



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 09:26 PM UTC

PDB ID : 7K0T / pdb_00007k0t
EMDB ID : EMD-22616
Title : Cryo-EM structure of rabbit RyR1 in the presence of AMP-PCP in nanodisc
Authors : Nayak, A.R.; Samso, M.
Deposited on : 2020-09-05
Resolution : 4.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

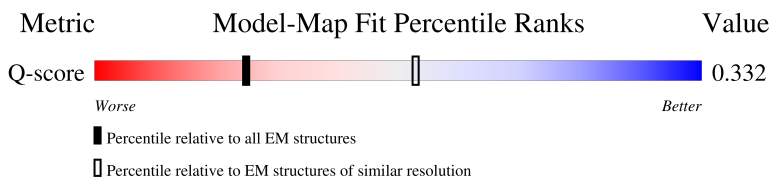
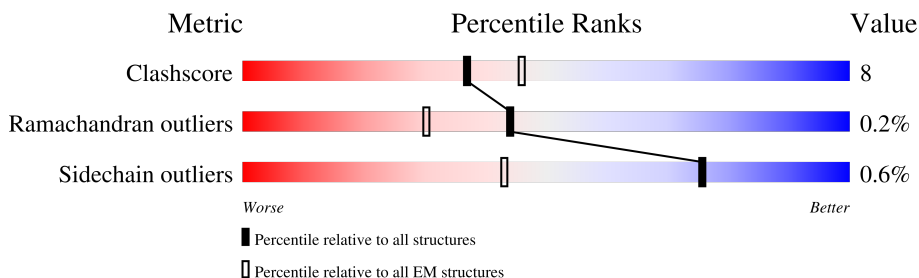
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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](#)

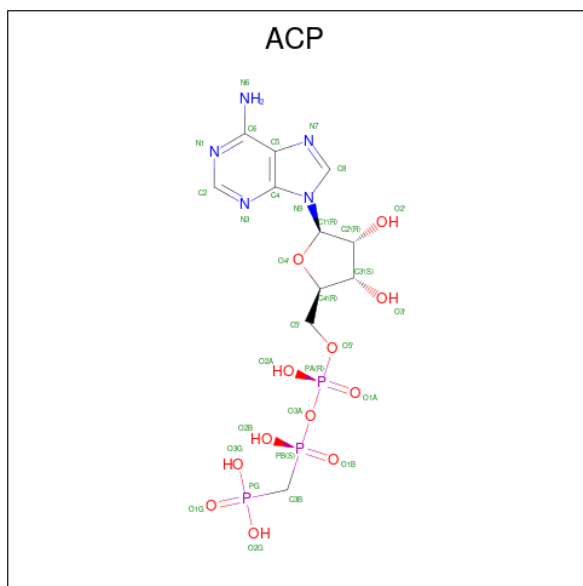
There are 3 unique types of molecules in this entry. The entry contains 115905 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	4105	Total	C	N	O	S	0	0
			28962	18349	5127	5329	157		
1	B	4105	Total	C	N	O	S	0	0
			28934	18331	5126	5320	157		
1	D	4105	Total	C	N	O	S	0	0
			28933	18332	5125	5319	157		
1	C	4105	Total	C	N	O	S	0	0
			28948	18340	5129	5322	157		

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



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 (CCD ID: 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	



[illegible]



Chain D: 69% 12% 19%









L4884	D4744	SER	PRO	PRO	ASP	PRO	LEU	GLU	P4106	M3999
M4887	F4760	TRP	PRO	GLU	GLY	ALA	TRP	ALA	Q4109	A4004
R4892	F4783	GLY	PRO	PRO	THR	THR	VAL	ALA	F4132	Q4005
P4904	D4786	ALA	LYS	LYS	THR	THR	ALA	ALA	Q4133	D4006
R4913	F4791	GLU	PRO	PRO	GLU	ASP	ARG	ALA	D4138	Q4009
E4942	F4794	GLU	PRO	PRO	PRO	GLY	GLY	ALA	M4142	I4010
L4943	F4795	GLU	PRO	PRO	THR	ALA	ALA	ALA	R4159	L4013
M4944	F4796	ASP	ALA	ALA	GLU	GLY	GLY	VAL	E4182	L4016
V4950	F4797	GLU	LYS	LYS	GLY	GLY	ALA	ALA	I4183	D4018
M4954	F4798	ASP	LYS	LYS	SER	SER	ALA	ALA	M4184	L4019
C4958	F4799	GLU	GLU	GLU	PRO	GLY	ALA	GLY	T4200	Q4020
D4966	F4812	GLU	GLU	GLU	ILE	GLY	GLY	ALA	T4190	Q4021
R4978	D4815	ALA	ALA	ALA	LEU	GLY	GLY	ALA	D4022	D4022
H4983	L4826	L4632	GLY	GLY	LYS	ASP	LEU	THR	S4198	M4034
L4985	S4828	A4654	GLY	GLY	ARG	ALA	LEU	ALA	V4024	V4023
I4996	T4831	A4661	ALA	ALA	LYS	ALA	ARG	ARG	V4025	V4025
K4997	V4831	L4663	GLY	GLY	LYS	LEU	LEU	ALA	M4201	L4030
K4998	V4848	R4673	MET	GLY	GLY	ASP	TRP	ALA	T4218	M4034
E5000	T4852	L4664	GLU	GLU	VAL	GLY	GLY	ALA	V4222	I4040
F5002	V4853	K4665	F4540	GLY	GLY	ASP	SER	ALA	E4227	D4046
H5003	V4854	A4666	R4563	GLU	GLU	GLY	PHI	ARG	A4238	M4047
M5013	A4855	P4667	L4567	GLU	GLU	GLY	GLY	LEU	E4229	S4051
R5017	F4859	L4688	N4574	VAL	VAL	HIS	LEU	LEU	C4238	I4058
C5018	Y4863	E4689	L4577	PRO	ALA	GLU	VAL	GLY	E4239	F4062
S5037	K4864	K4680	L4578	GLU	GLY	GLY	ALA	ARG	T4241	F4062
	S4866	I4688	K4581	PRO	GLY	GLY	LYS	SER	I4242	F4065
	D4867	E4690	P4587	PRO	PRO	GLU	VAL	ARG	E4253	K4069
	D4868	Q4691	GLY	PRO	PRO	GLY	THR	ARG	GLU	V4072
	E4869	D4696	ASP	PRO	PRO	VAL	THR	VAL	GLY	F4077
	D4870	V4697	ASP	PRO	PRO	VAL	GLU	ARG	GLU	Q4078
	F4871	G4698	MET	GLU	GLU	VAL	LEU	ARG	PRO	D4079
	L4872	G4699	GLY	GLU	VAL	VAL	ALA	LEU	GLU	Y4680
	D4873	D4868	LYS	ALA	LYS	ALA	ALA	ARG	ALA	V4081
	D4874	R4703	SER	ALA	ASP	GLY	GLY	ARG	ASP	
	K4875	L4704	ALA	ALA	GLY	MET	LEU	GLU	GLU	
	C4876	V4705	ALA	ALA	GLU	PRO	THR	ASP	ASP	
	D4877	L4706	GLY	GLY	GLY	GLY	ALA	GLU	GLY	I4088
	N4879	N4707	ASP	ASN	PHE	PRO	ARG	GLY	GLY	Q4094
	C4878	T4708	LEU	GLY	ARG	THR	THR	GLY	GLY	M4097
	D4879	Y4715	ALA	LYS	PRO	SER	ALA	ALA	GLU	K4101
	D4880	Y4716	GLY	GLU	GLY	ASP	THR	ALA	ALA	Q4102
	D4881	I4731	GLY	GLU	VAL	GLY	HIS	LEU	ALA	F4103
	D4882	L4732	SER	GLY	PRO	GLY	GLY	ALA	GLU	T4104
	Y4883	L4733	GLY	GLY	ALA	GLY	LEU	GLU	ALA	F4105

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	21551	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 ($e^-/\text{\AA}^2$)	70.3	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.128	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	462.24002, 462.24002, 462.24002	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.16	0/25009	0.41	4/33951 (0.0%)
1	B	0.18	1/24980 (0.0%)	0.44	8/33913 (0.0%)
1	C	0.17	0/24994	0.42	3/33929 (0.0%)
1	D	0.17	1/24979 (0.0%)	0.42	5/33913 (0.0%)
All	All	0.17	2/99962 (0.0%)	0.42	20/135706 (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	B	0	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	889	GLN	C-N	8.94	1.46	1.33
1	B	967	PRO	C-N	7.42	1.49	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	967	PRO	O-C-N	11.34	136.92	122.86
1	D	4872	PRO	N-CA-C	-9.10	102.24	113.98
1	B	4868	ASP	CB-CA-C	7.78	120.52	109.71
1	A	4690	GLU	CA-C-N	7.59	130.94	120.39
1	A	4690	GLU	C-N-CA	7.59	130.94	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	967	PRO	CA-C-N	-7.35	103.86	121.80
1	B	967	PRO	C-N-CA	-7.35	103.86	121.80
1	B	3768	SER	CA-C-N	6.38	128.83	120.28
1	B	3768	SER	C-N-CA	6.38	128.83	120.28
1	C	3662	ILE	N-CA-C	-6.35	106.26	111.91
1	C	2144	ILE	CA-C-N	6.02	129.04	120.49
1	C	2144	ILE	C-N-CA	6.02	129.04	120.49
1	B	2144	ILE	CA-C-N	5.45	128.23	120.49
1	B	2144	ILE	C-N-CA	5.45	128.23	120.49
1	A	2144	ILE	CA-C-N	5.22	127.91	120.49
1	A	2144	ILE	C-N-CA	5.22	127.91	120.49
1	D	3770	LEU	CA-C-N	5.17	131.41	121.54
1	D	3770	LEU	C-N-CA	5.17	131.41	121.54
1	D	889	GLN	CA-C-N	-5.08	111.53	121.53
1	D	889	GLN	C-N-CA	-5.08	111.53	121.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	883	ALA	Peptide
1	D	889	GLN	Mainchain

5.2 Too-close contacts [i](#)

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	28962	0	24423	420	0
1	B	28934	0	24389	415	0
1	C	28948	0	24429	399	0
1	D	28933	0	24401	416	0
2	A	31	0	14	6	0
2	B	31	0	14	4	0
2	C	31	0	14	7	0
2	D	31	0	14	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	115905	0	97698	1631	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 8.

All (1631) 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:B:4662:ASN:O	1:B:4666:VAL:HG11	1.38	1.23
1:B:3758:MET:HE2	1:B:3758:MET:HA	1.29	1.11
1:D:4662:ASN:O	1:D:4666:VAL:HG11	1.52	1.09
1:C:4865:LYS:HE2	1:C:4865:LYS:HA	1.37	1.06
1:D:3674:ILE:HB	1:D:3769:ARG:HH21	1.19	1.04
1:B:879:HIS:NE2	1:B:908:VAL:O	1.91	1.04
1:A:4867:GLU:CB	1:A:4871:GLU:CB	2.37	1.02
1:A:4867:GLU:CB	1:A:4871:GLU:HB2	1.89	1.02
1:B:880:GLU:OE2	1:B:965:TYR:CE2	2.12	1.00
1:A:3737:GLU:HA	1:A:3763:LEU:HD11	1.43	0.97
1:A:4874:MET:O	1:A:4875:LYS:HB2	1.64	0.95
1:A:3737:GLU:CA	1:A:3763:LEU:HD11	1.97	0.94
1:D:3955:MET:HE3	1:D:4019:LEU:HD13	1.51	0.89
1:B:4666:VAL:HG13	1:B:4667:PRO:HD3	1.53	0.89
1:D:1707:LEU:HG	1:D:1708:ARG:H	1.34	0.89
1:B:880:GLU:OE2	1:B:965:TYR:HE2	1.54	0.87
1:B:3758:MET:HA	1:B:3758:MET:CE	2.06	0.86
1:B:950:LEU:HD13	1:B:970:LEU:HD13	1.58	0.85
1:D:759:ILE:HG22	1:D:762:CYS:HB2	1.60	0.84
1:A:3737:GLU:N	1:A:3763:LEU:HD11	1.92	0.84
1:B:880:GLU:OE1	1:B:967:PRO:HA	1.76	0.84
1:C:3770:LEU:HD12	1:C:3770:LEU:O	1.77	0.83
1:B:4662:ASN:C	1:B:4666:VAL:HG11	2.05	0.82
1:D:4666:VAL:HG12	1:D:4667:PRO:HD3	1.60	0.82
1:B:4860:ARG:O	1:B:4876:CYS:SG	2.37	0.82
1:B:4662:ASN:O	1:B:4666:VAL:CG1	2.26	0.82
1:A:4867:GLU:CB	1:A:4871:GLU:HB3	2.09	0.81
1:B:4875:LYS:O	1:B:4877:ASP:N	2.13	0.81
1:B:759:ILE:HG22	1:B:762:CYS:HB2	1.62	0.80
1:D:4017:LEU:HD13	1:D:4020:GLN:HE21	1.46	0.80
1:D:4662:ASN:O	1:D:4666:VAL:CG1	2.29	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:759:ILE:HG22	1:C:762:CYS:HB2	1.67	0.76
1:B:880:GLU:OE2	1:B:965:TYR:CZ	2.39	0.76
1:D:879:HIS:NE2	1:D:908:VAL:O	2.15	0.76
1:A:759:ILE:HG22	1:A:762:CYS:HB2	1.68	0.76
1:B:173:SER:HB3	1:B:178:ARG:H	1.50	0.76
1:D:3674:ILE:HB	1:D:3769:ARG:NH2	1.99	0.76
1:C:670:GLU:HG3	1:C:788:LYS:H	1.51	0.75
1:C:4865:LYS:HD2	1:C:4865:LYS:N	2.01	0.75
1:C:4654:ALA:HB1	1:C:4796:MET:HE1	1.69	0.75
1:D:4871:GLU:N	1:D:4872:PRO:HD3	2.01	0.75
1:D:880:GLU:OE2	1:D:965:TYR:OH	2.02	0.74
1:D:3762:ARG:HH21	1:D:4754:ASN:HA	1.50	0.74
1:A:652:ARG:HB2	1:A:750:LEU:HD23	1.70	0.74
1:A:4871:GLU:O	1:A:4871:GLU:HG2	1.88	0.73
1:C:4870:ASP:OD2	1:C:4872:PRO:CG	2.37	0.73
1:A:620:LEU:O	1:A:624:ASN:HB2	1.89	0.73
1:D:2116:LEU:HG	1:D:2120:MET:HE1	1.70	0.73
1:B:3761:GLN:HA	1:B:3761:GLN:OE1	1.89	0.73
1:A:670:GLU:HG3	1:A:788:LYS:H	1.54	0.72
1:A:2116:LEU:HG	1:A:2120:MET:HE1	1.71	0.72
1:B:670:GLU:HG3	1:B:788:LYS:H	1.54	0.72
1:A:4954:MET:SD	2:A:5101:ACP:H1'	2.29	0.72
1:C:4954:MET:SD	2:C:5101:ACP:H1'	2.30	0.72
1:B:880:GLU:OE2	1:B:965:TYR:OH	2.06	0.72
1:C:4104:THR:HG22	1:C:4106:PRO:HD2	1.71	0.72
1:C:652:ARG:HB2	1:C:750:LEU:HD23	1.72	0.72
1:D:293:LEU:HD13	1:D:298:GLY:H	1.54	0.72
1:B:2116:LEU:HG	1:B:2120:MET:HE1	1.72	0.71
1:A:3736:GLU:C	1:A:3763:LEU:HD11	2.15	0.71
1:D:5003:HIS:HB3	1:D:5008:SER:HB3	1.72	0.71
1:C:4865:LYS:HA	1:C:4865:LYS:CE	2.15	0.71
1:A:293:LEU:HD13	1:A:298:GLY:H	1.56	0.71
1:C:2116:LEU:HG	1:C:2120:MET:HE1	1.71	0.71
1:A:590:LEU:HD13	1:A:599:VAL:HG21	1.72	0.71
1:B:875:ALA:HB1	1:B:910:PHE:CZ	2.26	0.71
1:A:4866:SER:C	1:A:4871:GLU:OE2	2.33	0.71
1:D:670:GLU:HG3	1:D:788:LYS:H	1.55	0.71
1:B:4662:ASN:C	1:B:4666:VAL:CG1	2.64	0.70
1:B:4791:TYR:HE1	1:B:4815:ASP:HB3	1.56	0.70
1:C:3761:GLN:OE1	1:C:3761:GLN:HA	1.91	0.70
1:C:4069:LYS:HD2	1:C:4133:GLN:HG2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3757:GLU:HA	1:B:3757:GLU:OE1	1.92	0.70
1:B:4995:LEU:HD11	1:B:5011:TRP:HB2	1.73	0.70
1:D:173:SER:HB3	1:D:178:ARG:H	1.57	0.69
1:C:560:ILE:HA	1:C:563:VAL:HG12	1.73	0.69
1:A:173:SER:HB3	1:A:178:ARG:H	1.55	0.69
1:C:293:LEU:HD13	1:C:298:GLY:H	1.57	0.69
1:B:2131:LEU:HB3	1:B:3662:ILE:HG21	1.74	0.69
1:B:875:ALA:HB1	1:B:910:PHE:CE1	2.28	0.69
1:A:4654:ALA:HB1	1:A:4796:MET:HE1	1.75	0.69
1:C:3986:TRP:HA	1:C:3989:VAL:HG22	1.73	0.69
1:A:755:ILE:HB	1:A:768:PHE:HB2	1.74	0.69
2:B:5101:ACP:O1A	2:B:5101:ACP:H3B2	1.93	0.68
1:D:590:LEU:HD13	1:D:599:VAL:HG21	1.75	0.68
1:D:955:LEU:HD12	1:D:967:PRO:O	1.93	0.68
1:C:4985:LEU:HB2	2:C:5101:ACP:HN61	1.59	0.68
1:A:3897:ASN:HD22	1:A:3897:ASN:C	1.99	0.68
1:B:977:LEU:HB3	1:B:1044:ARG:HG3	1.77	0.67
1:A:1653:LEU:HD11	1:A:1659:LEU:HB3	1.76	0.67
1:A:1679:ASN:ND2	1:A:1797:ARG:O	2.28	0.67
1:B:652:ARG:HB2	1:B:750:LEU:HD23	1.77	0.67
1:B:3755:GLU:OE2	1:B:3755:GLU:HA	1.94	0.67
1:A:111:HIS:HD2	1:A:114:SER:H	1.41	0.67
1:A:4995:LEU:HD11	1:A:5011:TRP:HB2	1.76	0.67
1:B:3674:ILE:HB	1:B:3769:ARG:HH21	1.59	0.67
1:A:2207:VAL:HG12	1:A:2211:MET:HE1	1.77	0.66
1:A:3737:GLU:HA	1:A:3763:LEU:CD1	2.21	0.66
1:A:197:GLN:NE2	1:A:198:THR:O	2.29	0.66
1:A:4921:PHE:O	1:B:4892:ARG:NH2	2.29	0.66
1:B:615:ARG:NH2	1:B:1677:GLY:O	2.29	0.66
1:B:4843:LEU:HD22	1:B:4928:LEU:HD11	1.78	0.66
1:D:197:GLN:NE2	1:D:198:THR:O	2.28	0.66
1:D:615:ARG:NH2	1:D:1677:GLY:O	2.29	0.66
1:A:1705:GLY:HA2	1:A:1709:ALA:HB3	1.78	0.66
1:B:594:GLY:H	1:B:1594:ARG:HD2	1.61	0.66
1:B:3753:PHE:HZ	1:B:4719:PHE:CE1	2.14	0.65
1:A:3674:ILE:HB	1:A:3769:ARG:HH21	1.61	0.65
1:D:4666:VAL:CG1	1:D:4667:PRO:HD3	2.26	0.65
1:B:907:LEU:HB3	1:B:963:ASN:HD22	1.62	0.65
1:B:4875:LYS:C	1:B:4877:ASP:H	2.02	0.65
1:D:567:VAL:HG13	1:D:568:LEU:HD12	1.79	0.65
1:D:2291:GLN:NE2	1:D:2349:ASN:OD1	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1232:ARG:NH1	1:B:1828:ASP:O	2.29	0.65
1:B:293:LEU:HD13	1:B:298:GLY:H	1.62	0.65
1:B:3758:MET:HE2	1:B:3758:MET:CA	2.15	0.65
1:C:4017:LEU:HD13	1:C:4020:GLN:HE21	1.62	0.65
1:A:19:GLU:HA	1:A:68:THR:HA	1.78	0.65
1:A:3897:ASN:O	1:A:3897:ASN:ND2	2.22	0.65
1:D:907:LEU:HB3	1:D:963:ASN:HD22	1.62	0.65
1:D:4104:THR:HG22	1:D:4106:PRO:HD2	1.77	0.65
2:D:5101:ACP:O1A	2:D:5101:ACP:H3B2	1.95	0.65
1:A:907:LEU:HB3	1:A:963:ASN:HD22	1.61	0.65
1:C:1974:ARG:HH21	1:C:3642:TYR:HB2	1.62	0.65
1:B:4666:VAL:CG1	1:B:4667:PRO:HD3	2.23	0.64
1:D:719:LEU:O	1:D:720:HIS:ND1	2.30	0.64
1:C:78:LEU:HA	1:C:81:MET:HE2	1.79	0.64
1:C:1115:LEU:HB3	1:C:1123:VAL:HG11	1.79	0.64
1:C:182:LEU:HD11	1:C:189:LEU:HD23	1.79	0.64
1:C:594:GLY:H	1:C:1594:ARG:HD2	1.61	0.64
1:B:19:GLU:HA	1:B:68:THR:HA	1.79	0.64
1:A:4924:VAL:HG23	1:A:4925:ILE:HG12	1.80	0.64
1:D:652:ARG:HB2	1:D:750:LEU:HD23	1.80	0.64
1:C:3648:ARG:HG2	1:C:3652:MET:HE1	1.80	0.63
1:B:4874:MET:SD	1:B:4876:CYS:HB2	2.38	0.63
1:C:1679:ASN:ND2	1:C:1797:ARG:O	2.31	0.63
1:C:2265:LEU:HD22	1:C:2330:ARG:HD3	1.80	0.63
1:B:1119:GLU:HG2	1:B:1134:LEU:HD21	1.80	0.63
1:D:322:LYS:HE3	1:D:322:LYS:HA	1.79	0.63
1:C:908:VAL:HG12	1:C:909:ASN:H	1.62	0.63
1:C:1698:LEU:HB3	1:C:1814:MET:HE1	1.80	0.63
1:A:560:ILE:HA	1:A:563:VAL:HG12	1.80	0.63
1:A:606:LEU:O	1:A:617:ASN:ND2	2.32	0.63
1:A:1119:GLU:OE2	1:A:1133:HIS:NE2	2.30	0.63
1:B:606:LEU:O	1:B:617:ASN:ND2	2.32	0.63
1:A:3648:ARG:HG2	1:A:3652:MET:HE1	1.81	0.63
1:C:606:LEU:O	1:C:617:ASN:ND2	2.32	0.63
1:A:3766:GLN:HA	1:A:3769:ARG:HB3	1.79	0.63
1:A:4864:ASN:O	1:A:4865:LYS:O	2.16	0.63
1:D:4871:GLU:C	1:D:4873:ASP:N	2.55	0.62
1:C:3773:ARG:HA	1:C:3815:LYS:HE3	1.79	0.62
1:D:3986:TRP:HA	1:D:3989:VAL:HG22	1.81	0.62
1:C:590:LEU:HD13	1:C:599:VAL:HG21	1.80	0.62
1:B:168:ASP:OD1	1:B:201:ASN:ND2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3761:GLN:NE2	1:B:4750:ILE:HD12	2.15	0.62
1:D:64:ILE:HG23	1:D:402:ARG:HH21	1.65	0.62
1:D:889:GLN:O	1:D:902:ARG:NH1	2.32	0.62
1:C:4738:ALA:HB1	1:C:4744:ASP:HA	1.80	0.62
1:C:4799:SER:HB2	1:C:4812:HIS:HE1	1.65	0.62
1:B:322:LYS:HE3	1:B:322:LYS:HA	1.81	0.62
1:C:22:LEU:HD11	1:C:37:LEU:HD12	1.82	0.62
1:C:3794:VAL:HG11	1:C:3835:LEU:HD21	1.82	0.62
1:A:2214:VAL:HG13	1:A:2215:LEU:HG	1.81	0.62
1:D:4871:GLU:C	1:D:4873:ASP:H	2.08	0.62
1:B:1229:ASN:HB3	1:B:1826:ALA:HB1	1.81	0.62
1:A:1931:LEU:HD22	1:A:1935:VAL:HG11	1.82	0.62
1:D:2248:ARG:HA	1:D:2286:LEU:HD21	1.82	0.62
1:A:4685:GLY:HA3	1:A:4689:THR:HB	1.81	0.62
1:B:491:ILE:O	1:B:495:ASN:N	2.33	0.62
1:B:883:ALA:HA	1:B:887:ILE:H	1.65	0.62
1:B:4920:PHE:O	1:B:4924:VAL:HG22	1.99	0.62
1:C:730:VAL:O	1:C:735:GLN:NE2	2.33	0.62
1:D:19:GLU:HA	1:D:68:THR:HA	1.81	0.61
1:D:606:LEU:O	1:D:617:ASN:ND2	2.34	0.61
1:D:3674:ILE:CG2	1:D:3769:ARG:HE	2.14	0.61
1:C:596:ASN:HD21	1:C:598:LYS:HB2	1.65	0.61
1:A:1215:ALA:HA	1:A:1219:LEU:HD13	1.83	0.61
1:B:4066:LEU:HD12	1:B:4133:GLN:HE22	1.66	0.61
1:A:2265:LEU:HD22	1:A:2330:ARG:HD3	1.81	0.61
1:D:3648:ARG:HG2	1:D:3652:MET:HE1	1.82	0.61
1:D:3808:GLY:O	1:D:3813:GLN:NE2	2.34	0.61
1:B:2288:LEU:O	1:B:3849:ARG:NH1	2.34	0.61
1:C:3989:VAL:HG12	1:C:4023:MET:HE1	1.81	0.61
1:A:4232:GLU:OE2	1:A:5017:ARG:NH2	2.34	0.60
1:B:22:LEU:HD11	1:B:37:LEU:HD12	1.83	0.60
1:C:615:ARG:NH2	1:C:1677:GLY:O	2.34	0.60
1:A:647:ASN:ND2	1:A:820:ARG:O	2.34	0.60
1:C:2170:MET:HE3	1:C:2171:GLY:H	1.66	0.60
1:D:3675:ASP:N	1:D:3769:ARG:NH2	2.50	0.60
1:D:3722:TYR:CZ	1:D:3782:MET:HE1	2.36	0.60
1:B:1703:LEU:HD12	1:B:1704:PRO:HD2	1.83	0.60
1:B:4666:VAL:HG13	1:B:4667:PRO:CD	2.29	0.60
1:A:1730:MET:O	1:A:1772:ARG:NH1	2.34	0.60
1:B:5003:HIS:HB3	1:B:5008:SER:HB2	1.83	0.60
1:D:2288:LEU:O	1:D:3849:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4679:ARG:NH1	1:B:4715:TYR:OH	2.33	0.60
1:C:838:HIS:HA	1:C:1201:HIS:HB3	1.83	0.60
1:C:1730:MET:O	1:C:1772:ARG:NH1	2.35	0.60
1:A:748:LEU:HD22	1:A:755:ILE:HG12	1.83	0.60
1:A:2288:LEU:O	1:A:3849:ARG:NH1	2.34	0.60
1:D:4101:LYS:HG3	1:C:4731:ILE:HA	1.82	0.60
1:C:19:GLU:HA	1:C:68:THR:HA	1.83	0.60
1:A:4182:GLU:OE2	1:A:4983:HIS:ND1	2.35	0.60
1:C:4182:GLU:OE2	1:C:4983:HIS:ND1	2.34	0.60
1:A:637:LEU:HD23	1:A:1637:MET:HE1	1.83	0.60
1:D:3794:VAL:HG11	1:D:3835:LEU:HD11	1.84	0.60
1:A:4137:ARG:NH2	1:A:4196:GLU:OE2	2.35	0.59
1:D:176:SER:OG	1:D:178:ARG:NH1	2.35	0.59
1:A:418:LEU:HD22	1:A:493:ARG:HD3	1.84	0.59
1:B:730:VAL:O	1:B:735:GLN:NE2	2.35	0.59
1:B:4184:MET:HB3	1:B:4190:ILE:HD13	1.84	0.59
1:B:4867:GLU:OE1	1:B:4869:GLU:O	2.20	0.59
1:D:2005:GLN:HE22	1:D:3641:LEU:HD22	1.67	0.59
1:B:556:ALA:HB1	1:B:560:ILE:HG12	1.83	0.59
1:D:3698:LEU:HD22	1:D:3770:LEU:O	2.02	0.59
1:B:2005:GLN:HE22	1:B:3641:LEU:HD22	1.66	0.59
1:C:1229:ASN:HB3	1:C:1826:ALA:HB1	1.85	0.59
1:C:4874:MET:O	1:C:4876:CYS:N	2.36	0.59
1:C:2816:MET:SD	1:C:2882:TYR:OH	2.59	0.59
1:A:684:VAL:HG12	1:A:781:VAL:HG23	1.84	0.59
1:A:4820:VAL:HB	1:A:4823:LEU:HD23	1.85	0.59
1:C:869:ARG:NH2	1:C:941:MET:SD	2.75	0.59
1:A:719:LEU:HD13	1:A:735:GLN:HG2	1.85	0.59
1:B:719:LEU:HD13	1:B:735:GLN:HG2	1.84	0.59
1:D:4924:VAL:HA	1:D:4928:LEU:HD23	1.84	0.59
1:C:2288:LEU:O	1:C:3849:ARG:NH1	2.34	0.59
1:A:1196:PRO:O	1:A:1198:GLN:NE2	2.33	0.59
1:D:61:ASP:OD2	1:D:402:ARG:NH2	2.36	0.59
1:C:4046:ASP:OD1	1:C:4159:ARG:NH2	2.35	0.59
1:A:182:LEU:HD11	1:A:189:LEU:HD23	1.84	0.59
1:A:4162:ASN:O	1:A:4166:LEU:HB2	2.03	0.59
1:B:1730:MET:O	1:B:1772:ARG:NH1	2.36	0.59
1:D:1732:SER:OG	1:D:2140:ARG:NH2	2.35	0.59
1:C:4094:GLN:NE2	1:C:4109:GLN:OE1	2.36	0.59
2:C:5101:ACP:O2B	2:C:5101:ACP:H5'2	2.03	0.59
1:A:4058:ILE:HG22	1:A:4062:PHE:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2208:MET:SD	1:D:2253:HIS:ND1	2.76	0.58
1:A:168:ASP:OD1	1:A:201:ASN:ND2	2.31	0.58
1:A:4003:LEU:HD21	1:A:4012:LEU:HD23	1.85	0.58
1:B:719:LEU:O	1:B:720:HIS:ND1	2.36	0.58
1:D:794:GLY:H	1:D:798:GLY:HA3	1.66	0.58
1:D:4791:TYR:HE1	1:D:4815:ASP:HB3	1.68	0.58
1:C:4874:MET:C	1:C:4876:CYS:H	2.09	0.58
1:B:2170:MET:HE3	1:B:2171:GLY:H	1.67	0.58
1:B:4666:VAL:N	1:B:4667:PRO:HD2	2.19	0.58
1:D:1703:LEU:HD11	1:D:1709:ALA:HB2	1.85	0.58
1:D:4871:GLU:N	1:D:4872:PRO:CD	2.65	0.58
1:B:560:ILE:HA	1:B:563:VAL:HG12	1.86	0.58
1:C:2742:THR:O	1:C:2814:LYS:NZ	2.34	0.58
1:A:730:VAL:O	1:A:735:GLN:NE2	2.35	0.58
1:A:1041:GLN:OE1	1:A:1044:ARG:NH1	2.36	0.58
1:B:4731:ILE:HA	1:C:4101:LYS:HG3	1.85	0.58
1:C:23:GLN:OE1	1:C:203:ASN:ND2	2.37	0.58
1:B:4661:TYR:OH	1:B:4786:ASP:OD2	2.22	0.58
1:D:2170:MET:HE3	1:D:2171:GLY:H	1.69	0.58
1:C:719:LEU:O	1:C:720:HIS:ND1	2.36	0.58
1:C:1041:GLN:HA	1:C:1044:ARG:HD3	1.85	0.58
1:B:649:PHE:HB3	1:B:776:LEU:HD13	1.85	0.58
1:B:3986:TRP:HA	1:B:3989:VAL:HG22	1.84	0.58
1:D:1383:UNK:HA	1:D:1398:UNK:HA	1.85	0.58
1:C:1866:ILE:HD11	1:C:1926:LEU:HD23	1.84	0.58
1:A:289:ARG:NE	1:A:303:ASP:OD1	2.37	0.58
1:D:4666:VAL:CG2	1:D:4783:ILE:CD1	2.81	0.58
1:D:22:LEU:HD11	1:D:37:LEU:HD12	1.86	0.58
1:D:2096:GLU:O	1:D:2100:HIS:ND1	2.34	0.58
1:A:4973:HIS:ND1	1:D:4227:GLU:OE2	2.33	0.57
1:B:883:ALA:HB2	1:B:886:ARG:HB2	1.86	0.57
1:D:719:LEU:HD13	1:D:735:GLN:HG2	1.86	0.57
1:D:4666:VAL:N	1:D:4667:PRO:HD2	2.18	0.57
1:A:838:HIS:HA	1:A:1201:HIS:HB3	1.86	0.57
1:B:1862:ILE:HA	1:B:1865:MET:HE1	1.86	0.57
1:B:2740:VAL:HG11	1:B:2815:ALA:HB2	1.86	0.57
1:C:763:PRO:O	1:C:765:GLN:NE2	2.37	0.57
1:A:210:GLU:OE1	1:A:273:HIS:NE2	2.37	0.57
1:A:4849:TYR:HA	1:A:4883:TYR:HE1	1.69	0.57
1:B:1041:GLN:OE1	1:B:1044:ARG:NH1	2.37	0.57
1:A:1074:ILE:HD12	1:A:1115:LEU:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1936:LYS:HB2	1:B:2116:LEU:HD11	1.85	0.57
1:C:1383:UNK:HA	1:C:1398:UNK:HA	1.86	0.57
1:A:323:LEU:HG	1:A:325:THR:H	1.69	0.57
1:A:483:MET:HE2	1:A:483:MET:H	1.68	0.57
1:A:4201:ASN:ND2	1:A:4993:MET:SD	2.78	0.57
1:D:2359:ARG:NH1	1:C:195:PHE:O	2.33	0.57
1:B:1383:UNK:HA	1:B:1398:UNK:HA	1.87	0.57
1:B:4849:TYR:HA	1:B:4883:TYR:HE1	1.69	0.57
1:D:182:LEU:HD11	1:D:189:LEU:HD23	1.85	0.57
1:C:1247:PRO:HA	1:C:1598:GLN:HG3	1.87	0.57
1:A:64:ILE:HG23	1:A:402:ARG:HH21	1.68	0.57
1:A:717:ASP:OD1	1:A:720:HIS:ND1	2.38	0.56
1:B:111:HIS:CD2	1:B:114:SER:H	2.23	0.56
1:D:103:TYR:HB3	1:D:152:PRO:HD3	1.87	0.56
1:D:560:ILE:HA	1:D:563:VAL:HG12	1.87	0.56
1:A:3737:GLU:N	1:A:3763:LEU:CD1	2.67	0.56
1:B:1703:LEU:HD21	1:B:1709:ALA:N	2.19	0.56
1:C:4004:ALA:HA	1:C:4013:LEU:HD11	1.87	0.56
1:A:4184:MET:HB2	1:A:4190:ILE:HD13	1.86	0.56
1:D:730:VAL:O	1:D:735:GLN:NE2	2.38	0.56
1:D:4046:ASP:OD1	1:D:4159:ARG:NH2	2.38	0.56
1:C:633:LEU:HB3	1:C:1639:LEU:HD11	1.88	0.56
1:C:755:ILE:HB	1:C:768:PHE:HB2	1.87	0.56
1:A:2107:GLN:O	1:A:3694:LYS:NZ	2.33	0.56
1:B:4874:MET:O	1:B:4876:CYS:N	2.38	0.56
1:D:745:SER:OG	1:D:758:ARG:O	2.21	0.56
1:D:1735:ILE:HG22	1:D:2142:TYR:HB3	1.87	0.56
1:B:243:ARG:NH1	1:B:301:VAL:O	2.39	0.56
1:A:23:GLN:HE21	1:A:34:LYS:HB3	1.70	0.56
1:A:2291:GLN:O	1:A:2292:GLU:HG3	2.06	0.56
1:A:2874:MET:HE1	1:A:2939:ARG:HH21	1.70	0.56
1:B:733:PRO:HD2	1:B:763:PRO:HD2	1.87	0.56
1:B:1735:ILE:HG22	1:B:2142:TYR:HB3	1.87	0.56
1:C:4985:LEU:HB2	2:C:5101:ACP:N6	2.19	0.56
2:C:5101:ACP:O1A	2:C:5101:ACP:H3B1	2.05	0.56
1:B:4100:GLN:O	1:B:4101:LYS:HG2	2.06	0.56
1:B:4867:GLU:O	1:B:4868:ASP:C	2.46	0.56
1:D:1041:GLN:OE1	1:D:1044:ARG:NH1	2.39	0.56
1:D:4061:PHE:HA	1:D:4064:MET:HE2	1.88	0.56
1:D:4574:ASN:HA	1:D:4577:LEU:HD12	1.88	0.56
1:D:4871:GLU:O	1:D:4874:MET:HE3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4151:SER:HB2	1:A:4164:LEU:HD21	1.86	0.55
1:B:120:CYS:HA	1:B:135:VAL:HA	1.88	0.55
1:B:3754:GLU:N	1:B:3754:GLU:OE1	2.39	0.55
1:B:4664:LEU:CD2	1:B:4665:LYS:HE3	2.36	0.55
1:D:221:ARG:NH2	1:D:255:HIS:O	2.39	0.55
1:D:880:GLU:OE2	1:D:965:TYR:CE2	2.59	0.55
1:C:1702:HIS:O	1:C:1708:ARG:NH2	2.39	0.55
1:C:2291:GLN:O	1:C:2292:GLU:HG3	2.06	0.55
1:A:331:VAL:HG22	1:A:333:GLY:H	1.70	0.55
1:B:3754:GLU:CD	1:B:3754:GLU:H	2.14	0.55
1:B:2291:GLN:O	1:B:2292:GLU:HG3	2.06	0.55
1:D:1155:LEU:HD23	1:D:1184:ILE:HG23	1.89	0.55
1:C:23:GLN:HE21	1:C:34:LYS:HB3	1.72	0.55
1:C:4865:LYS:HD2	1:C:4865:LYS:H	1.68	0.55
1:B:1105:ALA:HB1	1:B:1109:LEU:HD21	1.87	0.55
1:B:2265:LEU:HD22	1:B:2330:ARG:HD3	1.89	0.55
1:A:4046:ASP:OD1	1:A:4159:ARG:NH2	2.40	0.55
1:B:1866:ILE:HD11	1:B:1926:LEU:HD23	1.88	0.55
1:B:4191:GLU:OE1	1:B:5006:GLN:NE2	2.40	0.55
1:D:243:ARG:NH1	1:D:301:VAL:O	2.40	0.55
1:C:138:GLN:HG2	1:C:139:GLU:N	2.22	0.55
1:C:243:ARG:NH1	1:C:301:VAL:O	2.38	0.55
1:C:580:GLU:HG2	1:C:583:ILE:HD11	1.88	0.55
1:C:4875:LYS:N	1:C:4875:LYS:HD2	2.22	0.55
1:D:614:VAL:HG22	1:D:616:SER:H	1.72	0.55
1:D:1170:MET:HE1	1:D:1176:GLU:HG3	1.88	0.55
1:D:2236:LEU:HD22	1:D:2250:MET:HE1	1.87	0.55
1:D:4958:CYS:SG	1:D:4983:HIS:CD2	2.98	0.55
1:A:45:ARG:HG2	1:A:443:LEU:HD21	1.89	0.55
1:A:3753:PHE:HA	1:A:3756:LYS:HD2	1.87	0.55
1:B:590:LEU:HD13	1:B:599:VAL:HG21	1.88	0.55
1:B:1155:LEU:HD23	1:B:1184:ILE:HG23	1.89	0.55
1:D:1738:LEU:HB2	1:D:2146:PRO:HD3	1.89	0.55
1:A:4738:ALA:HB1	1:A:4744:ASP:HA	1.88	0.55
1:B:1384:UNK:O	1:B:1397:UNK:N	2.40	0.55
1:B:3842:LEU:O	1:B:3929:SER:OG	2.24	0.55
1:D:4567:LEU:HD12	1:D:4816:ILE:HG22	1.89	0.55
1:C:4875:LYS:HA	1:C:4875:LYS:CE	2.37	0.55
1:A:4578:LEU:HD23	1:D:4879:MET:HE1	1.89	0.55
1:C:4958:CYS:SG	1:C:4978:HIS:CD2	3.00	0.55
1:A:284:HIS:HB3	1:A:287:THR:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2877:GLN:OE1	1:B:2939:ARG:NH2	2.40	0.55
1:B:3767:GLN:HG3	1:B:3809:ASN:OD1	2.07	0.55
1:B:4687:TYR:OH	1:B:4699:GLY:O	2.24	0.55
1:B:4958:CYS:HA	2:B:5101:ACP:H2	1.88	0.55
1:D:4675:LYS:NZ	1:D:4715:TYR:OH	2.40	0.55
1:C:4865:LYS:HE2	1:C:4865:LYS:CA	2.22	0.55
1:A:16:THR:OG1	1:A:97:GLY:O	2.25	0.54
1:A:3878:ASP:OD1	1:A:3879:GLU:N	2.40	0.54
1:B:4708:THR:OG1	1:B:4772:ASP:OD2	2.20	0.54
1:B:4921:PHE:CD1	1:B:4921:PHE:C	2.85	0.54
1:B:4966:ASP:OD1	1:B:4967:TYR:N	2.40	0.54
1:D:3674:ILE:HG22	1:D:3769:ARG:HE	1.72	0.54
1:A:1232:ARG:NH1	1:A:1828:ASP:O	2.31	0.54
1:A:2205:GLU:O	1:A:2209:GLU:HG2	2.06	0.54
1:B:121:LEU:HG	1:B:136:GLY:HA3	1.89	0.54
1:D:1703:LEU:HD22	1:D:1708:ARG:HB3	1.88	0.54
1:D:1866:ILE:HD11	1:D:1926:LEU:HD23	1.90	0.54
1:C:2305:CYS:O	1:C:2324:ASN:ND2	2.40	0.54
1:C:3198:UNK:O	1:C:3200:UNK:N	2.40	0.54
1:A:1735:ILE:HG22	1:A:2142:TYR:HB3	1.88	0.54
1:B:4170:ILE:HG23	1:B:4171:LEU:HD12	1.90	0.54
2:C:5101:ACP:H3B1	2:C:5101:ACP:H5'1	1.88	0.54
1:A:664:PHE:HB2	1:A:746:CYS:H	1.72	0.54
1:D:4170:ILE:HG23	1:D:4171:LEU:HD12	1.88	0.54
1:C:13:PHE:HE1	1:C:164:ARG:HG3	1.71	0.54
1:C:647:ASN:ND2	1:C:820:ARG:O	2.35	0.54
1:B:4820:VAL:HB	1:B:4823:LEU:HD23	1.90	0.54
1:C:2005:GLN:HE22	1:C:3641:LEU:HD22	1.71	0.54
1:A:614:VAL:HG22	1:A:616:SER:H	1.72	0.54
1:A:4180:ARG:HH21	1:A:4981:GLU:HG3	1.72	0.54
1:B:4921:PHE:CZ	1:C:4892:ARG:HB2	2.42	0.54
1:D:23:GLN:HE21	1:D:34:LYS:HB3	1.72	0.54
1:D:1384:UNK:O	1:D:1397:UNK:N	2.41	0.54
1:D:4826:ILE:O	1:D:4829:SER:OG	2.25	0.54
1:C:1095:VAL:HB	1:C:1199:VAL:HG13	1.90	0.54
1:C:4563:ARG:HH22	1:C:4791:TYR:HE2	1.56	0.54
1:C:4874:MET:C	1:C:4876:CYS:N	2.66	0.54
1:D:4184:MET:HB3	1:D:4190:ILE:HD13	1.89	0.54
1:C:1155:LEU:HD23	1:C:1184:ILE:HG23	1.89	0.54
1:C:3808:GLY:O	1:C:3813:GLN:NE2	2.38	0.54
1:A:111:HIS:CD2	1:A:114:SER:H	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2131:LEU:HD13	1:B:3662:ILE:HG12	1.90	0.54
1:D:1730:MET:O	1:D:1772:ARG:NH1	2.40	0.54
1:D:3888:LEU:HD12	1:D:3891:LEU:HD12	1.90	0.54
1:C:16:THR:OG1	1:C:97:GLY:O	2.24	0.54
1:C:61:ASP:OD2	1:C:402:ARG:NH2	2.41	0.54
1:C:221:ARG:NH2	1:C:255:HIS:O	2.38	0.54
1:D:5004:THR:HG22	1:D:5007:GLU:HG3	1.90	0.54
1:A:4104:THR:HG22	1:A:4106:PRO:HD2	1.89	0.54
1:B:210:GLU:OE1	1:B:273:HIS:NE2	2.41	0.54
1:B:3888:LEU:HD12	1:B:3891:LEU:HD12	1.90	0.54
1:B:4879:MET:SD	1:C:4578:LEU:HD12	2.48	0.54
1:D:2452:ARG:NH2	1:C:177:GLU:OE1	2.37	0.54
1:D:4697:VAL:HA	1:D:4700:GLN:HB3	1.89	0.54
1:C:4679:ARG:NH1	1:C:4715:TYR:OH	2.40	0.54
1:A:1041:GLN:HA	1:A:1044:ARG:HH11	1.73	0.53
1:A:3657:TYR:HD2	1:A:3661:TRP:CD1	2.25	0.53
1:B:4839:MET:HE2	1:C:4822:THR:HG22	1.89	0.53
1:D:4871:GLU:O	1:D:4874:MET:CE	2.55	0.53
1:A:1859:VAL:HA	1:A:1862:ILE:HG22	1.90	0.53
1:A:4921:PHE:CE1	1:A:4925:ILE:HG13	2.43	0.53
1:A:650:VAL:O	1:A:777:PHE:N	2.34	0.53
1:A:4799:SER:HB2	1:A:4812:HIS:HE1	1.72	0.53
1:B:1159:THR:HG23	1:B:1178:ALA:HA	1.90	0.53
1:C:206:CYS:HB2	1:C:271:GLY:HA3	1.91	0.53
1:C:1724:CYS:HA	1:C:1851:MET:HE1	1.90	0.53
1:C:3946:GLN:HA	1:C:3949:ARG:HG2	1.90	0.53
1:A:627:PRO:O	1:A:629:ARG:NH1	2.41	0.53
1:D:4995:LEU:HD11	1:D:5011:TRP:HB2	1.90	0.53
1:A:23:GLN:OE1	1:A:203:ASN:ND2	2.41	0.53
1:A:221:ARG:NH2	1:A:255:HIS:O	2.39	0.53
1:B:758:ARG:NH1	1:B:760:ASN:O	2.42	0.53
1:D:3762:ARG:NH2	1:D:4754:ASN:HA	2.23	0.53
1:C:664:PHE:HB2	1:C:746:CYS:H	1.73	0.53
1:C:3657:TYR:HD2	1:C:3661:TRP:CD1	2.26	0.53
1:B:1288:UNK:HA	1:B:1327:UNK:HA	1.90	0.53
1:B:5004:THR:HG22	1:B:5007:GLU:HG3	1.90	0.53
1:D:4666:VAL:HG23	1:D:4783:ILE:HD11	1.91	0.53
1:C:650:VAL:O	1:C:777:PHE:N	2.35	0.53
1:C:1196:PRO:O	1:C:1198:GLN:NE2	2.33	0.53
1:C:4875:LYS:HA	1:C:4875:LYS:HE2	1.90	0.53
1:B:794:GLY:H	1:B:798:GLY:HA3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:ASP:O	1:A:1594:ARG:NH1	2.37	0.53
1:A:2005:GLN:HE22	1:A:3641:LEU:HD22	1.74	0.53
1:A:4687:TYR:OH	1:A:4699:GLY:O	2.27	0.53
1:A:4904:PRO:HB3	1:A:4913:ARG:HG2	1.90	0.53
1:B:3850:GLN:NE2	1:B:3870:ASN:O	2.42	0.53
1:B:4920:PHE:CD1	1:B:4920:PHE:C	2.85	0.53
1:D:1841:VAL:O	1:D:1845:VAL:HG23	2.09	0.53
1:D:4664:LEU:CD2	1:D:4665:LYS:HE3	2.39	0.53
1:C:695:TYR:OH	1:C:1073:ARG:NH2	2.42	0.53
1:B:162:LYS:O	1:B:164:ARG:NH1	2.42	0.53
1:B:1293:UNK:N	1:B:1324:UNK:O	2.42	0.53
1:B:23:GLN:OE1	1:B:203:ASN:ND2	2.42	0.53
1:B:3761:GLN:NE2	1:B:4750:ILE:CD1	2.72	0.53
1:B:5013:MET:HE3	1:B:5018:CYS:HB3	1.90	0.53
1:D:556:ALA:HB1	1:D:560:ILE:HG12	1.91	0.53
1:D:591:ASP:O	1:D:1594:ARG:NH1	2.37	0.53
1:D:1096:THR:HG23	1:D:1100:MET:HE1	1.91	0.53
1:A:4125:PHE:HA	1:A:4128:PHE:HB3	1.92	0.52
1:B:614:VAL:HG22	1:B:616:SER:H	1.73	0.52
1:B:2358:ILE:HA	1:B:2364:PHE:HZ	1.74	0.52
1:D:838:HIS:HA	1:D:1201:HIS:HB3	1.92	0.52
1:D:4690:GLU:HG2	1:D:4691:GLN:N	2.23	0.52
1:D:4820:VAL:HB	1:D:4823:LEU:HD23	1.90	0.52
1:D:4985:LEU:HB2	2:D:5101:ACP:N6	2.25	0.52
1:C:733:PRO:HD2	1:C:763:PRO:HD2	1.90	0.52
1:A:619:ASP:HA	1:A:622:THR:HG22	1.92	0.52
1:B:182:LEU:HD11	1:B:189:LEU:HD23	1.90	0.52
1:B:627:PRO:O	1:B:629:ARG:NH1	2.41	0.52
1:B:4720:VAL:HA	1:B:4723:LYS:HG2	1.90	0.52
1:B:4826:ILE:O	1:B:4829:SER:OG	2.25	0.52
1:D:169:LEU:HD21	1:D:202:MET:HG2	1.91	0.52
1:D:256:ALA:H	1:D:480:GLU:HG3	1.74	0.52
1:C:45:ARG:HG2	1:C:443:LEU:HD21	1.92	0.52
1:C:289:ARG:HG2	1:C:303:ASP:HA	1.90	0.52
1:C:1148:VAL:HB	1:C:1165:ASN:HA	1.90	0.52
1:C:1385:UNK:HA	1:C:1396:UNK:HA	1.90	0.52
1:A:103:TYR:OH	1:A:167:ASP:OD2	2.25	0.52
1:B:1839:VAL:HG13	1:B:1841:VAL:H	1.74	0.52
1:D:103:TYR:OH	1:D:167:ASP:OD2	2.27	0.52
1:D:500:ALA:HA	1:D:504:ALA:HB3	1.92	0.52
1:D:3946:GLN:HA	1:D:3949:ARG:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4232:GLU:OE2	1:D:5017:ARG:NH2	2.43	0.52
1:C:1735:ILE:HG22	1:C:2142:TYR:HB3	1.90	0.52
1:C:4875:LYS:CE	1:C:4875:LYS:CA	2.85	0.52
1:A:1693:GLN:HG3	1:A:1708:ARG:HH22	1.74	0.52
1:B:3657:TYR:HD2	1:B:3661:TRP:CD1	2.28	0.52
1:D:23:GLN:OE1	1:D:203:ASN:ND2	2.41	0.52
1:C:3850:GLN:NE2	1:C:3870:ASN:O	2.42	0.52
1:A:3842:LEU:O	1:A:3929:SER:OG	2.26	0.52
1:D:4871:GLU:H	1:D:4872:PRO:HD3	1.71	0.52
1:C:908:VAL:HG12	1:C:909:ASN:N	2.25	0.52
1:C:1243:PRO:HB2	1:C:1600:LEU:HD13	1.92	0.52
1:A:4710:SER:O	1:A:4713:SER:OG	2.25	0.52
1:D:2742:THR:HG23	1:D:2814:LYS:HD2	1.91	0.52
1:D:4578:LEU:HD12	1:C:4879:MET:SD	2.50	0.52
1:C:4690:GLU:HG2	1:C:4691:GLN:H	1.75	0.52
1:A:22:LEU:HD11	1:A:37:LEU:HD12	1.90	0.52
1:A:1293:UNK:N	1:A:1324:UNK:O	2.43	0.52
1:A:3757:GLU:OE1	1:A:4719:PHE:CZ	2.63	0.52
1:B:580:GLU:HG2	1:B:583:ILE:HD11	1.91	0.52
1:B:1385:UNK:HA	1:B:1396:UNK:HA	1.90	0.52
1:B:1387:UNK:HA	1:B:1394:UNK:HA	1.92	0.52
1:B:4094:GLN:HG2	1:B:4108:ILE:HG21	1.91	0.52
1:D:941:MET:HE1	1:D:1050:GLY:HA3	1.91	0.52
1:D:1694:LEU:O	1:D:1698:LEU:HG	2.10	0.52
1:C:1677:GLY:HA3	1:C:1721:GLU:HG2	1.90	0.52
1:A:1148:VAL:HB	1:A:1165:ASN:HA	1.91	0.52
1:A:4874:MET:O	1:A:4875:LYS:CB	2.44	0.52
1:A:4966:ASP:OD1	1:A:4966:ASP:N	2.43	0.52
1:B:650:VAL:O	1:B:777:PHE:N	2.42	0.52
1:D:650:VAL:O	1:D:777:PHE:N	2.36	0.52
1:D:3658:LYS:HA	1:D:3661:TRP:CD2	2.45	0.52
1:D:3767:GLN:HE22	1:D:3809:ASN:HD21	1.57	0.52
1:D:4079:ASP:N	1:D:4079:ASP:OD1	2.42	0.52
1:C:3760:LYS:HE3	1:C:3764:LEU:HB2	1.91	0.52
1:A:3733:CYS:SG	1:A:3803:SER:HB3	2.50	0.52
1:B:3753:PHE:HZ	1:B:4719:PHE:CZ	2.28	0.52
1:C:591:ASP:O	1:C:1594:ARG:NH1	2.38	0.52
1:A:1808:ARG:NH1	1:A:1858:ASP:OD2	2.43	0.51
1:A:3888:LEU:HD12	1:A:3891:LEU:HD12	1.92	0.51
1:B:103:TYR:OH	1:B:167:ASP:OD2	2.26	0.51
1:B:647:ASN:ND2	1:B:820:ARG:O	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3698:LEU:CD2	1:D:3770:LEU:O	2.59	0.51
1:D:3959:LYS:HB2	1:D:4019:LEU:HD12	1.92	0.51
1:C:4017:LEU:HD13	1:C:4020:GLN:NE2	2.25	0.51
1:C:4574:ASN:HA	1:C:4577:LEU:HD12	1.92	0.51
1:A:733:PRO:HD2	1:A:763:PRO:HD2	1.92	0.51
1:A:4060:LYS:O	1:A:4064:MET:HG2	2.10	0.51
1:B:181:HIS:CG	1:B:196:MET:HB2	2.45	0.51
1:B:1382:UNK:O	1:B:1399:UNK:N	2.43	0.51
1:B:4231:MET:HA	1:B:4234:PHE:HB3	1.93	0.51
1:D:888:GLU:C	1:D:890:GLY:H	2.17	0.51
1:D:1152:MET:HB3	1:D:1161:ILE:HB	1.92	0.51
1:D:3198:UNK:O	1:D:3200:UNK:N	2.44	0.51
1:D:3711:THR:O	1:D:3713:LYS:NZ	2.39	0.51
1:C:169:LEU:HD21	1:C:202:MET:HG2	1.92	0.51
1:C:3771:HIS:O	1:C:3775:ALA:N	2.43	0.51
1:D:627:PRO:O	1:D:629:ARG:NH1	2.43	0.51
1:C:3658:LYS:HD2	1:C:3661:TRP:CZ3	2.46	0.51
1:A:556:ALA:HB1	1:A:560:ILE:HG23	1.92	0.51
1:A:1101:ARG:HB3	1:A:1123:VAL:HG21	1.91	0.51
1:A:1243:PRO:HB2	1:A:1600:LEU:HD13	1.92	0.51
1:A:3999:MET:O	1:A:4003:LEU:HB3	2.10	0.51
1:D:4690:GLU:HG2	1:D:4691:GLN:H	1.76	0.51
1:C:3888:LEU:HD12	1:C:3891:LEU:HD12	1.92	0.51
1:A:3737:GLU:CA	1:A:3763:LEU:CD1	2.79	0.51
1:A:3877:ASP:HB3	1:A:3881:THR:HG23	1.91	0.51
1:B:16:THR:OG1	1:B:97:GLY:O	2.27	0.51
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.92	0.51
1:B:1694:LEU:O	1:B:1698:LEU:HG	2.11	0.51
1:B:1721:GLU:OE1	1:B:1725:ARG:NH1	2.41	0.51
1:B:2096:GLU:O	1:B:2100:HIS:ND1	2.35	0.51
1:B:3766:GLN:OE1	1:B:3766:GLN:HA	2.10	0.51
1:D:759:ILE:HG13	1:D:760:ASN:H	1.76	0.51
1:D:1041:GLN:HA	1:D:1044:ARG:HH11	1.75	0.51
1:D:1196:PRO:O	1:D:1198:GLN:NE2	2.37	0.51
1:C:1664:SER:HB3	1:C:1706:PRO:HB3	1.93	0.51
1:A:3986:TRP:HA	1:A:3989:VAL:HG12	1.92	0.51
1:A:4914:VAL:HG23	1:B:4888:TYR:HD1	1.76	0.51
1:B:4839:MET:HE1	1:C:4826:ILE:HG13	1.92	0.51
1:C:162:LYS:O	1:C:164:ARG:NH1	2.44	0.51
1:C:1150:GLY:O	1:C:1163:THR:OG1	2.28	0.51
1:C:1931:LEU:HD22	1:C:1935:VAL:HG11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:GLY:H	1:A:1594:ARG:HD2	1.75	0.51
1:A:3937:TYR:OH	1:A:3944:GLU:OE2	2.29	0.51
1:D:154:SER:OG	1:D:155:LYS:N	2.44	0.51
1:D:206:CYS:HB2	1:D:271:GLY:HA3	1.93	0.51
1:D:232:THR:HB	1:D:252:VAL:HG11	1.91	0.51
1:D:292:ALA:HB2	1:D:312:THR:HG22	1.93	0.51
1:D:4666:VAL:CG2	1:D:4783:ILE:HD11	2.39	0.51
1:C:1808:ARG:NH1	1:C:1858:ASP:OD2	2.43	0.51
1:C:1841:VAL:O	1:C:1845:VAL:HG23	2.11	0.51
1:C:4567:LEU:HD12	1:C:4816:ILE:HG22	1.92	0.51
1:A:61:ASP:OD2	1:A:402:ARG:NH2	2.42	0.51
1:A:292:ALA:HB2	1:A:312:THR:HG22	1.91	0.51
1:A:3198:UNK:O	1:A:3200:UNK:N	2.43	0.51
1:A:3897:ASN:C	1:A:3897:ASN:ND2	2.66	0.51
1:A:4944:ARG:NE	1:D:4942:GLU:OE2	2.44	0.51
1:C:977:LEU:HB3	1:C:1047:LEU:HD11	1.91	0.51
1:C:1936:LYS:HB2	1:C:2116:LEU:HD11	1.93	0.51
1:A:1101:ARG:NH2	1:A:1114:GLU:OE2	2.44	0.51
1:A:4865:LYS:CB	1:A:4873:ASP:OD2	2.59	0.51
1:B:4198:SER:OG	1:B:4199:GLU:N	2.44	0.51
1:D:3674:ILE:CB	1:D:3769:ARG:HH21	2.07	0.51
1:C:3955:MET:HE2	1:C:4019:LEU:HD13	1.93	0.51
1:A:1383:UNK:HA	1:A:1398:UNK:HA	1.93	0.51
1:B:1384:UNK:N	1:B:1397:UNK:O	2.44	0.51
1:B:4786:ASP:OD2	1:B:4788:SER:OG	2.24	0.51
1:D:206:CYS:SG	1:D:207:SER:N	2.84	0.51
1:D:647:ASN:ND2	1:D:820:ARG:O	2.33	0.51
1:C:3733:CYS:SG	1:C:3803:SER:HB3	2.51	0.51
1:A:1829:PRO:HB2	1:A:1837:GLN:HB2	1.93	0.50
1:A:1862:ILE:HA	1:A:1865:MET:HE1	1.93	0.50
1:A:2207:VAL:O	1:A:2210:VAL:HG12	2.10	0.50
1:A:2305:CYS:O	1:A:2324:ASN:ND2	2.45	0.50
1:B:793:LEU:HD13	1:B:821:LEU:HD13	1.92	0.50
1:C:154:SER:OG	1:C:155:LYS:N	2.44	0.50
1:C:1637:MET:HE1	1:C:1697:ALA:HB2	1.93	0.50
1:B:110:ARG:HA	1:B:117:TYR:HA	1.93	0.50
1:B:894:GLY:HA3	1:B:903:LEU:HB3	1.94	0.50
1:D:2740:VAL:HG11	1:D:2815:ALA:HB2	1.93	0.50
1:C:1717:SER:HA	1:C:1720:LEU:HD22	1.93	0.50
1:A:3946:GLN:HA	1:A:3949:ARG:HG2	1.93	0.50
1:B:2736:ASP:N	1:B:2736:ASP:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:GLU:OE1	1:D:273:HIS:NE2	2.32	0.50
1:D:880:GLU:OE2	1:D:965:TYR:CZ	2.64	0.50
1:D:4985:LEU:HB2	2:D:5101:ACP:HN61	1.75	0.50
1:A:4069:LYS:HD2	1:A:4133:GLN:HG2	1.94	0.50
1:B:154:SER:OG	1:B:155:LYS:N	2.45	0.50
1:B:3733:CYS:SG	1:B:3803:SER:HB3	2.50	0.50
1:D:1106:ARG:HD2	1:D:1120:LEU:HD13	1.93	0.50
1:D:4887:MET:HE2	1:D:4887:MET:HA	1.93	0.50
1:A:793:LEU:HD13	1:A:821:LEU:HD13	1.94	0.50
1:A:3850:GLN:NE2	1:A:3870:ASN:O	2.44	0.50
1:A:4864:ASN:C	1:A:4865:LYS:O	2.54	0.50
1:B:4045:VAL:HG22	1:B:4160:LEU:HD21	1.93	0.50
1:C:330:ASP:OD1	1:C:330:ASP:N	2.43	0.50
1:C:1382:UNK:O	1:C:1399:UNK:N	2.44	0.50
1:A:1936:LYS:HB2	1:A:2116:LEU:HD11	1.93	0.50
1:B:1653:LEU:HD21	1:B:1660:GLN:HA	1.94	0.50
1:B:3761:GLN:HE22	1:B:4750:ILE:HD12	1.75	0.50
1:B:4060:LYS:O	1:B:4064:MET:HG2	2.12	0.50
1:D:284:HIS:HB3	1:D:287:THR:HB	1.94	0.50
1:D:4666:VAL:CG2	1:D:4783:ILE:HD12	2.40	0.50
1:C:100:THR:HB	1:C:162:LYS:HE2	1.92	0.50
1:C:1148:VAL:O	1:C:1165:ASN:N	2.43	0.50
1:C:1163:THR:HG22	1:C:1168:VAL:HA	1.94	0.50
1:A:637:LEU:HA	1:A:1637:MET:HE1	1.94	0.50
1:A:638:ILE:HD12	1:A:1638:ALA:HB3	1.94	0.50
1:A:1838:PHE:HD2	1:A:1935:VAL:HG21	1.77	0.50
1:B:4874:MET:C	1:B:4876:CYS:N	2.70	0.50
1:D:2207:VAL:HG13	1:D:2232:CYS:HB2	1.94	0.50
1:C:1115:LEU:HD12	1:C:1193:SER:HB3	1.94	0.50
1:C:4222:VAL:HG11	1:C:4950:VAL:HA	1.93	0.50
1:C:4870:ASP:OD2	1:C:4872:PRO:CD	2.59	0.50
1:A:3765:TYR:CZ	1:A:4751:THR:HG22	2.46	0.50
1:A:4059:LEU:HA	1:A:4062:PHE:HD2	1.77	0.50
1:A:4242:ILE:HD12	1:A:4993:MET:HB2	1.93	0.50
1:B:1115:LEU:HB3	1:B:1123:VAL:HG11	1.94	0.50
1:D:684:VAL:HG12	1:D:781:VAL:HG23	1.93	0.50
1:C:331:VAL:HG12	1:C:333:GLY:H	1.77	0.50
1:A:206:CYS:SG	1:A:207:SER:N	2.85	0.50
1:B:615:ARG:NH1	1:B:1676:LEU:O	2.41	0.50
1:B:3794:VAL:HG11	1:B:3835:LEU:HD11	1.93	0.50
1:D:649:PHE:HB3	1:D:776:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1936:LYS:HB2	1:D:2116:LEU:HD11	1.93	0.50
1:D:4958:CYS:SG	1:D:4978:HIS:HD2	2.35	0.50
1:C:4985:LEU:CB	2:C:5101:ACP:HN61	2.24	0.50
1:B:533:ASN:ND2	1:B:536:ASN:OD1	2.45	0.49
1:B:883:ALA:H	1:B:886:ARG:H	1.60	0.49
1:B:1808:ARG:NH1	1:B:1858:ASP:OD2	2.45	0.49
1:B:3781:GLN:O	1:B:3784:SER:OG	2.29	0.49
1:B:4567:LEU:HD12	1:B:4816:ILE:HG22	1.94	0.49
1:D:894:GLY:HA3	1:D:903:LEU:HB3	1.94	0.49
1:D:1731:LEU:O	1:D:1772:ARG:NH2	2.43	0.49
1:A:894:GLY:HA3	1:A:903:LEU:HB3	1.94	0.49
1:A:2207:VAL:HG21	1:A:2235:PHE:HE2	1.75	0.49
1:B:1079:LYS:NZ	1:B:1107:PRO:O	2.46	0.49
1:B:4887:MET:HA	1:B:4887:MET:HE2	1.94	0.49
1:D:977:LEU:HD12	1:D:978:THR:N	2.27	0.49
1:D:3962:PHE:O	1:D:3966:THR:HG23	2.12	0.49
1:D:4182:GLU:O	1:D:4988:TYR:OH	2.26	0.49
1:D:5003:HIS:HD1	1:D:5007:GLU:CD	2.19	0.49
1:C:1103:GLY:HA3	1:C:1123:VAL:HA	1.94	0.49
1:C:4138:ASP:O	1:C:4142:ASN:ND2	2.43	0.49
1:A:207:SER:OG	1:A:208:CYS:N	2.45	0.49
1:A:4873:ASP:O	1:A:4874:MET:HB2	2.11	0.49
1:B:1243:PRO:HB2	1:B:1600:LEU:HD13	1.92	0.49
1:D:106:ALA:HA	1:D:149:THR:HA	1.94	0.49
1:D:1229:ASN:HB3	1:D:1826:ALA:HB1	1.94	0.49
1:C:2280:VAL:HG11	1:C:2290:LEU:HD12	1.94	0.49
1:B:2280:VAL:HG11	1:B:2290:LEU:HD12	1.94	0.49
1:B:4828:SER:HA	1:B:4831:THR:HG22	1.93	0.49
1:D:275:ARG:NH2	1:D:327:PRO:O	2.44	0.49
1:D:2271:THR:HG22	1:D:2273:LEU:H	1.77	0.49
1:A:2208:MET:O	1:A:2212:VAL:HG13	2.12	0.49
1:D:615:ARG:NH1	1:D:1676:LEU:O	2.34	0.49
1:D:4017:LEU:HD13	1:D:4020:GLN:NE2	2.22	0.49
1:C:2170:MET:HE3	1:C:2171:GLY:N	2.28	0.49
1:A:1695:LEU:HA	1:A:1698:LEU:HD23	1.93	0.49
1:B:206:CYS:HB2	1:B:271:GLY:HA3	1.93	0.49
1:B:475:GLN:HG2	1:B:529:LEU:HD12	1.95	0.49
1:D:150:MET:HG2	1:D:169:LEU:HD13	1.95	0.49
1:D:4101:LYS:O	1:D:4102:GLN:HG2	2.12	0.49
1:D:4134:GLU:HB2	1:D:4135:PRO:HD3	1.95	0.49
1:D:4162:ASN:O	1:D:4166:LEU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:HIS:HB3	1:C:480:GLU:HG3	1.94	0.49
1:C:615:ARG:NH1	1:C:1676:LEU:O	2.40	0.49
1:A:426:ARG:HA	1:A:431:PRO:HB3	1.95	0.49
1:A:1221:GLU:HB3	1:A:1223:PHE:HD1	1.77	0.49
1:B:317:ARG:HH12	1:B:323:LEU:HB3	1.77	0.49
1:D:491:ILE:O	1:D:495:ASN:HB2	2.13	0.49
1:D:888:GLU:C	1:D:890:GLY:N	2.71	0.49
1:D:4865:LYS:CB	1:D:4873:ASP:OD2	2.61	0.49
1:C:120:CYS:HA	1:C:136:GLY:H	1.77	0.49
1:C:719:LEU:HD13	1:C:735:GLN:HG2	1.95	0.49
1:C:1680:ARG:NH2	1:C:1785:ALA:O	2.45	0.49
1:C:1732:SER:OG	1:C:2140:ARG:NH2	2.45	0.49
1:C:4079:ASP:OD1	1:C:4079:ASP:N	2.46	0.49
1:A:953:THR:OG1	1:A:969:PRO:O	2.23	0.49
1:A:1095:VAL:HB	1:A:1199:VAL:HG13	1.93	0.49
1:B:759:ILE:HG13	1:B:760:ASN:H	1.78	0.49
1:D:3733:CYS:SG	1:D:3803:SER:HB3	2.52	0.49
1:C:206:CYS:SG	1:C:207:SER:N	2.84	0.49
1:C:315:CYS:SG	1:C:316:PHE:N	2.85	0.49
1:A:580:GLU:HG2	1:A:583:ILE:HD11	1.95	0.49
1:A:4079:ASP:OD1	1:A:4080:TYR:N	2.46	0.49
1:A:4207:MET:HE1	1:A:4209:GLN:HB3	1.95	0.49
1:B:669:ASP:N	1:B:669:ASP:OD1	2.45	0.49
1:B:3986:TRP:HD1	1:B:4047:MET:HG3	1.78	0.49
1:B:4673:ARG:HH22	1:B:4698:LYS:HB2	1.78	0.49
1:D:957:LYS:HA	1:D:966:LYS:NZ	2.28	0.49
1:D:4703:ARG:HA	1:D:4706:LEU:HD12	1.94	0.49
1:C:2191:PHE:HZ	1:C:2239:PHE:HB2	1.76	0.49
1:A:891:TRP:HE3	1:A:904:HIS:HB2	1.78	0.49
1:A:1079:LYS:NZ	1:A:1107:PRO:O	2.45	0.49
1:A:3658:LYS:HD2	1:A:3661:TRP:CZ3	2.48	0.49
1:A:4984:ASN:C	2:A:5101:ACP:HN61	2.21	0.49
1:B:4853:VAL:O	1:B:4857:ASN:ND2	2.46	0.49
1:D:891:TRP:HE3	1:D:904:HIS:HB2	1.78	0.49
1:C:627:PRO:O	1:C:629:ARG:NH1	2.46	0.49
1:C:1365:UNK:HA	1:C:1403:UNK:HA	1.95	0.49
1:C:4184:MET:HB2	1:C:4190:ILE:HD13	1.94	0.49
1:C:4690:GLU:HG2	1:C:4691:GLN:N	2.27	0.49
1:A:1936:LYS:HZ3	1:A:2105:TRP:CD1	2.30	0.48
1:A:3977:GLN:NE2	1:A:4030:LEU:O	2.45	0.48
1:A:4207:MET:HE3	1:A:4210:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:CYS:SG	1:B:316:PHE:N	2.86	0.48
1:B:2214:VAL:HG13	1:B:2215:LEU:HD23	1.94	0.48
1:D:331:VAL:HG12	1:D:333:GLY:H	1.78	0.48
1:D:977:LEU:HD12	1:D:978:THR:HG22	1.94	0.48
1:C:556:ALA:HB1	1:C:560:ILE:HG12	1.95	0.48
1:C:2042:CYS:SG	1:C:2043:GLY:N	2.79	0.48
1:C:2285:GLU:HG3	1:C:2286:LEU:HG	1.94	0.48
1:C:4240:ASP:OD1	1:C:4668:LEU:HD11	2.12	0.48
1:B:4875:LYS:C	1:B:4877:ASP:N	2.65	0.48
1:D:2291:GLN:O	1:D:2292:GLU:HG3	2.12	0.48
1:A:1288:UNK:HA	1:A:1327:UNK:HA	1.94	0.48
1:B:20:VAL:HG11	1:B:202:MET:HB3	1.94	0.48
1:B:2042:CYS:SG	1:B:2043:GLY:N	2.84	0.48
1:D:831:ARG:HD2	1:D:838:HIS:HB2	1.96	0.48
1:C:4198:SER:HB3	1:C:4201:ASN:HB2	1.94	0.48
1:A:3773:ARG:HA	1:A:3815:LYS:HE3	1.95	0.48
1:A:4892:ARG:HH22	1:D:4898:GLY:H	1.61	0.48
1:D:315:CYS:SG	1:D:316:PHE:N	2.86	0.48
1:D:594:GLY:H	1:D:1594:ARG:HD2	1.78	0.48
1:D:667:MET:HE2	1:D:667:MET:HA	1.95	0.48
1:C:4870:ASP:OD2	1:C:4872:PRO:HD3	2.13	0.48
1:C:4904:PRO:HB3	1:C:4913:ARG:HG2	1.96	0.48
1:A:1229:ASN:HB3	1:A:1826:ALA:HB1	1.95	0.48
1:A:3941:ASP:N	1:A:3941:ASP:OD1	2.44	0.48
1:B:3773:ARG:HA	1:B:3815:LYS:HE3	1.96	0.48
1:D:289:ARG:HG2	1:D:303:ASP:HA	1.95	0.48
1:D:1340:UNK:HA	1:D:1353:UNK:HA	1.95	0.48
1:D:1717:SER:HA	1:D:1720:LEU:HD22	1.95	0.48
1:D:4687:TYR:OH	1:D:4699:GLY:O	2.24	0.48
1:A:4054:ASN:O	1:A:4057:MET:HE3	2.12	0.48
1:A:4794:TRP:HH2	1:A:4811:ALA:HB1	1.78	0.48
1:D:3989:VAL:HG12	1:D:4023:MET:HE1	1.95	0.48
1:D:4666:VAL:CG1	1:D:4667:PRO:CD	2.91	0.48
1:D:4918:ILE:HG22	1:D:4922:PHE:CE1	2.49	0.48
1:C:4865:LYS:N	1:C:4873:ASP:OD2	2.46	0.48
1:D:755:ILE:HD13	1:D:768:PHE:HB2	1.96	0.48
1:C:567:VAL:HG13	1:C:568:LEU:HD12	1.96	0.48
1:C:1749:PRO:HB3	1:C:1760:HIS:HA	1.95	0.48
1:C:4017:LEU:HA	1:C:4020:GLN:HE21	1.78	0.48
1:A:192:ASP:N	1:A:192:ASP:OD1	2.47	0.48
1:A:686:TRP:CE3	1:A:777:PHE:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4922:PHE:HD1	1:B:4892:ARG:HH12	1.62	0.48
1:B:4874:MET:HE2	1:B:4876:CYS:HG	1.78	0.48
1:D:2736:ASP:OD1	1:D:2736:ASP:N	2.46	0.48
1:C:758:ARG:HH22	1:C:804:PRO:HA	1.79	0.48
1:C:3941:ASP:N	1:C:3941:ASP:OD1	2.45	0.48
1:C:4688:ILE:HD11	1:C:4737:ILE:HD12	1.96	0.48
1:A:2280:VAL:HG11	1:A:2290:LEU:HD12	1.96	0.48
1:A:4732:PHE:HB3	1:A:4736:ARG:HH11	1.79	0.48
1:B:1100:MET:HE3	1:B:1198:GLN:HB3	1.95	0.48
1:B:3809:ASN:HB3	1:B:3812:VAL:HG22	1.95	0.48
1:D:3999:MET:HE3	1:D:3999:MET:HA	1.96	0.48
1:D:4909:TYR:HB3	1:D:4912:TYR:HB2	1.95	0.48
1:C:1288:UNK:HA	1:C:1327:UNK:HA	1.96	0.48
1:C:3766:GLN:HA	1:C:3769:ARG:NH1	2.29	0.48
1:B:891:TRP:HE3	1:B:904:HIS:HB2	1.78	0.48
1:B:2332:LEU:HD22	1:B:2432:LEU:HD22	1.96	0.48
1:B:4690:GLU:HG2	1:B:4691:GLN:H	1.79	0.48
1:D:20:VAL:HG11	1:D:202:MET:HB3	1.96	0.48
1:D:911:HIS:O	1:D:918:ARG:NH2	2.47	0.48
1:D:1115:LEU:HB3	1:D:1123:VAL:HG11	1.95	0.48
1:D:4006:ASP:OD2	1:D:4009:GLN:NE2	2.47	0.48
1:C:500:ALA:HA	1:C:504:ALA:HB3	1.96	0.48
1:C:3652:MET:HA	1:C:3655:GLU:HG2	1.96	0.48
1:A:134:ASP:N	1:A:134:ASP:OD1	2.46	0.47
1:A:4985:LEU:HG	2:A:5101:ACP:HN61	1.79	0.47
1:B:207:SER:OG	1:B:208:CYS:N	2.46	0.47
1:B:4843:LEU:HA	1:B:4846:VAL:HG12	1.96	0.47
1:D:1677:GLY:N	1:D:1721:GLU:HG2	2.29	0.47
1:D:3874:VAL:HG12	1:D:3875:MET:HG2	1.95	0.47
1:D:4673:ARG:HH22	1:D:4698:LYS:HB2	1.79	0.47
1:C:138:GLN:HG2	1:C:139:GLU:H	1.79	0.47
1:C:173:SER:HB3	1:C:178:ARG:H	1.79	0.47
1:C:745:SER:OG	1:C:758:ARG:O	2.28	0.47
1:C:4703:ARG:HA	1:C:4706:LEU:HD12	1.95	0.47
1:C:4892:ARG:H	1:C:4892:ARG:HD3	1.79	0.47
1:A:202:MET:HE2	1:A:202:MET:N	2.29	0.47
1:A:911:HIS:O	1:A:918:ARG:NH2	2.47	0.47
1:A:913:LEU:O	1:A:918:ARG:NH2	2.48	0.47
1:A:3817:LEU:HD12	1:A:3899:PHE:HD1	1.78	0.47
1:A:4223:ASN:OD1	1:A:4224:GLU:N	2.48	0.47
1:B:911:HIS:O	1:B:918:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1839:VAL:HG22	1:B:1840:PRO:HD2	1.95	0.47
1:B:3962:PHE:O	1:B:3966:THR:HG23	2.14	0.47
1:D:660:GLY:HA2	1:D:750:LEU:HB2	1.96	0.47
1:D:2182:ILE:O	1:D:2185:ILE:HG22	2.14	0.47
1:C:52:THR:HA	1:C:60:PRO:HG3	1.96	0.47
1:C:4966:ASP:OD1	1:C:4966:ASP:N	2.46	0.47
1:A:131:LEU:HD22	1:A:178:ARG:HH22	1.79	0.47
1:A:3962:PHE:O	1:A:3966:THR:HG23	2.14	0.47
1:A:4909:TYR:HB3	1:A:4912:TYR:HB2	1.97	0.47
1:D:1679:ASN:ND2	1:D:1798:LEU:O	2.47	0.47
1:C:192:ASP:N	1:C:192:ASP:OD1	2.46	0.47
1:C:289:ARG:NE	1:C:303:ASP:OD1	2.38	0.47
1:C:894:GLY:HA3	1:C:903:LEU:HB3	1.96	0.47
1:C:2131:LEU:HD13	1:C:3662:ILE:HG21	1.95	0.47
1:A:2208:MET:HA	1:A:2211:MET:HE2	1.95	0.47
1:B:1247:PRO:HA	1:B:1598:GLN:HG3	1.95	0.47
1:B:2170:MET:HE3	1:B:2171:GLY:N	2.29	0.47
1:B:4134:GLU:HG2	1:B:4135:PRO:HD3	1.96	0.47
1:B:4703:ARG:HA	1:B:4706:LEU:HD12	1.97	0.47
1:D:192:ASP:OD1	1:D:192:ASP:N	2.47	0.47
1:D:348:VAL:HG13	1:D:357:LEU:HB2	1.96	0.47
1:D:1707:LEU:HG	1:D:1708:ARG:N	2.17	0.47
1:C:945:LYS:O	1:C:949:ASN:ND2	2.46	0.47
1:C:1166:GLY:HA2	1:C:1216:ILE:HD11	1.97	0.47
1:C:3770:LEU:HD12	1:C:3770:LEU:C	2.31	0.47
1:C:4863:TYR:N	1:C:4863:TYR:CD1	2.78	0.47
1:A:4170:ILE:HG23	1:A:4171:LEU:HD12	1.96	0.47
1:B:23:GLN:HE21	1:B:34:LYS:HB3	1.80	0.47
1:B:1150:GLY:O	1:B:1163:THR:OG1	2.29	0.47
1:B:3756:LYS:NZ	1:B:3760:LYS:HE3	2.30	0.47
1:D:111:HIS:CE1	1:D:113:HIS:HB3	2.50	0.47
1:D:1079:LYS:NZ	1:D:1107:PRO:O	2.48	0.47
1:C:202:MET:N	1:C:202:MET:HE2	2.29	0.47
1:C:1727:ARG:HH12	1:C:1773:PRO:HD2	1.80	0.47
1:C:4875:LYS:HE2	1:C:4875:LYS:CA	2.43	0.47
1:B:34:LYS:H	1:B:53:SER:HG	1.57	0.47
1:B:221:ARG:NH2	1:B:255:HIS:O	2.44	0.47
1:B:913:LEU:O	1:B:918:ARG:NH2	2.48	0.47
1:B:2182:ILE:O	1:B:2185:ILE:HG22	2.14	0.47
1:D:202:MET:HE2	1:D:202:MET:N	2.29	0.47
1:D:4222:VAL:HG11	1:D:4950:VAL:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:VAL:HG13	1:C:357:LEU:HB2	1.96	0.47
1:C:2674:UNK:O	1:C:2676:UNK:N	2.47	0.47
1:C:4791:TYR:OH	1:C:4815:ASP:O	2.27	0.47
1:A:169:LEU:HD21	1:A:202:MET:HG2	1.95	0.47
1:A:481:GLU:CD	1:A:483:MET:HE3	2.39	0.47
1:A:707:VAL:HB	1:A:713:SER:HB2	1.95	0.47
1:A:1717:SER:HA	1:A:1720:LEU:HD22	1.97	0.47
1:A:3969:ILE:HG21	1:A:4030:LEU:HA	1.96	0.47
1:A:4865:LYS:C	1:A:4871:GLU:OE2	2.57	0.47
1:B:206:CYS:SG	1:B:207:SER:N	2.86	0.47
1:B:838:HIS:HA	1:B:1201:HIS:HB3	1.97	0.47
1:B:1773:PRO:HA	1:B:2153:MET:HE1	1.97	0.47
1:B:4006:ASP:OD2	1:B:4009:GLN:NE2	2.48	0.47
1:D:580:GLU:HG2	1:D:583:ILE:HD11	1.97	0.47
1:D:973:SER:HA	1:D:1044:ARG:HH21	1.80	0.47
1:D:1770:SER:OG	1:D:1956:GLU:OE2	2.24	0.47
1:D:3767:GLN:NE2	1:D:3809:ASN:HD21	2.11	0.47
1:D:3927:GLN:HB2	1:D:3992:PHE:CE2	2.49	0.47
1:D:4794:TRP:HA	1:D:4797:VAL:HG22	1.97	0.47
1:C:134:ASP:N	1:C:134:ASP:OD1	2.47	0.47
1:C:3962:PHE:O	1:C:3966:THR:HG23	2.15	0.47
1:C:3999:MET:HA	1:C:3999:MET:HE2	1.96	0.47
1:C:4848:VAL:HG11	1:C:4887:MET:HE1	1.97	0.47
1:A:1106:ARG:HD2	1:A:1120:LEU:HD13	1.97	0.47
1:A:1839:VAL:HG13	1:A:1841:VAL:HG23	1.95	0.47
1:B:202:MET:N	1:B:202:MET:HE2	2.30	0.47
1:B:348:VAL:HG13	1:B:357:LEU:HB2	1.95	0.47
1:B:4702:ASP:N	1:B:4702:ASP:OD1	2.48	0.47
1:D:626:LEU:HD12	1:D:627:PRO:HD2	1.96	0.47
1:D:1859:VAL:HA	1:D:1862:ILE:HG22	1.95	0.47
1:D:3845:ASN:O	1:D:3849:ARG:HG2	2.15	0.47
1:D:4582:VAL:HG12	1:C:4877:ASP:HA	1.96	0.47
1:C:4696:ASP:O	1:C:4699:GLY:N	2.43	0.47
1:C:4874:MET:HE3	1:C:4874:MET:HB3	1.59	0.47
1:A:950:LEU:HD13	1:A:970:LEU:HD13	1.96	0.47
1:A:1651:LEU:HD13	1:A:1702:HIS:HE1	1.80	0.47
1:A:1728:ARG:HA	1:A:1731:LEU:HG	1.97	0.47
1:A:2736:ASP:OD1	1:A:2736:ASP:N	2.47	0.47
1:B:668:VAL:HG22	1:B:789:VAL:HA	1.96	0.47
1:B:1707:LEU:O	1:B:1709:ALA:N	2.48	0.47
1:D:162:LYS:O	1:D:164:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:733:PRO:HD2	1:D:763:PRO:HD2	1.97	0.47
1:D:959:TYR:HB2	1:D:966:LYS:HD3	1.95	0.47
1:D:3840:SER:OG	1:D:3877:ASP:OD2	2.30	0.47
2:D:5101:ACP:H5'1	2:D:5101:ACP:O1B	2.15	0.47
1:C:292:ALA:HB2	1:C:312:THR:HG22	1.96	0.47
1:C:896:VAL:HG13	1:C:903:LEU:HD13	1.97	0.47
1:C:5013:MET:SD	1:C:5018:CYS:HB3	2.55	0.47
1:A:154:SER:OG	1:A:155:LYS:N	2.47	0.47
1:A:4034:ASN:HD22	1:A:4040:ILE:HB	1.80	0.47
1:A:4198:SER:HB3	1:A:4201:ASN:HB2	1.95	0.47
1:B:323:LEU:H	1:B:323:LEU:HD23	1.80	0.47
1:B:977:LEU:HD12	1:B:1043:VAL:HB	1.95	0.47
1:B:4097:MET:HE2	1:B:4097:MET:N	2.30	0.47
1:D:118:LEU:HA	1:D:137:LEU:HB3	1.97	0.47
1:D:3969:ILE:HG21	1:D:4030:LEU:HA	1.96	0.47
1:D:4097:MET:HE2	1:D:4097:MET:N	2.30	0.47
1:C:3760:LYS:C	1:C:3760:LYS:CD	2.88	0.47
1:C:4875:LYS:HD2	1:C:4875:LYS:H	1.79	0.47
1:A:138:GLN:HG2	1:A:139:GLU:H	1.79	0.46
1:A:4231:MET:HE2	1:A:4231:MET:HA	1.97	0.46
1:B:755:ILE:HB	1:B:768:PHE:HB2	1.97	0.46
1:B:1041:GLN:HA	1:B:1044:ARG:HH11	1.80	0.46
1:D:4707:ASN:ND2	1:D:4740:LEU:O	2.48	0.46
1:D:5000:GLU:HA	1:D:5003:HIS:CD2	2.50	0.46
1:C:111:HIS:CE1	1:C:113:HIS:HB3	2.50	0.46
1:C:695:TYR:HB3	1:C:1240:LYS:HZ2	1.80	0.46
1:A:118:LEU:HA	1:A:137:LEU:HB3	1.96	0.46
1:A:315:CYS:SG	1:A:316:PHE:N	2.88	0.46
1:A:867:LEU:HD21	1:A:939:VAL:HG21	1.98	0.46
1:A:4001:MET:HE1	1:A:4057:MET:HG3	1.97	0.46
1:A:4879:MET:SD	1:B:4578:LEU:HD12	2.55	0.46
1:B:331:VAL:HG12	1:B:333:GLY:H	1.79	0.46
1:B:4155:PRO:HG3	1:B:5036:LEU:HD22	1.96	0.46
1:B:4245:MET:HE3	1:B:4245:MET:HA	1.97	0.46
1:D:708:GLY:HA3	1:D:722:TRP:HB3	1.96	0.46
1:D:4138:ASP:OD1	1:D:4138:ASP:N	2.46	0.46
1:C:118:LEU:HA	1:C:137:LEU:HB3	1.96	0.46
1:C:1980:LEU:HD23	1:C:1980:LEU:H	1.80	0.46
1:A:206:CYS:HB2	1:A:271:GLY:HA3	1.96	0.46
1:A:1079:LYS:HA	1:A:1189:LEU:HD11	1.96	0.46
1:B:61:ASP:OD2	1:B:402:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1717:SER:HA	1:B:1720:LEU:HD22	1.96	0.46
1:B:2447:LYS:HG3	1:B:2449:GLU:H	1.80	0.46
1:B:3883:ASP:OD1	1:B:3884:LEU:N	2.48	0.46
1:D:3941:ASP:OD1	1:D:3941:ASP:N	2.46	0.46
1:D:4661:TYR:HH	1:D:4788:SER:HG	1.46	0.46
1:C:348:VAL:HG22	1:C:357:LEU:HD13	1.97	0.46
1:C:869:ARG:NH1	1:C:870:ILE:HB	2.30	0.46
1:C:1384:UNK:N	1:C:1397:UNK:O	2.48	0.46
1:C:2740:VAL:HG21	1:C:2815:ALA:HA	1.97	0.46
1:C:3977:GLN:NE2	1:C:4030:LEU:O	2.47	0.46
1:C:4097:MET:N	1:C:4097:MET:HE2	2.29	0.46
1:C:4892:ARG:HG2	1:C:4892:ARG:HH11	1.81	0.46
1:A:523:TYR:O	1:A:526:LEU:HG	2.15	0.46
1:A:1119:GLU:HG2	1:A:1134:LEU:HD21	1.96	0.46
1:A:5011:TRP:NE1	1:A:5015:GLN:OE1	2.49	0.46
1:B:1859:VAL:HA	1:B:1862:ILE:HG22	1.96	0.46
1:B:3780:LEU:HA	1:B:3783:ILE:HG22	1.97	0.46
1:B:4909:TYR:HB3	1:B:4912:TYR:HB2	1.97	0.46
1:D:340:LYS:O	1:D:344:SER:OG	2.30	0.46
1:D:533:ASN:ND2	1:D:536:ASN:OD1	2.49	0.46
1:C:3877:ASP:HB3	1:C:3881:THR:HG23	1.97	0.46
1:A:3737:GLU:HA	1:A:3763:LEU:HD21	1.98	0.46
1:A:5013:MET:SD	1:A:5018:CYS:HB3	2.56	0.46
1:D:2025:GLU:HA	1:D:2028:ARG:HE	1.81	0.46
1:D:4013:LEU:O	1:D:4017:LEU:HD23	2.15	0.46
1:D:4985:LEU:CB	2:D:5101:ACP:HN61	2.28	0.46
1:C:322:LYS:HE3	1:C:322:LYS:HA	1.97	0.46
1:C:895:PRO:HA	1:C:905:PRO:HG3	1.97	0.46
1:C:1159:THR:HG23	1:C:1178:ALA:HA	1.98	0.46
1:C:1211:LEU:HB3	1:C:1214:PHE:CD2	2.50	0.46
1:C:4227:GLU:HB2	1:C:4229:GLU:HG2	1.97	0.46
1:A:275:ARG:NH1	1:A:278:GLN:HB2	2.30	0.46
1:A:1866:ILE:HD11	1:A:1926:LEU:HD23	1.97	0.46
1:B:2203:MET:SD	1:B:2203:MET:N	2.86	0.46
1:B:2458:ARG:NH2	1:B:2509:UNK:O	2.43	0.46
1:B:4069:LYS:HB2	1:B:4133:GLN:HG3	1.98	0.46
1:B:5000:GLU:HA	1:B:5003:HIS:CD2	2.51	0.46
1:D:913:LEU:O	1:D:918:ARG:NH2	2.48	0.46
1:D:1697:ALA:HB1	1:D:1708:ARG:HD2	1.97	0.46
1:D:2740:VAL:HG21	1:D:2815:ALA:HA	1.96	0.46
1:D:2761:TYR:OH	1:D:2925:GLU:OE1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:481:GLU:HB3	1:C:483:MET:HE3	1.98	0.46
1:C:541:SER:HA	1:C:574:VAL:HG22	1.97	0.46
1:C:3711:THR:O	1:C:3713:LYS:NZ	2.46	0.46
1:C:3883:ASP:OD1	1:C:3884:LEU:N	2.49	0.46
1:A:1384:UNK:O	1:A:1397:UNK:N	2.48	0.46
1:A:2107:GLN:HE22	1:A:3681:GLY:HA2	1.81	0.46
1:A:2740:VAL:HG11	1:A:2815:ALA:HB2	1.97	0.46
1:B:317:ARG:N	1:B:347:PHE:O	2.36	0.46
1:B:1980:LEU:H	1:B:1980:LEU:HD23	1.80	0.46
1:B:4034:ASN:HD22	1:B:4040:ILE:HB	1.81	0.46
1:D:4666:VAL:HG12	1:D:4667:PRO:CD	2.38	0.46
1:D:4938:ASP:O	1:D:4942:GLU:HG2	2.15	0.46
1:C:64:ILE:HG23	1:C:402:ARG:HH21	1.80	0.46
1:C:3963:ASN:O	1:C:3966:THR:OG1	2.26	0.46
1:C:4999:ASP:OD1	1:C:5001:THR:OG1	2.30	0.46
1:A:3757:GLU:OE1	1:A:4719:PHE:HZ	1.99	0.46
1:A:4759:ASP:OD1	1:A:4759:ASP:N	2.48	0.46
1:B:256:ALA:H	1:B:480:GLU:HG3	1.81	0.46
1:B:762:CYS:SG	1:B:764:VAL:HG23	2.56	0.46
1:B:1340:UNK:HA	1:B:1353:UNK:HA	1.98	0.46
1:B:1728:ARG:HA	1:B:1731:LEU:HG	1.98	0.46
1:D:2125:HIS:NE2	1:D:3724:ALA:HB1	2.31	0.46
1:D:2170:MET:HE3	1:D:2171:GLY:N	2.30	0.46
1:D:2214:VAL:HG13	1:D:2215:LEU:HD23	1.97	0.46
1:C:2198:MET:HA	1:C:2203:MET:HE1	1.96	0.46
1:A:4843:LEU:HD22	1:A:4928:LEU:HD11	1.97	0.46
1:B:4190:ILE:HG21	1:B:5028:PHE:HB2	1.98	0.46
1:D:172:VAL:HG22	1:D:179:TYR:HD1	1.81	0.46
1:C:1639:LEU:N	1:C:1648:MET:O	2.44	0.46
1:C:3722:TYR:CZ	1:C:3782:MET:HE3	2.51	0.46
1:C:4875:LYS:N	1:C:4875:LYS:CD	2.72	0.46
1:A:32:GLN:OE1	1:A:34:LYS:NZ	2.41	0.46
1:A:161:GLU:HB3	1:A:164:ARG:HH12	1.81	0.46
1:A:686:TRP:CD1	1:A:748:LEU:HD11	2.51	0.46
1:A:831:ARG:HD2	1:A:838:HIS:HB2	1.98	0.46
1:A:3808:GLY:O	1:A:3813:GLN:NE2	2.49	0.46
1:B:1679:ASN:ND2	1:B:1798:LEU:O	2.48	0.46
1:D:1980:LEU:H	1:D:1980:LEU:HD23	1.81	0.46
1:D:4901:ILE:HG21	1:D:4913:ARG:HH12	1.80	0.46
1:C:1866:ILE:HG12	1:C:1927:LEU:HD13	1.98	0.46
1:C:2272:PRO:HA	1:C:2275:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4034:ASN:HD22	1:C:4040:ILE:HB	1.81	0.46
1:A:201:ASN:C	1:A:202:MET:HE2	2.41	0.45
1:B:3877:ASP:HB3	1:B:3881:THR:HG23	1.98	0.45
1:B:4231:MET:HE1	1:B:5022:PHE:CD1	2.51	0.45
1:B:4581:LYS:HD2	1:B:4632:LEU:HD22	1.97	0.45
1:B:4837:LEU:HD23	1:B:4935:LEU:HD12	1.97	0.45
1:D:132:ALA:HA	1:D:194:SER:HB3	1.97	0.45
1:D:139:GLU:O	1:D:141:ALA:N	2.48	0.45
1:D:541:SER:HA	1:D:574:VAL:HG22	1.98	0.45
1:D:4581:LYS:HD2	1:D:4632:LEU:HD22	1.98	0.45
1:D:4666:VAL:HG23	1:D:4783:ILE:CD1	2.46	0.45
1:C:1689:VAL:HG13	1:C:1690:ASP:N	2.31	0.45
1:C:4058:ILE:HG23	1:C:4062:PHE:HE2	1.81	0.45
1:B:195:PHE:HE1	1:C:2359:ARG:HA	1.81	0.45
1:B:541:SER:HA	1:B:574:VAL:HG22	1.98	0.45
1:B:1103:GLY:HA3	1:B:1123:VAL:HA	1.98	0.45
1:D:265:LEU:HD11	1:D:279:PRO:HG2	1.99	0.45
1:D:626:LEU:HG	1:D:628:GLY:H	1.80	0.45
1:D:1115:LEU:HD11	1:D:1191:VAL:HG21	1.98	0.45
1:D:2025:GLU:HA	1:D:2028:ARG:NE	2.30	0.45
1:C:201:ASN:C	1:C:202:MET:HE2	2.40	0.45
1:A:162:LYS:O	1:A:164:ARG:NH1	2.48	0.45
1:A:220:LEU:HD12	1:A:390:LEU:HB3	1.98	0.45
1:A:1980:LEU:HD23	1:A:1980:LEU:H	1.82	0.45
1:A:3779:VAL:O	1:A:3783:ILE:HG12	2.16	0.45
1:B:484:LEU:O	1:B:488:LEU:HG	2.17	0.45
1:B:2207:VAL:HG13	1:B:2232:CYS:HB2	1.97	0.45
1:B:3561:UNK:O	1:B:3563:UNK:N	2.48	0.45
1:B:3754:GLU:N	1:B:3754:GLU:CD	2.73	0.45
1:B:4928:LEU:HD13	1:B:4931:ILE:HD11	1.97	0.45
1:D:110:ARG:HA	1:D:117:TYR:HA	1.98	0.45
1:D:1243:PRO:HB2	1:D:1600:LEU:HD13	1.98	0.45
1:A:3771:HIS:O	1:A:3775:ALA:N	2.49	0.45
1:C:1839:VAL:HG13	1:C:1841:VAL:HG23	1.98	0.45
1:C:2207:VAL:HG21	1:C:2235:PHE:HE2	1.82	0.45
1:B:201:ASN:C	1:B:202:MET:HE2	2.41	0.45
1:B:686:TRP:CE3	1:B:777:PHE:HB3	2.51	0.45
1:B:3518:UNK:O	1:B:3520:UNK:N	2.49	0.45
1:D:664:PHE:CZ	1:D:779:PRO:HB3	2.52	0.45
1:D:2748:PRO:HD2	1:D:2751:LEU:HD12	1.99	0.45
1:C:649:PHE:HB3	1:C:776:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:867:LEU:HD21	1:C:939:VAL:HG21	1.99	0.45
1:C:3829:PHE:HD1	1:C:3915:ILE:HD11	1.81	0.45
1:C:3969:ILE:HD11	1:C:3980:LEU:HD12	1.99	0.45
1:C:4081:VAL:HG21	1:C:4088:ILE:HG22	1.97	0.45
1:C:4661:TYR:OH	1:C:4786:ASP:OD2	2.30	0.45
1:A:110:ARG:HA	1:A:117:TYR:HA	1.99	0.45
1:A:289:ARG:HG2	1:A:303:ASP:HA	1.98	0.45
1:A:1384:UNK:N	1:A:1397:UNK:O	2.49	0.45
1:B:275:ARG:NH1	1:B:278:GLN:HB2	2.32	0.45
1:D:2262:GLY:HA3	1:D:2301:TYR:CZ	2.52	0.45
1:C:2101:MET:O	1:C:2104:ARG:HG2	2.17	0.45
1:C:4998:LYS:HD3	1:C:5003:HIS:HD2	1.82	0.45
1:A:355:LEU:HB3	1:A:378:LEU:HB3	1.98	0.45
1:A:495:ASN:C	1:A:495:ASN:HD22	2.25	0.45
1:A:541:SER:HA	1:A:574:VAL:HG22	1.99	0.45
1:A:667:MET:HE1	1:A:741:GLU:HA	1.98	0.45
1:A:2358:ILE:HA	1:A:2364:PHE:HZ	1.82	0.45
1:B:635:THR:HB	1:B:1639:LEU:HD23	1.99	0.45
1:B:1948:ASP:OD1	1:B:2126:ARG:NH2	2.44	0.45
1:B:4942:GLU:OE1	1:C:4944:ARG:NE	2.50	0.45
1:D:1653:LEU:HD21	1:D:1660:GLN:HA	1.99	0.45
1:D:4218:ILE:HD11	1:D:4985:LEU:HD21	1.98	0.45
1:C:1847:THR:O	1:C:1851:MET:HG2	2.17	0.45
1:C:3779:VAL:O	1:C:3783:ILE:HG12	2.16	0.45
1:C:4874:MET:CE	1:C:4877:ASP:OD1	2.65	0.45
1:B:1689:VAL:HG13	1:B:1690:ASP:N	2.32	0.45
1:B:1866:ILE:HG22	1:B:1866:ILE:O	2.17	0.45
1:B:3927:GLN:HB2	1:B:3992:PHE:CE2	2.51	0.45
1:B:4920:PHE:O	1:B:4920:PHE:CD1	2.70	0.45
1:D:275:ARG:NH1	1:D:278:GLN:HB2	2.31	0.45
1:D:1365:UNK:HA	1:D:1403:UNK:HA	1.99	0.45
1:D:4696:ASP:O	1:D:4699:GLY:N	2.46	0.45
1:D:4944:ARG:NE	1:C:4942:GLU:OE1	2.50	0.45
1:C:1217:CYS:O	1:C:1221:GLU:HB2	2.16	0.45
1:C:2908:TYR:O	1:C:2916:LYS:NZ	2.46	0.45
1:C:3874:VAL:HG12	1:C:3875:MET:HG2	1.98	0.45
1:A:2742:THR:HG23	1:A:2814:LYS:HD2	1.99	0.45
1:A:2751:LEU:O	1:A:2755:ILE:HG12	2.16	0.45
1:A:4581:LYS:HD2	1:A:4632:LEU:HD22	1.98	0.45
1:B:3875:MET:HE3	1:B:3875:MET:HB3	1.84	0.45
1:B:3941:ASP:OD1	1:B:3941:ASP:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:HIS:NE2	1:D:386:ASP:O	2.49	0.45
1:D:1110:ARG:HD3	1:D:1111:PRO:O	2.17	0.45
1:D:2267:MET:SD	1:D:2268:GLN:N	2.90	0.45
1:C:275:ARG:NH1	1:C:278:GLN:HB2	2.32	0.45
1:C:2212:VAL:HG12	1:C:2256:TYR:CZ	2.52	0.45
1:C:2802:LYS:HA	1:C:2802:LYS:HD3	1.80	0.45
1:C:4013:LEU:O	1:C:4017:LEU:HD23	2.16	0.45
1:C:4892:ARG:HG2	1:C:4892:ARG:NH1	2.32	0.45
1:A:2098:VAL:HG11	1:A:2127:GLN:HG3	1.99	0.45
1:B:3836:MET:HE2	1:B:3836:MET:HB3	1.85	0.45
1:B:4090:LYS:HE3	1:B:4090:LYS:HB2	1.81	0.45
1:D:886:ARG:O	1:D:891:TRP:N	2.43	0.45
1:D:2348:GLU:OE1	1:D:3849:ARG:NH2	2.50	0.45
1:D:4058:ILE:HG23	1:D:4062:PHE:HE2	1.82	0.45
1:C:533:ASN:ND2	1:C:536:ASN:OD1	2.49	0.45
1:C:3713:LYS:HD2	1:C:3716:LEU:HD23	1.98	0.45
1:A:867:LEU:HD11	1:A:933:LEU:HD22	2.00	0.44
1:A:2131:LEU:HD13	1:A:3662:ILE:HG21	1.99	0.44
1:A:3722:TYR:CZ	1:A:3782:MET:HE3	2.52	0.44
1:B:3845:ASN:O	1:B:3849:ARG:HG2	2.17	0.44
1:D:344:SER:HB2	1:D:389:PHE:HA	1.98	0.44
1:D:1103:GLY:HA3	1:D:1123:VAL:HA	1.98	0.44
1:D:1689:VAL:HG13	1:D:1690:ASP:N	2.32	0.44
1:D:2186:MET:HE1	1:D:2235:PHE:HA	1.99	0.44
1:C:1384:UNK:O	1:C:1397:UNK:N	2.50	0.44
1:A:2745:VAL:HB	1:A:2814:LYS:HD3	1.99	0.44
1:A:2807:TRP:N	1:A:2808:PRO:HD3	2.33	0.44
1:A:4202:ARG:HD2	1:A:4202:ARG:HA	1.76	0.44
1:A:4729:GLY:O	1:A:4734:ARG:NE	2.46	0.44
1:B:591:ASP:O	1:B:1594:ARG:NH1	2.45	0.44
1:B:742:ASP:HB3	1:B:759:ILE:HD11	1.99	0.44
1:B:1839:VAL:CG2	1:B:1840:PRO:HD2	2.47	0.44
1:B:3778:MET:HB3	1:B:3778:MET:HE2	1.83	0.44
1:B:4921:PHE:O	1:B:4921:PHE:CG	2.70	0.44
1:C:20:VAL:HG11	1:C:202:MET:HB3	1.99	0.44
1:C:264:PRO:HA	1:C:280:LEU:HG	1.99	0.44
1:C:835:ARG:NH2	1:C:1210:SER:O	2.50	0.44
1:C:3751:VAL:HG23	1:C:3756:LYS:HE2	1.99	0.44
1:C:4679:ARG:HE	1:C:5017:ARG:CZ	2.30	0.44
1:A:1704:PRO:HD2	1:A:1707:LEU:HD12	1.99	0.44
1:A:4691:GLN:NE2	1:A:4694:ASP:OD2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4848:VAL:HG21	1:A:4887:MET:HE3	1.99	0.44
1:B:5003:HIS:HD1	1:B:5007:GLU:CD	2.24	0.44
1:D:932:LEU:HD13	1:D:1046:LEU:HD22	1.98	0.44
1:D:3883:ASP:OD1	1:D:3884:LEU:N	2.50	0.44
1:C:614:VAL:HG22	1:C:616:SER:H	1.82	0.44
1:C:891:TRP:HE3	1:C:904:HIS:HB2	1.83	0.44
1:C:4034:ASN:ND2	1:C:4040:ILE:HB	2.33	0.44
1:C:4218:ILE:HD11	1:C:4985:LEU:HD21	2.00	0.44
1:A:1129:GLY:O	1:A:1139:PHE:N	2.40	0.44
1:A:1221:GLU:HB3	1:A:1223:PHE:CD1	2.52	0.44
1:A:3652:MET:HA	1:A:3655:GLU:HG2	2.00	0.44
1:A:4192:ARG:HG2	1:A:4194:TYR:CE1	2.53	0.44
1:A:4794:TRP:HA	1:A:4797:VAL:HG22	1.99	0.44
1:B:1691:GLN:HG2	1:B:1692:ALA:N	2.32	0.44
1:D:134:ASP:OD1	1:D:134:ASP:N	2.50	0.44
1:C:117:TYR:HD2	1:C:141:ALA:HA	1.81	0.44
1:C:786:GLY:HA2	1:C:1631:GLN:HA	1.99	0.44
1:C:908:VAL:CG1	1:C:909:ASN:H	2.30	0.44
1:B:348:VAL:HG22	1:B:357:LEU:HD13	1.98	0.44
1:B:4002:LYS:HA	1:B:4002:LYS:HD3	1.80	0.44
1:B:4031:LEU:HD23	1:B:4031:LEU:H	1.83	0.44
1:B:4041:ALA:O	1:B:4045:VAL:HG23	2.18	0.44
1:B:4221:VAL:HG23	1:B:4233:LEU:HD11	1.98	0.44
1:B:4707:ASN:ND2	1:B:4740:LEU:O	2.49	0.44
1:D:2807:TRP:N	1:D:2808:PRO:HD3	2.32	0.44
1:A:194:SER:O	1:B:2359:ARG:NH1	2.38	0.44
1:A:1948:ASP:OD1	1:A:2126:ARG:NH2	2.42	0.44
1:D:597:HIS:HB3	1:D:1665:HIS:CE1	2.53	0.44
1:D:1154:ASP:HB3	1:D:1157:GLU:HB2	1.99	0.44
1:D:2310:CYS:N	1:D:2324:ASN:OD1	2.51	0.44
1:D:3986:TRP:HD1	1:D:4047:MET:HG3	1.82	0.44
1:C:913:LEU:O	1:C:918:ARG:NH2	2.51	0.44
1:C:1948:ASP:OD1	1:C:2126:ARG:NH2	2.44	0.44
1:A:360:ALA:HB2	1:A:377:ILE:HG12	2.00	0.44
1:A:578:ILE:HD11	1:A:617:ASN:HB3	2.00	0.44
1:A:2042:CYS:SG	1:A:2043:GLY:N	2.85	0.44
1:A:3999:MET:HE2	1:A:4003:LEU:HD22	2.00	0.44
1:A:4661:TYR:OH	1:A:4786:ASP:OD2	2.36	0.44
1:A:4938:ASP:O	1:A:4942:GLU:HG2	2.17	0.44
1:B:292:ALA:HB2	1:B:312:THR:HG22	1.99	0.44
1:B:4938:ASP:O	1:B:4942:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:488:LEU:HD22	1:D:546:TRP:CH2	2.53	0.44
1:D:498:THR:HG23	1:D:499:THR:H	1.83	0.44
1:D:758:ARG:NH1	1:D:760:ASN:O	2.51	0.44
1:D:1707:LEU:O	1:D:1709:ALA:N	2.51	0.44
1:D:3889:GLN:HG3	1:D:3967:GLU:HG2	2.00	0.44
1:D:4661:TYR:OH	1:D:4786:ASP:OD2	2.36	0.44
1:A:794:GLY:H	1:A:798:GLY:HA3	1.82	0.44
1:A:869:ARG:NH1	1:A:870:ILE:HB	2.32	0.44
1:A:2203:MET:SD	1:A:2203:MET:N	2.88	0.44
1:A:3674:ILE:HG23	1:A:3698:LEU:HD21	2.00	0.44
1:A:4730:ASP:OD1	1:A:4730:ASP:N	2.47	0.44
1:D:45:ARG:HG2	1:D:443:LEU:HD21	1.98	0.44
1:D:118:LEU:HD12	1:D:137:LEU:HB3	1.99	0.44
1:D:360:ALA:HB2	1:D:377:ILE:HG12	2.00	0.44
1:D:4198:SER:OG	1:D:4199:GLU:N	2.51	0.44
1:C:1689:VAL:HG13	1:C:1690:ASP:H	1.81	0.44
1:C:3710:LEU:HD21	1:C:3781:GLN:NE2	2.33	0.44
1:C:4673:ARG:HH22	1:C:4698:LYS:HE3	1.83	0.44
1:A:786:GLY:HA2	1:A:1631:GLN:HA	1.99	0.44
1:A:1238:PHE:HB3	1:A:1608:MET:HE3	2.00	0.44
1:A:4236:SER:HA	1:A:4675:LYS:NZ	2.32	0.44
1:B:1716:ILE:HD11	1:B:1844:LEU:HG	1.99	0.44
1:D:1095:VAL:HG23	1:D:1200:GLY:HA2	2.00	0.44
1:C:426:ARG:HA	1:C:431:PRO:HB3	1.99	0.44
1:C:2107:GLN:HE22	1:C:3681:GLY:HA2	1.82	0.44
1:C:4780:PHE:HA	1:C:4783:ILE:HG12	1.99	0.44
1:A:42:PHE:HD2	1:A:447:ASP:HB3	1.83	0.43
1:A:745:SER:OG	1:A:758:ARG:O	2.26	0.43
1:A:4017:LEU:HD13	1:A:4135:PRO:HB2	2.00	0.43
1:B:42:PHE:HD2	1:B:447:ASP:HB3	1.83	0.43
1:B:1148:VAL:O	1:B:1165:ASN:N	2.45	0.43
1:D:4901:ILE:HG21	1:D:4913:ARG:NH1	2.33	0.43
1:C:4006:ASP:OD2	1:C:4009:GLN:NE2	2.51	0.43
1:A:1148:VAL:O	1:A:1165:ASN:N	2.39	0.43
1:A:2813:LEU:HD21	1:A:2930:LEU:HD11	2.00	0.43
1:A:3665:GLU:HG2	1:A:3667:HIS:HD2	1.83	0.43
1:B:710:ASP:OD1	1:B:710:ASP:N	2.50	0.43
1:B:2305:CYS:O	1:B:2324:ASN:ND2	2.52	0.43
1:B:4666:VAL:CG1	1:B:4667:PRO:CD	2.92	0.43
1:D:950:LEU:HD13	1:D:970:LEU:HD13	1.99	0.43
1:D:4666:VAL:N	1:D:4667:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3771:HIS:HB3	1:C:3773:ARG:NH1	2.33	0.43
1:C:4101:LYS:O	1:C:4102:GLN:HG2	2.18	0.43
1:C:4198:SER:OG	1:C:4199:GLU:N	2.51	0.43
1:A:52:THR:HA	1:A:60:PRO:HG3	2.00	0.43
1:A:1110:ARG:HD3	1:A:1111:PRO:O	2.18	0.43
1:A:3765:TYR:OH	1:A:4751:THR:HG22	2.17	0.43
1:A:4731:ILE:HD12	1:B:4101:LYS:HE3	2.01	0.43
1:B:4696:ASP:O	1:B:4699:GLY:N	2.46	0.43
1:D:1091:GLU:OE2	1:D:1212:ARG:HB2	2.18	0.43
1:D:4034:ASN:ND2	1:D:4040:ILE:HB	2.34	0.43
1:D:4060:LYS:NZ	1:D:4064:MET:HB3	2.34	0.43
1:D:4198:SER:HB3	1:D:4201:ASN:HB2	2.00	0.43
1:D:4577:LEU:HD23	1:D:4580:TYR:HE2	1.83	0.43
1:C:384:MET:SD	1:C:384:MET:N	2.91	0.43
1:C:1111:PRO:HD3	1:C:1605:TRP:HE1	1.83	0.43
1:C:4870:ASP:OD2	1:C:4872:PRO:HG2	2.18	0.43
1:A:734:GLY:O	1:A:736:HIS:ND1	2.41	0.43
1:A:1115:LEU:HD13	1:A:1193:SER:HB3	2.00	0.43
1:A:2188:ASN:O	1:A:2189:LYS:HG2	2.19	0.43
1:A:4892:ARG:NH1	1:D:4896:GLY:HA3	2.34	0.43
1:B:232:THR:HB	1:B:252:VAL:HG11	2.00	0.43
1:B:1089:TYR:HB3	1:B:1223:PHE:HB3	2.01	0.43
1:D:201:ASN:C	1:D:202:MET:HE2	2.43	0.43
1:D:786:GLY:HA2	1:D:1631:GLN:HA	2.00	0.43
1:D:4051:SER:O	1:D:4051:SER:OG	2.34	0.43
1:C:418:LEU:HB3	1:C:493:ARG:NH2	2.33	0.43
1:C:3959:LYS:HB2	1:C:4019:LEU:HD12	2.01	0.43
1:C:4680:LYS:HA	1:C:4680:LYS:HD2	1.80	0.43
1:A:20:VAL:HG11	1:A:202:MET:HB3	2.00	0.43
1:A:264:PRO:HA	1:A:280:LEU:HG	2.00	0.43
1:A:481:GLU:OE2	1:A:483:MET:HE3	2.19	0.43
1:A:1794:ALA:HA	1:A:1795:PRO:HD3	1.92	0.43
1:A:2012:PHE:HB3	1:A:2021:CYS:HA	2.01	0.43
1:B:134:ASP:OD1	1:B:134:ASP:N	2.50	0.43
1:B:3937:TYR:OH	1:B:3944:GLU:OE2	2.36	0.43
1:D:247:TYR:HE2	1:D:359:TYR:HB3	1.84	0.43
1:D:319:SER:OG	1:D:320:LYS:N	2.51	0.43
1:D:1217:CYS:O	1:D:1221:GLU:HB2	2.19	0.43
1:C:2211:MET:HE2	1:C:2211:MET:HA	1.99	0.43
1:C:4716:TRP:CH2	1:C:4996:ILE:HG13	2.54	0.43
1:A:4705:VAL:O	1:A:4708:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:HIS:O	1:B:354:GLY:N	2.50	0.43
1:B:2770:LYS:HA	1:B:2770:LYS:HD3	1.73	0.43
1:B:4985:LEU:CB	2:B:5101:ACP:HN61	2.31	0.43
1:D:52:THR:HA	1:D:60:PRO:HG3	2.00	0.43
1:D:769:GLU:O	1:D:1383:UNK:N	2.52	0.43
1:D:2469:ILE:HA	1:D:2472:LEU:HG	2.00	0.43
1:D:3145:UNK:HA	1:D:3191:UNK:HA	2.00	0.43
1:C:4664:LEU:HG	1:C:4665:LYS:HG3	2.01	0.43
1:A:3815:LYS:HE2	1:A:3815:LYS:HB2	1.81	0.43
1:B:2792:ARG:NH2	1:B:2801:ASP:OD2	2.52	0.43
1:D:419:ASP:HB2	1:D:493:ARG:HH12	1.84	0.43
1:D:1808:ARG:NH1	1:D:1858:ASP:OD2	2.52	0.43
1:C:116:MET:HE1	1:C:137:LEU:HG	2.00	0.43
1:C:911:HIS:O	1:C:918:ARG:NH2	2.48	0.43
1:C:4892:ARG:HG2	1:C:4892:ARG:O	2.18	0.43
1:A:500:ALA:HA	1:A:504:ALA:HB3	2.00	0.43
1:B:4090:LYS:NZ	1:B:4120:ASN:OD1	2.42	0.43
1:D:426:ARG:HA	1:D:431:PRO:HB3	1.99	0.43
1:D:565:TYR:HB2	1:D:602:VAL:HG22	2.01	0.43
1:D:663:TYR:HH	1:D:758:ARG:HH21	1.67	0.43
1:D:762:CYS:SG	1:D:764:VAL:HG23	2.59	0.43
1:A:973:SER:HA	1:A:1044:ARG:HH21	1.83	0.43
1:B:879:HIS:HE1	1:B:906:CYS:O	2.01	0.43
1:D:2142:TYR:HE1	1:D:2196:ASN:HB2	1.84	0.43
1:D:2297:LYS:HD2	1:D:2297:LYS:HA	1.86	0.43
1:D:3561:UNK:O	1:D:3563:UNK:N	2.52	0.43
1:D:4183:ILE:HG12	1:D:4193:ILE:HD11	2.00	0.43
1:C:523:TYR:O	1:C:526:LEU:HG	2.19	0.43
1:C:4010:ILE:HG22	1:C:4132:PHE:HZ	1.82	0.43
1:B:69:LEU:HD21	1:B:107:ILE:HD12	2.00	0.43
1:B:1238:PHE:HB3	1:B:1608:MET:HE3	2.01	0.43
1:B:1636:MET:HE1	1:B:1638:ALA:HB2	2.01	0.43
1:B:4046:ASP:OD1	1:B:4159:ARG:NH2	2.43	0.43
1:B:4058:ILE:HG23	1:B:4062:PHE:HE2	1.84	0.43
1:B:4138:ASP:O	1:B:4142:ASN:ND2	2.46	0.43
1:B:4863:TYR:CD1	1:B:4901:ILE:HG12	2.54	0.43
1:D:523:TYR:O	1:D:526:LEU:HG	2.19	0.43
1:D:1718:ILE:HG13	1:D:1719:HIS:CD2	2.54	0.43
1:D:3762:ARG:O	1:D:3766:GLN:HG2	2.18	0.43
1:D:4859:PHE:HE2	1:D:4913:ARG:HB2	1.84	0.43
1:D:5037:SER:O	1:D:5037:SER:OG	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1072:VAL:HG12	1:C:1195:GLY:HA2	2.00	0.43
1:A:531:ARG:NH2	1:A:562:GLU:OE2	2.48	0.42
1:A:3736:GLU:C	1:A:3763:LEU:CD1	2.88	0.42
1:A:3845:ASN:O	1:A:3849:ARG:HG2	2.19	0.42
1:A:4151:SER:HA	1:A:4160:LEU:HD21	2.01	0.42
1:A:4762:PRO:O	1:A:4766:THR:OG1	2.37	0.42
1:B:1178:ALA:HB1	1:B:1180:ARG:HE	1.84	0.42
1:B:2267:MET:SD	1:B:2268:GLN:N	2.92	0.42
1:B:2358:ILE:HG13	1:B:2359:ARG:HE	1.83	0.42
1:D:561:LEU:HD21	1:D:596:ASN:ND2	2.34	0.42
1:D:1164:LEU:HB3	1:D:1169:LEU:HD21	2.01	0.42
1:D:3675:ASP:N	1:D:3675:ASP:OD1	2.52	0.42
1:D:4572:ALA:O	1:D:4576:ILE:HG12	2.19	0.42
1:C:222:LEU:HG	1:C:390:LEU:HD11	1.99	0.42
1:A:221:ARG:NE	1:A:253:CYS:O	2.52	0.42
1:A:1749:PRO:HB3	1:A:1760:HIS:HA	2.01	0.42
1:A:1839:VAL:O	1:A:1841:VAL:N	2.52	0.42
1:A:2101:MET:O	1:A:2104:ARG:HG2	2.19	0.42
1:A:4105:GLY:HA2	1:A:4108:ILE:HD12	2.01	0.42
1:A:4925:ILE:O	1:A:4929:LEU:HB2	2.18	0.42
1:B:498:THR:HG23	1:B:499:THR:N	2.35	0.42
1:B:578:ILE:HD11	1:B:617:ASN:HB3	2.01	0.42
1:B:638:ILE:HG21	1:B:703:GLY:HA3	2.01	0.42
1:B:786:GLY:HA2	1:B:1631:GLN:HA	2.01	0.42
1:B:4662:ASN:C	1:B:4666:VAL:HG12	2.43	0.42
1:B:4716:TRP:CH2	1:B:4996:ILE:HG13	2.54	0.42
1:B:4875:LYS:H	1:B:4875:LYS:HG2	1.74	0.42
1:D:686:TRP:CE3	1:D:777:PHE:HB3	2.54	0.42
1:D:4022:ASP:HA	1:D:4025:VAL:HG12	2.01	0.42
1:D:4182:GLU:OE2	1:D:4983:HIS:ND1	2.33	0.42
1:C:710:ASP:OD1	1:C:710:ASP:N	2.52	0.42
1:C:2785:LEU:O	1:C:2785:LEU:HD23	2.19	0.42
1:C:3845:ASN:O	1:C:3849:ARG:HG2	2.19	0.42
1:A:484:LEU:HD23	1:A:540:PHE:HE1	1.83	0.42
1:A:1833:SER:HB3	1:A:1836:PHE:HD2	1.85	0.42
1:B:247:TYR:HE2	1:B:359:TYR:HB3	1.84	0.42
1:B:1100:MET:HB2	1:B:1143:TRP:CH2	2.54	0.42
1:C:495:ASN:C	1:C:495:ASN:HD22	2.26	0.42
1:C:3878:ASP:OD1	1:C:3879:GLU:N	2.52	0.42
1:A:1703:LEU:HD11	1:A:1709:ALA:H	1.84	0.42
1:A:2211:MET:HA	1:A:2214:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3887:PHE:CZ	1:A:3891:LEU:HD21	2.54	0.42
1:B:2149:VAL:O	1:B:2153:MET:HG2	2.19	0.42
1:B:2242:ILE:HG13	1:B:2242:ILE:O	2.20	0.42
1:B:3829:PHE:HD1	1:B:3915:ILE:HD11	1.84	0.42
1:D:34:LYS:N	1:D:53:SER:OG	2.48	0.42
1:D:1100:MET:H	1:D:1143:TRP:HH2	1.65	0.42
1:D:2474:LEU:HD23	1:D:2474:LEU:H	1.84	0.42
1:D:3778:MET:HE2	1:D:3778:MET:HB3	1.87	0.42
1:C:360:ALA:HB2	1:C:377:ILE:HG12	2.02	0.42
1:C:2310:CYS:N	1:C:2324:ASN:OD1	2.53	0.42
1:C:4855:ALA:HA	1:C:4859:PHE:HB2	2.01	0.42
1:A:719:LEU:O	1:A:720:HIS:ND1	2.53	0.42
1:A:2025:GLU:HA	1:A:2028:ARG:NE	2.35	0.42
1:B:734:GLY:O	1:B:736:HIS:ND1	2.43	0.42
1:B:3878:ASP:OD1	1:B:3879:GLU:N	2.52	0.42
1:B:3887:PHE:CZ	1:B:3891:LEU:HD21	2.55	0.42
1:B:4141:PHE:HB2	1:B:4174:PHE:HE2	1.85	0.42
1:B:4874:MET:CE	1:B:4876:CYS:HB2	2.50	0.42
1:D:207:SER:OG	1:D:208:CYS:N	2.49	0.42
1:D:4034:ASN:HD22	1:D:4040:ILE:HB	1.84	0.42
1:C:664:PHE:CZ	1:C:779:PRO:HB3	2.53	0.42
1:C:1704:PRO:HD2	1:C:1707:LEU:HD12	2.02	0.42
1:C:2474:LEU:HD23	1:C:2474:LEU:H	1.84	0.42
1:A:342:GLY:N	1:A:390:LEU:O	2.39	0.42
1:A:1973:GLN:HG2	1:A:3641:LEU:HD11	2.01	0.42
1:A:4958:CYS:HA	2:A:5101:ACP:H2	2.00	0.42
1:B:384:MET:SD	1:B:384:MET:N	2.91	0.42
1:B:755:ILE:HB	1:B:768:PHE:HD2	1.84	0.42
1:D:3887:PHE:CZ	1:D:3891:LEU:HD21	2.54	0.42
1:D:4705:VAL:O	1:D:4708:THR:HG22	2.18	0.42
1:C:1698:LEU:HD22	1:C:1712:TYR:CZ	2.54	0.42
1:C:3842:LEU:O	1:C:3929:SER:OG	2.36	0.42
1:C:4065:PHE:CZ	1:C:4132:PHE:HB2	2.54	0.42
1:A:14:LEU:HB2	1:A:101:LEU:HD12	2.02	0.42
1:A:565:TYR:HB2	1:A:602:VAL:HG22	2.02	0.42
1:D:418:LEU:HD22	1:D:493:ARG:HD3	2.02	0.42
1:D:521:LEU:HD23	1:D:524:GLU:OE2	2.20	0.42
1:D:886:ARG:HB3	1:D:891:TRP:HB2	2.02	0.42
1:D:1794:ALA:HA	1:D:1795:PRO:HD3	1.92	0.42
1:D:4003:LEU:HD22	1:D:4013:LEU:HG	2.02	0.42
1:D:4138:ASP:O	1:D:4142:ASN:ND2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3403:UNK:O	1:C:3407:UNK:N	2.53	0.42
1:A:1727:ARG:HH12	1:A:1773:PRO:HD2	1.85	0.42
1:A:3779:VAL:HG23	1:A:3797:THR:HG22	2.01	0.42
1:A:4034:ASN:ND2	1:A:4040:ILE:HB	2.35	0.42
1:B:1101:ARG:HB3	1:B:1123:VAL:HG21	2.02	0.42
1:B:1118:ASP:N	1:B:1118:ASP:OD1	2.52	0.42
1:B:2025:GLU:HA	1:B:2028:ARG:NE	2.34	0.42
1:D:1866:ILE:HG22	1:D:1866:ILE:O	2.20	0.42
1:C:708:GLY:HA3	1:C:722:TRP:HB3	2.01	0.42
1:C:1047:LEU:HD23	1:C:1047:LEU:HA	1.87	0.42
1:C:2025:GLU:HA	1:C:2028:ARG:NE	2.35	0.42
1:C:3702:VAL:HG11	1:C:3775:ALA:HA	2.02	0.42
1:C:4892:ARG:HD3	1:C:4892:ARG:C	2.44	0.42
1:A:4984:ASN:HA	2:A:5101:ACP:N6	2.35	0.42
1:B:111:HIS:HD2	1:B:114:SER:H	1.64	0.42
1:B:1867:GLU:N	1:B:1868:PRO:HD2	2.34	0.42
1:D:1095:VAL:HB	1:D:1199:VAL:HG13	2.01	0.42
1:D:4238:CYS:O	1:D:4242:ILE:HG12	2.20	0.42
1:C:243:ARG:HG2	1:C:301:VAL:HB	2.02	0.42
1:C:961:MET:HG2	1:C:962:SER:N	2.35	0.42
1:C:1698:LEU:HD22	1:C:1712:TYR:CE1	2.55	0.42
1:C:1724:CYS:SG	1:C:1728:ARG:NH1	2.93	0.42
1:C:1849:LEU:HG	1:C:1945:TYR:CE2	2.54	0.42
1:C:2267:MET:SD	1:C:2268:GLN:N	2.92	0.42
1:C:4238:CYS:O	1:C:4242:ILE:HG12	2.19	0.42
1:C:4705:VAL:O	1:C:4708:THR:HG22	2.20	0.42
1:C:4870:ASP:OD2	1:C:4872:PRO:HG3	2.15	0.42
1:A:2251:PHE:HZ	1:A:2290:LEU:HA	1.84	0.42
1:B:500:ALA:HA	1:B:504:ALA:HB3	2.02	0.42
1:B:4920:PHE:O	1:B:4920:PHE:CG	2.70	0.42
1:B:4954:MET:SD	2:B:5101:ACP:H1'	2.60	0.42
1:D:1723:ALA:HB1	1:D:1851:MET:SD	2.60	0.42
1:D:2042:CYS:SG	1:D:2043:GLY:N	2.86	0.42
1:D:2806:ARG:HA	1:D:2806:ARG:HD2	1.82	0.42
1:D:3877:ASP:HB3	1:D:3881:THR:HG23	2.02	0.42
1:D:4837:LEU:HA	1:D:4840:THR:HG22	2.02	0.42
1:C:1130:GLN:HA	1:C:1138:PRO:HA	2.00	0.42
1:C:4794:TRP:HA	1:C:4797:VAL:HG22	2.01	0.42
1:A:2773:ASN:HB3	1:A:2775:TRP:CD1	2.55	0.41
1:A:4134:GLU:HB2	1:A:4135:PRO:HD3	2.02	0.41
1:A:4795:TYR:HE1	1:A:4812:HIS:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2142:TYR:CD2	1:D:2197:LEU:HD12	2.55	0.41
1:A:2474:LEU:HD23	1:A:2474:LEU:H	1.84	0.41
2:A:5101:ACP:H3B1	2:A:5101:ACP:O1A	2.20	0.41
1:B:1749:PRO:HB3	1:B:1760:HIS:HA	2.02	0.41
1:B:4874:MET:SD	1:B:4874:MET:O	2.78	0.41
1:D:426:ARG:HG2	1:D:431:PRO:HB3	2.00	0.41
1:D:960:MET:HE3	1:D:960:MET:HB3	1.91	0.41
1:D:1238:PHE:HB3	1:D:1608:MET:HE3	2.02	0.41
1:D:1867:GLU:N	1:D:1868:PRO:HD2	2.35	0.41
1:C:738:LEU:HD23	1:C:738:LEU:HA	1.92	0.41
1:A:488:LEU:HD22	1:A:546:TRP:CH2	2.55	0.41
1:A:1600:LEU:O	1:A:1601:MET:HE2	2.20	0.41
1:A:2739:PRO:HB3	1:A:2888:ARG:HG2	2.02	0.41
1:A:3836:MET:HE2	1:A:3836:MET:HB3	1.84	0.41
1:B:1175:SER:OG	1:B:1176:GLU:N	2.52	0.41
1:B:1927:LEU:HD23	1:B:2101:MET:HG3	2.02	0.41
1:B:2474:LEU:H	1:B:2474:LEU:HD23	1.84	0.41
1:B:4863:TYR:HD1	1:B:4901:ILE:CG1	2.32	0.41
1:D:422:SER:OG	1:D:423:GLY:N	2.53	0.41
1:D:886:ARG:O	1:D:891:TRP:HB2	2.20	0.41
1:D:4702:ASP:OD1	1:D:4702:ASP:N	2.52	0.41
1:C:4666:VAL:N	1:C:4667:PRO:HD2	2.35	0.41
1:A:672:VAL:HB	1:A:680:THR:HG21	2.03	0.41
1:A:708:GLY:HA3	1:A:722:TRP:HB3	2.02	0.41
1:A:3702:VAL:HG21	1:A:3775:ALA:HB1	2.02	0.41
1:B:340:LYS:O	1:B:344:SER:OG	2.32	0.41
1:B:1794:ALA:HA	1:B:1795:PRO:HD3	1.92	0.41
1:B:4920:PHE:CZ	1:B:4924:VAL:HG21	2.56	0.41
1:D:475:GLN:HG2	1:D:529:LEU:HD12	2.02	0.41
1:D:1747:LEU:HB3	1:D:1760:HIS:HB3	2.02	0.41
1:C:110:ARG:HA	1:C:117:TYR:HA	2.03	0.41
1:A:330:ASP:OD1	1:A:330:ASP:N	2.43	0.41
1:A:941:MET:HE3	1:A:941:MET:HA	2.03	0.41
1:A:3809:ASN:O	1:A:3812:VAL:HG22	2.20	0.41
1:A:3986:TRP:HD1	1:A:4047:MET:HG3	1.86	0.41
1:B:64:ILE:HG23	1:B:402:ARG:HH21	1.86	0.41
1:B:1148:VAL:HB	1:B:1165:ASN:HA	2.03	0.41
1:B:1237:TRP:CZ3	1:B:1652:GLU:HG2	2.56	0.41
1:D:986:ASP:HA	1:D:1039:LEU:HD12	2.03	0.41
1:D:4563:ARG:HD2	1:D:4563:ARG:HA	1.87	0.41
1:C:571:SER:OG	1:C:573:GLU:OE1	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:684:VAL:HG12	1:C:781:VAL:HG23	2.02	0.41
1:C:1747:LEU:HB3	1:C:1760:HIS:HB3	2.01	0.41
1:A:556:ALA:O	1:A:560:ILE:HG12	2.20	0.41
1:A:567:VAL:HG13	1:A:568:LEU:HD12	2.01	0.41
1:A:1687:SER:HB3	1:A:1782:PHE:HD1	1.85	0.41
1:A:1810:LYS:HB2	1:A:1810:LYS:HE3	1.79	0.41
1:B:2101:MET:O	1:B:2104:ARG:HG2	2.21	0.41
1:B:2423:MET:HE3	1:B:2494:UNK:HA	2.03	0.41
1:B:4921:PHE:CD1	1:B:4921:PHE:O	2.73	0.41
1:D:734:GLY:O	1:D:736:HIS:ND1	2.41	0.41
1:D:3401:UNK:O	1:D:3406:UNK:N	2.54	0.41
1:D:4919:THR:O	1:D:4923:PHE:HB3	2.21	0.41
1:C:137:LEU:HD23	1:C:137:LEU:H	1.85	0.41
1:C:4852:THR:HG22	1:C:4853:VAL:N	2.36	0.41
1:A:1689:VAL:HG13	1:A:1690:ASP:N	2.35	0.41
1:A:1727:ARG:NH1	1:A:1772:ARG:HB3	2.36	0.41
1:A:1765:VAL:HG22	1:A:1766:GLY:H	1.86	0.41
1:A:1867:GLU:N	1:A:1868:PRO:HD2	2.35	0.41
1:A:2248:ARG:HA	1:A:2286:LEU:HD21	2.01	0.41
1:A:2310:CYS:N	1:A:2324:ASN:OD1	2.53	0.41
1:A:4152:GLU:OE1	1:A:4194:TYR:OH	2.39	0.41
1:A:5026:ASP:OD1	1:A:5027:CYS:N	2.53	0.41
1:B:1118:ASP:HA	1:B:1134:LEU:HD23	2.02	0.41
1:B:2770:LYS:HD2	1:B:2775:TRP:CE2	2.55	0.41
1:B:3731:LYS:HD2	1:B:3731:LYS:HA	1.89	0.41
1:C:110:ARG:HH21	1:C:115:ARG:HB3	1.86	0.41
1:C:617:ASN:OD1	1:C:618:GLN:N	2.54	0.41
1:C:663:TYR:CE2	1:C:665:GLU:HG3	2.55	0.41
1:C:1093:GLU:HA	1:C:1147:ASP:O	2.21	0.41
1:C:3804:ILE:HG22	1:C:3805:LEU:HD12	2.03	0.41
1:A:117:TYR:HD2	1:A:141:ALA:HA	1.86	0.41
1:A:533:ASN:ND2	1:A:536:ASN:OD1	2.53	0.41
1:A:805:PRO:HA	1:A:806:PRO:HD3	1.92	0.41
1:A:2802:LYS:HA	1:A:2802:LYS:HD3	1.85	0.41
1:A:3662:ILE:O	1:A:3662:ILE:HG22	2.21	0.41
1:A:4922:PHE:HD1	1:B:4892:ARG:NH1	2.19	0.41
1:B:143:GLY:HA3	1:B:147:TRP:HE1	1.86	0.41
1:B:4874:MET:C	1:B:4876:CYS:H	2.29	0.41
1:D:3997:ALA:HA	1:D:4058:ILE:HD11	2.03	0.41
1:D:4238:CYS:SG	1:D:4989:MET:HG2	2.61	0.41
1:C:960:MET:SD	1:C:961:MET:N	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2188:ASN:O	1:C:2189:LYS:HG2	2.21	0.41
1:C:4016:LEU:O	1:C:4020:GLN:HG2	2.21	0.41
1:C:4051:SER:O	1:C:4051:SER:OG	2.34	0.41
1:C:4072:VAL:HG12	1:C:4077:PHE:CD2	2.56	0.41
1:C:4875:LYS:H	1:C:4875:LYS:CD	2.33	0.41
1:A:172:VAL:HG22	1:A:179:TYR:HD1	1.85	0.41
1:A:340:LYS:O	1:A:344:SER:OG	2.36	0.41
1:A:491:ILE:O	1:A:495:ASN:HB2	2.21	0.41
1:A:2251:PHE:HB2	1:A:2286:LEU:HD23	2.02	0.41
1:A:2785:LEU:O	1:A:2785:LEU:HD23	2.20	0.41
1:A:3489:UNK:O	1:A:3494:UNK:N	2.54	0.41
1:A:3731:LYS:HD2	1:A:3731:LYS:HA	1.88	0.41
1:A:3927:GLN:HB2	1:A:3992:PHE:CE2	2.55	0.41
1:A:4238:CYS:O	1:A:4242:ILE:HG12	2.21	0.41
1:B:132:ALA:HA	1:B:194:SER:HB3	2.03	0.41
1:B:427:GLY:H	1:B:431:PRO:HB3	1.86	0.41
1:B:684:VAL:HG12	1:B:781:VAL:HG23	2.03	0.41
1:B:1656:ARG:O	1:B:1657:LEU:HG	2.20	0.41
1:B:1707:LEU:HB3	1:B:1708:ARG:H	1.63	0.41
1:B:1936:LYS:HA	1:B:1939:MET:HE2	2.02	0.41
1:B:2012:PHE:HB3	1:B:2021:CYS:HA	2.03	0.41
1:B:2273:LEU:HD23	1:B:2273:LEU:HA	1.91	0.41
1:B:2310:CYS:N	1:B:2324:ASN:OD1	2.54	0.41
1:B:4794:TRP:HA	1:B:4797:VAL:HG22	2.02	0.41
1:D:22:LEU:HD23	1:D:22:LEU:H	1.86	0.41
1:D:4160:LEU:O	1:D:4164:LEU:HD23	2.21	0.41
1:C:232:THR:HB	1:C:252:VAL:HG11	2.02	0.41
1:C:791:PHE:HE2	1:C:823:LEU:HD11	1.86	0.41
1:C:1118:ASP:HA	1:C:1134:LEU:HD23	2.03	0.41
1:C:1727:ARG:HH12	1:C:1772:ARG:HB3	1.85	0.41
1:C:1867:GLU:N	1:C:1868:PRO:HD2	2.35	0.41
1:C:2012:PHE:HB3	1:C:2022:PRO:HD3	2.03	0.41
1:C:2447:LYS:HG3	1:C:2449:GLU:H	1.86	0.41
1:C:3986:TRP:O	1:C:3990:VAL:HG22	2.21	0.41
1:C:4581:LYS:HD2	1:C:4632:LEU:HD22	2.03	0.41
1:C:4828:SER:HA	1:C:4831:THR:HG22	2.02	0.41
1:A:484:LEU:O	1:A:488:LEU:HG	2.21	0.41
1:A:1237:TRP:CZ3	1:A:1652:GLU:HG2	2.56	0.41
1:A:3725:TYR:O	1:A:3729:MET:HE2	2.20	0.41
1:A:3995:VAL:HG23	1:A:3996:PHE:CD1	2.56	0.41
1:B:960:MET:HE3	1:B:960:MET:HB3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1119:GLU:OE2	1:B:1133:HIS:NE2	2.52	0.41
1:B:1217:CYS:O	1:B:1221:GLU:HB2	2.20	0.41
1:B:4792:LEU:O	1:B:4796:MET:HG2	2.20	0.41
1:D:710:ASP:OD1	1:D:710:ASP:N	2.53	0.41
1:D:835:ARG:HH11	1:D:1212:ARG:HH11	1.68	0.41
1:D:3675:ASP:H	1:D:3769:ARG:NH2	2.16	0.41
1:D:4865:LYS:CB	1:D:4873:ASP:CG	2.93	0.41
1:C:645:ARG:O	1:C:824:GLU:N	2.49	0.41
1:C:867:LEU:HD11	1:C:933:LEU:HD22	2.02	0.41
1:C:1699:GLU:OE2	1:C:1813:ARG:NH1	2.54	0.41
1:C:1794:ALA:HA	1:C:1795:PRO:HD3	1.91	0.41
1:A:719:LEU:O	1:A:720:HIS:CG	2.73	0.40
1:B:360:ALA:HB2	1:B:377:ILE:HG12	2.03	0.40
1:B:1765:VAL:HG22	1:B:1766:GLY:H	1.86	0.40
1:B:1849:LEU:HG	1:B:1945:TYR:CE2	2.57	0.40
1:B:3817:LEU:HD12	1:B:3899:PHE:HD1	1.86	0.40
1:B:4892:ARG:CG	1:B:4892:ARG:O	2.70	0.40
1:D:619:ASP:HA	1:D:622:THR:HG22	2.02	0.40
1:D:1101:ARG:HB3	1:D:1123:VAL:HG21	2.03	0.40
1:D:1828:ASP:N	1:D:1829:PRO:HD2	2.36	0.40
1:D:4230:LYS:O	1:D:4233:LEU:HG	2.21	0.40
1:C:438:ILE:HD13	1:C:438:ILE:HA	1.94	0.40
1:C:3986:TRP:HD1	1:C:4047:MET:HG3	1.86	0.40
1:A:139:GLU:O	1:A:141:ALA:N	2.50	0.40
1:A:877:ASN:HD22	1:A:1045:THR:HG21	1.85	0.40
1:A:891:TRP:CG	1:A:902:ARG:HB3	2.57	0.40
1:A:977:LEU:HG	1:A:978:THR:HG22	2.03	0.40
1:A:2212:VAL:HG12	1:A:2256:TYR:OH	2.21	0.40
1:A:3674:ILE:HD11	1:A:3728:ILE:HG22	2.03	0.40
1:A:4578:LEU:HA	1:D:4879:MET:SD	2.61	0.40
1:A:4703:ARG:HA	1:A:4706:LEU:HD12	2.02	0.40
1:B:950:LEU:HB3	1:B:970:LEU:HD22	2.04	0.40
1:B:1111:PRO:HD3	1:B:1605:TRP:HE1	1.86	0.40
1:B:3658:LYS:HD2	1:B:3661:TRP:CZ3	2.56	0.40
1:D:35:LEU:HD13	1:D:49:LEU:HD13	2.03	0.40
1:D:763:PRO:O	1:D:765:GLN:NE2	2.55	0.40
1:D:4012:LEU:O	1:D:4015:GLU:HG3	2.20	0.40
1:C:139:GLU:O	1:C:141:ALA:N	2.53	0.40
1:C:350:HIS:O	1:C:354:GLY:N	2.51	0.40
1:C:488:LEU:HD22	1:C:546:TRP:CH2	2.57	0.40
1:C:869:ARG:HH11	1:C:870:ILE:HB	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4022:ASP:HA	1:C:4025:VAL:HG12	2.03	0.40
1:C:4716:TRP:HH2	1:C:4996:ILE:HG13	1.85	0.40
1:A:4180:ARG:HE	1:A:4981:GLU:HG3	1.85	0.40
1:A:4640:GLU:C	1:A:4642:ALA:H	2.29	0.40
1:B:181:HIS:NE2	1:B:182:LEU:O	2.54	0.40
1:B:445:LEU:HD23	1:B:521:LEU:HB3	2.02	0.40
1:B:1079:LYS:HA	1:B:1189:LEU:HD11	2.03	0.40
1:B:1221:GLU:HB3	1:B:1223:PHE:CD1	2.56	0.40
1:B:1810:LYS:HE3	1:B:1810:LYS:HB2	1.87	0.40
1:B:4081:VAL:HB	1:B:4088:ILE:HD13	2.04	0.40
1:B:4870:ASP:C	1:B:4872:PRO:HD3	2.47	0.40
1:D:498:THR:HG23	1:D:499:THR:N	2.37	0.40
1:D:941:MET:HA	1:D:941:MET:HE3	2.03	0.40
1:D:2802:LYS:HA	1:D:2802:LYS:HD2	1.83	0.40
1:D:2877:GLN:HE22	1:D:2939:ARG:HH22	1.68	0.40
1:D:4837:LEU:O	1:D:4841:VAL:HG23	2.21	0.40
1:A:1668:ARG:O	1:A:1671:ARG:HG2	2.22	0.40
1:A:2442:LEU:HD23	1:A:2442:LEU:H	1.85	0.40
1:A:2447:LYS:HG3	1:A:2449:GLU:H	1.87	0.40
1:B:45:ARG:HG2	1:B:443:LEU:HD21	2.03	0.40
1:B:192:ASP:OD1	1:B:192:ASP:N	2.51	0.40
1:B:567:VAL:HG13	1:B:568:LEU:HD12	2.03	0.40
1:D:765:GLN:HG3	1:D:1388:UNK:C	2.52	0.40
1:D:966:LYS:HB2	1:D:966:LYS:HE3	1.36	0.40
1:D:1948:ASP:OD1	1:D:2126:ARG:NH2	2.52	0.40
1:D:4873:ASP:O	1:D:4874:MET:HE2	2.21	0.40
1:C:758:ARG:HH22	1:C:805:PRO:HD3	1.86	0.40
1:C:1118:ASP:OD1	1:C:1118:ASP:N	2.55	0.40
1:C:1129:GLY:O	1:C:1139:PHE:N	2.39	0.40
1:C:1829:PRO:HB2	1:C:1837:GLN:HB2	2.03	0.40
1:C:4875:LYS:O	1:C:4882:CYS:HB2	2.21	0.40
1:A:118:LEU:HD12	1:A:137:LEU:HB3	2.02	0.40
1:A:349:GLN:HB2	1:A:356:TRP:CD1	2.57	0.40
1:A:876:GLU:O	1:A:880:GLU:HG2	2.22	0.40
1:A:1252:HIS:ND1	1:A:1255:TYR:HB2	2.37	0.40
1:A:3737:GLU:HA	1:A:3763:LEU:CG	2.51	0.40
1:A:3999:MET:O	1:A:4003:LEU:CB	2.70	0.40
1:A:4933:GLN:O	1:A:4937:ILE:HG12	2.22	0.40
1:B:492:ASP:OD2	1:B:546:TRP:NE1	2.48	0.40
1:B:3763:LEU:O	1:B:3767:GLN:HG2	2.21	0.40
1:B:4572:ALA:O	1:B:4576:ILE:HG12	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:719:LEU:O	1:D:719:LEU:HG	2.22	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	3172/5037 (63%)	2945 (93%)	222 (7%)	5 (0%)	43	77
1	B	3172/5037 (63%)	2926 (92%)	240 (8%)	6 (0%)	43	77
1	C	3172/5037 (63%)	2921 (92%)	246 (8%)	5 (0%)	43	77
1	D	3172/5037 (63%)	2930 (92%)	238 (8%)	4 (0%)	48	83
All	All	12688/20148 (63%)	11722 (92%)	946 (8%)	20 (0%)	44	77

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4865	LYS
1	B	4875	LYS
1	B	4876	CYS
1	D	3771	HIS
1	B	1708	ARG
1	B	4865	LYS
1	D	1708	ARG
1	C	3771	HIS
1	C	4875	LYS
1	D	4867	GLU
1	A	1840	PRO
1	A	4867	GLU
1	A	4875	LYS
1	C	4867	GLU

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Mol	Chain	Res	Type
1	B	4869	GLU
1	C	1840	PRO
1	A	4869	GLU
1	C	1708	ARG
1	B	1840	PRO
1	D	1840	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2464/3264 (76%)	2451 (100%)	13 (0%)	81	81
1	B	2455/3264 (75%)	2436 (99%)	19 (1%)	73	77
1	C	2459/3264 (75%)	2440 (99%)	19 (1%)	73	77
1	D	2455/3264 (75%)	2444 (100%)	11 (0%)	84	82
All	All	9833/13056 (75%)	9771 (99%)	62 (1%)	76	80

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3751	VAL
1	A	3753	PHE
1	A	3755	GLU
1	A	3758	MET
1	A	3759	GLU
1	A	3760	LYS
1	A	3762	ARG
1	A	3763	LEU
1	A	3897	ASN
1	A	4869	GLU
1	A	4871	GLU
1	A	4874	MET
1	A	4875	LYS
1	B	884	LEU
1	B	887	ILE

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Mol	Chain	Res	Type
1	B	888	GLU
1	B	3754	GLU
1	B	3755	GLU
1	B	3756	LYS
1	B	3757	GLU
1	B	3759	GLU
1	B	3760	LYS
1	B	3761	GLN
1	B	3763	LEU
1	B	3764	LEU
1	B	3766	GLN
1	B	3768	SER
1	B	4871	GLU
1	B	4875	LYS
1	B	4921	PHE
1	B	4922	PHE
1	B	4925	ILE
1	D	966	LYS
1	D	3759	GLU
1	D	3760	LYS
1	D	3762	ARG
1	D	3763	LEU
1	D	3767	GLN
1	D	3768	SER
1	D	3769	ARG
1	D	4867	GLU
1	D	4868	ASP
1	D	4870	ASP
1	C	3758	MET
1	C	3759	GLU
1	C	3760	LYS
1	C	3761	GLN
1	C	3762	ARG
1	C	3763	LEU
1	C	3769	ARG
1	C	3770	LEU
1	C	4852	THR
1	C	4865	LYS
1	C	4866	SER
1	C	4867	GLU
1	C	4868	ASP
1	C	4869	GLU

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Mol	Chain	Res	Type
1	C	4874	MET
1	C	4875	LYS
1	C	4884	LEU
1	C	4887	MET
1	C	4892	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	350	HIS
1	A	465	GLN
1	A	479	GLN
1	A	579	GLN
1	A	838	HIS
1	A	877	ASN
1	A	900	ASN
1	A	904	HIS
1	A	1035	ASN
1	A	1220	GLN
1	A	1254	HIS
1	A	1660	GLN
1	A	1973	GLN
1	A	2032	GLN
1	A	2107	GLN
1	A	2881	ASN
1	A	3700	GLN
1	A	3845	ASN
1	A	3895	HIS
1	A	3946	GLN
1	A	3998	HIS
1	A	4009	GLN
1	A	4078	GLN
1	A	4102	GLN
1	A	4156	HIS
1	A	4162	ASN
1	A	4707	ASN
1	A	4946	GLN
1	A	4997	ASN
1	B	12	GLN
1	B	111	HIS
1	B	380	GLN
1	B	597	HIS

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Mol	Chain	Res	Type
1	B	760	ASN
1	B	866	HIS
1	B	900	ASN
1	B	904	HIS
1	B	1220	GLN
1	B	1254	HIS
1	B	1665	HIS
1	B	2032	GLN
1	B	2107	GLN
1	B	2173	GLN
1	B	2184	ASN
1	B	2194	HIS
1	B	2420	HIS
1	B	3761	GLN
1	B	3771	HIS
1	B	3845	ASN
1	B	3895	HIS
1	B	3896	ASN
1	B	3998	HIS
1	B	4153	HIS
1	B	4162	ASN
1	B	4728	HIS
1	B	4803	HIS
1	B	4947	GLN
1	D	12	GLN
1	D	23	GLN
1	D	156	GLN
1	D	203	ASN
1	D	297	GLN
1	D	465	GLN
1	D	624	ASN
1	D	900	ASN
1	D	904	HIS
1	D	1220	GLN
1	D	1229	ASN
1	D	1254	HIS
1	D	1702	HIS
1	D	2184	ASN
1	D	2193	GLN
1	D	2420	HIS
1	D	2881	ASN
1	D	3761	GLN

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Mol	Chain	Res	Type
1	D	3771	HIS
1	D	3809	ASN
1	D	3845	ASN
1	D	3850	GLN
1	D	3895	HIS
1	D	3946	GLN
1	D	4020	GLN
1	D	4102	GLN
1	D	4109	GLN
1	D	4246	GLN
1	D	4776	GLN
1	D	4947	GLN
1	D	5015	GLN
1	C	23	GLN
1	C	54	ASN
1	C	201	ASN
1	C	203	ASN
1	C	297	GLN
1	C	465	GLN
1	C	576	ASN
1	C	582	HIS
1	C	838	HIS
1	C	949	ASN
1	C	1206	GLN
1	C	1220	GLN
1	C	1254	HIS
1	C	1274	HIS
1	C	2032	GLN
1	C	2107	GLN
1	C	2184	ASN
1	C	2194	HIS
1	C	2420	HIS
1	C	3771	HIS
1	C	3781	GLN
1	C	3814	GLN
1	C	3895	HIS
1	C	4009	GLN
1	C	4020	GLN
1	C	4250	GLN
1	C	4700	GLN
1	C	4707	ASN
1	C	4776	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACP	A	5101	-	31,33,33	1.66	8 (25%)	47,52,52	1.86	10 (21%)
2	ACP	C	5101	-	31,33,33	1.66	8 (25%)	47,52,52	1.83	10 (21%)
2	ACP	D	5101	-	31,33,33	1.66	8 (25%)	47,52,52	1.84	10 (21%)
2	ACP	B	5101	-	31,33,33	1.66	8 (25%)	47,52,52	1.85	10 (21%)

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	A	5101	-	-	4/19/38/38	0/3/3/3
2	ACP	C	5101	-	-	2/19/38/38	0/3/3/3
2	ACP	D	5101	-	-	2/19/38/38	0/3/3/3
2	ACP	B	5101	-	-	2/19/38/38	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5101	ACP	C5-C4	4.74	1.47	1.39
2	A	5101	ACP	C5-C4	4.72	1.47	1.39
2	C	5101	ACP	C5-C4	4.72	1.47	1.39
2	B	5101	ACP	C5-C4	4.70	1.47	1.39
2	A	5101	ACP	PG-O2G	2.92	1.61	1.55
2	A	5101	ACP	PG-O3G	2.90	1.61	1.55
2	D	5101	ACP	PG-O3G	2.90	1.61	1.55
2	D	5101	ACP	PG-O2G	2.90	1.61	1.55
2	B	5101	ACP	PG-O2G	2.89	1.61	1.55
2	B	5101	ACP	PG-O3G	2.89	1.61	1.55
2	C	5101	ACP	PG-O2G	2.88	1.61	1.55
2	C	5101	ACP	PG-O3G	2.87	1.61	1.55
2	C	5101	ACP	PB-O3A	2.79	1.61	1.58
2	B	5101	ACP	PB-O3A	2.76	1.61	1.58
2	B	5101	ACP	C5-C6	2.75	1.48	1.41
2	D	5101	ACP	C5-C6	2.75	1.48	1.41
2	D	5101	ACP	PB-O3A	2.74	1.61	1.58
2	C	5101	ACP	C5-C6	2.74	1.48	1.41
2	A	5101	ACP	PB-O3A	2.72	1.61	1.58
2	A	5101	ACP	C5-C6	2.71	1.48	1.41
2	C	5101	ACP	C8-N7	2.38	1.36	1.31
2	B	5101	ACP	C8-N7	2.37	1.36	1.31
2	D	5101	ACP	C8-N7	2.36	1.36	1.31
2	A	5101	ACP	C8-N7	2.34	1.36	1.31
2	D	5101	ACP	C5-N7	-2.26	1.35	1.39
2	A	5101	ACP	C5-N7	-2.25	1.35	1.39
2	B	5101	ACP	C5-N7	-2.24	1.35	1.39
2	C	5101	ACP	C5-N7	-2.21	1.35	1.39
2	B	5101	ACP	PB-O2B	2.08	1.61	1.56
2	D	5101	ACP	PB-O2B	2.08	1.61	1.56
2	C	5101	ACP	PB-O2B	2.08	1.61	1.56
2	A	5101	ACP	PB-O2B	2.06	1.61	1.56

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5101	ACP	C5-C4-N3	-5.85	118.66	126.72
2	B	5101	ACP	C5-C4-N3	-5.84	118.68	126.72
2	C	5101	ACP	C5-C4-N3	-5.83	118.68	126.72
2	D	5101	ACP	C5-C4-N3	-5.82	118.71	126.72
2	D	5101	ACP	N3-C4-N9	4.61	135.01	127.17
2	A	5101	ACP	N3-C4-N9	4.61	135.01	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5101	ACP	N3-C4-N9	4.60	134.99	127.17
2	C	5101	ACP	N3-C4-N9	4.60	134.99	127.17
2	A	5101	ACP	PB-O3A-PA	-3.78	120.05	132.37
2	D	5101	ACP	C2-N3-C4	3.70	120.88	111.83
2	B	5101	ACP	C2-N3-C4	3.70	120.87	111.83
2	A	5101	ACP	C2-N3-C4	3.69	120.83	111.83
2	C	5101	ACP	C2-N3-C4	3.67	120.80	111.83
2	D	5101	ACP	PB-O3A-PA	-3.67	120.40	132.37
2	B	5101	ACP	PB-O3A-PA	-3.57	120.73	132.37
2	A	5101	ACP	C4-C5-N7	-3.52	106.56	110.58
2	C	5101	ACP	C4-C5-N7	-3.49	106.60	110.58
2	B	5101	ACP	C4-C5-N7	-3.48	106.60	110.58
2	D	5101	ACP	C4-C5-N7	-3.44	106.64	110.58
2	C	5101	ACP	PB-O3A-PA	-3.41	121.25	132.37
2	D	5101	ACP	N3-C2-N1	-3.23	123.70	128.58
2	B	5101	ACP	N3-C2-N1	-3.22	123.71	128.58
2	A	5101	ACP	N3-C2-N1	-3.19	123.75	128.58
2	C	5101	ACP	N3-C2-N1	-3.18	123.76	128.58
2	A	5101	ACP	C4-N9-C8	2.63	108.50	105.74
2	C	5101	ACP	C4-N9-C8	2.62	108.49	105.74
2	B	5101	ACP	C4-N9-C8	2.62	108.49	105.74
2	D	5101	ACP	C4-N9-C8	2.61	108.48	105.74
2	A	5101	ACP	C5-N7-C8	2.57	107.49	103.45
2	B	5101	ACP	C5-N7-C8	2.55	107.46	103.45
2	C	5101	ACP	C5-N7-C8	2.54	107.44	103.45
2	D	5101	ACP	C5-N7-C8	2.51	107.40	103.45
2	D	5101	ACP	C3'-C2'-C1'	2.49	106.17	101.46
2	B	5101	ACP	C3'-C2'-C1'	2.47	106.13	101.46
2	A	5101	ACP	C3'-C2'-C1'	2.46	106.12	101.46
2	C	5101	ACP	C3'-C2'-C1'	2.45	106.10	101.46
2	A	5101	ACP	C6-C5-N7	2.08	136.10	132.09
2	D	5101	ACP	C6-C5-N7	2.07	136.09	132.09
2	C	5101	ACP	C6-C5-N7	2.07	136.08	132.09
2	B	5101	ACP	C6-C5-N7	2.07	136.08	132.09

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5101	ACP	C3'-C4'-C5'-O5'
2	A	5101	ACP	O4'-C4'-C5'-O5'
2	B	5101	ACP	C3'-C4'-C5'-O5'

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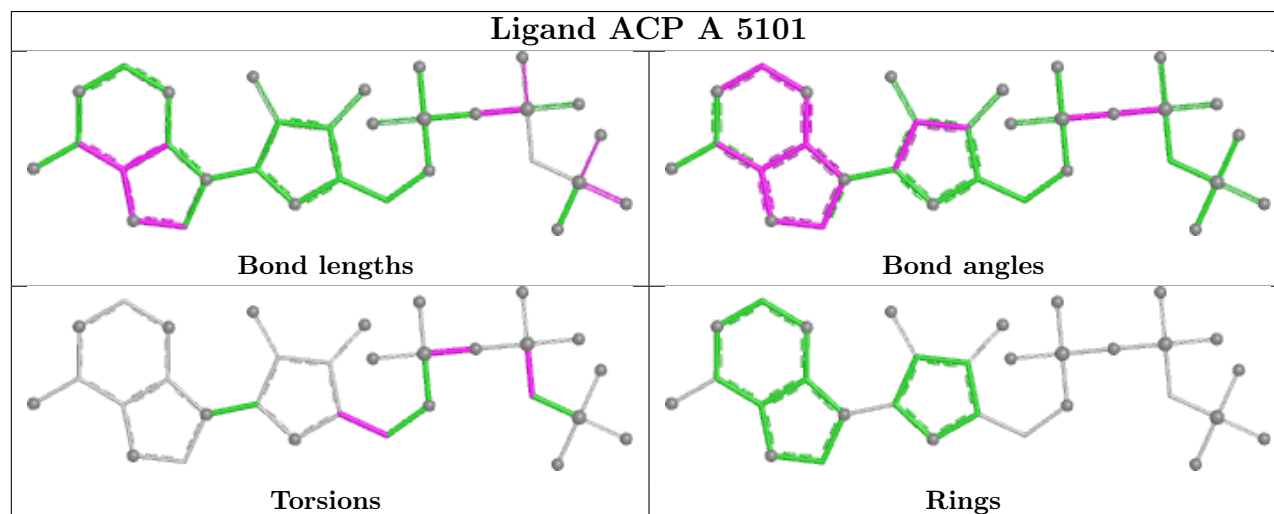
Mol	Chain	Res	Type	Atoms
2	C	5101	ACP	C3'-C4'-C5'-O5'
2	D	5101	ACP	C3'-C4'-C5'-O5'
2	C	5101	ACP	O4'-C4'-C5'-O5'
2	B	5101	ACP	O4'-C4'-C5'-O5'
2	D	5101	ACP	O4'-C4'-C5'-O5'
2	A	5101	ACP	PB-O3A-PA-O5'
2	A	5101	ACP	PG-C3B-PB-O2B

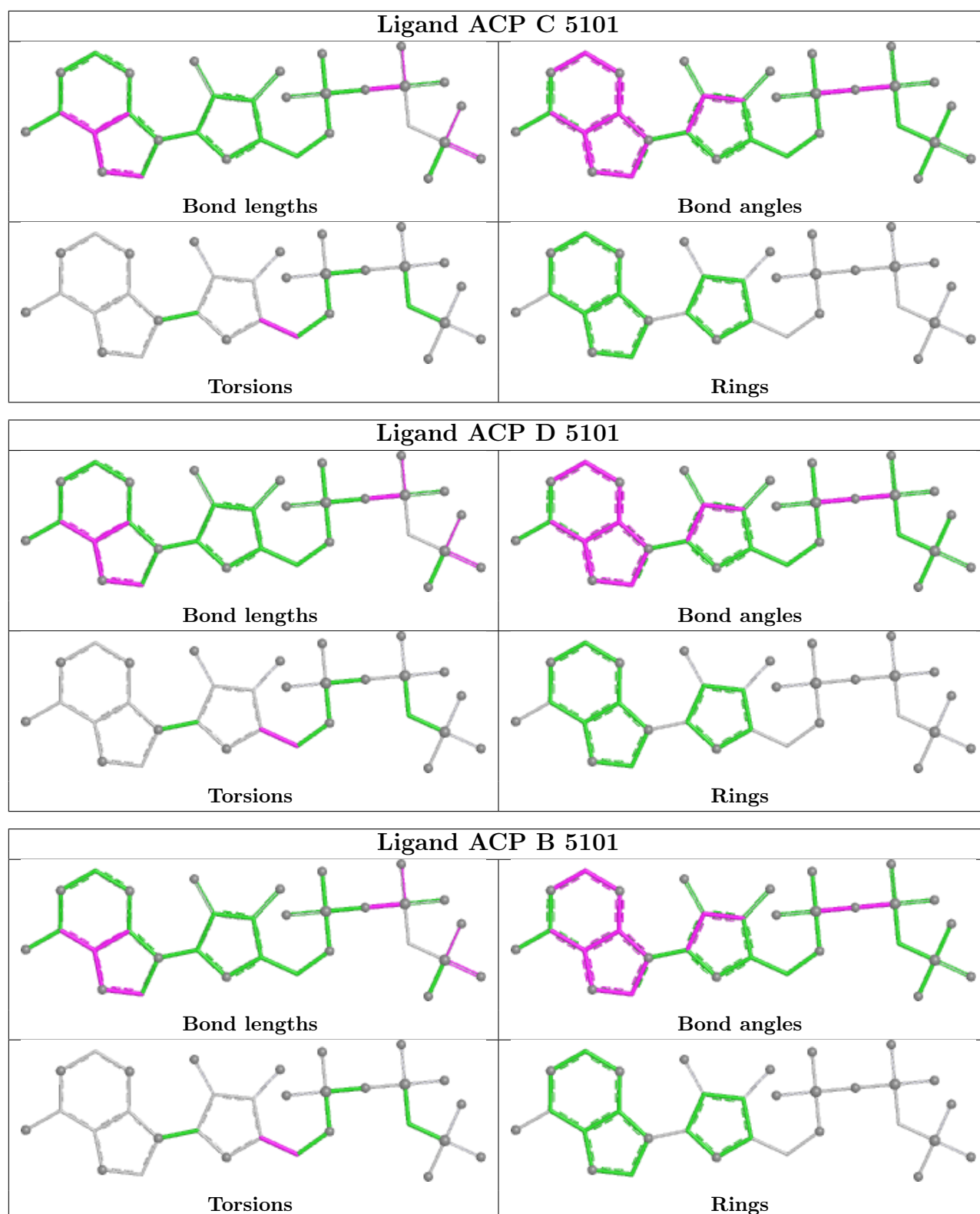
There are no ring outliers.

4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5101	ACP	6	0
2	C	5101	ACP	7	0
2	D	5101	ACP	5	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.





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	B	7
1	D	7
1	A	7
1	C	7

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3288:UNK	C	3289:UNK	N	19.38
1	B	3510:UNK	C	3511:UNK	N	17.00
1	D	3191:UNK	C	3192:UNK	N	16.39
1	D	3510:UNK	C	3511:UNK	N	15.09
1	D	3288:UNK	C	3289:UNK	N	14.70
1	A	3288:UNK	C	3289:UNK	N	14.08
1	C	3510:UNK	C	3511:UNK	N	13.93
1	A	3510:UNK	C	3511:UNK	N	13.83
1	A	3122:UNK	C	3123:UNK	N	13.57
1	C	3288:UNK	C	3289:UNK	N	13.56
1	B	3221:UNK	C	3222:UNK	N	13.41
1	B	3122:UNK	C	3123:UNK	N	12.73
1	C	3302:UNK	C	3303:UNK	N	12.41
1	C	3122:UNK	C	3123:UNK	N	12.11
1	B	3302:UNK	C	3303:UNK	N	11.72
1	D	3221:UNK	C	3222:UNK	N	11.53
1	A	3221:UNK	C	3222:UNK	N	11.22
1	D	3122:UNK	C	3123:UNK	N	9.79
1	A	3191:UNK	C	3192:UNK	N	9.57
1	A	3302:UNK	C	3303:UNK	N	9.25
1	D	3302:UNK	C	3303:UNK	N	8.00
1	B	3191:UNK	C	3192:UNK	N	7.85
1	C	3221:UNK	C	3222:UNK	N	7.69
1	C	3191:UNK	C	3192:UNK	N	6.76
1	A	1297:UNK	C	1298:UNK	N	5.81
1	D	1297:UNK	C	1298:UNK	N	5.36
1	C	1297:UNK	C	1298:UNK	N	5.21
1	B	1297:UNK	C	1298:UNK	N	4.61

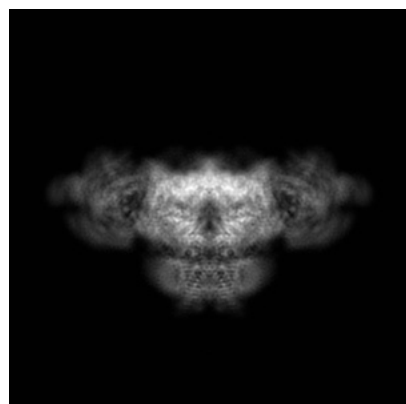
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22616. These allow visual inspection of the internal detail of the map and identification of artifacts.

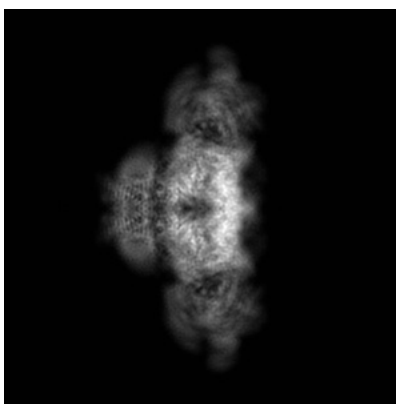
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

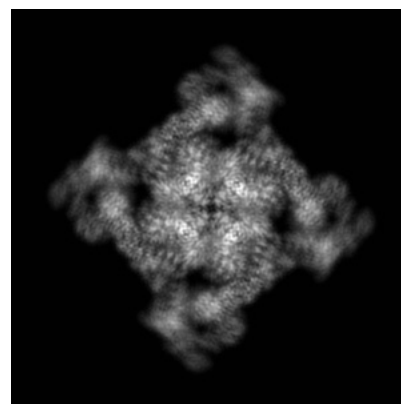
6.1.1 Primary map



X

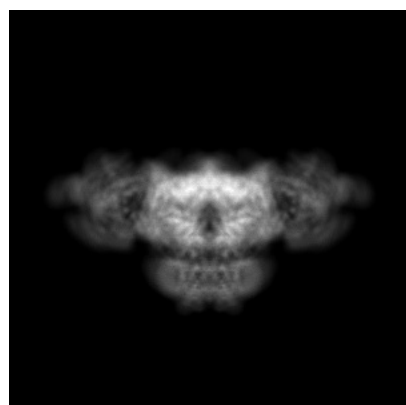


Y

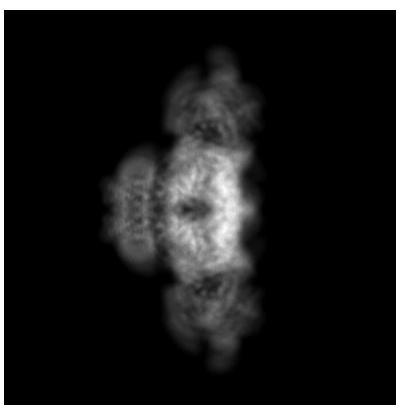


Z

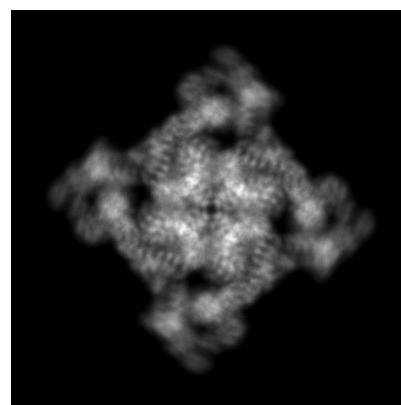
6.1.2 Raw map



X



Y

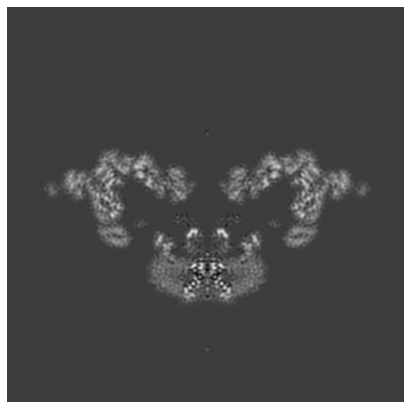


Z

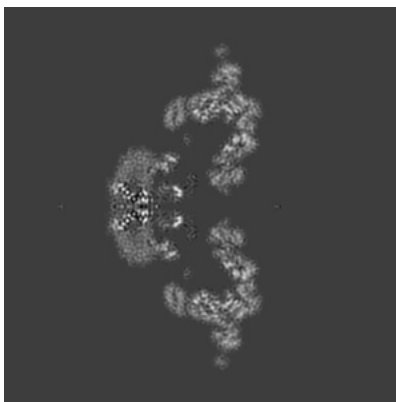
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

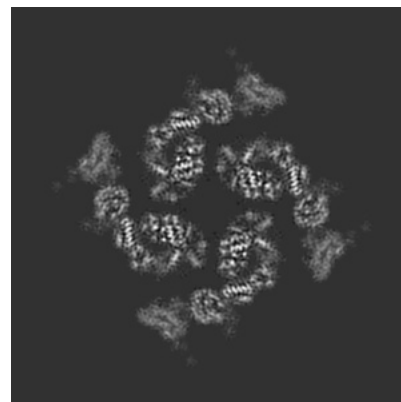
6.2.1 Primary map



X Index: 216

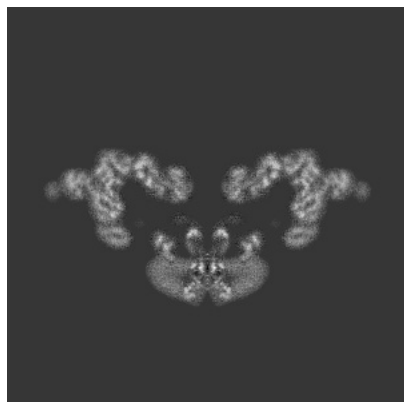


Y Index: 216

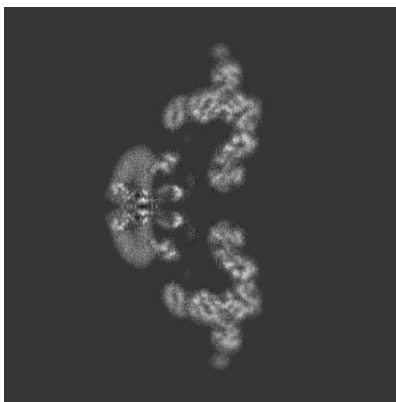


Z Index: 216

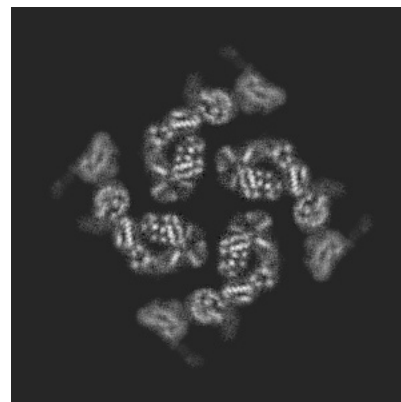
6.2.2 Raw map



X Index: 216



Y Index: 216

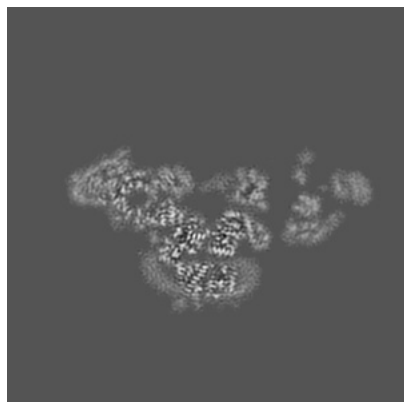


Z Index: 216

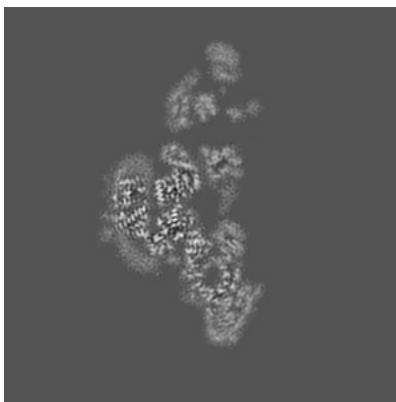
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

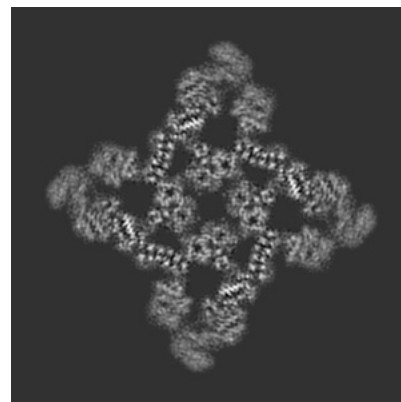
6.3.1 Primary map



X Index: 233

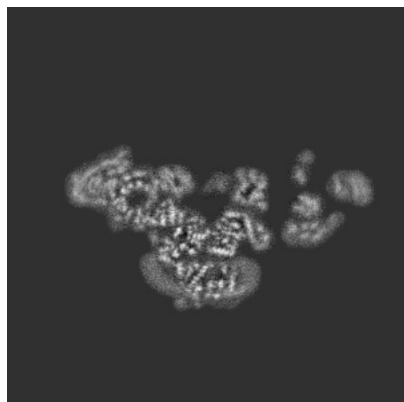


Y Index: 199

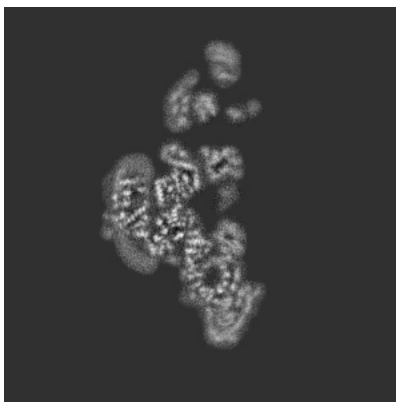


Z Index: 233

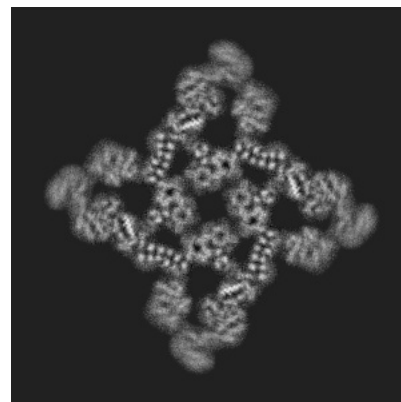
6.3.2 Raw map



X Index: 233



Y Index: 199

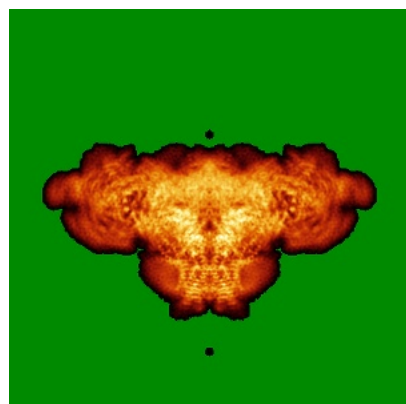


Z Index: 233

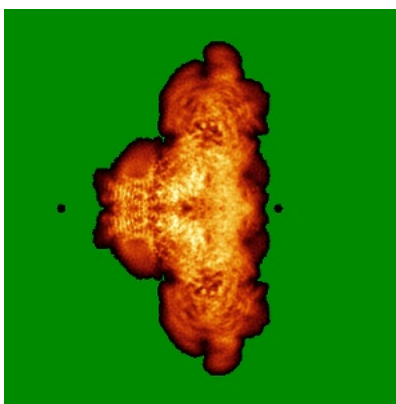
The images above show the largest variance slices of the map in three orthogonal directions.

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

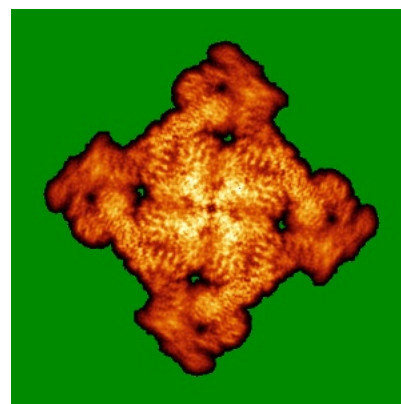
6.4.1 Primary map



X

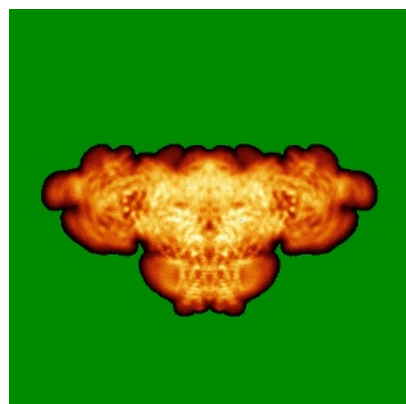


Y

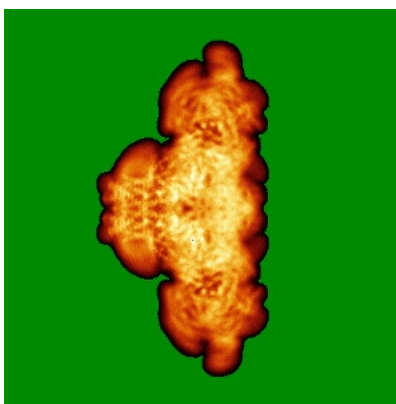


Z

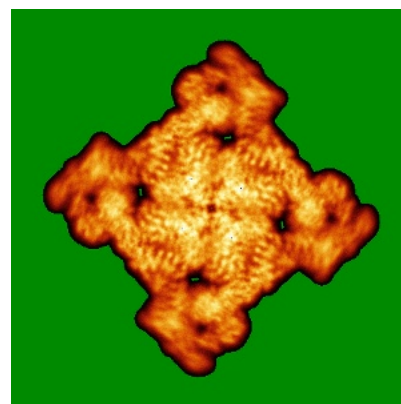
6.4.2 Raw map



X



Y

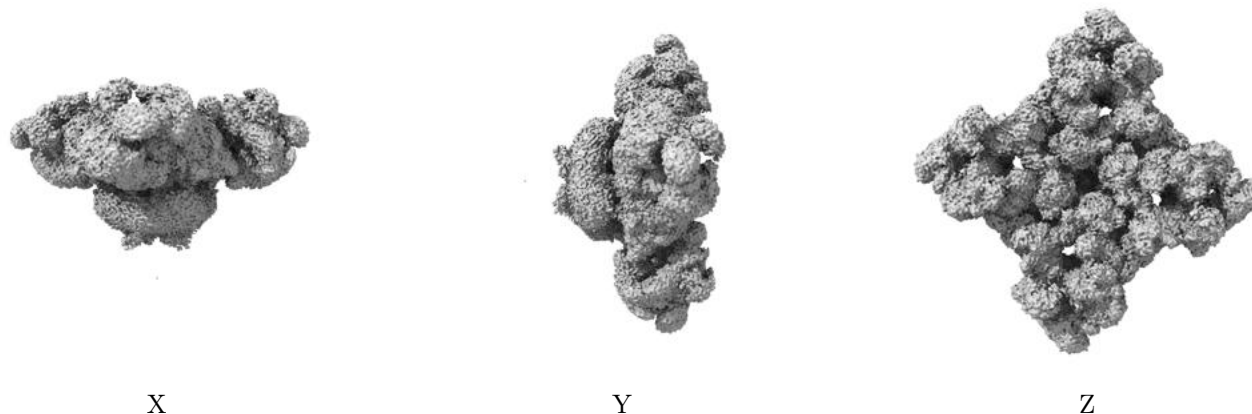


Z

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

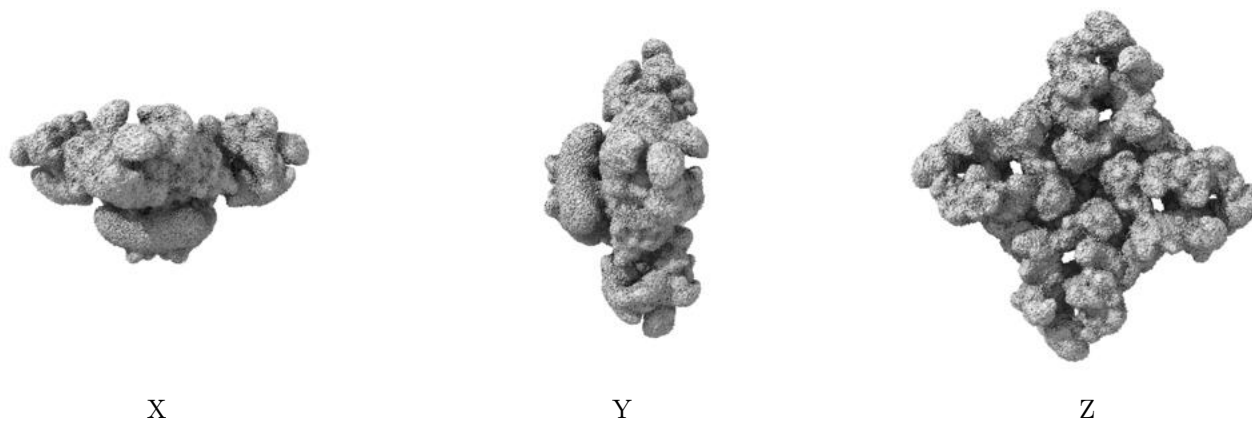
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

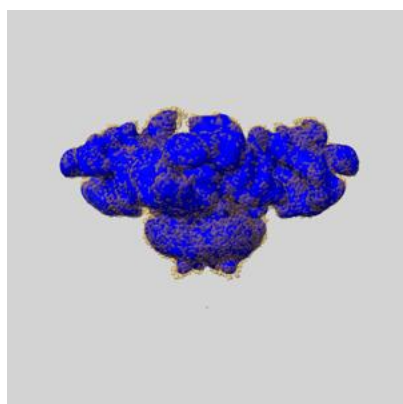
6.6 Mask visualisation [i](#)

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

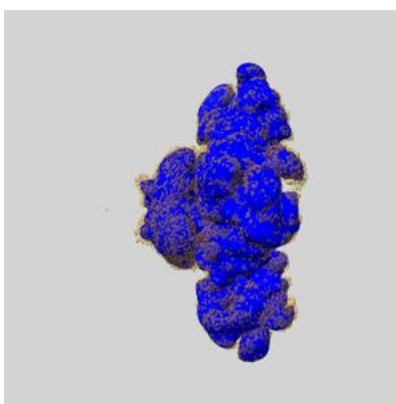
A mask typically either:

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

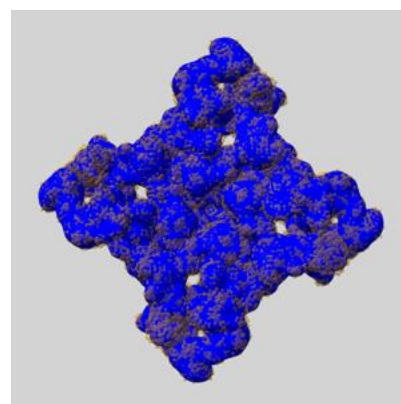
6.6.1 emd_22616_msk_1.map [i](#)



X



Y

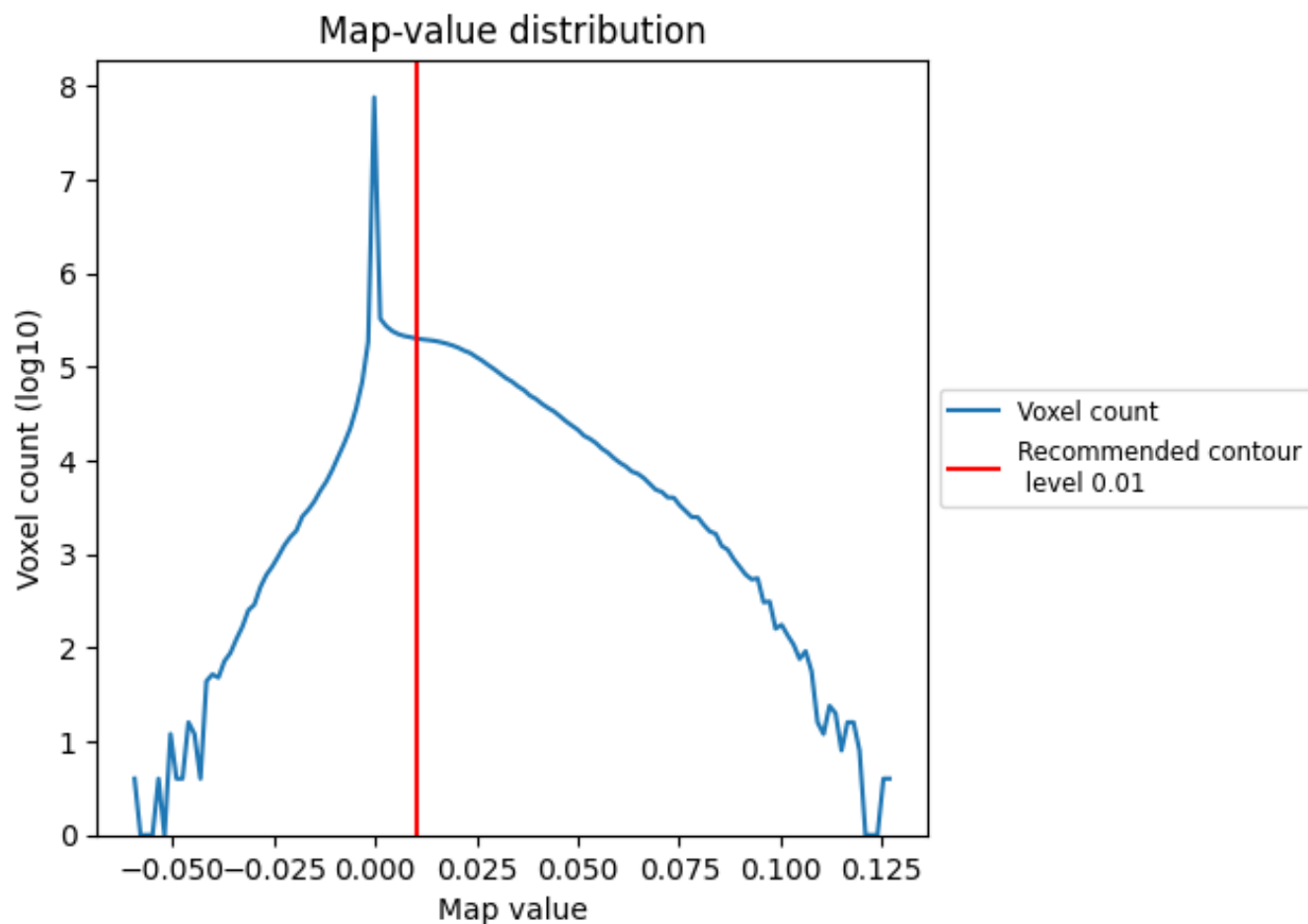


Z

7 Map analysis [i](#)

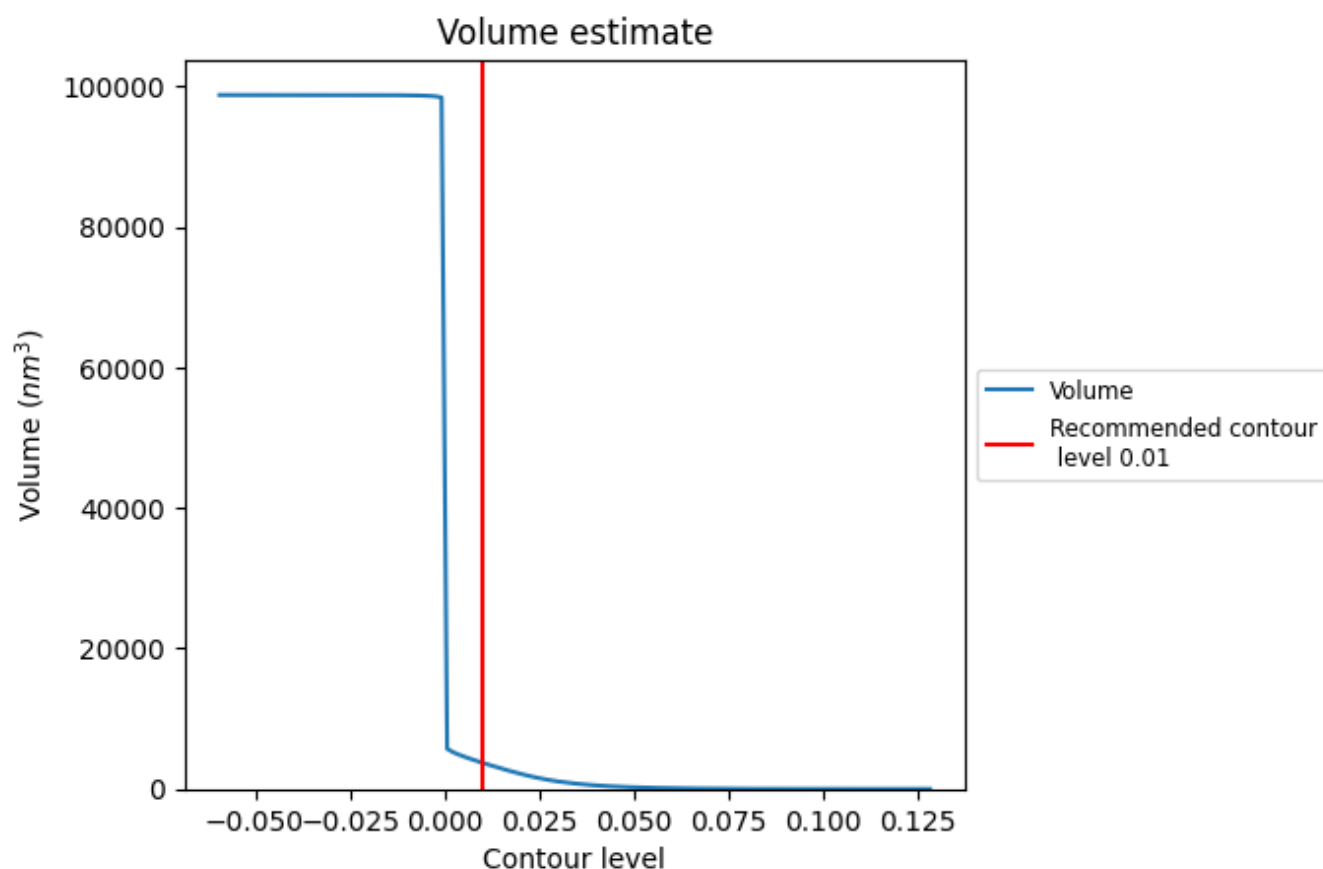
This section contains the results of statistical analysis of the map.

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.

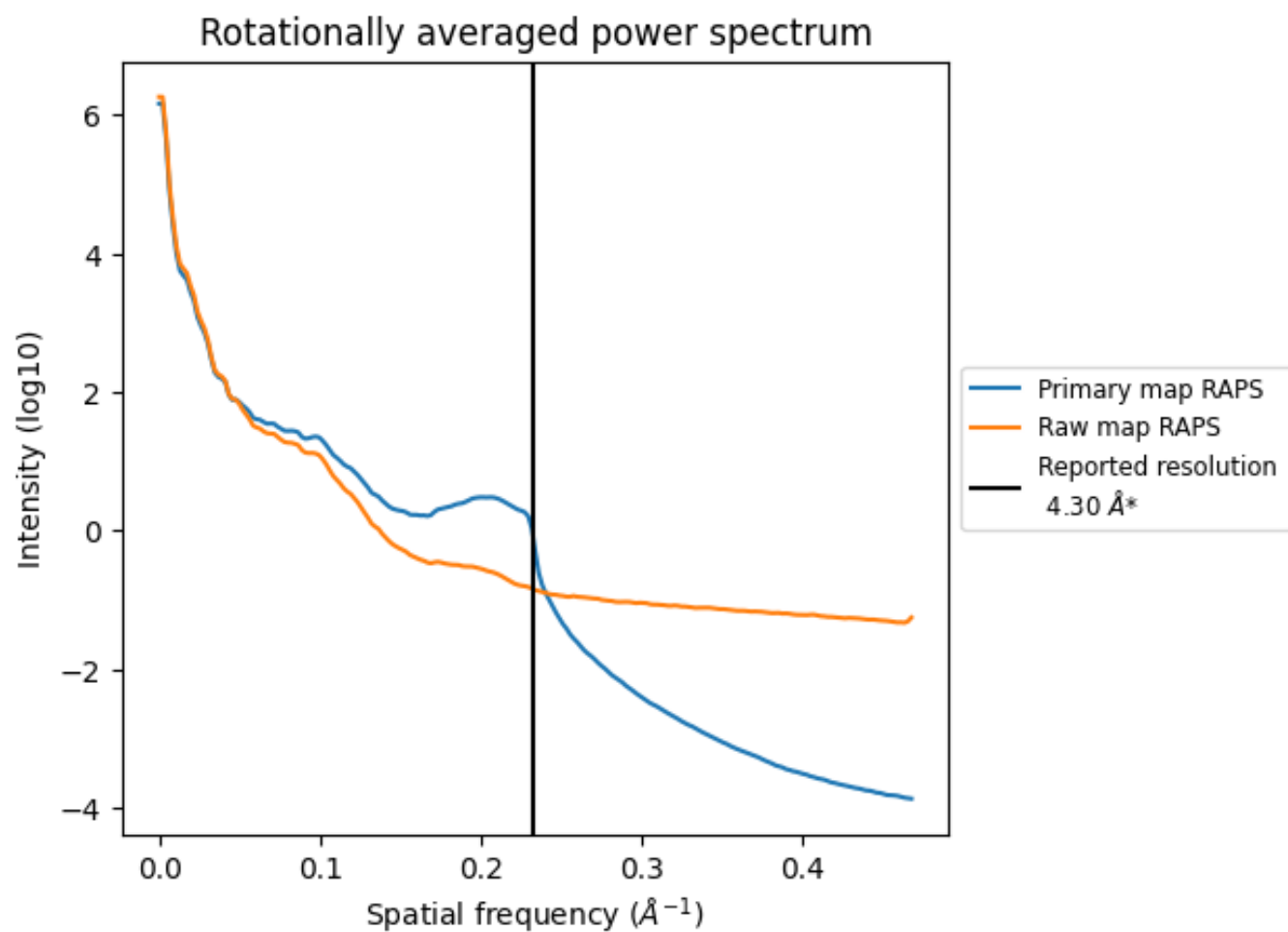
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3741 nm^3 ; this corresponds to an approximate mass of 3379 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 ⓘ

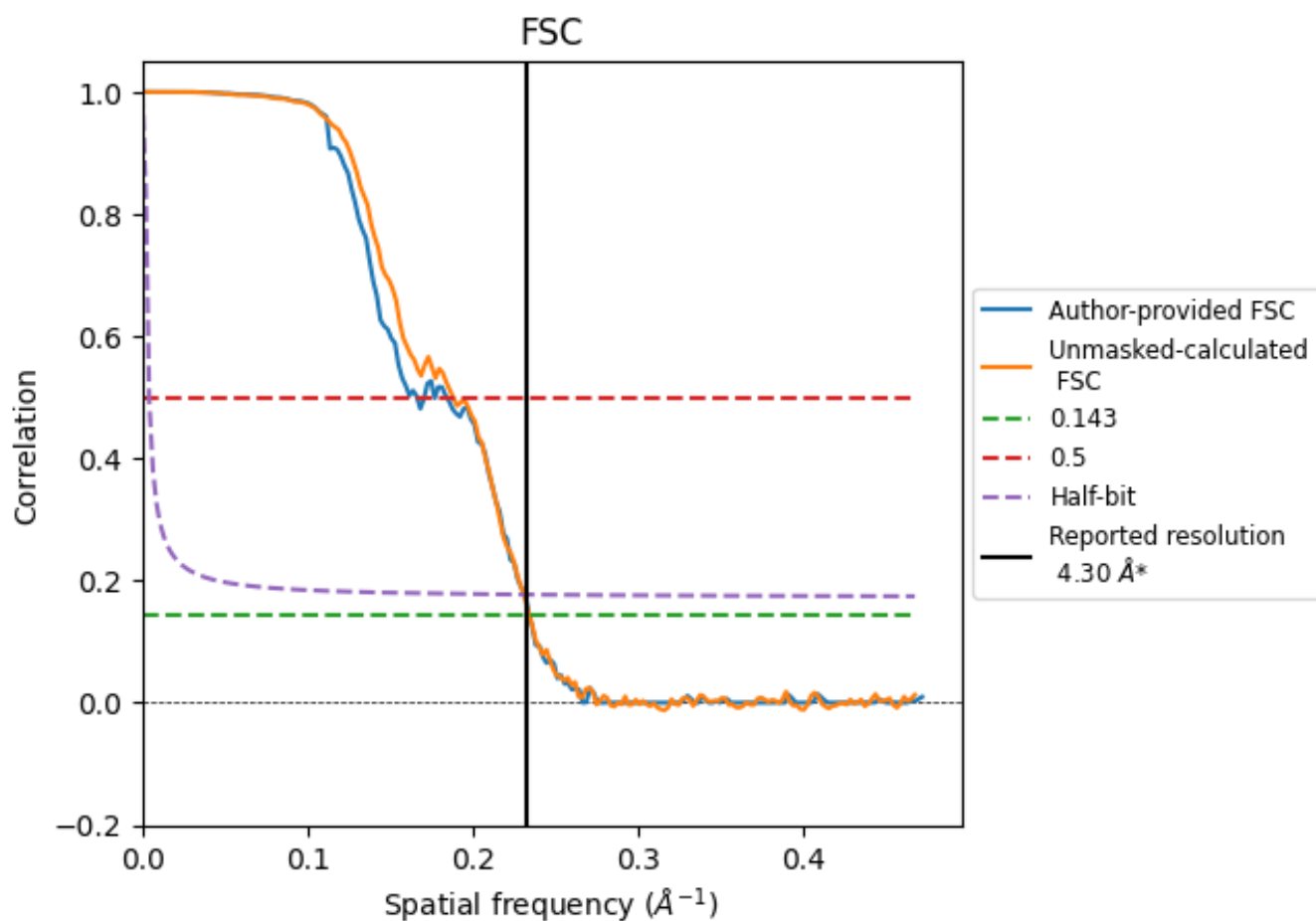


*Reported resolution corresponds to spatial frequency of 0.233 $\text{\AA}^{-1}$

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

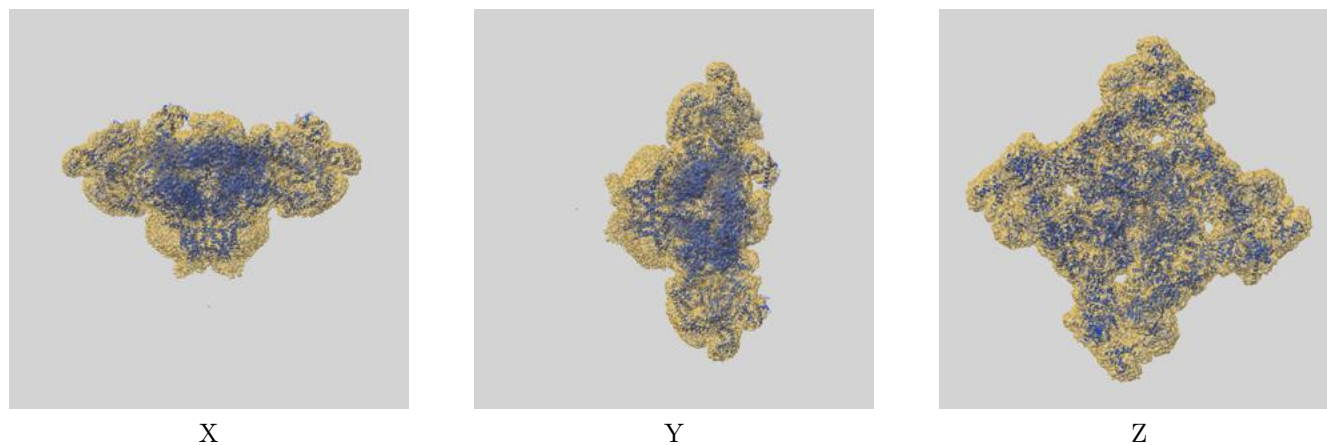
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.27	6.02	4.32
Unmasked-calculated*	4.27	5.31	4.33

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

9 Map-model fit [i](#)

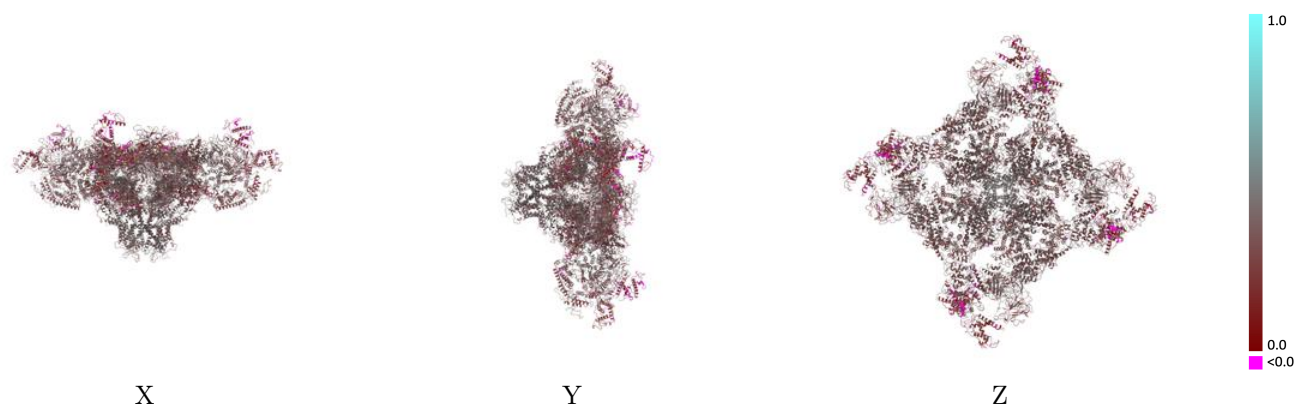
This section contains information regarding the fit between EMDB map EMD-22616 and PDB model 7K0T. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



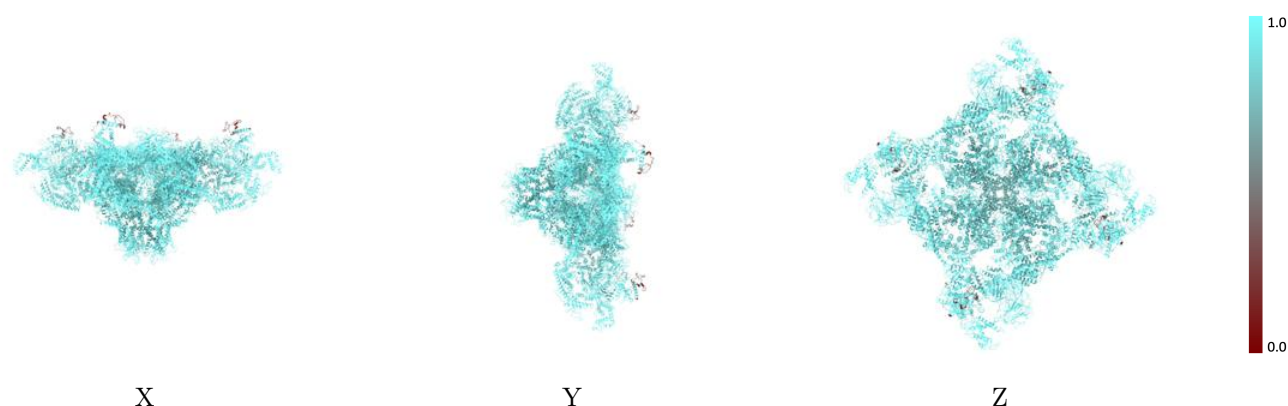
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



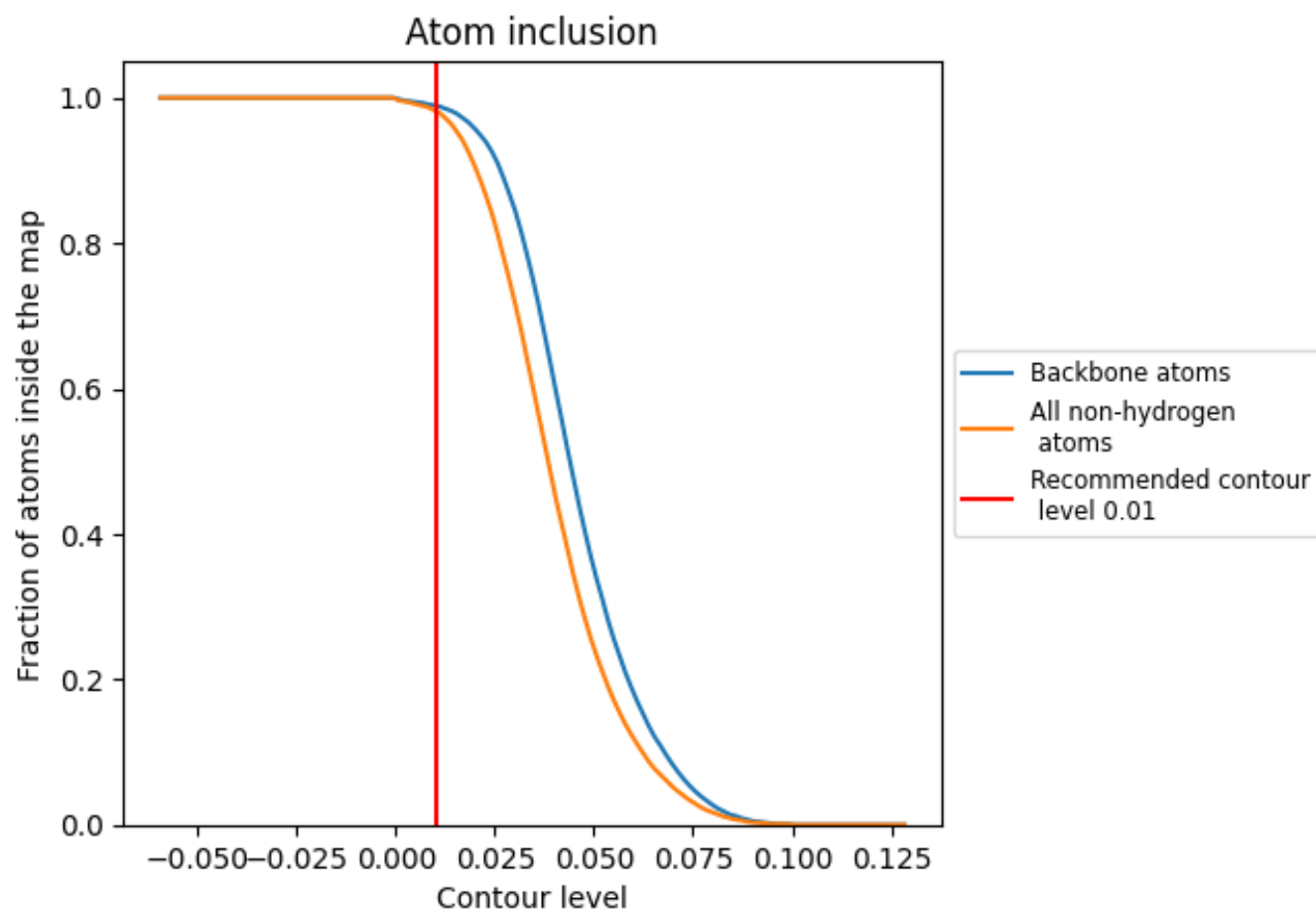
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9820	0.3320
A	0.9820	0.3320
B	0.9820	0.3310
C	0.9830	0.3320
D	0.9820	0.3320

