HA	1:D:1743:ARG:HG2	1.95	0.49
1:D:1747:LEU:HB3	1:D:1760:HIS:HB3	1.95	0.49
1:C:4689:THR:HA	1:C:4732:PHE:HE2	1.78	0.49
1:A:4244:GLU:HG2	1:A:4668:LEU:CD1	2.43	0.49
1:B:24:CYS:HB3	1:B:200:TRP:CE3	2.48	0.49
1:B:2178:MET:SD	1:B:2228:MET:HE1	2.53	0.49
1:B:4872:PRO:CD	1:B:4873:ASP:N	2.76	0.49
1:D:1580:PHE:HE2	1:D:1592:PRO:HG2	1.78	0.49
1:D:3886:ARG:NH1	1:D:3889:GLN:OE1	2.46	0.49
1:C:2810:LYS:HG2	1:C:2814:LYS:HE3	1.94	0.49
1:C:4066:LEU:HD21	1:C:4173:TYR:CE2	2.48	0.49
1:B:1639:LEU:N	1:B:1648:MET:O	2.44	0.48
1:B:4812:HIS:ND1	1:B:4812:HIS:C	2.67	0.48
1:C:483:MET:HA	1:C:486:LEU:HD13	1.95	0.48
1:C:1698:LEU:HD22	1:C:1810:LYS:HG2	1.93	0.48
1:C:4944:ARG:NH1	1:C:4944:ARG:CG	2.76	0.48
1:A:786:GLY:HA2	1:A:1631:GLN:HA	1.95	0.48
1:A:3889:GLN:HG3	1:A:3964:SER:HA	1.95	0.48
1:D:154:SER:OG	1:D:155:LYS:N	2.45	0.48
1:C:567:VAL:HG13	1:C:568:LEU:HD12	1.94	0.48
1:C:3723:MET:HE1	1:C:3793:MET:HA	1.94	0.48
1:A:790:ARG:HD3	1:A:1627:ALA:HB2	1.96	0.48
1:A:1649:ASP:N	1:A:1649:ASP:OD1	2.45	0.48
1:A:1703:LEU:HB2	1:A:1707:LEU:HB3	1.94	0.48
1:A:2736:ASP:N	1:A:2736:ASP:OD1	2.46	0.48
1:B:650:VAL:HB	1:B:777:PHE:HD2	1.77	0.48
1:D:19:GLU:HB3	1:D:68:THR:HG22	1.95	0.48
1:D:1240:LYS:HZ1	1:D:1242:LEU:HB3	1.77	0.48
1:D:2248:ARG:NH2	1:D:3865:VAL:O	2.46	0.48
1:D:3670:GLU:OE1	1:D:3670:GLU:N	2.44	0.48
1:D:4003:LEU:HD11	1:D:4009:GLN:HG2	1.96	0.48
1:D:4141:PHE:CE2	1:D:4196:GLU:HB2	2.48	0.48
1:C:426:ARG:NE	1:C:505:GLU:O	2.41	0.48
1:C:1857:GLU:HA	1:C:1860:LYS:HE2	1.95	0.48
1:C:2022:PRO:HB2	1:C:2024:PRO:HD2	1.95	0.48
1:C:3778:MET:HA	1:C:3781:GLN:HG2	1.96	0.48
1:B:116:MET:HG3	1:B:137:LEU:HD12	1.94	0.48
1:D:149:THR:HG23	1:D:151:HIS:HE1	1.78	0.48
1:D:1075:PHE:HB2	1:D:1192:CYS:SG	2.53	0.48
1:D:2022:PRO:HB2	1:D:2024:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3968:TYR:O	1:C:3976:ASN:ND2	2.46	0.48
1:A:4238:CYS:HA	1:A:4989:MET:HE1	1.94	0.48
1:B:149:THR:HG23	1:B:151:HIS:CE1	2.49	0.48
1:B:1676:LEU:HD22	1:B:2167:ILE:HG22	1.95	0.48
1:B:1740:PRO:HA	1:B:1743:ARG:HG2	1.95	0.48
1:B:2368:LEU:HD13	1:B:2376:LEU:HD21	1.94	0.48
1:B:4852:THR:HG21	1:B:4883:TYR:HA	1.95	0.48
1:D:248:GLU:HG2	1:D:252:VAL:HG23	1.96	0.48
1:D:1237:TRP:HH2	1:D:1652:GLU:HA	1.78	0.48
1:D:3805:LEU:O	1:D:3890:LEU:HD23	2.14	0.48
1:B:3972:PRO:HB3	1:B:4032:GLU:HG3	1.96	0.48
1:B:4865:LYS:CG	1:B:4875:LYS:CG	2.91	0.48
1:D:1707:LEU:O	1:D:1709:ALA:N	2.47	0.48
1:D:3767:GLN:HE22	1:D:3804:ILE:CD1	2.27	0.48
1:D:4095:LYS:HE2	1:D:4095:LYS:HB3	1.68	0.48
1:C:138:GLN:HG2	1:C:139:GLU:H	1.78	0.48
1:B:138:GLN:HG2	1:B:139:GLU:H	1.78	0.48
1:B:143:GLY:HA2	1:B:146:CYS:SG	2.54	0.48
1:D:455:PRO:HG3	1:D:467:LYS:HB3	1.95	0.48
1:D:1689:VAL:HG13	1:D:1690:ASP:N	2.28	0.48
1:B:2736:ASP:OD1	1:B:2736:ASP:N	2.46	0.48
1:B:4851:TYR:HD2	1:B:4920:PHE:HD1	1.61	0.48
1:D:243:ARG:NH1	1:D:301:VAL:O	2.47	0.48
1:D:1712:TYR:O	1:D:1716:ILE:HG12	2.13	0.48
1:C:3944:GLU:HG2	1:C:3947:GLY:H	1.79	0.48
1:A:664:PHE:CZ	1:A:779:PRO:HG3	2.49	0.48
1:A:1697:ALA:HB1	1:A:1708:ARG:HH11	1.78	0.48
1:A:1712:TYR:O	1:A:1716:ILE:HG12	2.14	0.48
1:A:1747:LEU:HB3	1:A:1760:HIS:HB3	1.94	0.48
1:A:4183:ILE:HD13	1:A:5010:VAL:HG21	1.96	0.48
1:A:4927:ILE:N	1:A:4927:ILE:HD13	2.29	0.48
1:B:700:GLU:HA	1:B:1646:ARG:HA	1.96	0.48
1:C:220:LEU:HD12	1:C:390:LEU:HB3	1.95	0.48
1:A:1689:VAL:HG13	1:A:1690:ASP:N	2.29	0.48
1:A:1740:PRO:HA	1:A:1743:ARG:HG2	1.96	0.48
1:D:2113:SER:OG	1:D:2113:SER:O	2.31	0.48
1:D:2871:LEU:HD12	1:D:2927:LEU:HD21	1.95	0.48
1:C:1698:LEU:HD21	1:C:1814:MET:HB2	1.95	0.48
1:C:3765:TYR:CD1	1:C:4750:ILE:HD12	2.49	0.48
1:B:216:GLY:HA2	1:B:262:LEU:HD11	1.96	0.47
1:B:3835:LEU:HD21	1:B:3880:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1580:PHE:HE2	1:C:1592:PRO:HG2	1.78	0.47
1:C:1929:MET:N	1:C:1929:MET:SD	2.87	0.47
1:C:2248:ARG:NH2	1:C:3865:VAL:O	2.47	0.47
1:A:24:CYS:HB3	1:A:200:TRP:CE3	2.49	0.47
1:A:273:HIS:H	1:A:334:MET:HB3	1.80	0.47
1:A:978:THR:HG22	1:A:981:GLN:H	1.79	0.47
1:A:2477:PRO:HB2	1:A:2488:UNK:HA	1.95	0.47
1:A:4244:GLU:HG3	1:A:4668:LEU:HD11	1.96	0.47
1:B:213:TYR:CG	1:B:337:PRO:HB2	2.49	0.47
1:D:3945:GLU:OE1	1:D:3946:GLN:NE2	2.47	0.47
1:D:4892:ARG:HH22	1:C:4897:ILE:N	2.12	0.47
1:D:4929:LEU:N	1:D:4929:LEU:CD2	2.77	0.47
1:C:449:ILE:HG13	1:C:525:LEU:HD12	1.95	0.47
1:C:455:PRO:HG3	1:C:467:LYS:HB3	1.96	0.47
1:C:3763:LEU:O	1:C:3767:GLN:OE1	2.31	0.47
1:C:4555:LEU:HD22	1:C:4656:LEU:HD11	1.95	0.47
1:A:1707:LEU:O	1:A:1709:ALA:N	2.47	0.47
1:A:2113:SER:O	1:A:2113:SER:OG	2.30	0.47
1:B:1703:LEU:HB2	1:B:1707:LEU:HB3	1.97	0.47
1:D:2930:LEU:HD13	1:D:2937:VAL:HG21	1.96	0.47
1:D:3889:GLN:NE2	1:D:3963:ASN:OD1	2.47	0.47
1:D:4582:VAL:HG11	1:C:4860:ARG:HH11	1.80	0.47
1:C:3924:LEU:HD22	1:C:3984:ARG:HD2	1.95	0.47
1:C:4671:PHE:HE1	1:C:4716:TRP:HB2	1.78	0.47
1:A:2742:THR:HG21	1:A:2814:LYS:HD3	1.96	0.47
1:A:3962:PHE:O	1:A:3966:THR:HG23	2.14	0.47
1:D:1077:ALA:HB3	1:D:1189:LEU:HD11	1.96	0.47
1:C:3729:MET:O	1:C:3732:SER:OG	2.30	0.47
1:A:219:VAL:HG12	1:A:261:ARG:HB2	1.96	0.47
1:A:313:SER:HB2	1:A:350:HIS:CE1	2.50	0.47
1:A:2299:VAL:HG11	1:A:2356:LEU:HB3	1.95	0.47
1:A:4865:LYS:HA	1:A:4865:LYS:CE	2.42	0.47
1:A:4921:PHE:HD2	1:B:4892:ARG:HD2	1.79	0.47
1:B:1707:LEU:O	1:B:1709:ALA:N	2.48	0.47
1:D:219:VAL:HG12	1:D:261:ARG:HB2	1.97	0.47
1:C:1707:LEU:O	1:C:1709:ALA:N	2.47	0.47
1:A:670:GLU:HG3	1:A:787:VAL:HA	1.95	0.47
1:A:1026:LEU:HA	1:A:1032:LYS:HE2	1.96	0.47
1:A:1840:PRO:HB3	1:A:1843:LYS:HD3	1.97	0.47
1:B:1580:PHE:HE2	1:B:1592:PRO:HG2	1.78	0.47
1:B:2474:LEU:HD23	1:B:2474:LEU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2257:LEU:HD11	1:D:2276:ALA:HB2	1.94	0.47
1:C:2192:TYR:HD1	1:C:2242:ILE:HD13	1.79	0.47
1:C:2809:ILE:HD11	1:C:2926:LEU:HD13	1.96	0.47
1:A:192:ASP:OD1	1:A:192:ASP:N	2.46	0.47
1:A:646:PRO:HD2	1:A:779:PRO:HB2	1.97	0.47
1:A:3236:UNK:N	1:A:3240:UNK:N	2.61	0.47
1:A:4158:PRO:HA	1:A:4161:ARG:HD3	1.96	0.47
1:B:2181:SER:O	1:B:2185:ILE:HG23	2.14	0.47
1:B:4690:GLU:HG2	1:B:4691:GLN:H	1.78	0.47
1:B:4946:GLN:O	1:B:4949:GLN:N	2.47	0.47
1:D:723:THR:H	1:D:726:VAL:HG12	1.79	0.47
1:D:1026:LEU:HA	1:D:1032:LYS:HE2	1.96	0.47
1:D:1839:VAL:HG13	1:D:1841:VAL:HG22	1.97	0.47
1:D:2192:TYR:HD1	1:D:2242:ILE:HD13	1.80	0.47
1:D:2474:LEU:HD23	1:D:2474:LEU:H	1.80	0.47
1:D:4866:SER:OG	1:D:4867:GLU:N	2.45	0.47
1:C:4011:GLU:HG2	1:C:4012:LEU:HD12	1.97	0.47
1:C:4869:GLU:HB3	1:C:4870:ASP:H	1.36	0.47
1:A:2287:ALA:O	1:A:2349:ASN:ND2	2.43	0.47
1:A:3957:VAL:O	1:A:3961:VAL:HG23	2.15	0.47
1:A:4690:GLU:HG2	1:A:4691:GLN:H	1.78	0.47
1:B:154:SER:OG	1:B:155:LYS:N	2.47	0.47
1:B:1857:GLU:HA	1:B:1860:LYS:HE2	1.97	0.47
1:B:3906:GLN:HE22	1:B:3913:ILE:HB	1.80	0.47
1:D:213:TYR:CD1	1:D:337:PRO:HB2	2.50	0.47
1:D:661:LYS:HB3	1:D:808:TYR:CD2	2.50	0.47
1:D:3937:TYR:OH	1:D:3944:GLU:OE2	2.32	0.47
1:C:978:THR:HG22	1:C:981:GLN:H	1.80	0.47
1:C:1747:LEU:HB3	1:C:1760:HIS:HB3	1.96	0.47
1:C:4716:TRP:HZ2	1:C:4996:ILE:HG21	1.79	0.47
1:A:138:GLN:HG2	1:A:139:GLU:H	1.79	0.47
1:A:1124:PHE:HE1	1:A:1139:PHE:HB3	1.79	0.47
1:D:1194:LEU:HB3	1:D:1198:GLN:HB2	1.96	0.47
1:D:4629:TYR:HE1	1:C:4860:ARG:HH12	1.62	0.47
1:C:2335:LEU:HD22	1:C:2353:VAL:HG21	1.96	0.47
1:C:3758:MET:C	1:C:3758:MET:SD	2.93	0.47
1:A:1204:LEU:HD23	1:A:1227:ALA:HB2	1.97	0.47
1:A:4917:ASP:OD2	1:B:4892:ARG:NH1	2.48	0.47
1:B:4865:LYS:HG3	1:B:4875:LYS:HG2	1.95	0.47
1:D:45:ARG:HD2	1:D:137:LEU:O	2.15	0.47
1:D:2449:GLU:OE2	1:D:2452:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4019:LEU:O	1:D:4023:MET:HG2	2.15	0.47
1:C:1740:PRO:HA	1:C:1743:ARG:HG2	1.97	0.47
1:C:2474:LEU:HD23	1:C:2474:LEU:H	1.80	0.47
1:A:3887:PHE:O	1:A:3891:LEU:HG	2.15	0.46
1:D:669:ASP:N	1:D:669:ASP:OD1	2.48	0.46
1:D:4978:HIS:HE1	1:D:5027:CYS:HB2	1.80	0.46
1:C:1119:GLU:HA	1:C:1133:HIS:CD2	2.49	0.46
1:C:1960:ALA:O	1:C:1963:GLU:HG3	2.14	0.46
1:C:2736:ASP:OD1	1:C:2736:ASP:N	2.46	0.46
1:A:102:LEU:HD13	1:A:160:GLY:HA2	1.96	0.46
1:A:1727:ARG:HH21	1:A:1772:ARG:HG3	1.79	0.46
1:B:106:ALA:HA	1:B:149:THR:HA	1.97	0.46
1:B:707:VAL:HG12	1:B:713:SER:HB2	1.97	0.46
1:B:4031:LEU:HD23	1:B:4031:LEU:H	1.81	0.46
1:B:4832:HIS:NE2	1:B:4942:GLU:OE1	2.48	0.46
1:A:4017:LEU:HD12	1:A:4139:ILE:HG13	1.98	0.46
1:B:224:HIS:N	1:B:229:GLU:O	2.39	0.46
1:B:1026:LEU:HA	1:B:1032:LYS:HE2	1.96	0.46
1:B:4022:ASP:O	1:B:4025:VAL:HG12	2.15	0.46
1:B:4654:ALA:CB	1:B:4795:TYR:CE1	2.98	0.46
1:D:4689:THR:HA	1:D:4732:PHE:HE2	1.81	0.46
1:C:1026:LEU:HA	1:C:1032:LYS:HE2	1.96	0.46
1:C:1667:LEU:HD21	1:C:1710:GLY:HA3	1.97	0.46
1:C:4219:PHE:CE1	1:C:4946:GLN:OE1	2.69	0.46
1:C:4662:ASN:HA	1:C:4666:VAL:HG23	1.97	0.46
1:A:1867:GLU:O	1:A:1871:PHE:N	2.38	0.46
1:A:2674:UNK:HA	1:A:2679:UNK:CB	2.45	0.46
1:B:358:THR:HG1	1:B:383:HIS:HD1	1.64	0.46
1:B:1667:LEU:HD21	1:B:1710:GLY:HA3	1.97	0.46
1:B:4864:ASN:HA	1:B:4874:MET:SD	2.55	0.46
1:B:4865:LYS:CG	1:B:4875:LYS:HG2	2.45	0.46
1:D:2348:GLU:HG2	1:D:3849:ARG:HE	1.81	0.46
1:D:3889:GLN:HG3	1:D:3964:SER:HA	1.96	0.46
1:A:669:ASP:N	1:A:669:ASP:OD1	2.48	0.46
1:A:2271:THR:HG22	1:A:2273:LEU:H	1.80	0.46
1:B:414:PHE:HE1	1:B:436:LEU:HD12	1.80	0.46
1:B:1851:MET:HB2	1:B:1853:ILE:HG12	1.97	0.46
1:B:2159:LEU:HD13	1:B:2201:LEU:HD23	1.97	0.46
1:B:4818:MET:C	1:B:4818:MET:SD	2.94	0.46
1:C:5000:GLU:HA	1:C:5003:HIS:ND1	2.31	0.46
1:A:560:ILE:HA	1:A:563:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2095:GLN:HE21	1:A:2128:TYR:HD1	1.63	0.46
1:A:3491:UNK:O	1:A:3495:UNK:CB	2.64	0.46
1:B:197:GLN:NE2	1:B:198:THR:O	2.48	0.46
1:B:1194:LEU:HB3	1:B:1198:GLN:HB2	1.97	0.46
1:B:5000:GLU:HA	1:B:5003:HIS:ND1	2.31	0.46
1:D:1850:VAL:HA	1:D:1945:TYR:CE1	2.51	0.46
1:C:1194:LEU:HB3	1:C:1198:GLN:HB2	1.97	0.46
1:C:1240:LYS:HZ1	1:C:1242:LEU:HB3	1.80	0.46
1:C:1712:TYR:O	1:C:1716:ILE:HG12	2.15	0.46
1:C:3906:GLN:HE22	1:C:3913:ILE:HB	1.81	0.46
1:C:4223:ASN:ND2	1:C:4946:GLN:NE2	2.63	0.46
1:C:4844:LEU:HD12	1:C:4928:LEU:HG	1.96	0.46
1:A:108:LEU:HD13	1:A:147:TRP:NE1	2.31	0.46
1:A:795:GLY:H	1:A:811:CYS:HB2	1.80	0.46
1:A:1077:ALA:HB3	1:A:1189:LEU:HD11	1.97	0.46
1:A:2337:PHE:HA	1:A:2340:PHE:HB2	1.98	0.46
2:A:5101:ACP:O2G	2:A:5101:ACP:O2B	2.33	0.46
1:B:758:ARG:HG2	1:B:759:ILE:O	2.16	0.46
1:B:4654:ALA:CB	1:B:4795:TYR:HE1	2.29	0.46
1:D:4184:MET:HB2	1:D:4190:ILE:HG22	1.97	0.46
1:C:257:ARG:O	1:C:284:HIS:NE2	2.44	0.46
1:C:1685:LEU:HD23	1:C:1718:ILE:HD12	1.97	0.46
1:C:3771:HIS:O	1:C:3775:ALA:N	2.49	0.46
1:A:710:ASP:OD1	1:A:713:SER:OG	2.31	0.46
1:A:1228:ILE:HD11	1:B:3573:UNK:HA	1.97	0.46
1:A:3941:ASP:OD1	1:A:3941:ASP:N	2.47	0.46
1:B:592:LYS:O	1:B:1594:ARG:HB2	2.16	0.46
1:D:149:THR:HG23	1:D:151:HIS:CE1	2.50	0.46
1:D:4895:GLY:HA2	1:D:4921:PHE:HE1	1.81	0.46
1:C:1141:ARG:NH2	1:C:1144:GLN:OE1	2.49	0.46
1:A:700:GLU:HA	1:A:1646:ARG:HA	1.98	0.46
1:A:1101:ARG:HH21	1:A:1115:LEU:HG	1.79	0.46
1:A:3944:GLU:HG2	1:A:3947:GLY:H	1.81	0.46
1:B:669:ASP:N	1:B:669:ASP:OD1	2.49	0.46
1:B:978:THR:HG22	1:B:981:GLN:H	1.80	0.46
1:B:1712:TYR:O	1:B:1716:ILE:HG12	2.15	0.46
1:B:4816:ILE:HD12	1:B:4816:ILE:HA	1.65	0.46
1:B:4818:MET:HA	1:B:4823:LEU:CG	2.41	0.46
1:D:661:LYS:HE3	1:D:750:LEU:HB3	1.98	0.46
1:D:978:THR:HG22	1:D:981:GLN:H	1.80	0.46
1:D:1072:VAL:HG22	1:D:1195:GLY:HA2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1203:ASN:ND2	1:D:1210:SER:O	2.43	0.46
1:D:1639:LEU:N	1:D:1648:MET:O	2.46	0.46
1:D:2182:ILE:O	1:D:2185:ILE:HG12	2.15	0.46
1:C:3733:CYS:SG	1:C:3803:SER:OG	2.52	0.46
1:A:213:TYR:CD2	1:A:337:PRO:HB2	2.51	0.46
1:A:3888:LEU:HD13	1:A:3891:LEU:HD12	1.97	0.46
1:B:1934:SER:O	1:B:1937:LEU:HG	2.16	0.46
1:D:358:THR:HG1	1:D:383:HIS:HD1	1.64	0.46
1:D:700:GLU:HA	1:D:1646:ARG:HA	1.98	0.46
1:D:4180:ARG:HG2	1:D:4194:TYR:CE1	2.51	0.46
1:D:4235:VAL:HG21	1:D:5019:TRP:CH2	2.51	0.46
1:D:4828:SER:HA	1:D:4831:THR:HG22	1.98	0.46
1:D:4904:PRO:HG3	1:D:4913:ARG:HE	1.81	0.46
1:C:3759:GLU:O	1:C:3762:ARG:N	2.49	0.46
1:A:4914:VAL:HG23	1:B:4888:TYR:HD2	1.80	0.45
1:B:313:SER:HB2	1:B:350:HIS:CE1	2.51	0.45
1:B:4638:TYR:O	1:B:4641:PRO:HD2	2.16	0.45
1:D:2012:PHE:HB3	1:D:2021:CYS:HA	1.98	0.45
1:D:4017:LEU:HA	1:D:4020:GLN:OE1	2.16	0.45
1:C:3996:PHE:HA	1:C:3999:MET:SD	2.56	0.45
1:C:4666:VAL:N	1:C:4667:PRO:HD2	2.31	0.45
1:C:4985:LEU:O	1:C:4989:MET:HG2	2.17	0.45
1:A:1720:LEU:HB2	1:A:1724:CYS:SG	2.57	0.45
1:A:4654:ALA:O	1:A:4658:ILE:HG12	2.16	0.45
1:D:138:GLN:HG2	1:D:139:GLU:N	2.31	0.45
1:D:330:ASP:OD1	1:D:330:ASP:N	2.49	0.45
1:D:652:ARG:HD3	1:D:773:LEU:HD12	1.98	0.45
1:D:1119:GLU:HA	1:D:1133:HIS:CD2	2.51	0.45
1:D:2736:ASP:OD1	1:D:2736:ASP:N	2.46	0.45
1:D:4865:LYS:HZ3	1:D:4865:LYS:CB	2.27	0.45
1:C:1676:LEU:HD22	1:C:2167:ILE:HG22	1.97	0.45
1:C:2012:PHE:HB3	1:C:2021:CYS:HA	1.99	0.45
1:A:162:LYS:O	1:A:164:ARG:NH1	2.49	0.45
1:A:1580:PHE:CE2	1:A:1592:PRO:HG2	2.51	0.45
1:A:3804:ILE:HG22	1:A:3805:LEU:HD12	1.97	0.45
1:A:4716:TRP:HZ2	1:A:4996:ILE:HG21	1.81	0.45
1:B:1101:ARG:HH21	1:B:1115:LEU:HG	1.80	0.45
1:B:2272:PRO:HA	1:B:2275:VAL:HG12	1.98	0.45
1:B:3676:ASP:OD1	1:B:3677:LEU:N	2.50	0.45
1:B:3832:ILE:O	1:B:3836:MET:HG2	2.16	0.45
1:D:759:ILE:HG13	1:D:760:ASN:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:TYR:CD1	1:C:337:PRO:HB2	2.51	0.45
1:A:543:ASN:O	1:A:547:VAL:HG23	2.17	0.45
1:A:1931:LEU:HD22	1:A:1935:VAL:HG11	1.99	0.45
1:B:3840:SER:OG	1:B:3877:ASP:OD2	2.32	0.45
1:B:4573:ILE:HD13	1:B:4809:PHE:CD2	2.45	0.45
1:B:4821:LYS:HA	1:B:4824:ARG:NH2	2.31	0.45
1:C:214:VAL:HG21	1:C:390:LEU:HD12	1.98	0.45
1:C:4063:ASP:OD2	1:C:4067:LYS:NZ	2.46	0.45
1:A:1857:GLU:HA	1:A:1860:LYS:HE2	1.98	0.45
1:A:2474:LEU:HD23	1:A:2474:LEU:H	1.80	0.45
1:A:3963:ASN:O	1:A:3966:THR:OG1	2.30	0.45
1:A:4221:VAL:HG22	1:A:4233:LEU:HD11	1.98	0.45
1:A:4901:ILE:CB	1:A:4913:ARG:HH21	2.27	0.45
1:A:5017:ARG:HH21	1:A:5019:TRP:HE1	1.63	0.45
1:B:2812:SER:HB2	1:B:2926:LEU:HD22	1.98	0.45
1:B:3845:ASN:O	1:B:3849:ARG:HG2	2.17	0.45
1:B:4024:VAL:HG23	1:B:4142:ASN:ND2	2.32	0.45
1:D:294:THR:HG23	1:D:295:GLU:N	2.32	0.45
1:D:313:SER:HB2	1:D:350:HIS:CE1	2.52	0.45
1:D:3769:ARG:O	1:D:3771:HIS:CE1	2.70	0.45
1:C:293:LEU:HD13	1:C:298:GLY:N	2.31	0.45
1:C:647:ASN:HB3	1:C:822:ARG:NH1	2.31	0.45
1:C:2348:GLU:HG3	1:C:3849:ARG:HH21	1.80	0.45
1:C:4869:GLU:C	1:C:4870:ASP:O	2.55	0.45
1:C:4904:PRO:HB3	1:C:4913:ARG:HD3	1.98	0.45
1:A:119:SER:OG	1:A:120:CYS:N	2.49	0.45
1:B:144:GLU:HG2	1:B:145:ALA:N	2.32	0.45
1:B:1677:GLY:HA2	1:B:1721:GLU:HG2	1.99	0.45
1:B:1866:ILE:HG22	1:B:1870:VAL:HG23	1.99	0.45
1:C:719:LEU:O	1:C:719:LEU:HD12	2.17	0.45
1:C:1677:GLY:HA2	1:C:1721:GLU:HG2	1.99	0.45
1:C:2182:ILE:O	1:C:2185:ILE:HG12	2.16	0.45
1:A:693:SER:N	1:A:694:PRO:HD2	2.31	0.45
1:A:758:ARG:HG2	1:A:759:ILE:O	2.17	0.45
1:A:3763:LEU:C	1:A:3763:LEU:CD1	2.85	0.45
1:D:257:ARG:O	1:D:284:HIS:NE2	2.50	0.45
1:D:1098:GLY:HA3	1:D:1198:GLN:HE22	1.80	0.45
1:C:119:SER:OG	1:C:120:CYS:N	2.50	0.45
1:A:505:GLU:HA	1:A:511:ALA:HB3	1.98	0.45
1:A:1194:LEU:HB3	1:A:1198:GLN:HB2	1.98	0.45
1:A:4937:ILE:CD1	1:D:4934:GLY:HA2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1240:LYS:NZ	1:B:1244:GLN:OE1	2.49	0.45
1:D:2272:PRO:HA	1:D:2275:VAL:HG12	1.98	0.45
1:C:700:GLU:HA	1:C:1646:ARG:HA	1.98	0.45
1:A:22:LEU:HD11	1:A:200:TRP:HB3	1.99	0.45
1:A:131:LEU:HD21	1:B:2456:ILE:HA	1.99	0.45
1:A:1839:VAL:HG13	1:A:1841:VAL:HG22	1.98	0.45
1:A:2367:ALA:HB3	1:A:2379:ALA:HB2	1.98	0.45
1:B:330:ASP:OD1	1:B:330:ASP:N	2.49	0.45
1:B:1143:TRP:CD1	1:B:1164:LEU:HD13	2.52	0.45
1:B:4865:LYS:C	1:B:4865:LYS:CD	2.85	0.45
1:D:24:CYS:SG	1:D:35:LEU:HB2	2.57	0.45
1:D:272:SER:HB2	1:D:334:MET:HA	1.98	0.45
1:D:416:LYS:HA	1:D:416:LYS:HD3	1.77	0.45
1:C:795:GLY:H	1:C:811:CYS:HB2	1.82	0.45
1:C:1101:ARG:HH21	1:C:1115:LEU:HG	1.81	0.45
1:C:1730:MET:SD	1:C:1772:ARG:NH1	2.90	0.45
1:C:3801:GLY:HA2	1:C:3804:ILE:HG22	1.99	0.45
1:C:3842:LEU:HD21	1:C:3954:ALA:HB2	1.99	0.45
1:A:723:THR:H	1:A:726:VAL:HG12	1.82	0.45
1:A:2012:PHE:HB3	1:A:2021:CYS:HA	1.99	0.45
1:A:3937:TYR:O	1:A:4002:LYS:NZ	2.50	0.45
1:A:4926:VAL:HG12	1:A:4927:ILE:CD1	2.47	0.45
1:B:1000:ARG:O	1:B:1005:TRP:N	2.50	0.45
1:B:2734:ASN:HB3	1:B:2735:PHE:H	1.59	0.45
1:B:2781:VAL:HG22	1:B:2789:PRO:HD2	1.99	0.45
1:D:1857:GLU:HA	1:D:1860:LYS:HE2	1.98	0.45
1:D:2794:TYR:HA	1:D:2797:PHE:HD2	1.82	0.45
1:D:4024:VAL:HG13	1:D:4142:ASN:ND2	2.32	0.45
1:D:4101:LYS:HG3	1:C:4731:ILE:HA	1.98	0.45
1:D:4705:VAL:HG22	1:D:4711:PHE:HD1	1.82	0.45
1:C:213:TYR:CG	1:C:337:PRO:HB2	2.51	0.45
1:C:3779:VAL:HG23	1:C:3797:THR:HG22	1.99	0.45
1:C:3845:ASN:O	1:C:3849:ARG:HG2	2.17	0.45
1:C:4922:PHE:CD2	1:C:4922:PHE:O	2.70	0.45
1:A:179:TYR:HB3	1:A:197:GLN:HB2	1.99	0.44
1:A:3808:GLY:HA2	1:A:3893:GLU:OE2	2.17	0.44
1:B:495:ASN:HD21	1:B:550:LYS:HB3	1.82	0.44
1:B:1119:GLU:HB3	1:B:1134:LEU:HD11	2.00	0.44
1:B:1935:VAL:O	1:B:1939:MET:HG2	2.17	0.44
1:B:4183:ILE:HD13	1:B:5010:VAL:HG21	1.99	0.44
1:D:134:ASP:N	1:D:134:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:592:LYS:O	1:D:1594:ARG:HB2	2.16	0.44
1:D:1622:GLU:HA	1:D:1626:TRP:CD2	2.52	0.44
1:D:1867:GLU:O	1:D:1871:PHE:N	2.37	0.44
1:D:2191:PHE:HZ	1:D:2239:PHE:HA	1.82	0.44
1:D:2781:VAL:HG22	1:D:2789:PRO:HD2	1.99	0.44
1:C:313:SER:HB2	1:C:350:HIS:CE1	2.52	0.44
1:C:614:VAL:O	1:C:618:GLN:NE2	2.50	0.44
1:C:1840:PRO:HB3	1:C:1843:LYS:HD3	1.98	0.44
1:C:4812:HIS:O	1:C:4816:ILE:HG12	2.17	0.44
1:A:78:LEU:HD11	1:A:147:TRP:CG	2.52	0.44
1:A:1237:TRP:HH2	1:A:1652:GLU:HA	1.81	0.44
1:A:1661:ARG:HA	1:A:1661:ARG:HD2	1.85	0.44
1:A:3729:MET:HG3	1:A:3770:LEU:CD1	2.42	0.44
1:B:213:TYR:CD1	1:B:337:PRO:HB2	2.52	0.44
1:B:3765:TYR:CE1	1:B:4750:ILE:HG22	2.41	0.44
1:B:4869:GLU:CD	1:B:4869:GLU:N	2.71	0.44
1:B:4958:CYS:SG	1:B:4978:HIS:HD2	2.37	0.44
1:D:615:ARG:NH2	1:D:1677:GLY:O	2.48	0.44
1:D:2165:LEU:HD13	1:D:2178:MET:HB3	1.97	0.44
1:D:4868:ASP:HB3	1:D:4869:GLU:H	1.66	0.44
1:C:543:ASN:O	1:C:547:VAL:HG23	2.17	0.44
1:C:4550:LYS:HA	1:C:4553:ASN:HD21	1.81	0.44
1:A:35:LEU:HD23	1:A:49:LEU:HD22	2.00	0.44
1:A:1738:LEU:HD11	1:A:1963:GLU:HG3	1.99	0.44
1:A:4865:LYS:CE	1:A:4865:LYS:CA	2.96	0.44
1:B:35:LEU:HD23	1:B:49:LEU:HD22	1.99	0.44
1:B:119:SER:OG	1:B:120:CYS:N	2.50	0.44
1:B:294:THR:HG23	1:B:295:GLU:N	2.32	0.44
1:B:693:SER:N	1:B:694:PRO:HD2	2.33	0.44
1:B:1736:VAL:HG21	1:B:1956:GLU:HG3	1.99	0.44
1:B:4158:PRO:HA	1:B:4161:ARG:HD3	1.98	0.44
1:D:4205:TRP:O	1:D:4205:TRP:CG	2.70	0.44
1:D:4865:LYS:HD3	1:D:4866:SER:N	2.32	0.44
1:C:150:MET:HE1	1:C:163:VAL:HG11	1.98	0.44
1:C:751:SER:OG	1:C:752:VAL:N	2.50	0.44
1:C:758:ARG:HG2	1:C:759:ILE:O	2.18	0.44
1:C:1851:MET:HB2	1:C:1853:ILE:HG12	1.98	0.44
1:C:2794:TYR:HA	1:C:2797:PHE:HD2	1.82	0.44
1:C:3763:LEU:C	1:C:3763:LEU:CD1	2.85	0.44
1:A:3670:GLU:OE1	1:A:3670:GLU:N	2.44	0.44
1:A:3767:GLN:HG3	1:A:3809:ASN:ND2	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:VAL:HG12	1:B:261:ARG:HB2	2.00	0.44
1:B:795:GLY:H	1:B:811:CYS:HB2	1.83	0.44
1:B:4142:ASN:HA	1:B:4145:VAL:HG12	1.99	0.44
1:B:4654:ALA:O	1:B:4658:ILE:HG12	2.17	0.44
1:D:1931:LEU:HD22	1:D:1935:VAL:HG11	1.99	0.44
1:C:629:ARG:HD2	1:C:634:GLN:HG2	1.98	0.44
1:C:1736:VAL:HG21	1:C:1956:GLU:HG3	2.00	0.44
1:C:2348:GLU:HG2	1:C:3849:ARG:HE	1.81	0.44
1:C:4219:PHE:CZ	1:C:4946:GLN:OE1	2.70	0.44
1:B:1158:ASN:HB3	1:B:1182:ILE:HG13	1.99	0.44
1:B:4631:PHE:HE2	1:B:4640:GLU:HA	1.83	0.44
1:B:4895:GLY:O	1:C:4892:ARG:CG	2.65	0.44
1:D:181:HIS:N	1:D:192:ASP:O	2.49	0.44
1:D:2236:LEU:HB3	1:D:2275:VAL:HG21	2.00	0.44
1:C:312:THR:OG1	1:C:313:SER:N	2.51	0.44
1:C:723:THR:H	1:C:726:VAL:HG12	1.82	0.44
1:A:1000:ARG:O	1:A:1005:TRP:N	2.50	0.44
1:A:3772:THR:HG23	1:A:3773:ARG:N	2.32	0.44
1:A:4850:LEU:CD1	1:B:4814:LEU:HD22	2.48	0.44
1:B:668:VAL:O	1:B:741:GLU:N	2.50	0.44
1:D:299:LEU:HG	1:D:378:LEU:HG	1.99	0.44
1:D:426:ARG:NE	1:D:505:GLU:O	2.45	0.44
1:D:4662:ASN:O	1:D:4666:VAL:HB	2.18	0.44
1:C:138:GLN:HG2	1:C:139:GLU:N	2.33	0.44
1:C:219:VAL:HG12	1:C:261:ARG:HB2	1.99	0.44
1:C:675:LEU:HD12	1:C:675:LEU:HA	1.89	0.44
1:C:1961:PHE:HA	1:C:1964:ARG:HG2	2.00	0.44
1:C:2159:LEU:HD22	1:C:2201:LEU:HD23	2.00	0.44
1:C:4095:LYS:HB3	1:C:4095:LYS:HE2	1.68	0.44
1:A:1225:PRO:HG2	1:A:1228:ILE:HB	1.99	0.44
1:A:2115:GLU:H	1:A:2115:GLU:CD	2.20	0.44
1:A:3775:ALA:O	1:A:3778:MET:HG3	2.17	0.44
1:B:312:THR:OG1	1:B:313:SER:N	2.51	0.44
1:B:455:PRO:HG3	1:B:467:LYS:HB3	1.99	0.44
1:B:723:THR:H	1:B:726:VAL:HG12	1.82	0.44
1:D:4666:VAL:N	1:D:4667:PRO:HD2	2.30	0.44
1:D:4818:MET:HE3	1:D:4818:MET:C	2.38	0.44
1:C:1077:ALA:HB3	1:C:1189:LEU:HD11	1.98	0.44
1:C:1239:SER:OG	1:C:1240:LYS:N	2.51	0.44
1:C:4702:ASP:HA	1:C:4778:TRP:HE1	1.83	0.44
1:C:4866:SER:O	1:C:4867:GLU:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:LYS:HD3	1:A:416:LYS:HA	1.78	0.44
1:A:1737:PRO:HD3	1:A:1771:LEU:HD21	2.00	0.44
1:A:4828:SER:HA	1:A:4831:THR:HG22	2.00	0.44
1:A:4928:LEU:HD22	1:A:4928:LEU:HA	1.78	0.44
1:B:214:VAL:HG22	1:B:341:TYR:HE1	1.83	0.44
1:B:2005:GLN:HE22	1:B:3641:LEU:HD22	1.83	0.44
1:B:2012:PHE:HB3	1:B:2021:CYS:HA	2.00	0.44
1:A:184:THR:HA	1:A:189:LEU:HG	2.00	0.44
1:A:1639:LEU:N	1:A:1648:MET:O	2.45	0.44
1:A:2781:VAL:HG22	1:A:2789:PRO:HD2	2.00	0.44
1:A:3773:ARG:HA	1:A:3815:LYS:HE3	1.97	0.44
1:B:109:LEU:HD23	1:B:148:TRP:HD1	1.82	0.44
1:B:3895:HIS:HE1	1:B:3970:GLN:HB3	1.82	0.44
1:B:4011:GLU:HG2	1:B:4012:LEU:HD12	1.99	0.44
1:B:4821:LYS:HG3	1:B:4822:THR:N	2.33	0.44
1:D:421:PHE:HE1	1:D:436:LEU:HD21	1.83	0.44
1:D:3720:TYR:HA	1:D:3723:MET:HB2	2.00	0.44
1:D:3903:LEU:HD12	1:D:3903:LEU:HA	1.88	0.44
1:D:4180:ARG:NH1	1:D:4981:GLU:HB3	2.33	0.44
1:D:4820:VAL:CG1	1:D:4823:LEU:H	2.31	0.44
1:C:273:HIS:CD2	1:C:337:PRO:HB3	2.53	0.44
1:C:693:SER:N	1:C:694:PRO:HD2	2.33	0.44
1:A:3845:ASN:O	1:A:3849:ARG:HG2	2.16	0.43
1:B:1961:PHE:HA	1:B:1964:ARG:HG2	2.00	0.43
1:D:20:VAL:HG11	1:D:202:MET:HB3	2.00	0.43
1:D:312:THR:OG1	1:D:313:SER:N	2.51	0.43
1:D:1689:VAL:HG13	1:D:1690:ASP:H	1.82	0.43
1:D:4011:GLU:HG2	1:D:4012:LEU:HD12	1.99	0.43
1:C:1839:VAL:HG13	1:C:1841:VAL:HG22	2.00	0.43
1:C:2734:ASN:HB3	1:C:2735:PHE:H	1.57	0.43
1:A:1119:GLU:HA	1:A:1133:HIS:CD2	2.53	0.43
1:A:2003:GLN:O	1:A:2007:ASN:ND2	2.51	0.43
1:B:670:GLU:H	1:B:740:PRO:HB3	1.83	0.43
1:B:1661:ARG:HD2	1:B:1661:ARG:HA	1.85	0.43
1:D:1158:ASN:HB3	1:D:1182:ILE:HG13	1.99	0.43
1:D:4037:ASN:HB2	1:D:5035:GLN:NE2	2.33	0.43
1:D:4960:ILE:HG12	1:D:4985:LEU:CD2	2.49	0.43
1:D:5000:GLU:HA	1:D:5003:HIS:ND1	2.34	0.43
1:C:294:THR:HG23	1:C:295:GLU:N	2.33	0.43
1:C:299:LEU:HG	1:C:378:LEU:HG	1.99	0.43
1:C:2766:TRP:HA	1:C:2769:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5017:ARG:HH21	1:C:5019:TRP:HE1	1.64	0.43
1:A:4642:ALA:HB1	1:A:4645:CYS:SG	2.59	0.43
1:B:233:ILE:HG22	1:B:257:ARG:HB3	2.00	0.43
1:B:615:ARG:NH2	1:B:1677:GLY:O	2.50	0.43
1:B:3663:LEU:N	1:B:3663:LEU:HD12	2.33	0.43
1:B:3765:TYR:HE2	1:B:3769:ARG:HH22	1.66	0.43
1:B:4654:ALA:HB2	1:B:4795:TYR:HE1	1.82	0.43
1:D:747:CYS:SG	1:D:756:SER:HB2	2.58	0.43
1:D:1118:ASP:OD1	1:D:1118:ASP:N	2.52	0.43
1:D:1961:PHE:HA	1:D:1964:ARG:HG2	2.01	0.43
1:D:4866:SER:HB3	1:D:4871:GLU:CD	2.38	0.43
1:C:252:VAL:HA	1:C:255:HIS:ND1	2.33	0.43
1:C:617:ASN:OD1	1:C:618:GLN:HG3	2.18	0.43
1:A:294:THR:HG23	1:A:295:GLU:N	2.32	0.43
1:A:664:PHE:HB2	1:A:746:CYS:HB2	2.01	0.43
1:A:721:LEU:HD12	1:A:721:LEU:HA	1.89	0.43
1:A:1119:GLU:HB3	1:A:1134:LEU:HD11	1.99	0.43
1:A:4235:VAL:HG21	1:A:5019:TRP:CH2	2.53	0.43
1:A:4687:TYR:OH	1:A:4699:GLY:O	2.30	0.43
1:B:1119:GLU:HA	1:B:1133:HIS:CD2	2.53	0.43
1:D:137:LEU:O	1:D:137:LEU:HD12	2.18	0.43
1:D:2348:GLU:HG3	1:D:3849:ARG:HH21	1.84	0.43
1:D:2874:MET:N	1:D:2874:MET:SD	2.92	0.43
1:D:4158:PRO:HA	1:D:4161:ARG:HD3	2.00	0.43
1:D:4177:TYR:HE2	1:D:4199:GLU:HB2	1.84	0.43
1:D:4572:ALA:O	1:D:4576:ILE:HG12	2.18	0.43
1:C:707:VAL:HG12	1:C:713:SER:HB2	2.00	0.43
1:C:1118:ASP:N	1:C:1118:ASP:OD1	2.51	0.43
1:C:3670:GLU:OE1	1:C:3670:GLU:N	2.44	0.43
1:C:3765:TYR:HH	1:C:4750:ILE:HG22	1.82	0.43
1:C:3887:PHE:O	1:C:3891:LEU:HG	2.18	0.43
1:A:181:HIS:CD2	1:A:196:MET:HB3	2.54	0.43
1:A:2248:ARG:HG3	1:A:2286:LEU:HD21	2.00	0.43
1:A:3821:LYS:O	1:A:3824:LYS:NZ	2.37	0.43
1:A:4865:LYS:O	1:A:4867:GLU:N	2.51	0.43
1:B:76:ARG:HB2	1:B:79:GLN:NE2	2.33	0.43
1:D:649:PHE:HB3	1:D:776:LEU:HD22	2.01	0.43
1:D:1000:ARG:O	1:D:1005:TRP:N	2.50	0.43
1:D:4020:GLN:HA	1:D:4023:MET:HE3	2.01	0.43
1:C:1000:ARG:O	1:C:1005:TRP:N	2.51	0.43
1:C:1580:PHE:CE2	1:C:1592:PRO:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3965:LEU:HA	1:C:3968:TYR:CD1	2.53	0.43
1:B:719:LEU:HD22	1:B:735:GLN:HG2	2.01	0.43
1:B:1124:PHE:HE1	1:B:1139:PHE:HB3	1.84	0.43
1:B:3944:GLU:HG2	1:B:3947:GLY:H	1.83	0.43
1:D:614:VAL:O	1:D:618:GLN:NE2	2.51	0.43
1:D:3674:ILE:CD1	1:D:3769:ARG:HD2	2.43	0.43
1:D:4794:TRP:HA	1:D:4797:VAL:HG12	1.99	0.43
1:A:4671:PHE:HE1	1:A:4716:TRP:HB2	1.84	0.43
1:A:4904:PRO:HG3	1:A:4913:ARG:HH12	1.72	0.43
1:B:3957:VAL:O	1:B:3961:VAL:HG23	2.19	0.43
1:B:4586:PRO:HB3	1:B:4628:VAL:HG21	1.99	0.43
1:B:4935:LEU:HD23	1:B:4935:LEU:HA	1.72	0.43
1:D:119:SER:OG	1:D:120:CYS:N	2.50	0.43
1:D:664:PHE:CD2	1:D:746:CYS:HB2	2.53	0.43
1:D:693:SER:N	1:D:694:PRO:HD2	2.33	0.43
1:C:1720:LEU:HB2	1:C:1724:CYS:SG	2.58	0.43
1:C:4838:VAL:HA	1:C:4841:VAL:HG12	2.01	0.43
1:A:138:GLN:HG2	1:A:139:GLU:N	2.34	0.43
1:A:426:ARG:NE	1:A:505:GLU:O	2.42	0.43
1:A:2158:CYS:O	1:A:2162:ILE:HG12	2.19	0.43
1:A:4929:LEU:HD22	1:A:4929:LEU:HA	1.79	0.43
1:B:1580:PHE:CE2	1:B:1592:PRO:HG2	2.54	0.43
1:B:2766:TRP:HA	1:B:2769:ASP:OD2	2.18	0.43
1:D:2105:TRP:HB3	1:D:2120:MET:HE1	2.01	0.43
1:C:110:ARG:HA	1:C:117:TYR:HA	2.00	0.43
1:C:330:ASP:N	1:C:330:ASP:OD1	2.49	0.43
1:C:2005:GLN:HE22	1:C:3641:LEU:HD22	1.84	0.43
1:C:4716:TRP:CZ2	1:C:4996:ILE:HG21	2.54	0.43
1:A:213:TYR:CG	1:A:337:PRO:HB2	2.53	0.43
1:A:617:ASN:OD1	1:A:618:GLN:HG3	2.19	0.43
1:A:4716:TRP:CZ2	1:A:4996:ILE:HG12	2.54	0.43
1:B:138:GLN:HG2	1:B:139:GLU:N	2.33	0.43
1:B:670:GLU:OE2	1:B:788:LYS:HB2	2.18	0.43
1:B:1719:HIS:NE2	1:B:1802:ILE:HD11	2.34	0.43
1:B:2113:SER:O	1:B:2113:SER:OG	2.31	0.43
1:D:1580:PHE:CE2	1:D:1592:PRO:HG2	2.54	0.43
1:D:2030:ASP:N	1:D:2030:ASP:OD1	2.52	0.43
1:D:2766:TRP:HA	1:D:2769:ASP:OD2	2.19	0.43
1:C:142:THR:OG1	1:C:144:GLU:OE1	2.29	0.43
1:C:635:THR:HB	1:C:1639:LEU:HD23	2.00	0.43
1:C:2030:ASP:N	1:C:2030:ASP:OD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2781:VAL:HG22	1:C:2789:PRO:HD2	2.00	0.43
1:C:4013:LEU:O	1:C:4017:LEU:HD23	2.18	0.43
1:C:4065:PHE:CZ	1:C:4132:PHE:HB2	2.53	0.43
1:C:4158:PRO:HA	1:C:4161:ARG:HD3	2.00	0.43
1:C:4705:VAL:HG22	1:C:4711:PHE:HD1	1.83	0.43
1:C:4922:PHE:O	1:C:4922:PHE:CG	2.70	0.43
1:A:580:GLU:HG2	1:A:583:ILE:HD11	2.00	0.43
1:A:1736:VAL:HG21	1:A:1956:GLU:HG3	2.00	0.43
1:A:1961:PHE:HA	1:A:1964:ARG:HG2	2.00	0.43
1:A:3760:LYS:HZ2	1:A:3760:LYS:CA	2.20	0.43
1:A:3927:GLN:HA	1:A:3930:ILE:HG22	2.00	0.43
1:B:293:LEU:HD13	1:B:298:GLY:N	2.33	0.43
1:B:527:ALA:HA	1:B:563:VAL:HG23	2.01	0.43
1:B:5036:LEU:HD12	1:B:5036:LEU:HA	1.91	0.43
1:D:3804:ILE:HG22	1:D:3805:LEU:HD12	2.00	0.43
1:A:719:LEU:N	1:A:719:LEU:HD23	2.33	0.42
1:A:2030:ASP:N	1:A:2030:ASP:OD1	2.51	0.42
1:B:181:HIS:NE2	1:B:183:SER:HB2	2.34	0.42
1:B:675:LEU:HD12	1:B:675:LEU:HA	1.89	0.42
1:B:1237:TRP:HH2	1:B:1652:GLU:HA	1.84	0.42
1:B:2030:ASP:OD1	1:B:2030:ASP:N	2.52	0.42
1:B:2291:GLN:HG3	1:B:2295:LEU:HG	2.00	0.42
1:B:2794:TYR:HA	1:B:2797:PHE:HD2	1.84	0.42
1:B:4921:PHE:CD1	1:B:4925:ILE:HG21	2.53	0.42
1:D:839:LEU:HD13	1:D:1075:PHE:CZ	2.54	0.42
1:C:695:TYR:O	1:C:697:GLY:N	2.49	0.42
1:C:1072:VAL:HG22	1:C:1195:GLY:HA2	1.99	0.42
1:A:2766:TRP:HA	1:A:2769:ASP:OD2	2.19	0.42
1:A:4060:LYS:NZ	1:A:4064:MET:HB3	2.34	0.42
1:B:1288:UNK:O	1:B:1598:GLN:N	2.45	0.42
1:B:3655:GLU:O	1:B:3658:LYS:HG2	2.19	0.42
1:B:4584:ASP:HA	1:B:4627:MET:HA	1.99	0.42
1:B:4865:LYS:CG	1:B:4875:LYS:HG3	2.48	0.42
1:D:299:LEU:HD23	1:D:299:LEU:HA	1.92	0.42
1:D:2335:LEU:HD22	1:D:2353:VAL:HG21	2.01	0.42
1:D:3767:GLN:NE2	1:D:3804:ILE:HA	2.18	0.42
1:D:3845:ASN:O	1:D:3849:ARG:HG2	2.18	0.42
1:D:4017:LEU:HD12	1:D:4139:ILE:HG13	2.02	0.42
1:C:2738:ARG:HD2	1:C:2819:TRP:HZ2	1.84	0.42
1:C:3964:SER:O	1:C:3968:TYR:CD1	2.72	0.42
1:C:4921:PHE:O	1:C:4925:ILE:HG22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LEU:O	1:A:194:SER:OG	2.25	0.42
1:A:2794:TYR:HA	1:A:2797:PHE:HD2	1.85	0.42
1:A:3754:GLU:OE1	1:A:3754:GLU:CA	2.67	0.42
1:A:3906:GLN:HE22	1:A:3913:ILE:HB	1.83	0.42
1:A:5000:GLU:HA	1:A:5003:HIS:ND1	2.34	0.42
1:B:614:VAL:O	1:B:618:GLN:NE2	2.52	0.42
1:B:4889:VAL:HG12	1:B:4897:ILE:HG22	2.01	0.42
1:D:2773:ASN:OD1	1:D:2775:TRP:NE1	2.50	0.42
1:D:4998:LYS:HB3	1:D:5003:HIS:NE2	2.34	0.42
1:C:560:ILE:HA	1:C:563:VAL:HG12	2.01	0.42
1:C:1158:ASN:HB3	1:C:1182:ILE:HG13	2.00	0.42
1:C:2367:ALA:HB3	1:C:2379:ALA:HB2	2.00	0.42
1:C:4184:MET:HB2	1:C:4190:ILE:HG22	2.00	0.42
1:A:3965:LEU:HA	1:A:3968:TYR:CD1	2.55	0.42
1:A:4674:GLU:HG2	1:A:4715:TYR:HB2	2.02	0.42
1:B:252:VAL:HA	1:B:255:HIS:CG	2.54	0.42
1:B:1087:ARG:HB3	1:B:1223:PHE:CG	2.54	0.42
1:B:2890:LYS:HA	1:B:2890:LYS:HD2	1.81	0.42
1:B:3842:LEU:HD21	1:B:3954:ALA:HB2	2.00	0.42
1:B:4017:LEU:HA	1:B:4020:GLN:HE21	1.85	0.42
1:B:4235:VAL:HG21	1:B:5019:TRP:CH2	2.55	0.42
1:D:15:ARG:HG3	1:D:18:ASP:OD2	2.20	0.42
1:D:3992:PHE:HD2	1:D:3996:PHE:CE2	2.37	0.42
1:D:4222:VAL:HG11	1:D:4950:VAL:HG23	2.00	0.42
1:C:293:LEU:HD13	1:C:298:GLY:H	1.82	0.42
1:C:2737:PRO:HG3	1:C:2891:LYS:HD3	2.00	0.42
1:A:1992:ALA:O	1:A:1996:ARG:HG2	2.20	0.42
1:B:195:PHE:HE2	1:C:2361:PRO:HB3	1.84	0.42
1:B:650:VAL:HB	1:B:777:PHE:CD2	2.54	0.42
1:B:2215:LEU:HD23	1:B:2215:LEU:HA	1.89	0.42
1:B:2243:SER:OG	1:B:2244:ARG:N	2.52	0.42
1:B:4654:ALA:HB2	1:B:4795:TYR:CE1	2.54	0.42
1:C:839:LEU:HD13	1:C:1075:PHE:CZ	2.53	0.42
1:C:1661:ARG:HA	1:C:1661:ARG:HD2	1.85	0.42
1:C:3830:GLN:O	1:C:3833:GLN:HG2	2.19	0.42
1:C:3941:ASP:OD1	1:C:3941:ASP:N	2.49	0.42
1:A:580:GLU:HG3	1:A:620:LEU:HD22	2.02	0.42
1:A:1624:LEU:HD12	1:A:1624:LEU:HA	1.91	0.42
1:A:2737:PRO:HG3	1:A:2891:LYS:HD3	2.01	0.42
1:A:2810:LYS:HG2	1:A:2814:LYS:HE2	2.02	0.42
1:A:4040:ILE:O	1:A:4044:MET:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3809:ASN:O	1:B:3812:VAL:HG12	2.20	0.42
1:B:4552:LEU:HD12	1:B:4552:LEU:HA	1.90	0.42
1:B:4705:VAL:HG22	1:B:4711:PHE:HD1	1.84	0.42
1:D:719:LEU:O	1:D:720:HIS:CG	2.73	0.42
1:D:3988:ALA:O	1:D:3992:PHE:HD1	2.02	0.42
1:D:4679:ARG:NH1	1:D:5017:ARG:HD3	2.34	0.42
1:C:110:ARG:HH21	1:C:115:ARG:HB3	1.85	0.42
1:C:517:GLU:O	1:C:521:LEU:HD23	2.19	0.42
1:C:3888:LEU:HD13	1:C:3891:LEU:HD12	2.01	0.42
1:C:3901:ASN:OD1	1:C:3904:ARG:NH1	2.47	0.42
1:A:1622:GLU:HA	1:A:1626:TRP:CD2	2.54	0.42
1:A:1719:HIS:NE2	1:A:1802:ILE:HD11	2.34	0.42
1:A:2747:ILE:HD13	1:A:2814:LYS:HA	2.01	0.42
1:A:3835:LEU:HD21	1:A:3880:PHE:CZ	2.55	0.42
1:A:4705:VAL:HG22	1:A:4711:PHE:HD1	1.85	0.42
1:B:3771:HIS:O	1:B:3775:ALA:N	2.52	0.42
1:D:162:LYS:O	1:D:164:ARG:NH1	2.52	0.42
1:D:721:LEU:HB3	1:D:728:ARG:HB2	2.01	0.42
1:D:1649:ASP:OD1	1:D:1652:GLU:HB2	2.20	0.42
1:D:3771:HIS:HB3	1:D:3773:ARG:NH1	2.35	0.42
1:D:3989:VAL:HA	1:D:3992:PHE:HB2	2.00	0.42
1:D:4689:THR:HA	1:D:4732:PHE:CE2	2.55	0.42
1:C:2158:CYS:O	1:C:2162:ILE:HG12	2.20	0.42
1:C:4027:LEU:HA	1:C:4030:LEU:HG	2.02	0.42
1:A:614:VAL:O	1:A:618:GLN:NE2	2.53	0.42
1:A:1667:LEU:HD21	1:A:1710:GLY:HA3	2.00	0.42
1:A:1939:MET:N	1:A:1939:MET:SD	2.92	0.42
1:A:4180:ARG:HH21	1:A:4192:ARG:HD3	1.84	0.42
1:A:4960:ILE:HB	1:A:4983:HIS:CD2	2.55	0.42
1:B:416:LYS:HA	1:B:416:LYS:HD3	1.78	0.42
1:B:1720:LEU:HB2	1:B:1724:CYS:SG	2.60	0.42
1:B:2880:GLU:O	1:B:2884:ASN:ND2	2.53	0.42
1:B:4818:MET:SD	1:B:4818:MET:O	2.78	0.42
1:B:4925:ILE:O	1:B:4925:ILE:HD12	2.20	0.42
1:B:4940:PHE:O	1:B:4944:ARG:HB2	2.20	0.42
1:D:213:TYR:CG	1:D:337:PRO:HB2	2.54	0.42
1:D:1939:MET:N	1:D:1939:MET:SD	2.92	0.42
1:D:2142:TYR:CE2	1:D:2197:LEU:HB2	2.55	0.42
1:D:3655:GLU:O	1:D:3658:LYS:HG2	2.19	0.42
1:D:3965:LEU:HA	1:D:3968:TYR:CD1	2.54	0.42
1:D:4093:PHE:O	1:D:4097:MET:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2121:PHE:O	1:C:3725:TYR:OH	2.34	0.42
1:C:2126:ARG:HE	1:C:2126:ARG:HB3	1.73	0.42
1:A:293:LEU:HD13	1:A:298:GLY:N	2.34	0.42
1:A:719:LEU:HD22	1:A:736:HIS:C	2.40	0.42
1:A:1098:GLY:HA3	1:A:1198:GLN:HE22	1.85	0.42
1:A:3793:MET:O	1:A:3797:THR:OG1	2.26	0.42
1:B:277:GLY:HA2	1:B:315:CYS:SG	2.60	0.42
1:B:1098:GLY:HA3	1:B:1198:GLN:HE22	1.85	0.42
1:B:1225:PRO:HG2	1:B:1228:ILE:HB	2.00	0.42
1:B:1622:GLU:HA	1:B:1626:TRP:CD2	2.55	0.42
1:B:1867:GLU:O	1:B:1871:PHE:N	2.37	0.42
1:B:2292:GLU:H	1:B:2295:LEU:HG	1.85	0.42
1:B:2792:ARG:HD2	1:B:2796:THR:HG21	2.01	0.42
1:B:3535:UNK:O	1:B:3537:UNK:N	2.53	0.42
1:B:3804:ILE:HA	1:B:3804:ILE:HD13	1.93	0.42
1:B:3893:GLU:HG3	1:B:3894:GLY:N	2.34	0.42
1:D:1624:LEU:HD12	1:D:1624:LEU:HA	1.92	0.42
1:C:1095:VAL:HB	1:C:1199:VAL:HG13	2.02	0.42
1:C:2880:GLU:O	1:C:2884:ASN:ND2	2.52	0.42
1:C:3662:ILE:O	1:C:3664:THR:N	2.52	0.42
1:C:4978:HIS:O	1:C:4982:GLU:HB2	2.20	0.42
1:A:214:VAL:HG22	1:A:341:TYR:HE1	1.84	0.42
1:A:2175:GLU:O	1:A:2179:ILE:HG12	2.20	0.42
1:A:2182:ILE:O	1:A:2185:ILE:HG12	2.19	0.42
1:A:2881:ASN:HA	1:A:2884:ASN:ND2	2.35	0.42
1:A:3719:ASP:HB3	1:A:3722:TYR:HB3	2.01	0.42
1:B:20:VAL:HG11	1:B:202:MET:HB3	2.02	0.42
1:B:491:ILE:O	1:B:495:ASN:HB2	2.20	0.42
1:B:595:ARG:HH21	1:B:633:LEU:HD21	1.85	0.42
1:B:617:ASN:OD1	1:B:618:GLN:HG3	2.20	0.42
1:B:1143:TRP:HD1	1:B:1164:LEU:HD13	1.84	0.42
1:B:2158:CYS:O	1:B:2162:ILE:HG12	2.20	0.42
1:B:3965:LEU:HA	1:B:3968:TYR:CD1	2.55	0.42
1:B:4218:ILE:HD11	1:B:4985:LEU:HD11	2.01	0.42
1:D:664:PHE:CZ	1:D:779:PRO:HB3	2.55	0.42
1:D:695:TYR:O	1:D:697:GLY:N	2.48	0.42
1:D:1720:LEU:HB2	1:D:1724:CYS:SG	2.60	0.42
1:D:2871:LEU:HA	1:D:2874:MET:HG2	2.02	0.42
1:D:3662:ILE:O	1:D:3664:THR:N	2.52	0.42
1:D:3721:LEU:HD12	1:D:3722:TYR:N	2.35	0.42
1:D:3842:LEU:HD21	1:D:3954:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4892:ARG:NH1	1:C:4896:GLY:HA3	2.34	0.42
1:C:926:GLY:O	1:C:929:LEU:HG	2.20	0.42
1:C:3535:UNK:O	1:C:3537:UNK:N	2.53	0.42
1:C:3986:TRP:HA	1:C:3989:VAL:HG22	2.01	0.42
1:C:4549:VAL:O	1:C:4553:ASN:ND2	2.53	0.42
1:A:262:LEU:HB3	1:A:280:LEU:HD23	2.02	0.41
1:A:357:LEU:HD11	1:A:388:LEU:HD11	2.02	0.41
1:A:717:ASP:OD1	1:A:720:HIS:HB2	2.20	0.41
1:A:719:LEU:O	1:A:720:HIS:CG	2.73	0.41
1:A:2099:SER:O	1:A:2103:VAL:HG23	2.20	0.41
1:A:2330:ARG:HA	1:A:2330:ARG:HD2	1.81	0.41
1:A:2368:LEU:HD13	1:A:2376:LEU:HG	2.02	0.41
1:A:4095:LYS:HB3	1:A:4095:LYS:HE2	1.69	0.41
1:A:4184:MET:HB2	1:A:4190:ILE:HG22	2.01	0.41
1:B:482:GLY:O	1:B:484:LEU:HD12	2.18	0.41
1:B:647:ASN:HB3	1:B:822:ARG:NH1	2.35	0.41
1:B:717:ASP:OD1	1:B:720:HIS:HB2	2.20	0.41
1:B:1730:MET:SD	1:B:1772:ARG:NH1	2.93	0.41
1:B:2191:PHE:HZ	1:B:2239:PHE:HA	1.85	0.41
1:B:4572:ALA:O	1:B:4576:ILE:HG12	2.20	0.41
1:B:4936:ILE:HD12	1:B:4936:ILE:HA	1.79	0.41
1:D:138:GLN:HG2	1:D:139:GLU:H	1.85	0.41
1:D:1228:ILE:HG23	1:D:1229:ASN:N	2.34	0.41
1:D:1685:LEU:HD23	1:D:1718:ILE:HD12	2.02	0.41
1:D:2005:GLN:HE22	1:D:3641:LEU:HD22	1.85	0.41
1:D:3890:LEU:HA	1:D:3893:GLU:HB3	2.02	0.41
1:C:197:GLN:NE2	1:C:198:THR:O	2.53	0.41
1:C:322:LYS:HD2	1:C:322:LYS:HA	1.88	0.41
1:C:421:PHE:HE1	1:C:436:LEU:HD21	1.84	0.41
1:C:523:TYR:O	1:C:526:LEU:HG	2.20	0.41
1:C:1225:PRO:HG2	1:C:1228:ILE:HB	2.02	0.41
1:C:1622:GLU:HA	1:C:1626:TRP:CD2	2.55	0.41
1:C:1624:LEU:HD12	1:C:1624:LEU:HA	1.91	0.41
1:C:4093:PHE:O	1:C:4097:MET:HG2	2.19	0.41
1:C:4572:ALA:O	1:C:4576:ILE:HG12	2.20	0.41
1:C:4959:PHE:HE2	1:C:4985:LEU:HD21	1.84	0.41
1:C:4998:LYS:HB3	1:C:5003:HIS:NE2	2.35	0.41
1:A:20:VAL:HG11	1:A:202:MET:HB3	2.02	0.41
1:A:1186:ASP:OD1	1:A:1186:ASP:N	2.50	0.41
1:A:1689:VAL:HG13	1:A:1690:ASP:H	1.84	0.41
1:B:4040:ILE:O	1:B:4044:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4063:ASP:OD2	1:B:4067:LYS:NZ	2.47	0.41
1:B:4878:ASP:O	1:B:4881:THR:OG1	2.29	0.41
1:B:4957:LYS:HA	1:B:4957:LYS:HD2	1.87	0.41
1:B:4993:MET:SD	1:B:4997:ASN:ND2	2.93	0.41
1:D:229:GLU:HG2	1:D:247:TYR:HB3	2.02	0.41
1:D:1288:UNK:O	1:D:1598:GLN:N	2.44	0.41
1:D:2737:PRO:HG3	1:D:2891:LYS:HD3	2.02	0.41
1:C:40:GLU:OE2	1:C:44:ASN:N	2.48	0.41
1:C:104:GLY:H	1:C:150:MET:HB3	1.85	0.41
1:C:181:HIS:CD2	1:C:196:MET:HB2	2.55	0.41
1:C:221:ARG:HB3	1:C:391:THR:HG22	2.02	0.41
1:C:688:LEU:HD21	1:C:777:PHE:HE1	1.83	0.41
1:C:1078:GLU:HG3	1:C:1237:TRP:HE1	1.85	0.41
1:C:2881:ASN:HA	1:C:2884:ASN:ND2	2.36	0.41
1:C:4010:ILE:HG13	1:C:4011:GLU:N	2.35	0.41
1:C:4031:LEU:HD23	1:C:4031:LEU:H	1.85	0.41
1:C:4946:GLN:O	1:C:4949:GLN:N	2.53	0.41
1:A:1574:PRO:HD2	1:A:1577:ALA:HB2	2.01	0.41
1:A:4577:LEU:HD11	1:A:4807:PHE:HD1	1.86	0.41
1:A:4794:TRP:HA	1:A:4797:VAL:HG12	2.02	0.41
1:A:4867:GLU:CG	1:A:4867:GLU:O	2.68	0.41
1:B:24:CYS:SG	1:B:35:LEU:HB2	2.60	0.41
1:B:1240:LYS:NZ	1:B:1242:LEU:HB3	2.35	0.41
1:B:4794:TRP:HA	1:B:4797:VAL:HG12	2.02	0.41
1:D:260:TRP:CZ3	1:D:284:HIS:HD2	2.38	0.41
1:D:3723:MET:HE1	1:D:3793:MET:HA	2.02	0.41
1:D:3927:GLN:O	1:D:3930:ILE:HG22	2.20	0.41
1:C:564:LEU:HA	1:C:567:VAL:HG12	2.02	0.41
1:C:670:GLU:H	1:C:740:PRO:HB3	1.85	0.41
1:C:710:ASP:OD1	1:C:713:SER:OG	2.31	0.41
1:C:750:LEU:HD21	1:C:777:PHE:HE2	1.85	0.41
1:C:3655:GLU:O	1:C:3658:LYS:HG2	2.20	0.41
1:A:1847:THR:O	1:A:1850:VAL:HG12	2.19	0.41
1:B:70:GLU:HG2	1:B:108:LEU:HD23	2.03	0.41
1:B:505:GLU:HA	1:B:511:ALA:HB3	2.01	0.41
1:B:4207:MET:HE1	1:B:4209:GLN:HB3	2.03	0.41
1:B:4577:LEU:HD11	1:B:4807:PHE:CD1	2.55	0.41
1:B:4966:ASP:N	1:B:4966:ASP:OD1	2.53	0.41
1:D:76:ARG:H	1:D:76:ARG:HD3	1.86	0.41
1:D:1719:HIS:NE2	1:D:1802:ILE:HD11	2.35	0.41
1:D:3996:PHE:HA	1:D:3999:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1749:PRO:HA	1:C:1750:PRO:HD3	1.96	0.41
1:C:1931:LEU:HD22	1:C:1935:VAL:HG11	2.03	0.41
1:C:1992:ALA:O	1:C:1996:ARG:HG2	2.19	0.41
1:C:4863:TYR:CE2	1:C:4876:CYS:SG	3.13	0.41
1:C:4966:ASP:OD1	1:C:4966:ASP:N	2.54	0.41
1:A:299:LEU:HG	1:A:378:LEU:HG	2.02	0.41
1:A:4037:ASN:HB2	1:A:5035:GLN:NE2	2.35	0.41
1:A:4550:LYS:HA	1:A:4553:ASN:HD21	1.86	0.41
1:A:4679:ARG:NH1	1:A:5017:ARG:HD3	2.35	0.41
1:A:4869:GLU:O	1:A:4870:ASP:O	2.38	0.41
1:B:2099:SER:O	1:B:2103:VAL:HG23	2.21	0.41
1:B:2182:ILE:O	1:B:2185:ILE:HG12	2.19	0.41
1:B:2287:ALA:HA	1:B:2290:LEU:HG	2.01	0.41
1:B:2775:TRP:CE2	1:B:2786:LYS:HE3	2.56	0.41
1:B:3406:UNK:O	1:B:3410:UNK:N	2.54	0.41
1:D:926:GLY:O	1:D:929:LEU:HG	2.20	0.41
1:D:2099:SER:O	1:D:2103:VAL:HG23	2.21	0.41
1:D:4674:GLU:HG2	1:D:4715:TYR:HB2	2.02	0.41
1:C:221:ARG:NH1	1:C:253:CYS:O	2.46	0.41
1:C:686:TRP:CZ3	1:C:777:PHE:HB3	2.54	0.41
1:C:4223:ASN:ND2	1:C:4946:GLN:CD	2.74	0.41
1:A:2252:ASP:N	1:A:2252:ASP:OD1	2.53	0.41
1:A:2606:UNK:O	1:A:2608:UNK:N	2.53	0.41
1:B:149:THR:CG2	1:B:151:HIS:HE1	2.33	0.41
1:B:515:TRP:HA	1:B:518:ILE:HG22	2.03	0.41
1:B:517:GLU:O	1:B:521:LEU:HD23	2.20	0.41
1:B:1083:VAL:HG21	1:B:1088:TRP:NE1	2.35	0.41
1:B:1574:PRO:HD2	1:B:1577:ALA:HB2	2.01	0.41
1:B:1649:ASP:OD1	1:B:1652:GLU:HB2	2.20	0.41
1:B:2881:ASN:HA	1:B:2884:ASN:ND2	2.35	0.41
1:B:3644:LEU:HG	1:B:3645:PRO:HD2	2.03	0.41
1:B:4553:ASN:HA	1:B:4556:SER:HB3	2.02	0.41
1:B:4821:LYS:CG	1:B:4822:THR:N	2.83	0.41
1:B:4872:PRO:CD	1:B:4873:ASP:H	2.34	0.41
1:D:1667:LEU:HD12	1:D:1714:LEU:HD12	2.02	0.41
1:D:1854:PHE:HD1	1:D:1858:ASP:HB3	1.85	0.41
1:D:4181:ILE:HG12	1:D:4195:PHE:CE1	2.55	0.41
1:C:705:ASN:ND2	1:C:709:ASP:OD2	2.53	0.41
1:C:873:LYS:HA	1:C:873:LYS:HD3	1.93	0.41
1:C:3644:LEU:HG	1:C:3645:PRO:HD2	2.02	0.41
1:A:4093:PHE:O	1:A:4097:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4572:ALA:O	1:A:4576:ILE:HG12	2.20	0.41
1:B:926:GLY:O	1:B:929:LEU:HG	2.20	0.41
1:B:4068:LEU:O	1:B:4071:ILE:HG22	2.20	0.41
1:D:648:ILE:HD13	1:D:779:PRO:HG2	2.02	0.41
1:D:2880:GLU:O	1:D:2884:ASN:ND2	2.53	0.41
1:D:3406:UNK:O	1:D:3410:UNK:N	2.54	0.41
1:D:4091:LYS:HD3	1:D:4091:LYS:HA	1.91	0.41
1:C:2890:LYS:HA	1:C:2890:LYS:HD2	1.80	0.41
1:C:3843:ASP:HB3	1:C:3846:ALA:HB3	2.03	0.41
1:A:517:GLU:O	1:A:521:LEU:HD23	2.20	0.41
1:A:1087:ARG:HB3	1:A:1223:PHE:CG	2.56	0.41
1:A:4207:MET:HE1	1:A:4209:GLN:HB3	2.03	0.41
1:D:1101:ARG:HH21	1:D:1115:LEU:HG	1.85	0.41
1:D:1658:ASP:OD1	1:D:1658:ASP:N	2.54	0.41
1:D:2368:LEU:HD13	1:D:2376:LEU:HD21	2.03	0.41
1:D:3941:ASP:OD1	1:D:3941:ASP:N	2.46	0.41
1:D:4207:MET:HE1	1:D:4210:VAL:HG23	2.02	0.41
1:C:24:CYS:SG	1:C:35:LEU:HB2	2.60	0.41
1:C:1087:ARG:HD3	1:C:1223:PHE:CE1	2.56	0.41
1:C:3668:SER:O	1:C:3672:ARG:NH2	2.46	0.41
1:C:3903:LEU:HD12	1:C:3903:LEU:HA	1.91	0.41
1:C:4798:MET:HB3	1:C:4812:HIS:NE2	2.35	0.41
1:C:4863:TYR:CD2	1:C:4876:CYS:SG	3.14	0.41
1:A:926:GLY:O	1:A:929:LEU:HG	2.20	0.41
1:A:1072:VAL:HG22	1:A:1195:GLY:HA2	2.02	0.41
1:A:2348:GLU:OE1	1:A:3849:ARG:NE	2.54	0.41
1:A:3406:UNK:O	1:A:3410:UNK:N	2.54	0.41
1:A:3535:UNK:O	1:A:3537:UNK:N	2.53	0.41
1:A:3760:LYS:HZ3	1:A:3760:LYS:CB	2.28	0.41
1:A:3761:GLN:OE1	1:A:3764:LEU:HG	2.21	0.41
1:A:4691:GLN:NE2	1:A:4692:PRO:HD2	2.36	0.41
1:A:4860:ARG:HD2	1:A:4861:LYS:N	2.36	0.41
1:B:77:ALA:HA	1:B:80:GLU:CD	2.40	0.41
1:B:1072:VAL:HG22	1:B:1195:GLY:HA2	2.02	0.41
1:B:1866:ILE:HG22	1:B:1866:ILE:O	2.21	0.41
1:B:2310:CYS:O	1:B:2314:LEU:HG	2.21	0.41
1:B:3889:GLN:HB2	1:B:3964:SER:HA	2.03	0.41
1:B:4020:GLN:O	1:B:4024:VAL:HG22	2.21	0.41
1:B:4691:GLN:NE2	1:B:4692:PRO:HD2	2.36	0.41
1:B:4918:ILE:HD13	1:B:4918:ILE:HA	1.89	0.41
1:B:4985:LEU:CB	2:B:5101:ACP:N1	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:617:ASN:OD1	1:D:618:GLN:HG3	2.20	0.41
1:D:1866:ILE:O	1:D:1866:ILE:HG22	2.21	0.41
1:D:2881:ASN:HA	1:D:2884:ASN:ND2	2.35	0.41
1:D:3535:UNK:O	1:D:3537:UNK:N	2.53	0.41
1:D:3809:ASN:O	1:D:3812:VAL:HG12	2.21	0.41
1:D:4031:LEU:HD23	1:D:4031:LEU:H	1.85	0.41
1:D:4065:PHE:CZ	1:D:4132:PHE:HB2	2.56	0.41
1:D:4937:ILE:HD11	1:C:4934:GLY:HA2	1.97	0.41
1:C:621:ILE:HD13	1:C:621:ILE:HA	1.92	0.41
1:C:649:PHE:HD1	1:C:776:LEU:HD13	1.86	0.41
1:C:956:PRO:HB2	1:C:958:THR:HG22	2.03	0.41
1:C:1039:LEU:HD23	1:C:1039:LEU:HA	1.85	0.41
1:C:2191:PHE:HZ	1:C:2239:PHE:HB2	1.86	0.41
1:C:2606:UNK:O	1:C:2608:UNK:N	2.54	0.41
1:C:3896:ASN:O	1:C:3896:ASN:ND2	2.51	0.41
1:C:4700:GLN:HE21	1:C:4703:ARG:HE	1.68	0.41
1:C:4859:PHE:HZ	1:C:4912:TYR:HD1	1.69	0.41
1:C:4929:LEU:O	1:C:4933:GLN:HB2	2.21	0.41
1:A:523:TYR:O	1:A:526:LEU:HG	2.21	0.41
1:A:695:TYR:O	1:A:697:GLY:N	2.48	0.41
1:A:705:ASN:ND2	1:A:709:ASP:OD2	2.53	0.41
1:A:1608:MET:HA	1:A:1609:PRO:HD3	1.97	0.41
1:A:3913:ILE:HD13	1:A:3913:ILE:HA	1.91	0.41
1:A:4049:VAL:HA	1:A:4163:PHE:HZ	1.86	0.41
1:B:19:GLU:HB2	1:B:206:CYS:HB3	2.02	0.41
1:B:4700:GLN:HE21	1:B:4703:ARG:HE	1.69	0.41
1:D:108:LEU:HD13	1:D:147:TRP:NE1	2.36	0.41
1:D:372:LEU:HD11	1:D:374:LYS:HZ2	1.85	0.41
1:D:551:LEU:HD21	1:D:589:LEU:HD22	2.03	0.41
1:D:2355:ARG:O	1:D:2358:ILE:HG22	2.21	0.41
1:C:464:LYS:HE3	1:C:464:LYS:HB2	1.96	0.41
1:C:1166:GLY:HA3	1:C:1216:ILE:HD13	2.03	0.41
1:C:3677:LEU:HD22	1:C:3697:PRO:HB2	2.02	0.41
1:C:3751:VAL:HG23	1:C:3755:GLU:HB3	2.03	0.41
1:A:1866:ILE:HG22	1:A:1866:ILE:O	2.21	0.40
1:A:2310:CYS:O	1:A:2314:LEU:HG	2.21	0.40
1:A:2880:GLU:O	1:A:2884:ASN:ND2	2.55	0.40
1:A:3986:TRP:HA	1:A:3989:VAL:HG22	2.02	0.40
1:B:614:VAL:HG12	1:B:2169:GLN:HG2	2.03	0.40
1:B:1118:ASP:OD1	1:B:1118:ASP:N	2.53	0.40
1:B:4027:LEU:HA	1:B:4030:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4674:GLU:HG2	1:B:4715:TYR:HB2	2.04	0.40
1:D:1225:PRO:HG2	1:D:1228:ILE:HB	2.03	0.40
1:D:1749:PRO:HA	1:D:1750:PRO:HD3	1.96	0.40
1:D:4160:LEU:HA	1:D:4163:PHE:HD1	1.86	0.40
1:D:4582:VAL:HG21	1:C:4860:ARG:NH1	2.35	0.40
1:D:4838:VAL:HA	1:D:4841:VAL:HG12	2.04	0.40
1:C:3406:UNK:O	1:C:3410:UNK:N	2.54	0.40
1:C:3712:GLU:O	1:C:3712:GLU:HG2	2.21	0.40
1:C:4662:ASN:O	1:C:4666:VAL:HB	2.21	0.40
1:A:661:LYS:HG2	1:A:749:ASP:HA	2.01	0.40
1:A:1676:LEU:HA	1:A:1725:ARG:HH22	1.86	0.40
1:A:3492:UNK:O	1:A:3495:UNK:O	2.40	0.40
1:A:4702:ASP:HA	1:A:4778:TRP:HE1	1.86	0.40
1:B:1929:MET:SD	1:B:1929:MET:N	2.94	0.40
1:B:2447:LYS:HD2	1:B:2447:LYS:HA	1.80	0.40
1:B:4068:LEU:HD12	1:B:4111:LEU:HD11	2.03	0.40
1:B:4865:LYS:HA	1:B:4865:LYS:CE	2.23	0.40
1:D:14:LEU:HD23	1:D:14:LEU:HA	1.86	0.40
1:D:573:GLU:O	1:D:577:ILE:HG12	2.20	0.40
1:D:595:ARG:HH21	1:D:633:LEU:HD21	1.87	0.40
1:D:635:THR:HB	1:D:1639:LEU:HD23	2.03	0.40
1:D:2878:LEU:HD13	1:D:2926:LEU:HD23	2.03	0.40
1:C:717:ASP:OD1	1:C:720:HIS:HB2	2.21	0.40
1:C:2175:GLU:O	1:C:2179:ILE:HG12	2.21	0.40
1:C:4011:GLU:HG2	1:C:4012:LEU:N	2.37	0.40
1:C:4055:VAL:HG22	1:C:4059:LEU:HG	2.02	0.40
1:A:82:LEU:HD21	1:A:143:GLY:C	2.41	0.40
1:A:1220:GLN:NE2	1:B:3527:UNK:O	2.47	0.40
1:A:1224:GLU:HG3	1:A:1225:PRO:HD2	2.04	0.40
1:A:3754:GLU:OE1	1:A:3754:GLU:HA	2.21	0.40
1:A:3887:PHE:CZ	1:A:3891:LEU:HD21	2.57	0.40
1:A:3935:TRP:HD1	1:D:76:ARG:NH1	2.14	0.40
1:B:584:LYS:HE3	1:B:584:LYS:HB2	1.88	0.40
1:B:2192:TYR:CD1	1:B:2242:ILE:HD13	2.56	0.40
1:B:4095:LYS:HB3	1:B:4095:LYS:HE2	1.69	0.40
1:B:4838:VAL:HA	1:B:4841:VAL:HG12	2.04	0.40
1:B:4859:PHE:HZ	1:B:4912:TYR:HD1	1.70	0.40
1:D:2158:CYS:O	1:D:2162:ILE:HG12	2.21	0.40
1:D:2386:ILE:HD13	1:D:2386:ILE:HA	1.92	0.40
1:D:2606:UNK:O	1:D:2608:UNK:N	2.54	0.40
1:D:3771:HIS:O	1:D:3775:ALA:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3835:LEU:HD21	1:D:3880:PHE:CZ	2.57	0.40
1:D:4920:PHE:CZ	1:D:4924:VAL:HG11	2.55	0.40
1:D:4937:ILE:CD1	1:C:4934:GLY:CA	2.95	0.40
1:C:28:VAL:HG11	1:C:189:LEU:HD21	2.03	0.40
1:C:1676:LEU:HA	1:C:1725:ARG:HH22	1.86	0.40
1:C:1731:LEU:HA	1:C:1772:ARG:HH12	1.86	0.40
1:C:4022:ASP:O	1:C:4025:VAL:HG12	2.20	0.40
1:C:4104:THR:OG1	1:C:4107:GLU:OE1	2.37	0.40
1:A:4869:GLU:HB3	1:A:4870:ASP:H	1.35	0.40
1:B:221:ARG:NH2	1:B:253:CYS:HA	2.33	0.40
1:B:2296:GLU:HA	1:B:2299:VAL:HG12	2.02	0.40
1:B:2606:UNK:O	1:B:2608:UNK:N	2.54	0.40
1:B:3887:PHE:O	1:B:3891:LEU:HG	2.22	0.40
1:D:523:TYR:O	1:D:526:LEU:HG	2.21	0.40
1:D:649:PHE:HD1	1:D:776:LEU:HD13	1.86	0.40
1:D:664:PHE:HD2	1:D:746:CYS:HB2	1.87	0.40
1:D:3887:PHE:CZ	1:D:3891:LEU:HD21	2.57	0.40
1:C:1128:ARG:HG3	1:C:1130:GLN:HG2	2.03	0.40
1:A:661:LYS:HB3	1:A:808:TYR:CD2	2.57	0.40
1:A:2191:PHE:HZ	1:A:2239:PHE:HB2	1.86	0.40
1:A:3804:ILE:HD13	1:A:3804:ILE:HA	1.92	0.40
1:A:4838:VAL:O	1:A:4841:VAL:HG12	2.21	0.40
1:A:4933:GLN:HE21	1:D:4930:ALA:HA	1.86	0.40
1:B:299:LEU:HD23	1:B:299:LEU:HA	1.91	0.40
1:B:652:ARG:HH11	1:B:773:LEU:HD12	1.87	0.40
1:B:695:TYR:O	1:B:697:GLY:N	2.51	0.40
1:B:1252:HIS:HE1	1:B:1254:HIS:CE1	2.40	0.40
1:B:2348:GLU:OE1	1:B:3849:ARG:NE	2.53	0.40
1:B:3771:HIS:HB3	1:B:3773:ARG:NH1	2.36	0.40
1:B:3778:MET:HA	1:B:3781:GLN:HG2	2.03	0.40
1:B:4716:TRP:CH2	1:B:4996:ILE:HG12	2.56	0.40
1:B:4936:ILE:HG22	1:B:4937:ILE:HD13	2.03	0.40
1:B:4998:LYS:HB3	1:B:5003:HIS:NE2	2.37	0.40
1:D:80:GLU:OE2	1:D:80:GLU:N	2.54	0.40
1:D:479:GLN:HE21	1:D:539:LEU:HD22	1.87	0.40
1:D:744:VAL:HG13	1:D:757:PHE:HE1	1.86	0.40
1:D:1139:PHE:HZ	1:D:1177:THR:HG22	1.87	0.40
1:D:2126:ARG:HE	1:D:2126:ARG:HB3	1.73	0.40
1:D:4142:ASN:HA	1:D:4145:VAL:HG12	2.04	0.40
1:D:4183:ILE:HG23	1:D:5021:PHE:HB2	2.04	0.40
1:D:4838:VAL:O	1:D:4841:VAL:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:GLY:HA2	1:C:315:CYS:SG	2.62	0.40
1:C:3830:GLN:HA	1:C:3833:GLN:HG2	2.04	0.40
1:C:5031:GLN:HE21	1:C:5031:GLN:HB3	1.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3191/5037 (63%)	2943 (92%)	243 (8%)	5 (0%)	47	81
1	B	3191/5037 (63%)	2934 (92%)	247 (8%)	10 (0%)	41	76
1	C	3191/5037 (63%)	2929 (92%)	254 (8%)	8 (0%)	41	76
1	D	3191/5037 (63%)	2932 (92%)	253 (8%)	6 (0%)	47	81
All	All	12764/20148 (63%)	11738 (92%)	997 (8%)	29 (0%)	50	81

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4866	SER
1	A	4870	ASP
1	B	3662	ILE
1	B	3666	ASP
1	B	4867	GLU
1	D	2292	GLU
1	D	3751	VAL
1	D	4867	GLU
1	C	2292	GLU
1	C	4870	ASP
1	C	4875	LYS
1	A	1708	ARG

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Mol	Chain	Res	Type
1	B	1708	ARG
1	B	3668	SER
1	B	4869	GLU
1	D	1708	ARG
1	C	1708	ARG
1	C	3685	GLU
1	C	4867	GLU
1	B	4868	ASP
1	B	3751	VAL
1	B	4866	SER
1	D	1840	PRO
1	B	1840	PRO
1	A	1840	PRO
1	C	1840	PRO
1	A	3774	GLY
1	D	4666	VAL
1	C	4666	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2452/3264 (75%)	2421 (99%)	31 (1%)	69	82
1	B	2452/3264 (75%)	2419 (99%)	33 (1%)	69	82
1	C	2455/3264 (75%)	2425 (99%)	30 (1%)	71	84
1	D	2458/3264 (75%)	2431 (99%)	27 (1%)	73	85
All	All	9817/13056 (75%)	9696 (99%)	121 (1%)	72	84

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	ARG
1	A	719	LEU
1	A	822	ARG
1	A	830	ARG

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Mol	Chain	Res	Type
1	A	2773	ASN
1	A	3752	SER
1	A	3758	MET
1	A	3759	GLU
1	A	3760	LYS
1	A	3766	GLN
1	A	3769	ARG
1	A	3770	LEU
1	A	3771	HIS
1	A	4668	LEU
1	A	4859	PHE
1	A	4860	ARG
1	A	4861	LYS
1	A	4865	LYS
1	A	4867	GLU
1	A	4868	ASP
1	A	4921	PHE
1	A	4924	VAL
1	A	4925	ILE
1	A	4927	ILE
1	A	4928	LEU
1	A	4929	LEU
1	A	4931	ILE
1	A	4932	ILE
1	A	4933	GLN
1	A	4938	ASP
1	A	5031	GLN
1	B	76	ARG
1	B	151	HIS
1	B	275	ARG
1	B	822	ARG
1	B	3663	LEU
1	B	3664	THR
1	B	3666	ASP
1	B	3751	VAL
1	B	3758	MET
1	B	3760	LYS
1	B	3769	ARG
1	B	3773	ARG
1	B	3928	GLU
1	B	4000	MET
1	B	4180	ARG

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Mol	Chain	Res	Type
1	B	4795	TYR
1	B	4808	PHE
1	B	4809	PHE
1	B	4816	ILE
1	B	4861	LYS
1	B	4865	LYS
1	B	4867	GLU
1	B	4869	GLU
1	B	4923	PHE
1	B	4925	ILE
1	B	4935	LEU
1	B	4936	ILE
1	B	4937	ILE
1	B	4938	ASP
1	B	4943	LEU
1	B	4944	ARG
1	B	4957	LYS
1	B	5031	GLN
1	D	76	ARG
1	D	275	ARG
1	D	822	ARG
1	D	830	ARG
1	D	2355	ARG
1	D	3675	ASP
1	D	3676	ASP
1	D	3759	GLU
1	D	3773	ARG
1	D	4085	ARG
1	D	4820	VAL
1	D	4821	LYS
1	D	4861	LYS
1	D	4865	LYS
1	D	4867	GLU
1	D	4869	GLU
1	D	4871	GLU
1	D	4918	ILE
1	D	4928	LEU
1	D	4929	LEU
1	D	4931	ILE
1	D	4932	ILE
1	D	4933	GLN
1	D	4935	LEU

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Mol	Chain	Res	Type
1	D	4936	ILE
1	D	4985	LEU
1	D	5031	GLN
1	C	163	VAL
1	C	275	ARG
1	C	822	ARG
1	C	830	ARG
1	C	3755	GLU
1	C	3759	GLU
1	C	3760	LYS
1	C	3761	GLN
1	C	3773	ARG
1	C	3896	ASN
1	C	3928	GLU
1	C	3965	LEU
1	C	4180	ARG
1	C	4574	ASN
1	C	4719	PHE
1	C	4861	LYS
1	C	4863	TYR
1	C	4865	LYS
1	C	4868	ASP
1	C	4875	LYS
1	C	4923	PHE
1	C	4931	ILE
1	C	4932	ILE
1	C	4933	GLN
1	C	4936	ILE
1	C	4937	ILE
1	C	4938	ASP
1	C	4944	ARG
1	C	4946	GLN
1	C	5031	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	536	ASN
1	A	634	GLN
1	A	735	GLN
1	A	2095	GLN
1	A	4223	ASN

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Mol	Chain	Res	Type
1	A	4933	GLN
1	A	4946	GLN
1	B	536	ASN
1	B	634	GLN
1	B	3809	ASN
1	B	3927	GLN
1	B	4020	GLN
1	B	4574	ASN
1	B	5035	GLN
1	D	151	HIS
1	D	536	ASN
1	D	2180	GLN
1	D	3761	GLN
1	D	3767	GLN
1	D	3927	GLN
1	D	4574	ASN
1	C	536	ASN
1	C	2107	GLN
1	C	3761	GLN
1	C	4223	ASN
1	C	4574	ASN
1	C	4933	GLN
1	C	4946	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 9 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	ACP	C	5101	4	27,33,33	1.33	5 (18%)	32,52,52	1.50	4 (12%)
2	ACP	A	5101	4	27,33,33	1.35	5 (18%)	32,52,52	1.51	5 (15%)
2	ACP	D	5101	4	27,33,33	1.37	5 (18%)	32,52,52	1.46	4 (12%)
2	ACP	B	5101	4	27,33,33	0.89	1 (3%)	32,52,52	0.84	2 (6%)

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	ACP	C	5101	4	-	7/15/38/38	0/3/3/3
2	ACP	A	5101	4	-	5/15/38/38	0/3/3/3
2	ACP	D	5101	4	-	9/15/38/38	0/3/3/3
2	ACP	B	5101	4	-	8/15/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5101	ACP	PG-O3G	2.87	1.61	1.54
2	C	5101	ACP	PG-O3G	2.86	1.61	1.54
2	C	5101	ACP	PG-O2G	2.85	1.61	1.54
2	D	5101	ACP	PG-O3G	2.83	1.61	1.54
2	D	5101	ACP	PG-O2G	2.83	1.61	1.54
2	A	5101	ACP	PG-O2G	2.83	1.61	1.54
2	D	5101	ACP	PB-O3A	2.75	1.61	1.58
2	A	5101	ACP	PB-O3A	2.61	1.61	1.58
2	D	5101	ACP	C5-C4	2.49	1.47	1.40
2	B	5101	ACP	PB-O2B	-2.40	1.50	1.56
2	C	5101	ACP	PB-O3A	2.39	1.61	1.58
2	A	5101	ACP	C5-C4	2.31	1.47	1.40
2	C	5101	ACP	C5-C4	2.26	1.46	1.40
2	D	5101	ACP	PB-O2B	2.15	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5101	ACP	PB-O2B	2.14	1.61	1.56
2	C	5101	ACP	PB-O2B	2.12	1.61	1.56

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5101	ACP	PB-O3A-PA	-4.14	119.42	132.56
2	A	5101	ACP	PB-O3A-PA	-4.07	119.65	132.56
2	D	5101	ACP	PB-O3A-PA	-3.87	120.27	132.56
2	A	5101	ACP	N3-C2-N1	-3.70	122.90	128.68
2	C	5101	ACP	N3-C2-N1	-3.65	122.98	128.68
2	D	5101	ACP	C3'-C2'-C1'	3.43	106.14	100.98
2	C	5101	ACP	C3'-C2'-C1'	3.33	105.99	100.98
2	A	5101	ACP	C3'-C2'-C1'	3.31	105.97	100.98
2	D	5101	ACP	N3-C2-N1	-3.20	123.68	128.68
2	D	5101	ACP	C4-C5-N7	-2.72	106.57	109.40
2	A	5101	ACP	C4-C5-N7	-2.52	106.77	109.40
2	C	5101	ACP	C4-C5-N7	-2.51	106.78	109.40
2	B	5101	ACP	O1G-PG-C3B	-2.28	106.32	111.24
2	B	5101	ACP	C5-C6-N6	2.26	123.79	120.35
2	A	5101	ACP	C2-N1-C6	2.05	122.25	118.75

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5101	ACP	C5'-O5'-PA-O1A
2	A	5101	ACP	C5'-O5'-PA-O3A
2	B	5101	ACP	PG-C3B-PB-O1B
2	B	5101	ACP	PG-C3B-PB-O3A
2	B	5101	ACP	C5'-O5'-PA-O2A
2	B	5101	ACP	C5'-O5'-PA-O3A
2	B	5101	ACP	C4'-C5'-O5'-PA
2	D	5101	ACP	PG-C3B-PB-O1B
2	D	5101	ACP	PG-C3B-PB-O3A
2	D	5101	ACP	C5'-O5'-PA-O1A
2	D	5101	ACP	C5'-O5'-PA-O2A
2	D	5101	ACP	C5'-O5'-PA-O3A
2	D	5101	ACP	C4'-C5'-O5'-PA
2	C	5101	ACP	PB-C3B-PG-O1G
2	C	5101	ACP	PB-C3B-PG-O2G
2	C	5101	ACP	PB-C3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
2	C	5101	ACP	PG-C3B-PB-O1B
2	C	5101	ACP	PG-C3B-PB-O2B
2	C	5101	ACP	PG-C3B-PB-O3A
2	B	5101	ACP	O4'-C4'-C5'-O5'
2	B	5101	ACP	C3'-C4'-C5'-O5'
2	C	5101	ACP	O4'-C4'-C5'-O5'
2	B	5101	ACP	PG-C3B-PB-O2B
2	D	5101	ACP	PG-C3B-PB-O2B
2	D	5101	ACP	C3'-C4'-C5'-O5'
2	A	5101	ACP	C4'-C5'-O5'-PA
2	A	5101	ACP	PG-C3B-PB-O1B
2	D	5101	ACP	O4'-C4'-C5'-O5'
2	A	5101	ACP	C3'-C4'-C5'-O5'

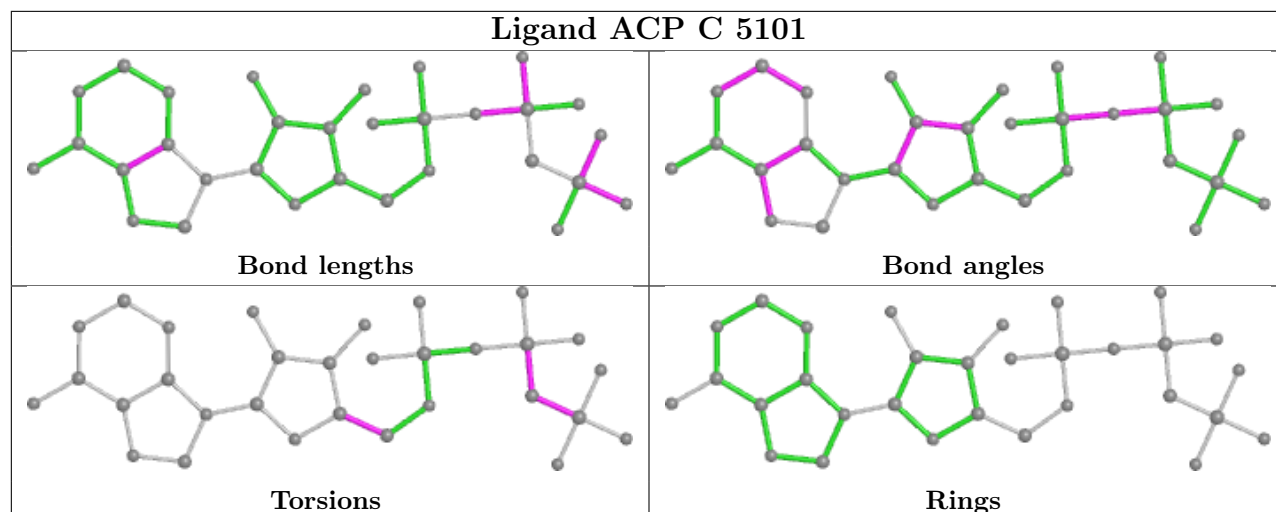
There are no ring outliers.

4 monomers are involved in 22 short contacts:

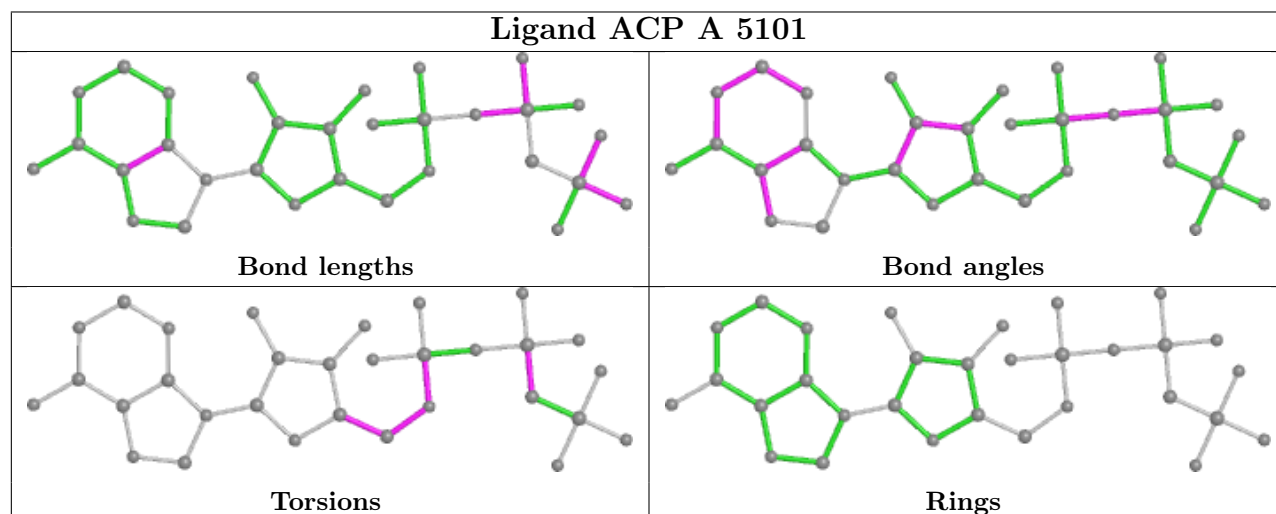
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	5101	ACP	3	0
2	A	5101	ACP	7	0
2	D	5101	ACP	8	0
2	B	5101	ACP	4	0

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.

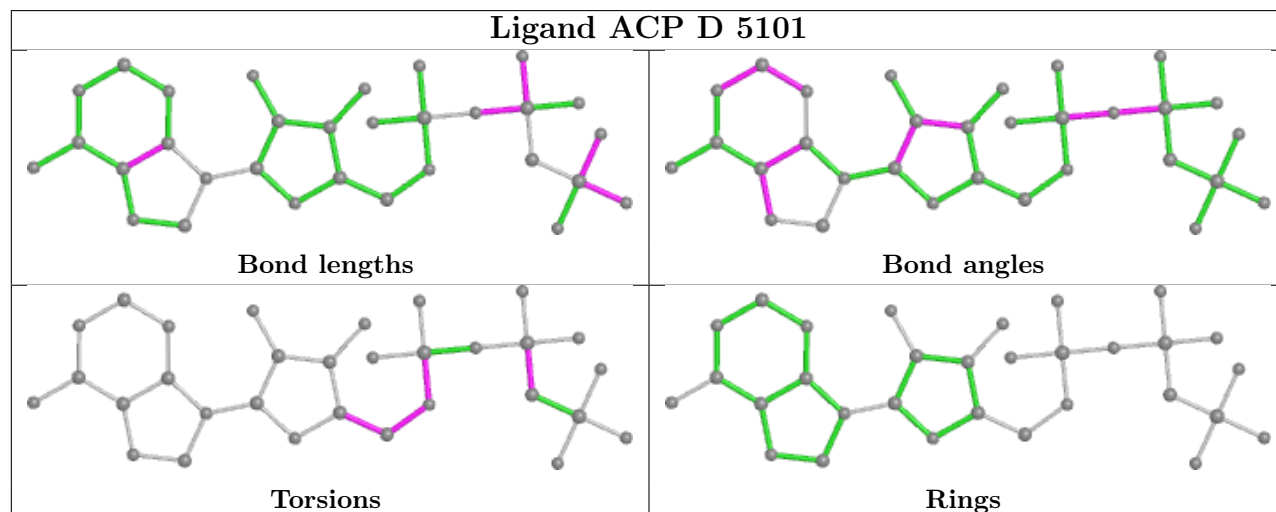
Ligand ACP C 5101

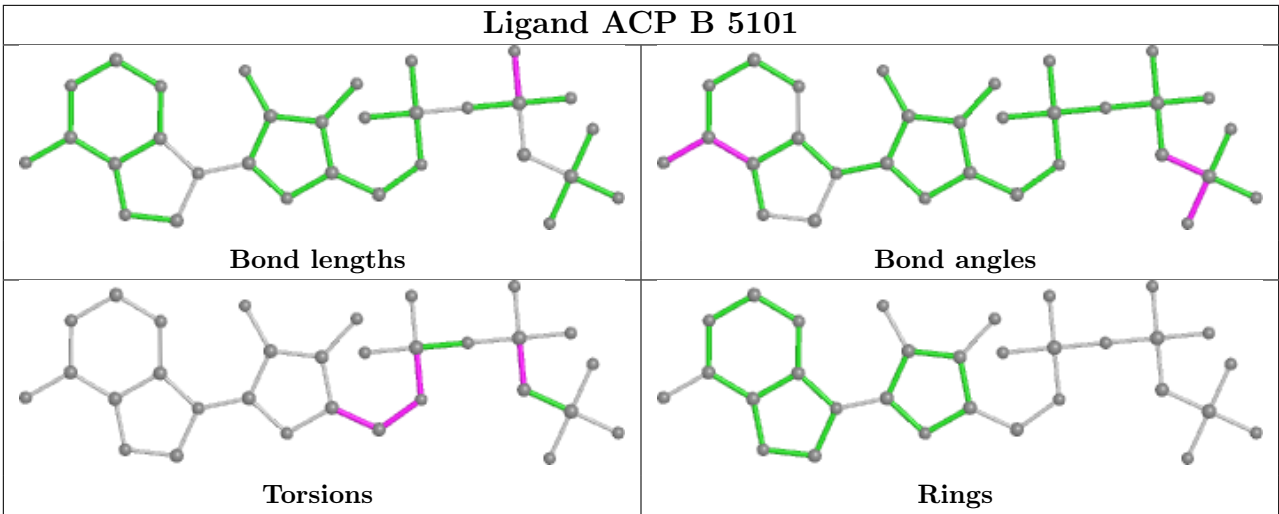


Ligand ACP A 5101



Ligand ACP D 5101





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	6
1	B	6
1	C	6
1	A	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	3302:UNK	C	3303:UNK	N	17.16
1	B	3302:UNK	C	3303:UNK	N	17.15
1	C	3302:UNK	C	3303:UNK	N	17.10
1	A	3302:UNK	C	3303:UNK	N	17.01
1	A	3510:UNK	C	3511:UNK	N	16.97
1	C	3510:UNK	C	3511:UNK	N	16.95
1	B	3510:UNK	C	3511:UNK	N	16.94
1	D	3510:UNK	C	3511:UNK	N	16.94
1	A	3136:UNK	C	3137:UNK	N	13.76
1	C	3136:UNK	C	3137:UNK	N	13.74
1	B	3136:UNK	C	3137:UNK	N	13.71
1	D	3136:UNK	C	3137:UNK	N	13.71
1	A	3235:UNK	C	3236:UNK	N	12.12

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	3235:UNK	C	3236:UNK	N	11.05
1	D	3235:UNK	C	3236:UNK	N	11.02
1	B	3235:UNK	C	3236:UNK	N	11.01
1	B	3205:UNK	C	3206:UNK	N	5.74
1	D	3205:UNK	C	3206:UNK	N	5.73
1	C	3205:UNK	C	3206:UNK	N	5.67
1	A	3205:UNK	C	3206:UNK	N	5.65
1	C	1297:UNK	C	1298:UNK	N	5.21
1	A	1297:UNK	C	1298:UNK	N	5.20
1	B	1297:UNK	C	1298:UNK	N	5.20
1	D	1297:UNK	C	1298:UNK	N	5.19

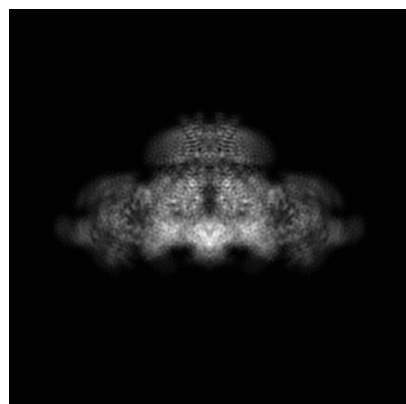
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22615. These allow visual inspection of the internal detail of the map and identification of artifacts.

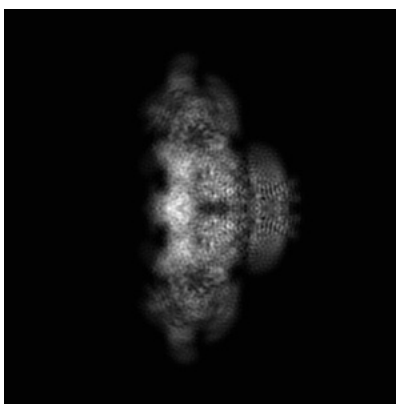
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

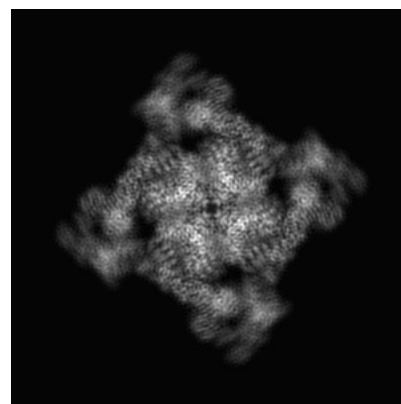
6.1.1 Primary map



X

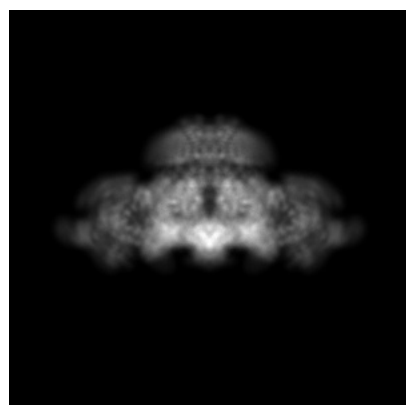


Y

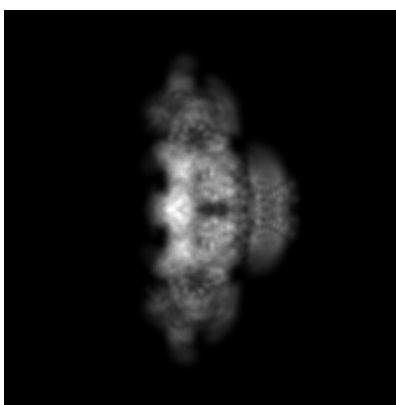


Z

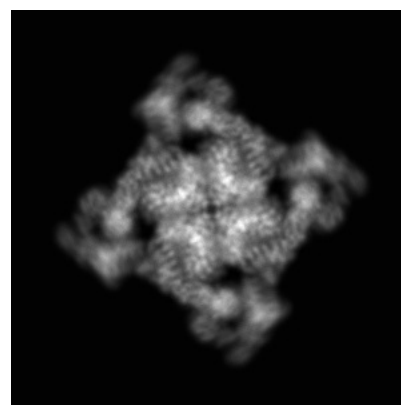
6.1.2 Raw map



X



Y

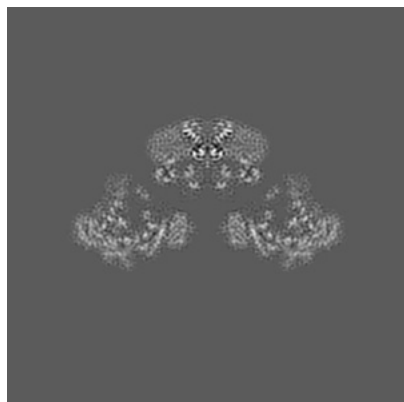


Z

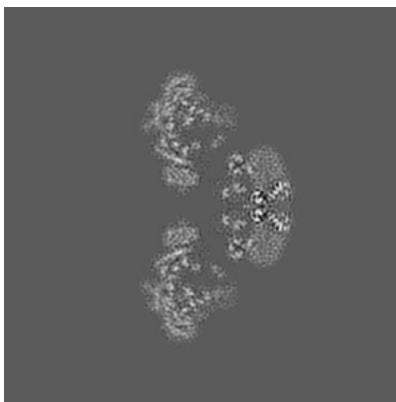
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

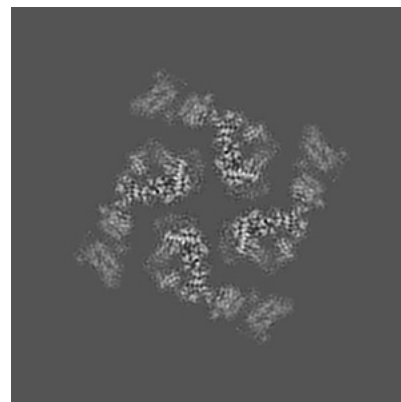
6.2.1 Primary map



X Index: 176

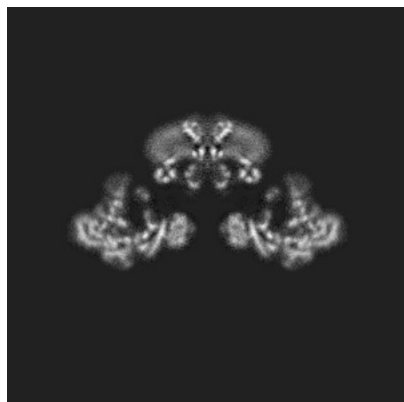


Y Index: 176

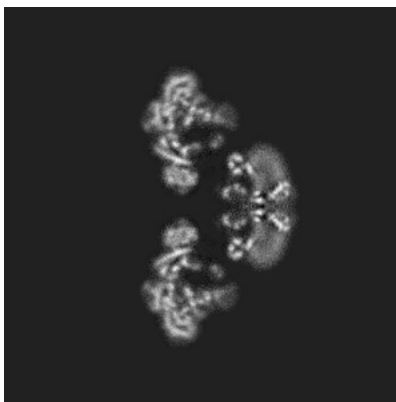


Z Index: 176

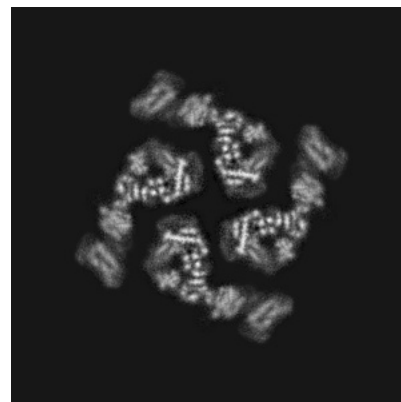
6.2.2 Raw map



X Index: 176



Y Index: 176

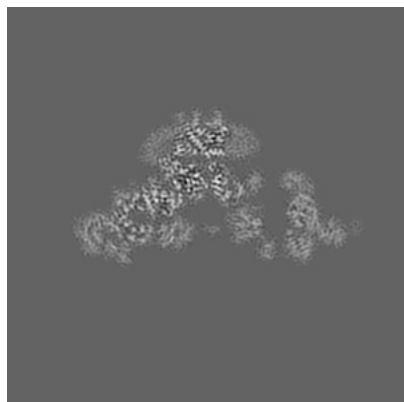


Z Index: 176

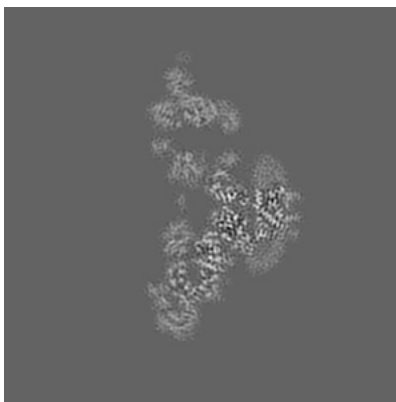
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

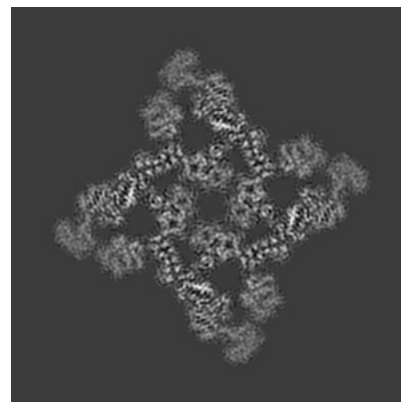
6.3.1 Primary map



X Index: 165

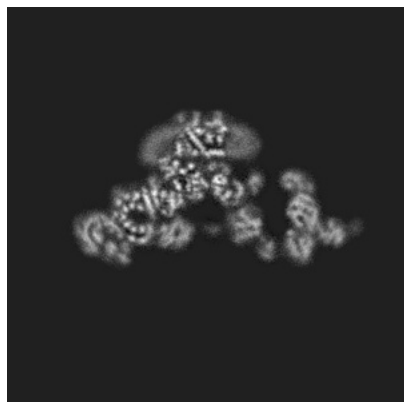


Y Index: 187

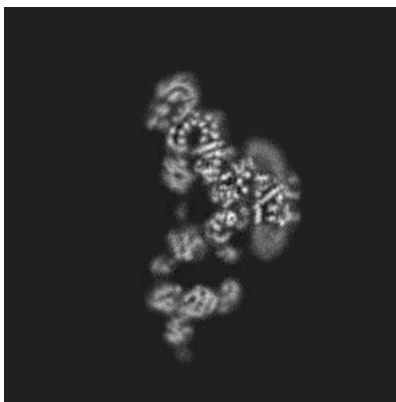


Z Index: 160

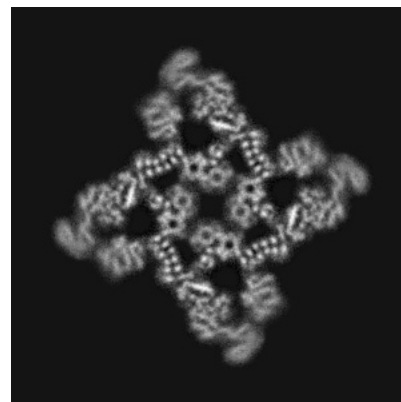
6.3.2 Raw map



X Index: 165



Y Index: 165

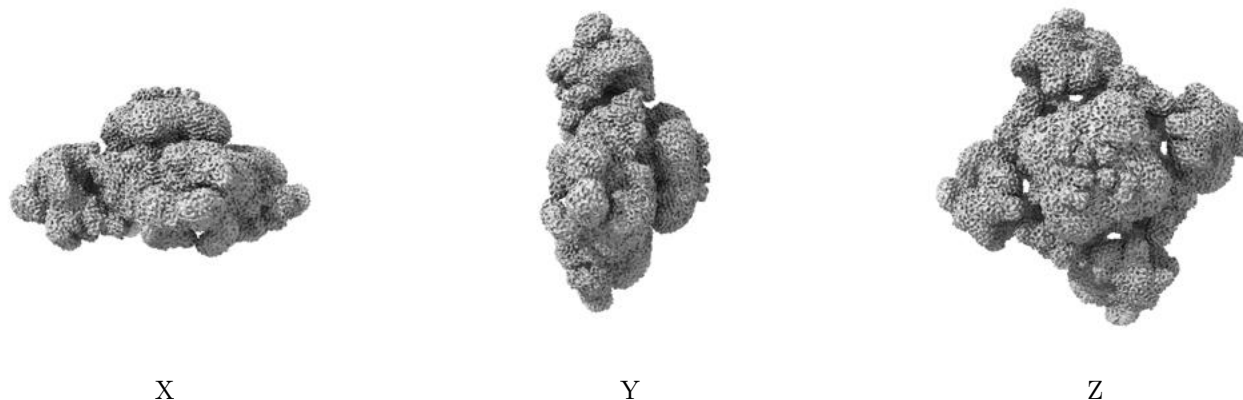


Z Index: 160

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

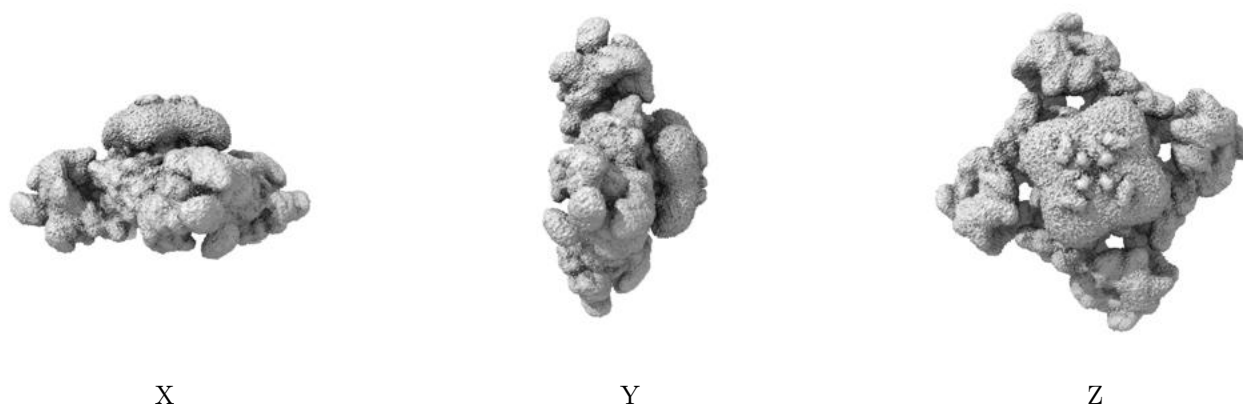
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

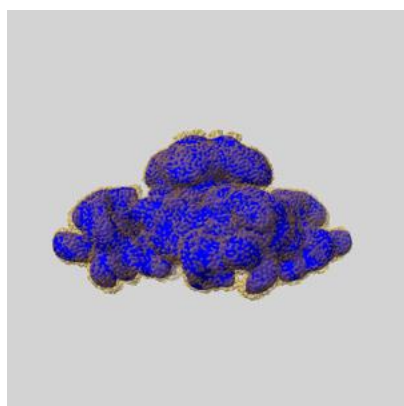
6.5 Mask visualisation [i](#)

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

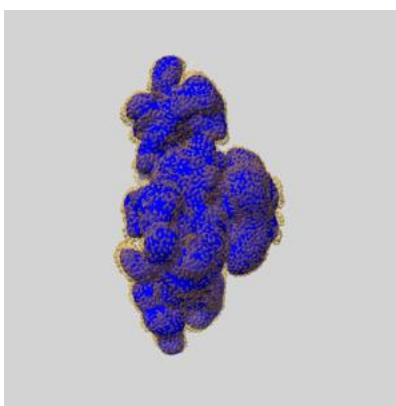
A mask typically either:

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

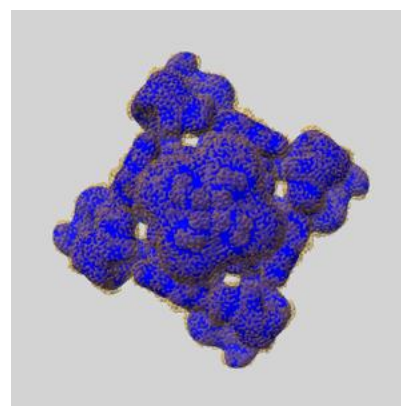
6.5.1 emd_22615_msk_1.map [i](#)



X



Y

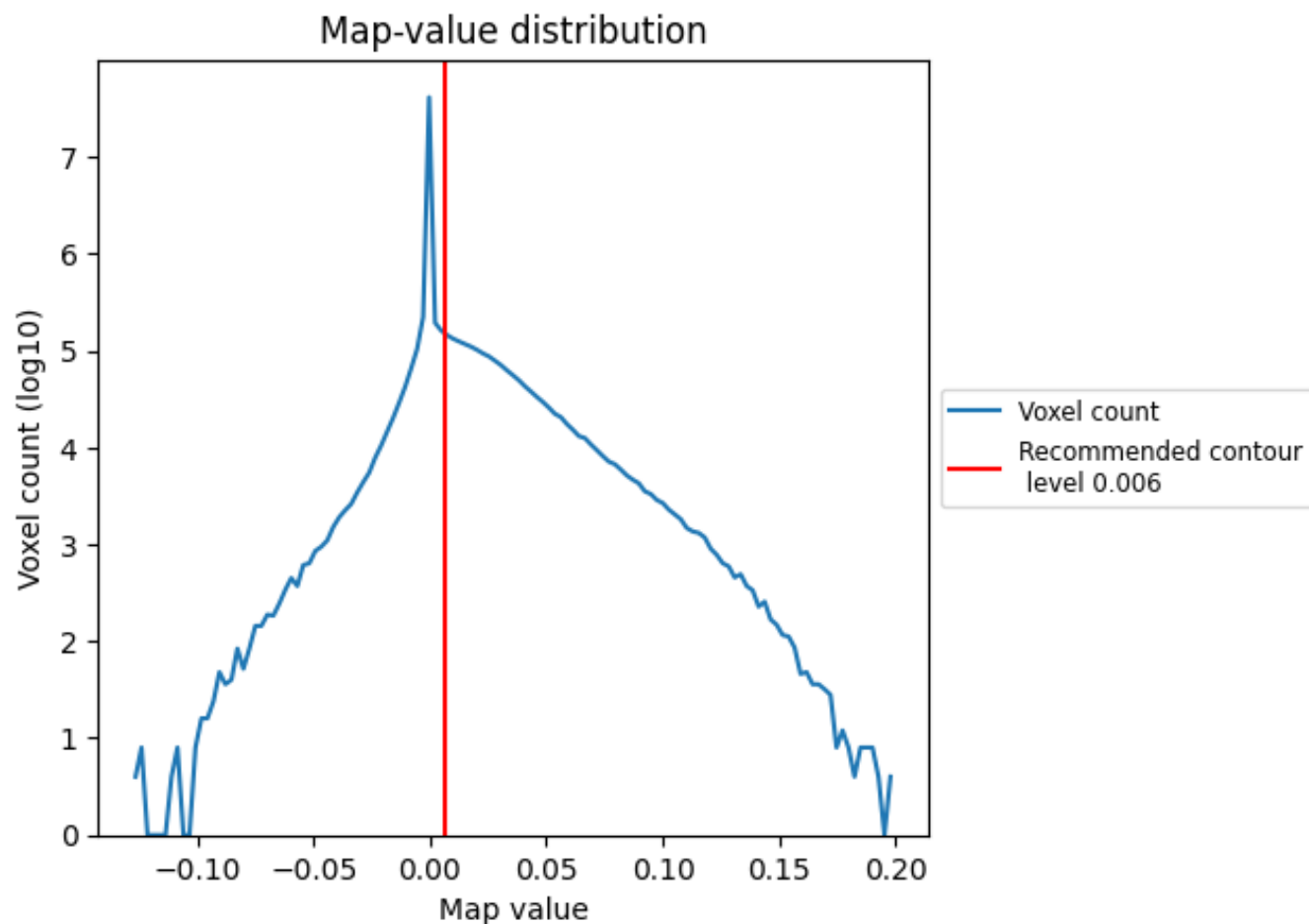


Z

7 Map analysis [i](#)

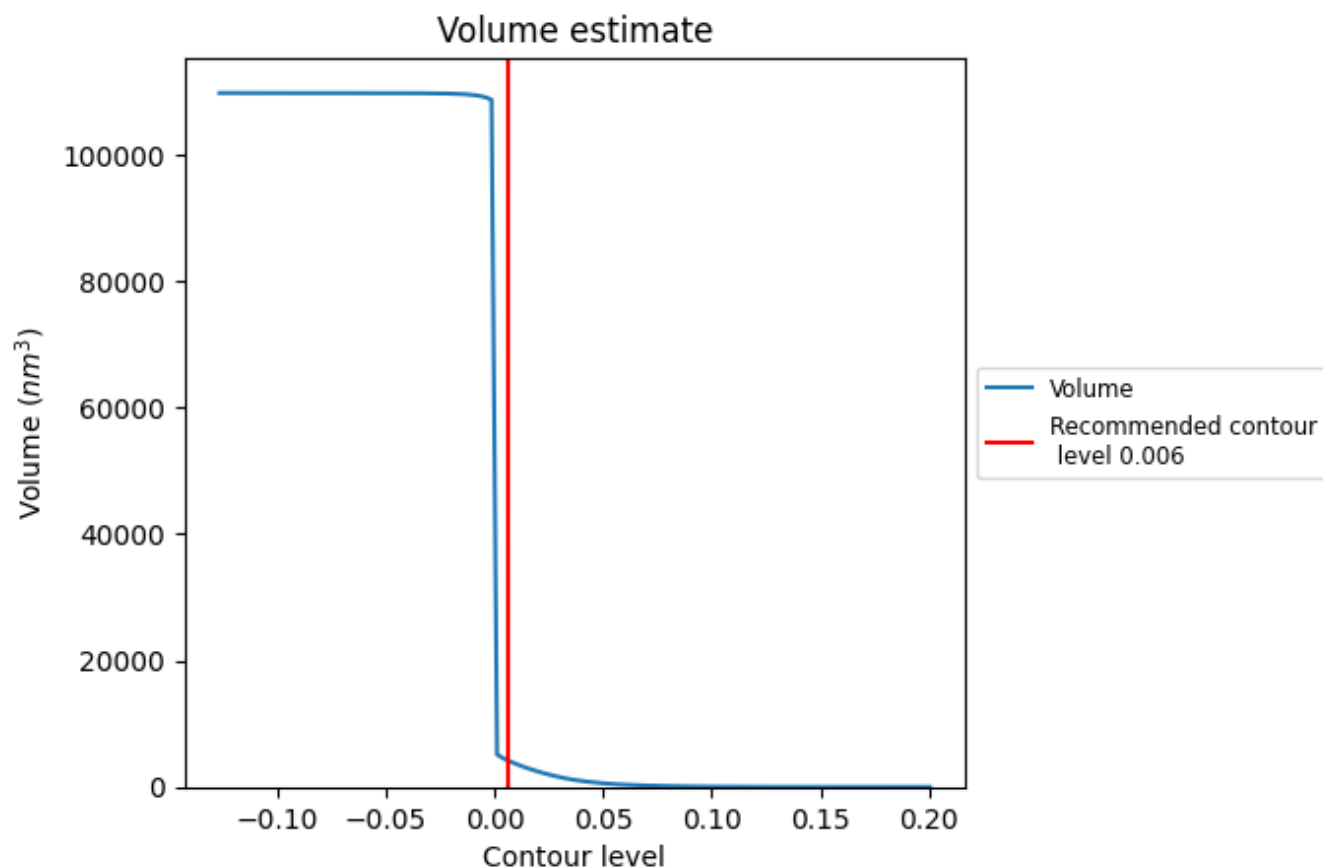
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

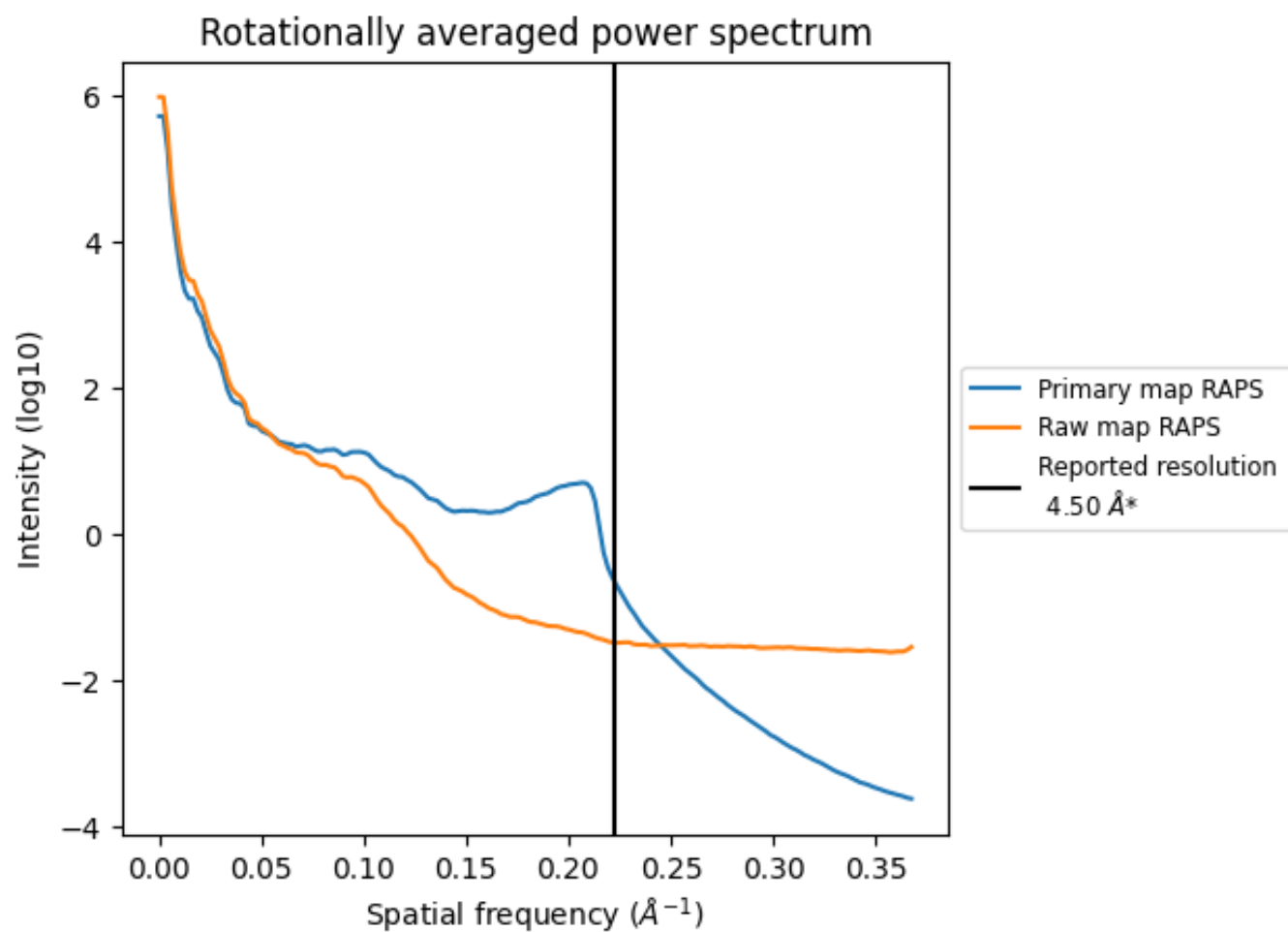
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4210 nm^3 ; this corresponds to an approximate mass of 3803 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 ⓘ

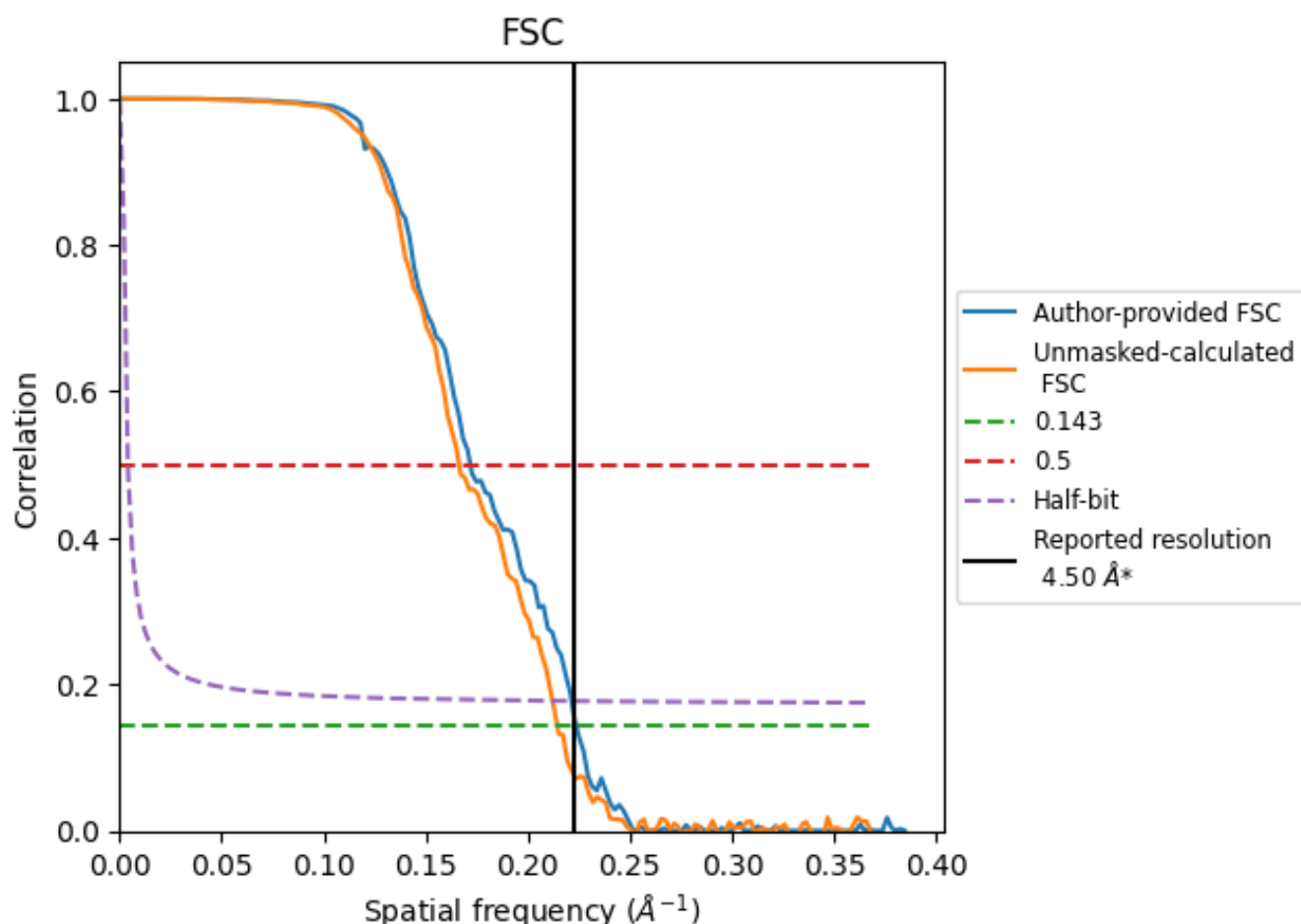


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

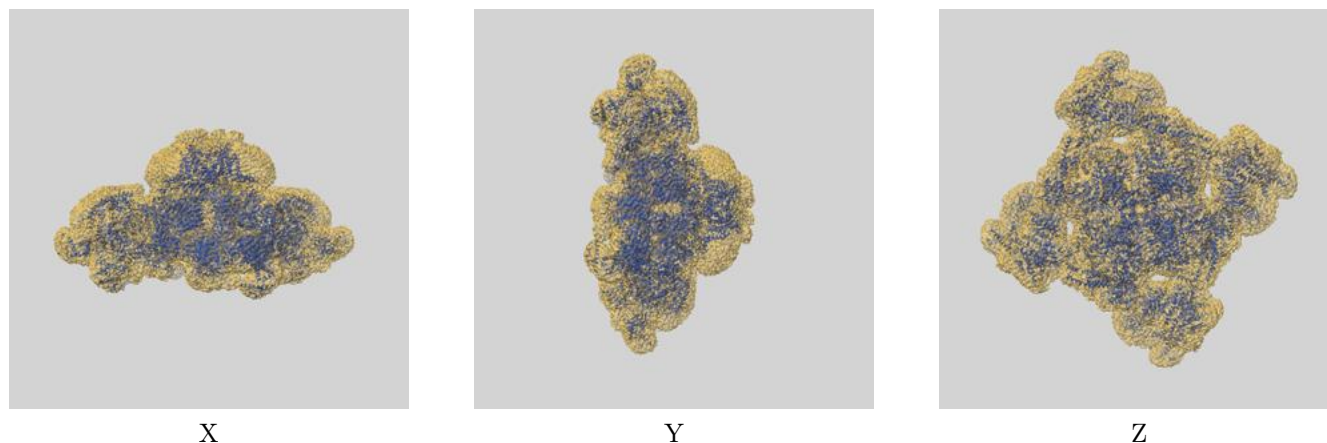
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.47	5.82	4.52
Unmasked-calculated*	4.66	6.01	4.71

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

9 Map-model fit [i](#)

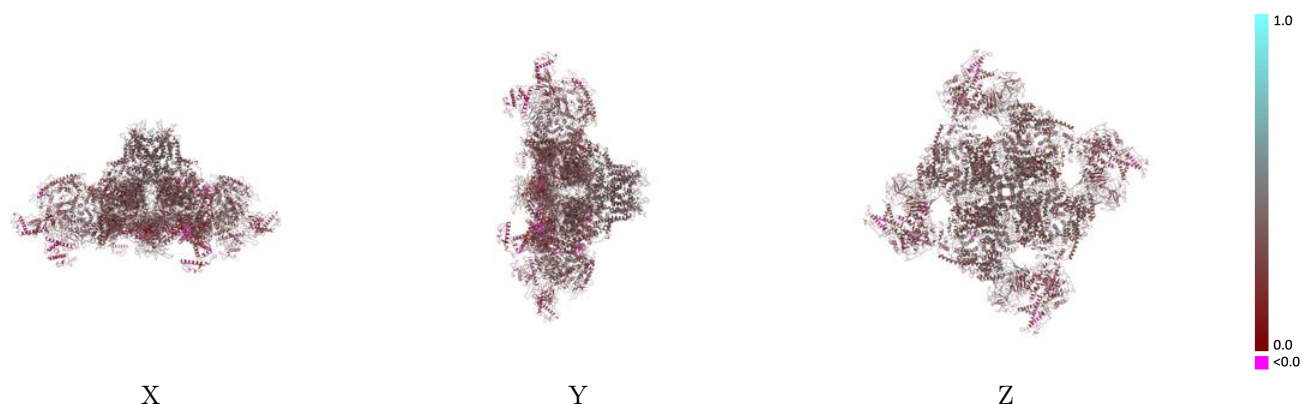
This section contains information regarding the fit between EMDB map EMD-22615 and PDB model 7K0S. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



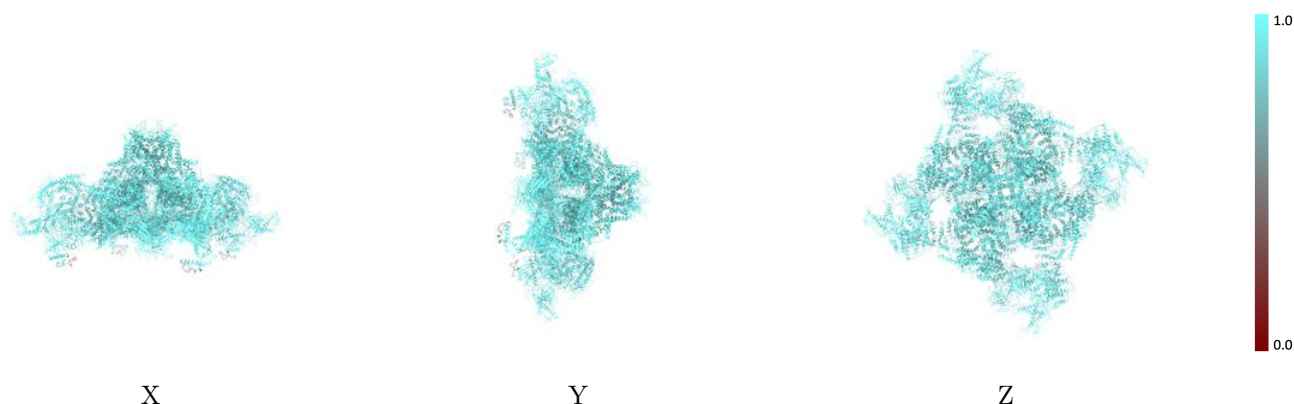
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



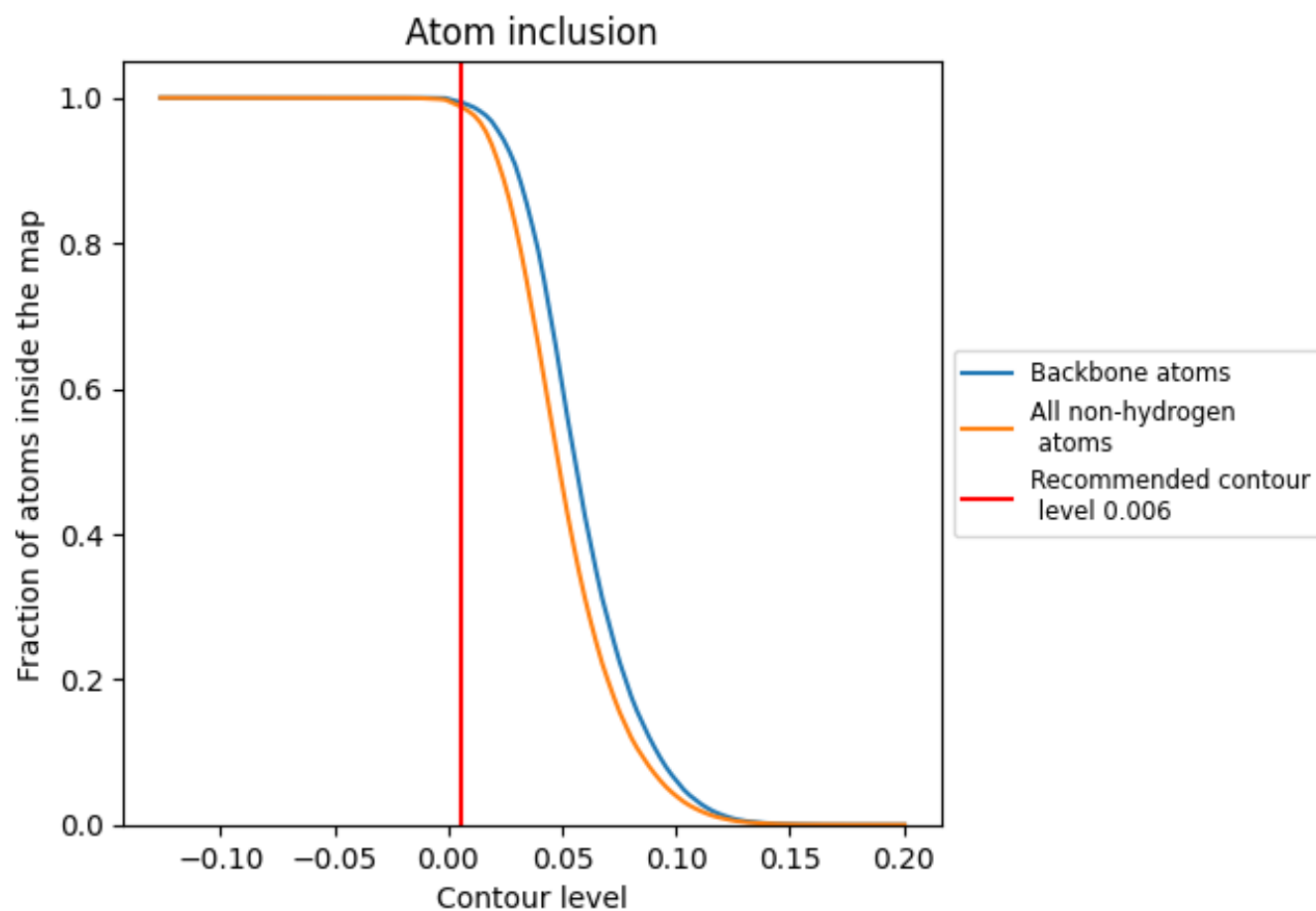
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9871	<div></div> 0.3120
A	<div></div> 0.9872	<div></div> 0.3110
B	<div></div> 0.9873	<div></div> 0.3120
C	<div></div> 0.9873	<div></div> 0.3120
D	<div></div> 0.9865	<div></div> 0.3110

