



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 08:03 AM UTC

PDB ID : 7TDG / pdb_00007tdg
EMDB ID : EMD-25828
Title : Rabbit RyR1 with AMP-PCP and high Ca²⁺ embedded in nanodisc in inactivated conformation (Dataset-A)
Authors : Nayak, A.R.; Samso, M.
Deposited on : 2021-12-31
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

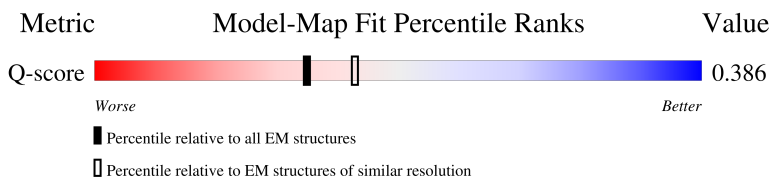
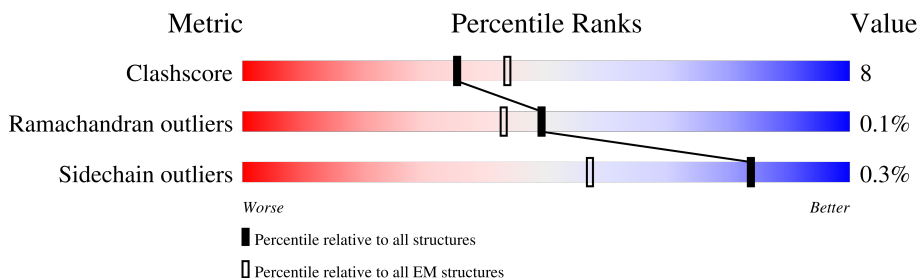
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



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

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

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

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 117345 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ryanodine receptor 1,RyR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4134	Total	C	N	O	S	0	0
			29247	18513	5182	5395	157		
1	C	4134	Total	C	N	O	S	0	0
			29244	18513	5179	5395	157		
1	D	4134	Total	C	N	O	S	0	0
			29228	18502	5176	5393	157		
1	B	4134	Total	C	N	O	S	0	0
			29246	18514	5182	5393	157		

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

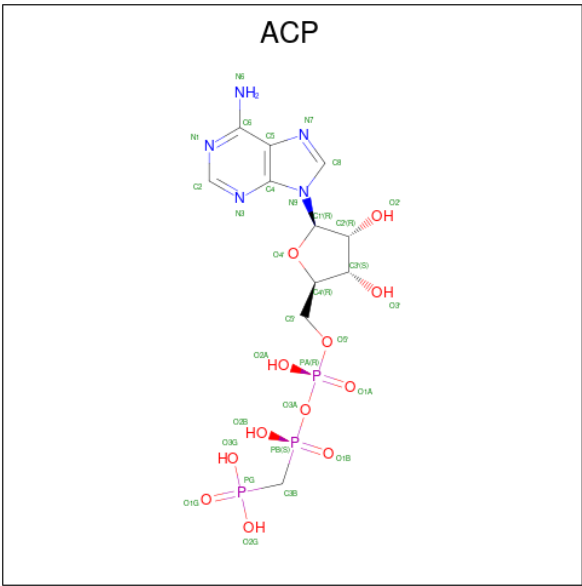
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	

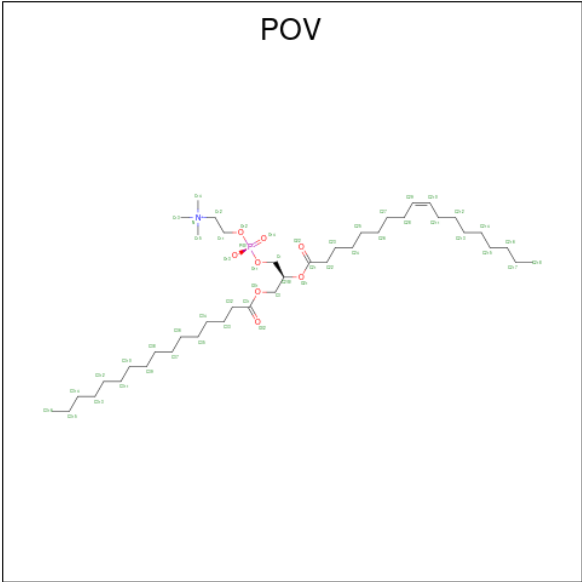
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Ca	0
			2	2	
3	C	2	Total	Ca	0
			2	2	
3	D	2	Total	Ca	0
			2	2	
3	B	2	Total	Ca	0
			2	2	

- Molecule 4 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID:

ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



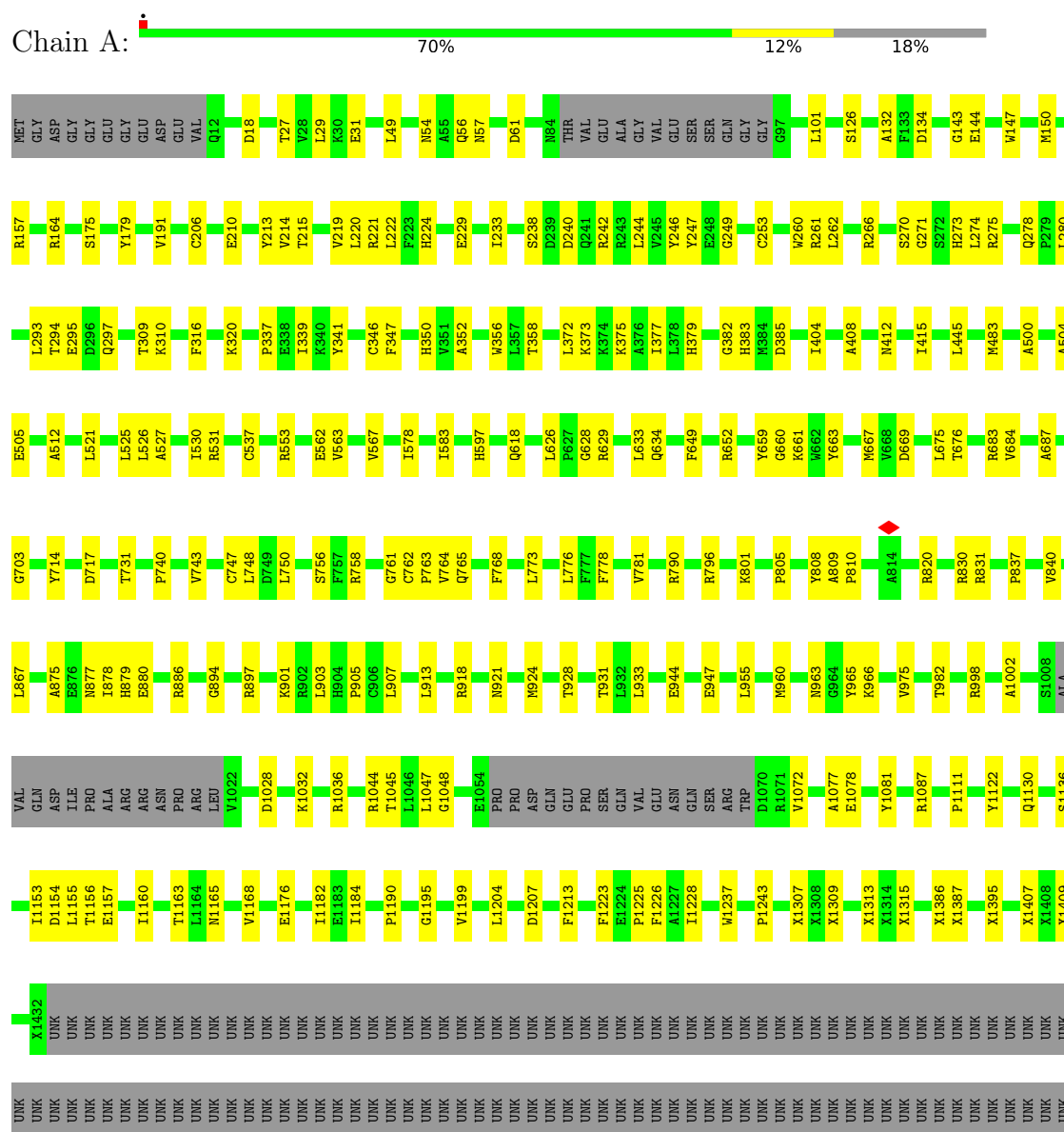


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C				0
			16	16				
5	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
5	C	1	Total	C				0
			16	16				
5	C	1	Total	C	N	O	P	0
			45	35	1	8	1	
5	C	1	Total	C				0
			16	16				
5	D	1	Total	C	N	O	P	0
			45	35	1	8	1	
5	B	1	Total	C				0
			16	16				
5	B	1	Total	C	N	O	P	0
			45	35	1	8	1	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Ryanodine receptor 1, RyR1







- Molecule 1: Ryanodine receptor 1, RyR1

Frequency	Percentage
Daily	70%
Weekly	12%
Monthly	18%









M4874	V4628	ALA	LEU	ASP	ALA	THR	R4175
K4875	Y4629	GLY	LYS	ALA	ALA	ALA	F4176
C4876	Y4630	GLY	ARG	ALA	ARG	ARG	Y4177
	F4631	ALA	LYS	ALA	LEU	LEU	
M4880	L4632	GLY	LEU	GLY	LEU	ALA	R4180
T4881	L4639	MET	GLY	ASP	TRP	ALA	
C4882	M4639	GLY	VAL	GLY	GLY	ALA	Y4194
			ASP	ASP	SER	ALA	
V4891	L4656	GLY	GLY	GLU	LEU	ALA	S4198
R4892		GLU	GLU	GLU	LEU	ALA	E4199
A4893	R4679	GLU	GLU	VAL	PHE	ARG	T4200
C4894		GLU	GLU	ALA	GLY	ALA	N4201
	D4684	GLY	GLY	GLY	GLY	ARG	
D4907		LEU	LEU	HIS	LEU	GLY	C4238
E4908	T4708	VAL	VAL	GLU	VAL	GLY	E4239
Y4909		PRO	PRO	ALA	GLU	SER	
E4910	G4733	GLY	GLY	GLY	GLY	TYR	I4242
L4911		PRO	PRO	PRO	ALA	ARG	
Y4912	R4736	GLY	GLY	GLY	LYS	SER	I4251
R4913		PRO	PRO	GLY	LYS	LEU	S4282
	E4739	GLY	GLY	ALA	VAL	ARG	E4283
F4916		GLU	GLU	VAL	THR	ARG	PRO
E4942	L4745	ASP	GLU	VAL	VAL	GLY	GLU
	K4757	MET	GLY	GLY	GLY	GLY	GLY
D4953		GLY	GLY	ALA	LEU	PRO	GLY
T4956	P4760	GLY	GLY	VAL	LEU	ARG	PRO
		SER	LYS	VAL	GLU	ARG	GLU
H4978	L4764	ALA	ALA	ASP	ALA	ALA	ALA
	L4765	ALA	ASP	GLY	GLY	ASP	GLY
E4981		GLY	GLY	GLY	PRO	LEU	GLY
E4982	Y4775	ASP	GLY	PRO	ASP	THR	ASP
H4983		LEU	ASN	PHE	GLY	ALA	GLY
N4984	G4793	ALA	GLY	ARG	THR	GLY	GLY
L4985		GLY	GLY	PRO	SER	ALA	GLY
A4986	V4797	ALA	LYS	ASP	ASP	GLY	GLY
		GLY	GLY	GLY	GLY	THR	ALA
M4993	F4808	SER	GLY	ALA	VAL	ALA	ALA
Y4994		GLY	VAL	GLY	HIS	LEU	ALA
L4995	I4816	GLY	PRO	GLY	GLY	GLY	GLY
		SER	ALA	ALA	GLY	LEU	ALA
D4999	H4832	GLY	PRO	ASP	PRO	LEU	ALA
		TRP	PRO	MET	ALA	GLY	GLY
E5002	M4839	GLY	GLY	GLY	GLY	TRP	ALA
H5003		SER	PRO	ASP	PRO	ALA	GLY
T5004	Y4849	GLY	PRO	THR	GLY	VAL	ALA
G5005	L4850	ALA	LYS	THR	GLY	VAL	ALA
	Y4851	GLY	LYS	PRO	ASP	ARG	ALA
Y5009	T4852	GLY	ALA	ALA	ALA	ALA	GLY
	V4853	GLY	PRO	GLY	ASP	GLY	GLY
M5013		GLU	ALA	GLU	ASP	GLY	GLY
		ALA	ALA	PRO	PRO	ALA	ALA
C5027	F4858	GLY	GLY	SER	GLY	ALA	ALA
F5028	F4859	GLY	GLY	PRO	THR	GLY	GLY
R5029		ASP	PRO	PRO	THR	ALA	THR
	N4864	GLY	ALA	GLY	GLY	GLY	VAL
	K4865	ASP	LYS	GLY	GLY	ALA	ALA
L5036		GLU	LYS	SER	GLY	ALA	ALA
S5037	E4871	GLY	LYS	PRO	GLY	ALA	ALA
	P4872	GLY	GLY	GLY	GLY	GLY	GLY
	M4873	M4826	M4827	ILE			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	90530	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	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.283	Depositor
Minimum map value	-0.147	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	477.36002, 477.36002, 477.36002	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.105, 1.105, 1.105	Depositor

5 Model quality

5.1 Standard geometry

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

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	0/25300	0.39	0/34345
1	B	0.16	0/25299	0.39	1/34344 (0.0%)
1	C	0.17	0/25297	0.40	1/34342 (0.0%)
1	D	0.17	0/25281	0.41	5/34322 (0.0%)
All	All	0.16	0/101177	0.40	7/137353 (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	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1618	ARG	O-C-N	-19.86	100.89	123.33
1	D	4895	GLY	CA-C-N	-7.34	111.09	122.69
1	D	4895	GLY	C-N-CA	-7.34	111.09	122.69
1	C	1618	ARG	O-C-N	-6.81	113.53	122.59
1	D	821	LEU	CA-C-N	6.55	130.44	120.82
1	D	821	LEU	C-N-CA	6.55	130.44	120.82
1	B	1795	PRO	N-CA-C	-6.38	101.21	111.03

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1617	THR	Mainchain
1	C	1618	ARG	Mainchain
1	D	1618	ARG	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	29247	0	24751	425	0
1	B	29246	0	24757	448	0
1	C	29244	0	24747	412	0
1	D	29228	0	24714	434	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	31	0	14	1	0
4	B	31	0	14	1	0
4	C	31	0	14	2	0
4	D	31	0	14	1	0
5	A	61	0	85	18	0
5	B	61	0	85	19	0
5	C	77	0	105	17	0
5	D	45	0	65	16	0
All	All	117345	0	99365	1711	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 (1711) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4858:PHE:CE2	5:A:5106:POV:H33A	1.60	1.36
1:B:4858:PHE:CE2	5:B:5106:POV:H33A	1.60	1.36
1:D:4858:PHE:CE2	5:D:5105:POV:H33A	1.59	1.36
1:D:1618:ARG:O	1:D:1626:TRP:HA	1.12	1.29
1:D:1618:ARG:O	1:D:1626:TRP:CA	1.91	1.17
1:A:1680:ARG:HB2	1:A:1796:ALA:HB1	1.29	1.12
1:A:1619:ARG:HA	1:A:1626:TRP:HA	1.31	1.04
1:A:3722:TYR:CZ	1:A:3782:MET:HE3	1.94	1.02
1:D:648:ILE:HD11	1:D:821:LEU:HD11	1.40	1.02
1:D:647:ASN:OD1	1:D:821:LEU:HA	1.59	1.01
1:A:4858:PHE:CE2	5:A:5106:POV:C33	2.45	1.00
1:A:3722:TYR:CZ	1:A:3782:MET:CE	2.45	0.99
1:B:4858:PHE:CE2	5:B:5106:POV:C33	2.45	0.99
1:D:4858:PHE:CE2	5:D:5105:POV:C33	2.44	0.98
1:A:1619:ARG:C	1:A:1626:TRP:H	1.70	0.98
1:B:1680:ARG:HB2	1:B:1796:ALA:CB	1.94	0.97
1:B:4858:PHE:CD2	5:B:5106:POV:H33A	2.02	0.95
1:A:4858:PHE:CD2	5:A:5106:POV:H33A	2.02	0.94
5:A:5106:POV:H13A	1:B:4629:TYR:CZ	2.02	0.94
1:A:4629:TYR:CZ	5:D:5105:POV:H13A	2.03	0.93
1:D:4858:PHE:CD2	5:D:5105:POV:H33A	2.02	0.93
1:C:4629:TYR:CZ	5:B:5106:POV:H13A	2.03	0.92
1:A:1680:ARG:HB2	1:A:1796:ALA:CB	2.01	0.90
1:A:3722:TYR:CE2	1:A:3782:MET:CE	2.54	0.90
1:A:1618:ARG:O	1:A:1627:ALA:N	2.04	0.90
1:A:3722:TYR:CE2	1:A:3782:MET:HE3	2.06	0.89
5:C:5106:POV:H13A	1:D:4629:TYR:CZ	2.05	0.89
1:A:4808:PHE:CE1	5:A:5105:POV:H35	2.08	0.87
1:B:1618:ARG:O	1:B:1626:TRP:HA	1.74	0.87
1:A:2867:LEU:CB	1:A:2872:GLN:CD	2.48	0.87
1:A:2867:LEU:CB	1:A:2872:GLN:OE1	2.22	0.86
1:C:1795:PRO:O	1:C:1797:ARG:N	2.09	0.85
1:C:1786:LEU:HD23	1:C:1786:LEU:H	1.42	0.83
1:A:3722:TYR:CE1	1:A:3782:MET:HE2	2.14	0.83
1:C:4808:PHE:CE1	5:C:5105:POV:H35	2.13	0.82
1:C:633:LEU:HD23	1:C:1639:LEU:HD21	1.62	0.82
1:B:4858:PHE:CD2	5:B:5106:POV:C33	2.63	0.82
5:C:5107:POV:H35	1:D:4808:PHE:CE1	2.15	0.82
1:A:4858:PHE:CD2	5:A:5106:POV:C33	2.63	0.81
1:D:4858:PHE:CD2	5:D:5105:POV:C33	2.63	0.81
1:C:4851:TYR:HE1	5:C:5106:POV:H312	1.46	0.81
1:D:4888:TYR:O	1:D:4892:ARG:NH1	2.13	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2581:UNK:HA	1:A:2895:GLU:HG3	1.64	0.80
1:C:4858:PHE:CD2	5:C:5106:POV:H33A	2.16	0.80
1:A:4808:PHE:HE1	5:A:5105:POV:H35	1.45	0.80
1:B:2581:UNK:HA	1:B:2895:GLU:HG3	1.64	0.80
1:C:2581:UNK:HA	1:C:2895:GLU:HG3	1.64	0.79
1:D:2581:UNK:HA	1:D:2895:GLU:HG3	1.64	0.79
1:C:2806:ARG:HH21	1:C:2808:PRO:HG3	1.48	0.79
1:D:4865:LYS:H	1:D:4875:LYS:HE2	1.47	0.79
1:B:4808:PHE:CE1	5:B:5105:POV:H35	2.18	0.79
1:A:2806:ARG:HH21	1:A:2808:PRO:HG3	1.48	0.78
1:A:293:LEU:HD11	1:A:297:GLN:H	1.49	0.78
1:A:1796:ALA:O	1:A:1797:ARG:HB2	1.82	0.78
1:D:2806:ARG:HH21	1:D:2808:PRO:HG3	1.48	0.78
1:B:1619:ARG:HA	1:B:1626:TRP:HA	1.66	0.77
1:B:2874:MET:HA	1:B:2877:GLN:HB3	1.65	0.77
1:B:293:LEU:HD11	1:B:297:GLN:H	1.49	0.77
1:D:293:LEU:HD11	1:D:297:GLN:H	1.49	0.77
1:B:2806:ARG:HH21	1:B:2808:PRO:HG3	1.48	0.77
1:A:2874:MET:HA	1:A:2877:GLN:HB3	1.65	0.77
1:C:293:LEU:HD11	1:C:297:GLN:H	1.49	0.76
1:D:793:LEU:HD13	1:D:821:LEU:HD21	1.67	0.76
1:A:1619:ARG:CA	1:A:1626:TRP:HA	2.14	0.76
1:B:3722:TYR:CE2	1:B:3782:MET:HE3	2.21	0.75
1:D:648:ILE:CD1	1:D:821:LEU:HD11	2.17	0.75
5:C:5106:POV:C13	1:D:4629:TYR:CZ	2.68	0.75
1:A:1680:ARG:CB	1:A:1796:ALA:HB1	2.13	0.75
1:B:4858:PHE:HE2	5:B:5106:POV:H33A	1.49	0.75
1:A:4578:LEU:HG	1:D:4880:MET:HE1	1.70	0.74
1:C:4808:PHE:HE1	5:C:5105:POV:H35	1.50	0.74
1:A:2867:LEU:O	1:A:2868:SER:O	2.06	0.73
1:C:1680:ARG:HB2	1:C:1796:ALA:HB1	1.71	0.73
1:B:1781:CYS:SG	1:B:1783:VAL:HG23	2.27	0.73
1:B:3722:TYR:CE2	1:B:3782:MET:CE	2.71	0.73
1:C:894:GLY:HA3	1:C:903:LEU:HB3	1.70	0.73
1:C:1078:GLU:OE2	1:C:1237:TRP:NE1	2.21	0.73
1:A:1078:GLU:OE2	1:A:1237:TRP:NE1	2.21	0.73
1:C:1619:ARG:C	1:C:1626:TRP:HA	2.13	0.73
1:B:4851:TYR:HE1	5:B:5106:POV:H312	1.52	0.73
1:D:894:GLY:HA3	1:D:903:LEU:HB3	1.70	0.72
1:A:894:GLY:HA3	1:A:903:LEU:HB3	1.70	0.72
1:C:4865:LYS:H	1:C:4875:LYS:HE2	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2873:ALA:HB1	1:B:2874:MET:HE2	1.71	0.72
1:B:2868:SER:O	1:B:2872:GLN:NE2	2.21	0.72
1:C:1616:GLU:O	1:C:1628:VAL:HA	1.90	0.72
1:B:894:GLY:HA3	1:B:903:LEU:HB3	1.70	0.72
1:B:4865:LYS:H	1:B:4875:LYS:HE2	1.54	0.72
1:A:2868:SER:O	1:A:2872:GLN:NE2	2.23	0.72
1:D:1679:ASN:CG	1:D:1798:LEU:O	2.32	0.72
5:A:5106:POV:C13	1:B:4629:TYR:CZ	2.72	0.72
1:C:1786:LEU:HD23	1:C:1786:LEU:N	2.04	0.72
1:C:4629:TYR:CZ	5:B:5106:POV:C13	2.73	0.72
5:C:5107:POV:H35	1:D:4808:PHE:HE1	1.54	0.71
1:A:1619:ARG:C	1:A:1626:TRP:N	2.47	0.71
4:A:5104:ACP:O2B	4:A:5104:ACP:O3G	2.09	0.70
4:C:5104:ACP:O2B	4:C:5104:ACP:O3G	2.09	0.70
1:B:4808:PHE:HE1	5:B:5105:POV:H35	1.56	0.70
1:D:2868:SER:O	1:D:2872:GLN:NE2	2.25	0.70
1:B:982:THR:O	1:B:1036:ARG:NH1	2.25	0.70
1:B:1618:ARG:O	1:B:1626:TRP:CA	2.40	0.70
1:D:982:THR:O	1:D:1036:ARG:NH1	2.25	0.70
4:D:5104:ACP:O2B	4:D:5104:ACP:O3G	2.09	0.70
1:A:982:THR:O	1:A:1036:ARG:NH1	2.25	0.69
1:A:4629:TYR:CZ	5:D:5105:POV:C13	2.73	0.69
1:C:2868:SER:O	1:C:2872:GLN:NE2	2.25	0.69
1:A:840:VAL:HG12	1:A:1199:VAL:HG22	1.74	0.69
1:D:2874:MET:HA	1:D:2877:GLN:HB3	1.74	0.69
1:C:982:THR:O	1:C:1036:ARG:NH1	2.25	0.69
1:A:4858:PHE:HE2	5:A:5106:POV:H33A	1.49	0.69
1:C:2874:MET:HA	1:C:2877:GLN:HB3	1.74	0.69
4:B:5104:ACP:O2B	4:B:5104:ACP:O3G	2.09	0.69
1:A:1618:ARG:O	1:A:1626:TRP:C	2.36	0.69
1:A:3722:TYR:CE1	1:A:3782:MET:CE	2.75	0.69
1:D:4851:TYR:HE1	5:D:5105:POV:H312	1.57	0.69
1:B:840:VAL:HG12	1:B:1199:VAL:HG22	1.75	0.69
1:C:4851:TYR:CE1	5:C:5106:POV:H312	2.28	0.69
1:D:647:ASN:OD1	1:D:821:LEU:CA	2.39	0.68
1:D:633:LEU:HD23	1:D:1639:LEU:HD21	1.75	0.68
1:A:1796:ALA:O	1:A:1797:ARG:CB	2.40	0.68
1:A:633:LEU:HD23	1:A:1639:LEU:HD21	1.76	0.68
1:C:247:TYR:O	1:C:373:LYS:NZ	2.27	0.68
1:C:684:VAL:HG12	1:C:781:VAL:HG22	1.76	0.68
1:D:684:VAL:HG12	1:D:781:VAL:HG22	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1786:LEU:H	1:C:1786:LEU:CD2	2.06	0.68
1:C:2581:UNK:N	1:C:2899:GLY:O	2.27	0.68
1:D:1078:GLU:OE2	1:D:1237:TRP:NE1	2.27	0.68
1:B:684:VAL:HG12	1:B:781:VAL:HG22	1.76	0.68
1:A:2581:UNK:N	1:A:2899:GLY:O	2.28	0.67
1:C:840:VAL:HG12	1:C:1199:VAL:HG22	1.75	0.67
1:D:623:GLU:CB	1:D:1786:LEU:O	2.43	0.67
1:D:840:VAL:HG12	1:D:1199:VAL:HG22	1.75	0.67
1:B:1078:GLU:OE2	1:B:1237:TRP:NE1	2.28	0.67
1:C:4555:LEU:HD22	1:C:4656:LEU:HD11	1.77	0.67
1:B:3722:TYR:CZ	1:B:3782:MET:CE	2.78	0.66
1:D:2581:UNK:N	1:D:2899:GLY:O	2.28	0.66
1:B:633:LEU:HD23	1:B:1639:LEU:HD21	1.78	0.66
1:B:2581:UNK:N	1:B:2899:GLY:O	2.28	0.66
1:A:537:CYS:HB2	1:A:567:VAL:HG23	1.78	0.66
5:C:5106:POV:H13A	1:D:4629:TYR:CE1	2.29	0.66
1:B:537:CYS:HB2	1:B:567:VAL:HG23	1.78	0.66
1:A:684:VAL:HG12	1:A:781:VAL:HG22	1.78	0.66
1:A:1653:LEU:HD12	1:A:1656:ARG:HG3	1.78	0.66
1:A:4555:LEU:HD22	1:A:4656:LEU:HD11	1.77	0.65
1:A:4880:MET:HE1	1:B:4578:LEU:HG	1.77	0.65
1:B:500:ALA:H	1:B:504:ALA:HB3	1.60	0.65
1:C:4578:LEU:HG	1:B:4880:MET:HE1	1.78	0.65
1:B:2809:ILE:HD12	1:B:2813:LEU:HD11	1.79	0.65
1:C:1653:LEU:HD12	1:C:1656:ARG:HG3	1.78	0.65
1:D:247:TYR:O	1:D:373:LYS:NZ	2.30	0.65
1:D:537:CYS:HB2	1:D:567:VAL:HG23	1.78	0.65
1:B:247:TYR:O	1:B:373:LYS:NZ	2.30	0.65
1:C:537:CYS:HB2	1:C:567:VAL:HG23	1.79	0.65
1:A:247:TYR:O	1:A:373:LYS:NZ	2.30	0.64
1:D:2809:ILE:HD12	1:D:2813:LEU:HD11	1.79	0.64
1:A:3722:TYR:CD2	1:A:3782:MET:HE1	2.31	0.64
1:C:2809:ILE:HD12	1:C:2813:LEU:HD11	1.79	0.64
1:D:669:ASP:HA	1:D:740:PRO:HA	1.80	0.64
1:D:1619:ARG:C	1:D:1626:TRP:H	2.05	0.64
1:B:4555:LEU:HD22	1:B:4656:LEU:HD11	1.80	0.64
1:B:1653:LEU:HD12	1:B:1656:ARG:HG3	1.80	0.64
1:B:1786:LEU:HD13	1:B:1786:LEU:H	1.61	0.64
1:D:500:ALA:H	1:D:504:ALA:HB3	1.63	0.64
1:D:4858:PHE:HE2	5:D:5105:POV:H33A	1.48	0.64
1:B:669:ASP:HA	1:B:740:PRO:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2582:UNK:O	1:A:2899:GLY:N	2.31	0.64
1:D:1653:LEU:HD12	1:D:1656:ARG:HG3	1.80	0.64
1:A:669:ASP:HA	1:A:740:PRO:HA	1.80	0.64
1:A:4832:HIS:NE2	1:A:4942:GLU:OE1	2.31	0.64
1:A:4851:TYR:HE1	5:A:5106:POV:H312	1.62	0.64
1:C:667:MET:HG3	1:C:790:ARG:HH21	1.63	0.64
1:D:4115:SER:HB2	1:D:4123:ILE:HG21	1.80	0.64
1:C:4880:MET:HE1	1:D:4578:LEU:HG	1.80	0.64
1:B:2928:LYS:O	1:B:2931:GLN:NE2	2.31	0.64
1:A:944:GLU:HA	1:A:947:GLU:HB2	1.80	0.64
1:D:4555:LEU:HD22	1:D:4656:LEU:HD11	1.80	0.64
1:B:206:CYS:HB3	1:B:271:GLY:HA3	1.80	0.64
1:C:669:ASP:HA	1:C:740:PRO:HA	1.80	0.63
1:C:2582:UNK:O	1:C:2899:GLY:N	2.31	0.63
1:C:2928:LYS:O	1:C:2931:GLN:NE2	2.31	0.63
1:C:49:LEU:HD11	1:C:191:VAL:HG13	1.79	0.63
1:C:500:ALA:H	1:C:504:ALA:HB3	1.63	0.63
1:D:2582:UNK:O	1:D:2899:GLY:N	2.31	0.63
1:B:1680:ARG:CB	1:B:1796:ALA:CB	2.75	0.63
1:A:531:ARG:NH2	1:A:562:GLU:OE1	2.32	0.63
1:D:531:ARG:NH2	1:D:562:GLU:OE1	2.31	0.63
1:B:1680:ARG:HB2	1:B:1796:ALA:HB2	1.80	0.63
1:A:2809:ILE:HD12	1:A:2813:LEU:HD11	1.79	0.63
1:D:944:GLU:HA	1:D:947:GLU:HB2	1.80	0.63
1:D:2928:LYS:O	1:D:2931:GLN:NE2	2.31	0.63
1:A:4115:SER:HB2	1:A:4123:ILE:HG21	1.81	0.63
1:B:4832:HIS:NE2	1:B:4942:GLU:OE1	2.31	0.63
1:A:49:LEU:HD11	1:A:191:VAL:HG13	1.80	0.63
1:A:2928:LYS:O	1:A:2931:GLN:NE2	2.31	0.63
1:A:206:CYS:HB3	1:A:271:GLY:HA3	1.81	0.63
1:B:531:ARG:NH2	1:B:562:GLU:OE1	2.32	0.63
1:A:4629:TYR:OH	5:D:5105:POV:H13A	1.98	0.63
1:C:531:ARG:NH2	1:C:562:GLU:OE1	2.31	0.63
1:B:1786:LEU:C	1:B:1786:LEU:HD22	2.23	0.63
1:C:3770:LEU:HD22	1:C:3804:ILE:HD11	1.80	0.62
1:C:4832:HIS:NE2	1:C:4942:GLU:OE1	2.31	0.62
1:D:667:MET:HG3	1:D:790:ARG:HH21	1.63	0.62
1:D:4832:HIS:NE2	1:D:4942:GLU:OE1	2.32	0.62
1:B:667:MET:HG3	1:B:790:ARG:HH21	1.62	0.62
1:B:4892:ARG:HH21	1:B:4892:ARG:HG3	1.63	0.62
1:B:4115:SER:HB2	1:B:4123:ILE:HG21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3770:LEU:HD22	1:A:3804:ILE:HD11	1.80	0.62
1:C:4925:ILE:O	1:C:4929:LEU:HB2	2.00	0.62
1:D:3770:LEU:HD22	1:D:3804:ILE:HD11	1.80	0.62
1:B:3770:LEU:HD22	1:B:3804:ILE:HD11	1.80	0.62
1:A:500:ALA:H	1:A:504:ALA:HB3	1.63	0.62
1:A:527:ALA:HB2	1:A:563:VAL:HG22	1.82	0.62
1:D:49:LEU:HD11	1:D:191:VAL:HG13	1.79	0.62
1:D:1618:ARG:CB	1:D:1627:ALA:O	2.48	0.62
1:C:944:GLU:HA	1:C:947:GLU:HB2	1.80	0.62
1:D:527:ALA:HB2	1:D:563:VAL:HG22	1.82	0.62
5:A:5106:POV:H13A	1:B:4629:TYR:OH	1.99	0.62
1:C:4629:TYR:CE1	5:B:5106:POV:H13A	2.34	0.62
1:B:49:LEU:HD11	1:B:191:VAL:HG13	1.81	0.62
1:C:206:CYS:HB3	1:C:271:GLY:HA3	1.82	0.62
1:B:3722:TYR:CE1	1:B:3782:MET:HE2	2.35	0.62
1:C:358:THR:HG21	1:C:383:HIS:HB2	1.82	0.62
1:B:2582:UNK:O	1:B:2899:GLY:N	2.32	0.62
1:A:4238:CYS:O	1:A:4242:ILE:HG12	2.00	0.61
1:D:206:CYS:HB3	1:D:271:GLY:HA3	1.81	0.61
1:A:280:LEU:HD11	1:A:316:PHE:HE1	1.65	0.61
1:A:1163:THR:HG22	1:A:1168:VAL:HA	1.82	0.61
1:C:1619:ARG:C	1:C:1626:TRP:CA	2.72	0.61
1:D:358:THR:HG21	1:D:383:HIS:HB2	1.82	0.61
1:B:652:ARG:HD3	1:B:750:LEU:HD13	1.82	0.61
1:C:652:ARG:HD3	1:C:750:LEU:HD13	1.82	0.61
1:C:280:LEU:HD11	1:C:316:PHE:HE1	1.64	0.61
1:D:5013:MET:HE1	1:D:5021:PHE:HB3	1.82	0.61
1:D:4889:VAL:O	1:D:4893:ALA:HB2	2.01	0.61
1:B:1163:THR:HG22	1:B:1168:VAL:HA	1.83	0.61
1:A:358:THR:HG21	1:A:383:HIS:HB2	1.83	0.60
1:C:527:ALA:HB2	1:C:563:VAL:HG22	1.82	0.60
1:D:1163:THR:HG22	1:D:1168:VAL:HA	1.83	0.60
1:B:280:LEU:HD11	1:B:316:PHE:HE1	1.65	0.60
1:A:652:ARG:HD3	1:A:750:LEU:HD13	1.82	0.60
1:D:280:LEU:HD11	1:D:316:PHE:HE1	1.65	0.60
1:D:652:ARG:HD3	1:D:750:LEU:HD13	1.82	0.60
1:C:1163:THR:HG22	1:C:1168:VAL:HA	1.83	0.60
1:C:4857:ASN:ND2	5:C:5106:POV:H14B	2.15	0.60
1:D:3889:GLN:HG3	1:D:3967:GLU:HG3	1.84	0.60
1:B:527:ALA:HB2	1:B:563:VAL:HG22	1.82	0.60
1:B:3722:TYR:CZ	1:B:3782:MET:HE3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2192:TYR:HA	1:D:2242:ILE:HD11	1.84	0.60
1:C:731:THR:OG1	1:C:765:GLN:NE2	2.35	0.60
1:C:2192:TYR:HA	1:C:2242:ILE:HD11	1.83	0.60
1:B:358:THR:HG21	1:B:383:HIS:HB2	1.83	0.60
1:A:2192:TYR:HA	1:A:2242:ILE:HD11	1.83	0.60
1:D:244:LEU:HD12	1:D:375:LYS:HE2	1.83	0.60
1:C:4629:TYR:OH	5:B:5106:POV:H13A	2.01	0.60
1:D:1739:THR:HG23	1:D:1742:THR:H	1.67	0.60
1:A:1739:THR:HG23	1:A:1742:THR:H	1.67	0.60
1:A:3889:GLN:HG3	1:A:3967:GLU:HG3	1.84	0.60
1:C:2155:LEU:HB2	1:C:2188:ASN:HD21	1.67	0.60
1:A:1028:ASP:OD2	1:A:1032:LYS:N	2.35	0.59
5:A:5106:POV:H13A	1:B:4629:TYR:CE1	2.36	0.59
1:C:4915:VAL:HA	1:C:4918:ILE:HG22	1.84	0.59
1:B:244:LEU:HD12	1:B:375:LYS:HE2	1.83	0.59
1:A:897:ARG:HG2	1:A:905:PRO:HD2	1.84	0.59
1:A:1619:ARG:HA	1:A:1626:TRP:CA	2.20	0.59
1:C:294:THR:HG23	1:C:295:GLU:H	1.68	0.59
1:C:1748:PHE:O	1:C:1750:PRO:HD3	2.02	0.59
1:D:3772:THR:HG23	1:D:3812:VAL:HG22	1.84	0.59
1:B:3772:THR:HG23	1:B:3812:VAL:HG22	1.84	0.59
1:A:1943:LEU:HD21	1:A:2098:VAL:HG22	1.84	0.59
1:A:4629:TYR:CE2	5:D:5105:POV:H13A	2.37	0.59
1:C:244:LEU:HD12	1:C:375:LYS:HE2	1.84	0.59
1:D:731:THR:OG1	1:D:765:GLN:NE2	2.35	0.59
1:B:1748:PHE:O	1:B:1750:PRO:HD3	2.02	0.59
1:D:897:ARG:HG2	1:D:905:PRO:HD2	1.84	0.59
1:D:3722:TYR:CZ	1:D:3782:MET:HE3	2.36	0.59
1:B:1943:LEU:HD21	1:B:2098:VAL:HG22	1.85	0.59
1:B:4239:GLU:OE2	1:B:4679:ARG:NH2	2.34	0.59
1:A:3772:THR:HG23	1:A:3812:VAL:HG22	1.84	0.59
1:A:4198:SER:OG	1:A:4201:ASN:ND2	2.35	0.59
1:C:4579:PHE:HB2	1:C:4639:MET:SD	2.42	0.59
1:B:1028:ASP:OD2	1:B:1032:LYS:N	2.35	0.59
1:A:1748:PHE:O	1:A:1750:PRO:HD3	2.02	0.59
1:C:3889:GLN:HG3	1:C:3967:GLU:HG3	1.84	0.59
1:B:897:ARG:HG2	1:B:905:PRO:HD2	1.85	0.59
1:D:1616:GLU:O	1:D:1628:VAL:HA	2.02	0.59
1:D:2665:UNK:C	1:D:2922:LYS:HZ3	2.15	0.59
1:C:4708:THR:HG21	1:C:4775:TYR:HB2	1.85	0.59
1:C:4858:PHE:CE2	5:C:5106:POV:H33A	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:THR:HG23	1:D:295:GLU:H	1.68	0.59
1:D:1072:VAL:HG12	1:D:1195:GLY:HA2	1.85	0.59
1:D:4708:THR:HG21	1:D:4775:TYR:HB2	1.85	0.59
1:B:294:THR:HG23	1:B:295:GLU:H	1.68	0.59
1:B:1739:THR:HG23	1:B:1742:THR:H	1.67	0.59
1:B:2192:TYR:HA	1:B:2242:ILE:HD11	1.84	0.59
1:C:1739:THR:HG23	1:C:1742:THR:H	1.67	0.59
1:C:2359:ARG:NH2	1:B:179:TYR:OH	2.36	0.59
1:D:2155:LEU:HB2	1:D:2188:ASN:HD21	1.68	0.59
1:D:2770:LYS:HD2	1:D:2775:TRP:HB2	1.85	0.59
1:A:244:LEU:HD12	1:A:375:LYS:HE2	1.84	0.59
1:A:731:THR:OG1	1:A:765:GLN:NE2	2.34	0.59
1:A:4865:LYS:HG2	1:A:4875:LYS:HE3	1.84	0.59
1:A:4892:ARG:NH1	1:D:4917:ASP:OD2	2.36	0.59
1:C:29:LEU:HG	1:C:31:GLU:H	1.68	0.59
1:B:2155:LEU:HB2	1:B:2188:ASN:HD21	1.68	0.59
1:A:294:THR:HG23	1:A:295:GLU:H	1.68	0.58
1:A:4067:LYS:HD3	1:A:4102:GLN:HG3	1.84	0.58
1:C:4239:GLU:OE2	1:C:4679:ARG:NH2	2.34	0.58
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	1.84	0.58
1:C:830:ARG:HD2	1:C:1608:MET:HE1	1.84	0.58
1:C:2196:ASN:OD1	1:C:2199:ARG:NH2	2.37	0.58
1:D:1748:PHE:O	1:D:1750:PRO:HD3	2.02	0.58
1:B:2770:LYS:HD2	1:B:2775:TRP:HB2	1.85	0.58
1:C:897:ARG:HG2	1:C:905:PRO:HD2	1.84	0.58
1:D:1028:ASP:OD2	1:D:1032:LYS:N	2.36	0.58
1:D:4864:ASN:OD1	1:D:4875:LYS:NZ	2.33	0.58
1:C:1943:LEU:HD21	1:C:2098:VAL:HG22	1.84	0.58
1:B:731:THR:OG1	1:B:765:GLN:NE2	2.35	0.58
1:B:1786:LEU:H	1:B:1786:LEU:CD1	2.16	0.58
1:A:1072:VAL:HG12	1:A:1195:GLY:HA2	1.86	0.58
1:C:3772:THR:HG23	1:C:3812:VAL:HG22	1.84	0.58
1:B:4978:HIS:CE1	1:B:4983:HIS:NE2	2.71	0.58
1:A:29:LEU:HG	1:A:31:GLU:H	1.69	0.58
1:A:2196:ASN:OD1	1:A:2199:ARG:NH2	2.36	0.58
1:A:2770:LYS:HD2	1:A:2775:TRP:HB2	1.85	0.58
1:A:4799:SER:HB2	1:A:4812:HIS:HE1	1.68	0.58
1:C:4115:SER:HB2	1:C:4123:ILE:HG21	1.85	0.58
1:B:29:LEU:HG	1:B:31:GLU:H	1.69	0.58
1:A:667:MET:HG3	1:A:790:ARG:HH21	1.67	0.58
1:C:3874:VAL:HG11	1:C:3950:ASN:ND2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1243:PRO:HB2	1:D:1600:LEU:HD11	1.86	0.58
1:D:4799:SER:HB2	1:D:4812:HIS:HE1	1.67	0.58
1:D:4858:PHE:HE2	5:D:5105:POV:C33	2.10	0.58
1:B:224:HIS:NE2	1:B:385:ASP:O	2.37	0.58
1:B:408:ALA:HB2	1:B:483:MET:HE1	1.86	0.58
1:A:179:TYR:OH	1:B:2359:ARG:NH2	2.37	0.58
1:C:3770:LEU:O	1:C:3770:LEU:HD23	2.04	0.58
1:A:101:LEU:HD12	1:A:150:MET:HE1	1.85	0.58
1:A:3874:VAL:HG11	1:A:3950:ASN:ND2	2.19	0.58
1:A:4239:GLU:OE2	1:A:4679:ARG:NH2	2.34	0.58
1:C:101:LEU:HD12	1:C:150:MET:HE1	1.85	0.58
1:C:1028:ASP:OD2	1:C:1032:LYS:N	2.36	0.58
1:B:1072:VAL:HG12	1:B:1195:GLY:HA2	1.85	0.58
1:B:4198:SER:OG	1:B:4201:ASN:ND2	2.37	0.58
1:A:4708:THR:HG21	1:A:4775:TYR:HB2	1.85	0.58
1:D:29:LEU:HG	1:D:31:GLU:H	1.69	0.58
1:D:408:ALA:HB2	1:D:483:MET:HE1	1.86	0.58
1:D:1943:LEU:HD21	1:D:2098:VAL:HG22	1.84	0.58
1:D:4239:GLU:OE2	1:D:4679:ARG:NH2	2.33	0.58
1:B:56:GLN:O	1:B:309:THR:OG1	2.22	0.58
1:B:4708:THR:HG21	1:B:4775:TYR:HB2	1.85	0.58
1:A:830:ARG:HH21	1:A:837:PRO:HB3	1.69	0.57
1:A:2155:LEU:HB2	1:A:2188:ASN:HD21	1.69	0.57
1:A:2589:UNK:O	1:A:2734:ASN:ND2	2.37	0.57
1:C:179:TYR:OH	1:D:2359:ARG:NH2	2.36	0.57
1:D:2589:UNK:O	1:D:2734:ASN:ND2	2.37	0.57
1:D:4859:PHE:HE1	1:D:4909:TYR:HD2	1.52	0.57
1:A:3770:LEU:HD23	1:A:3770:LEU:O	2.04	0.57
1:A:4865:LYS:H	1:A:4875:LYS:HE2	1.69	0.57
1:B:663:TYR:HB3	1:B:809:ALA:HB2	1.86	0.57
1:B:2178:MET:HE2	1:B:2210:VAL:HG21	1.87	0.57
1:A:2506:UNK:O	1:A:2511:UNK:N	2.38	0.57
1:C:1243:PRO:HB2	1:C:1600:LEU:HD11	1.86	0.57
1:C:2589:UNK:O	1:C:2734:ASN:ND2	2.37	0.57
1:C:2770:LYS:HD2	1:C:2775:TRP:HB2	1.85	0.57
1:D:1044:ARG:HA	1:D:1047:LEU:HD22	1.86	0.57
1:D:3874:VAL:HG11	1:D:3950:ASN:ND2	2.19	0.57
1:D:4184:MET:HB3	1:D:4190:ILE:HD13	1.85	0.57
1:C:408:ALA:HB2	1:C:483:MET:HE1	1.86	0.57
1:B:861:ILE:HG23	1:B:862:VAL:HG13	1.85	0.57
1:B:2196:ASN:OD1	1:B:2199:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3874:VAL:HG11	1:B:3950:ASN:ND2	2.20	0.57
1:A:663:TYR:HB3	1:A:809:ALA:HB2	1.86	0.57
1:C:2506:UNK:O	1:C:2511:UNK:N	2.38	0.57
1:D:2506:UNK:O	1:D:2511:UNK:N	2.38	0.57
1:B:1781:CYS:SG	1:B:1783:VAL:CG2	2.92	0.57
1:B:2642:UNK:N	1:B:2872:GLN:HB2	2.19	0.57
1:B:2644:UNK:H	1:B:2872:GLN:HA	1.69	0.57
1:B:2916:LYS:HG3	1:B:2920:ARG:HE	1.70	0.57
1:B:3722:TYR:CZ	1:B:3782:MET:HE2	2.40	0.57
1:A:1044:ARG:HA	1:A:1047:LEU:HD22	1.86	0.57
1:A:2291:GLN:O	1:A:2292:GLU:HG3	2.05	0.57
1:D:224:HIS:NE2	1:D:385:ASP:O	2.37	0.57
1:B:2589:UNK:O	1:B:2734:ASN:ND2	2.37	0.57
1:B:3806:ASN:HA	1:B:3890:LEU:HD21	1.86	0.57
1:B:4859:PHE:HE1	1:B:4909:TYR:HD2	1.53	0.57
1:A:408:ALA:HB2	1:A:483:MET:HE1	1.86	0.57
1:B:1793:GLU:CB	1:B:2173:GLN:CG	2.83	0.57
1:A:4859:PHE:HE1	1:A:4909:TYR:HD2	1.53	0.57
1:C:1155:LEU:HD13	1:C:1184:ILE:HD12	1.86	0.57
1:D:663:TYR:HB3	1:D:809:ALA:HB2	1.86	0.57
1:D:2291:GLN:O	1:D:2292:GLU:HG3	2.05	0.57
1:B:1619:ARG:HA	1:B:1626:TRP:CA	2.35	0.57
1:C:663:TYR:HB3	1:C:809:ALA:HB2	1.86	0.57
1:D:830:ARG:HH21	1:D:837:PRO:HB3	1.70	0.57
1:D:3806:ASN:HA	1:D:3890:LEU:HD21	1.87	0.57
1:A:1155:LEU:HD13	1:A:1184:ILE:HD12	1.86	0.56
1:A:3806:ASN:HA	1:A:3890:LEU:HD21	1.87	0.56
1:C:1072:VAL:HG12	1:C:1195:GLY:HA2	1.85	0.56
1:C:2291:GLN:O	1:C:2292:GLU:HG3	2.05	0.56
1:D:1798:LEU:N	1:D:1798:LEU:HD22	2.20	0.56
1:B:2291:GLN:O	1:B:2292:GLU:HG3	2.05	0.56
1:A:379:HIS:CD2	1:A:382:GLY:H	2.24	0.56
1:C:830:ARG:HH21	1:C:837:PRO:HB3	1.70	0.56
1:C:1933:GLU:HA	1:C:1936:LYS:HD3	1.87	0.56
1:C:4198:SER:OG	1:C:4201:ASN:ND2	2.39	0.56
1:A:379:HIS:HD2	1:A:382:GLY:H	1.53	0.56
1:A:1243:PRO:HB2	1:A:1600:LEU:HD11	1.86	0.56
1:A:4631:PHE:HE2	1:A:4639:MET:HE3	1.70	0.56
1:C:2742:THR:HG23	1:C:2811:GLU:HG2	1.88	0.56
1:C:3806:ASN:HA	1:C:3890:LEU:HD21	1.87	0.56
1:D:379:HIS:CD2	1:D:382:GLY:H	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2196:ASN:OD1	1:D:2199:ARG:NH2	2.37	0.56
1:B:578:ILE:HD12	1:B:583:ILE:HD11	1.87	0.56
1:B:830:ARG:HH21	1:B:837:PRO:HB3	1.69	0.56
1:B:2364:PHE:HB3	1:B:2368:LEU:HD23	1.87	0.56
1:A:3752:SER:N	1:A:3755:GLU:OE2	2.39	0.56
1:C:2880:GLU:HA	1:C:2883:HIS:NE2	2.21	0.56
1:B:1044:ARG:HA	1:B:1047:LEU:HD22	1.86	0.56
1:B:1793:GLU:CB	1:B:2173:GLN:HG3	2.35	0.56
1:A:56:GLN:O	1:A:309:THR:OG1	2.23	0.56
1:C:56:GLN:O	1:C:309:THR:OG1	2.23	0.56
1:C:3752:SER:N	1:C:3755:GLU:OE2	2.38	0.56
1:D:56:GLN:O	1:D:309:THR:OG1	2.23	0.56
1:D:1155:LEU:HD13	1:D:1184:ILE:HD12	1.87	0.56
1:B:1155:LEU:HD13	1:B:1184:ILE:HD12	1.87	0.56
1:B:4912:TYR:CD2	5:B:5106:POV:H34	2.41	0.56
1:C:379:HIS:HD2	1:C:382:GLY:H	1.53	0.56
1:C:4857:ASN:HD22	5:C:5107:POV:H34	1.70	0.56
1:C:886:ARG:HH21	1:C:907:LEU:HD13	1.71	0.56
1:D:379:HIS:HD2	1:D:382:GLY:H	1.53	0.56
1:B:886:ARG:HH21	1:B:907:LEU:HD13	1.71	0.56
1:C:346:CYS:SG	1:C:347:PHE:N	2.79	0.56
1:C:379:HIS:CD2	1:C:382:GLY:H	2.24	0.56
1:C:1078:GLU:HB2	1:C:1081:TYR:HD2	1.71	0.56
1:C:2364:PHE:HB3	1:C:2368:LEU:HD23	1.88	0.56
1:C:2916:LYS:HG3	1:C:2920:ARG:HE	1.70	0.56
1:D:2178:MET:HE2	1:D:2210:VAL:HG21	1.87	0.56
1:A:877:ASN:HD22	1:A:1045:THR:HG21	1.70	0.56
1:A:1933:GLU:HA	1:A:1936:LYS:HD3	1.87	0.56
1:A:2665:UNK:C	1:A:2922:LYS:HZ3	2.19	0.56
1:C:4858:PHE:CD2	5:C:5106:POV:C33	2.88	0.56
1:D:578:ILE:HD12	1:D:583:ILE:HD11	1.87	0.56
1:D:886:ARG:HH21	1:D:907:LEU:HD13	1.71	0.56
1:B:2506:UNK:O	1:B:2511:UNK:N	2.38	0.56
1:B:2742:THR:HG23	1:B:2811:GLU:HG2	1.88	0.56
1:B:4238:CYS:O	1:B:4242:ILE:HG12	2.06	0.56
1:B:4631:PHE:HE2	1:B:4639:MET:HE3	1.69	0.56
1:A:886:ARG:HH21	1:A:907:LEU:HD13	1.71	0.56
1:A:2916:LYS:HG3	1:A:2920:ARG:HE	1.70	0.56
1:D:1165:ASN:HA	1:D:1213:PHE:HE2	1.71	0.56
1:D:2916:LYS:HG3	1:D:2920:ARG:HE	1.70	0.56
1:A:830:ARG:HD2	1:A:1608:MET:HE1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2364:PHE:HB3	1:D:2368:LEU:HD23	1.88	0.55
1:D:4839:MET:HA	1:D:4839:MET:HE3	1.88	0.55
1:D:4912:TYR:CD2	5:D:5105:POV:H34	2.41	0.55
1:B:4892:ARG:HG3	1:B:4892:ARG:NH2	2.22	0.55
1:A:2364:PHE:HB3	1:A:2368:LEU:HD23	1.88	0.55
1:C:1044:ARG:HA	1:C:1047:LEU:HD22	1.87	0.55
1:D:244:LEU:HG	1:D:246:TYR:HE1	1.71	0.55
1:D:913:LEU:HB2	1:D:918:ARG:HD2	1.88	0.55
1:B:346:CYS:SG	1:B:347:PHE:N	2.79	0.55
1:B:4839:MET:HA	1:B:4839:MET:HE3	1.89	0.55
1:C:913:LEU:HB2	1:C:918:ARG:HD2	1.88	0.55
1:B:2665:UNK:C	1:B:2922:LYS:HZ3	2.19	0.55
1:A:2742:THR:HG23	1:A:2811:GLU:HG2	1.87	0.55
1:A:4839:MET:HA	1:A:4839:MET:HE3	1.88	0.55
1:D:877:ASN:HD22	1:D:1045:THR:HG21	1.70	0.55
1:A:244:LEU:HG	1:A:246:TYR:HE1	1.71	0.55
1:C:649:PHE:HB3	1:C:776:LEU:HD13	1.89	0.55
1:D:830:ARG:HD2	1:D:1608:MET:HE1	1.88	0.55
1:D:4631:PHE:HE2	1:D:4639:MET:HE3	1.71	0.55
1:B:379:HIS:HD2	1:B:382:GLY:H	1.53	0.55
1:A:3450:UNK:O	1:A:3454:UNK:N	2.40	0.55
1:C:2155:LEU:HB2	1:C:2188:ASN:ND2	2.21	0.55
1:C:4851:TYR:CD1	1:C:4916:PHE:HE1	2.24	0.55
1:D:346:CYS:SG	1:D:347:PHE:N	2.79	0.55
1:D:2880:GLU:HA	1:D:2883:HIS:NE2	2.21	0.55
1:B:1165:ASN:HA	1:B:1213:PHE:HE2	1.71	0.55
1:B:2155:LEU:HB2	1:B:2188:ASN:ND2	2.21	0.55
1:A:913:LEU:HB2	1:A:918:ARG:HD2	1.88	0.55
1:A:2770:LYS:HE3	1:A:2775:TRP:HE3	1.72	0.55
1:A:2880:GLU:HA	1:A:2883:HIS:NE2	2.21	0.55
1:D:2155:LEU:HB2	1:D:2188:ASN:ND2	2.21	0.55
1:B:649:PHE:HB3	1:B:776:LEU:HD13	1.89	0.55
1:C:3805:LEU:HD12	1:C:3890:LEU:HG	1.89	0.55
1:C:4839:MET:HE3	1:C:4839:MET:HA	1.89	0.55
1:D:2770:LYS:HE3	1:D:2775:TRP:HE3	1.71	0.55
1:B:877:ASN:HD22	1:B:1045:THR:HG21	1.71	0.55
1:B:3450:UNK:O	1:B:3454:UNK:N	2.40	0.55
1:B:5009:TYR:CZ	1:B:5013:MET:HE2	2.42	0.55
1:A:346:CYS:SG	1:A:347:PHE:N	2.79	0.55
1:A:1078:GLU:HB2	1:A:1081:TYR:HD2	1.71	0.55
1:C:2665:UNK:C	1:C:2922:LYS:HZ3	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2695:UNK:H	1:D:2761:TYR:HH	1.52	0.55
1:C:3450:UNK:O	1:C:3454:UNK:N	2.40	0.55
1:D:901:LYS:HE3	1:D:903:LEU:HD12	1.89	0.55
1:D:3752:SER:N	1:D:3755:GLU:OE2	2.39	0.55
1:A:3676:ASP:HA	1:A:3679:LYS:HB2	1.89	0.54
1:C:126:SER:HB3	1:C:132:ALA:HB2	1.90	0.54
1:C:320:LYS:HA	1:C:356:TRP:HH2	1.72	0.54
1:C:877:ASN:HD22	1:C:1045:THR:HG21	1.71	0.54
1:C:4238:CYS:O	1:C:4242:ILE:HG12	2.07	0.54
1:B:379:HIS:CD2	1:B:382:GLY:H	2.24	0.54
1:B:913:LEU:HB2	1:B:918:ARG:HD2	1.88	0.54
1:C:901:LYS:HE3	1:C:903:LEU:HD12	1.90	0.54
1:B:3752:SER:N	1:B:3755:GLU:OE2	2.39	0.54
1:A:2155:LEU:HB2	1:A:2188:ASN:ND2	2.22	0.54
1:A:3722:TYR:CD2	1:A:3782:MET:CE	2.90	0.54
1:B:244:LEU:HG	1:B:246:TYR:HE1	1.71	0.54
1:A:901:LYS:HE3	1:A:903:LEU:HD12	1.89	0.54
1:C:1165:ASN:HA	1:C:1213:PHE:HE2	1.71	0.54
1:D:661:LYS:HG2	1:D:808:TYR:CD1	2.43	0.54
1:B:320:LYS:HA	1:B:356:TRP:HH2	1.73	0.54
1:B:901:LYS:HE3	1:B:903:LEU:HD12	1.89	0.54
1:B:1243:PRO:HB2	1:B:1600:LEU:HD11	1.88	0.54
1:B:1679:ASN:HB3	1:B:1797:ARG:O	2.08	0.54
1:A:649:PHE:HB3	1:A:776:LEU:HD13	1.89	0.54
1:A:3442:UNK:O	1:A:3446:UNK:N	2.41	0.54
1:C:2162:ILE:HG23	1:C:2178:MET:HE1	1.90	0.54
1:B:2770:LYS:HE3	1:B:2775:TRP:HE3	1.71	0.54
1:A:320:LYS:HA	1:A:356:TRP:HH2	1.72	0.54
1:C:2695:UNK:H	1:C:2761:TYR:HH	1.53	0.54
1:D:144:GLU:O	1:D:175:SER:OG	2.24	0.54
1:D:649:PHE:HB3	1:D:776:LEU:HD13	1.89	0.54
1:D:3450:UNK:O	1:D:3454:UNK:N	2.40	0.54
1:B:944:GLU:HA	1:B:947:GLU:HB2	1.88	0.54
1:B:2644:UNK:C	1:B:2873:ALA:H	2.21	0.54
1:A:249:GLY:HA2	1:A:372:LEU:HD23	1.90	0.54
1:C:244:LEU:HG	1:C:246:TYR:HE1	1.72	0.54
1:C:661:LYS:HG2	1:C:808:TYR:CD1	2.43	0.54
1:B:830:ARG:HD2	1:B:1608:MET:HE1	1.89	0.54
1:B:661:LYS:HG2	1:B:808:TYR:CD1	2.43	0.54
1:B:1153:ILE:HG22	1:B:1160:ILE:HG23	1.90	0.54
1:A:2095:GLN:HA	1:A:2127:GLN:NE2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2162:ILE:HG23	1:A:2178:MET:HE1	1.89	0.54
1:A:3805:LEU:HD12	1:A:3890:LEU:HG	1.89	0.54
1:D:2742:THR:HG23	1:D:2811:GLU:HG2	1.88	0.54
1:D:4238:CYS:O	1:D:4242:ILE:HG12	2.08	0.54
1:B:144:GLU:O	1:B:175:SER:OG	2.24	0.54
1:B:2921:GLU:O	1:B:2924:GLN:NE2	2.40	0.54
1:A:2099:SER:HB2	1:A:2128:TYR:HE1	1.73	0.54
1:A:2128:TYR:HB3	1:A:3669:PHE:HZ	1.73	0.54
1:C:224:HIS:NE2	1:C:385:ASP:O	2.40	0.54
1:C:2770:LYS:HE3	1:C:2775:TRP:HE3	1.72	0.54
1:C:2868:SER:N	1:C:2872:GLN:HE22	2.06	0.53
1:C:3442:UNK:O	1:C:3446:UNK:N	2.41	0.53
1:B:126:SER:HB3	1:B:132:ALA:HB2	1.90	0.53
1:A:661:LYS:HG2	1:A:808:TYR:CD1	2.43	0.53
1:A:1153:ILE:HG22	1:A:1160:ILE:HG23	1.90	0.53
1:A:2642:UNK:N	1:A:2872:GLN:HB2	2.23	0.53
1:D:350:HIS:HE1	1:D:352:ALA:HB3	1.73	0.53
1:D:2812:SER:O	1:D:2882:TYR:OH	2.26	0.53
1:D:3770:LEU:HD23	1:D:3770:LEU:O	2.09	0.53
1:A:1407:UNK:O	1:A:1409:UNK:N	2.42	0.53
1:D:126:SER:HB3	1:D:132:ALA:HB2	1.90	0.53
1:D:320:LYS:HA	1:D:356:TRP:HH2	1.72	0.53
1:D:2868:SER:N	1:D:2872:GLN:HE22	2.06	0.53
1:D:3442:UNK:O	1:D:3446:UNK:N	2.41	0.53
1:D:4892:ARG:HG3	1:D:4892:ARG:O	2.08	0.53
1:B:3442:UNK:O	1:B:3446:UNK:N	2.41	0.53
1:A:578:ILE:HD12	1:A:583:ILE:HD11	1.90	0.53
1:A:758:ARG:HH12	1:A:764:VAL:H	1.57	0.53
1:A:1165:ASN:HA	1:A:1213:PHE:HE2	1.72	0.53
1:C:1407:UNK:O	1:C:1409:UNK:N	2.42	0.53
1:C:1618:ARG:O	1:C:1619:ARG:C	2.51	0.53
1:C:2095:GLN:HA	1:C:2127:GLN:NE2	2.24	0.53
1:D:2921:GLU:O	1:D:2924:GLN:NE2	2.41	0.53
1:D:3805:LEU:HD12	1:D:3890:LEU:HG	1.91	0.53
1:B:2867:LEU:HD22	1:B:2872:GLN:HG3	1.90	0.53
1:A:18:ASP:OD1	1:A:18:ASP:N	2.42	0.53
1:A:3722:TYR:CE2	1:A:3782:MET:HE1	2.38	0.53
1:C:1639:LEU:N	1:C:1648:MET:O	2.41	0.53
1:D:2867:LEU:O	1:D:2868:SER:O	2.27	0.53
1:D:3722:TYR:CE2	1:D:3782:MET:HE3	2.44	0.53
1:B:2644:UNK:O	1:B:2873:ALA:N	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1639:LEU:N	1:A:1648:MET:O	2.42	0.53
1:A:3446:UNK:O	1:A:3451:UNK:N	2.42	0.53
1:A:3985:LEU:HD21	1:A:4026:MET:HE1	1.90	0.53
1:A:4912:TYR:CD2	5:A:5106:POV:H34	2.43	0.53
1:C:144:GLU:O	1:C:175:SER:OG	2.24	0.53
1:D:2124:LEU:HD11	1:D:2128:TYR:CZ	2.44	0.53
1:B:207:SER:HB3	1:B:334:MET:HE2	1.90	0.53
1:B:1407:UNK:O	1:B:1409:UNK:N	2.42	0.53
1:B:3770:LEU:O	1:B:3770:LEU:HD23	2.09	0.53
1:C:350:HIS:HE1	1:C:352:ALA:HB3	1.73	0.53
1:C:1386:UNK:O	1:C:1395:UNK:N	2.42	0.53
1:C:4152:GLU:OE1	1:C:4194:TYR:OH	2.26	0.53
1:D:1577:ALA:HB1	1:D:1584:ARG:HA	1.91	0.53
1:B:1386:UNK:O	1:B:1395:UNK:N	2.42	0.53
1:B:2162:ILE:HG23	1:B:2178:MET:HE1	1.91	0.53
1:A:126:SER:HB3	1:A:132:ALA:HB2	1.90	0.53
1:A:350:HIS:HE1	1:A:352:ALA:HB3	1.73	0.53
1:C:1577:ALA:HB1	1:C:1584:ARG:HA	1.91	0.53
1:D:3985:LEU:HD21	1:D:4026:MET:HE1	1.91	0.53
1:B:1577:ALA:HB1	1:B:1584:ARG:HA	1.91	0.53
1:A:667:MET:SD	1:A:743:VAL:HG12	2.49	0.53
1:C:575:LEU:HD22	1:C:609:CYS:HB3	1.91	0.53
1:B:18:ASP:OD1	1:B:18:ASP:N	2.42	0.53
1:A:4152:GLU:OE1	1:A:4194:TYR:OH	2.26	0.52
1:C:3676:ASP:HA	1:C:3679:LYS:HB2	1.90	0.52
1:D:1153:ILE:HG22	1:D:1160:ILE:HG23	1.90	0.52
1:D:1407:UNK:O	1:D:1409:UNK:N	2.42	0.52
1:D:2867:LEU:C	1:D:2872:GLN:HE22	2.17	0.52
1:B:2880:GLU:HA	1:B:2883:HIS:NE2	2.24	0.52
1:C:3446:UNK:O	1:C:3451:UNK:N	2.42	0.52
1:A:275:ARG:H	1:A:278:GLN:HE22	1.57	0.52
1:B:758:ARG:HH12	1:B:764:VAL:H	1.57	0.52
1:B:3446:UNK:O	1:B:3451:UNK:N	2.42	0.52
1:B:2356:LEU:HA	1:B:2359:ARG:HG2	1.91	0.52
1:B:2812:SER:O	1:B:2882:TYR:OH	2.27	0.52
1:B:3805:LEU:HD12	1:B:3890:LEU:HG	1.90	0.52
1:A:215:THR:OG1	1:A:271:GLY:O	2.28	0.52
1:A:3944:GLU:HG2	1:A:3947:GLY:H	1.75	0.52
1:C:2812:SER:O	1:C:2882:TYR:OH	2.27	0.52
1:C:2921:GLU:O	1:C:2924:GLN:NE2	2.41	0.52
1:C:4579:PHE:HA	1:B:4880:MET:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:LEU:HB3	1:D:339:ILE:HD12	1.92	0.52
1:D:3944:GLU:HG2	1:D:3947:GLY:H	1.75	0.52
1:B:3761:GLN:NE2	1:B:3762:ARG:HG2	2.24	0.52
1:C:274:LEU:HB3	1:C:339:ILE:HD12	1.92	0.52
1:C:963:ASN:ND2	1:C:965:TYR:O	2.43	0.52
1:D:4152:GLU:OE1	1:D:4194:TYR:OH	2.26	0.52
1:B:249:GLY:HA2	1:B:372:LEU:HD23	1.91	0.52
1:B:1122:TYR:CZ	1:B:1182:ILE:HD11	2.45	0.52
1:B:2128:TYR:HB3	1:B:3669:PHE:HZ	1.75	0.52
1:A:963:ASN:ND2	1:A:965:TYR:O	2.43	0.52
1:A:1386:UNK:O	1:A:1395:UNK:N	2.42	0.52
1:C:4856:PHE:CZ	1:D:4580:TYR:HE2	2.28	0.52
1:D:18:ASP:OD1	1:D:18:ASP:N	2.43	0.52
1:D:1122:TYR:CZ	1:D:1182:ILE:HD11	2.45	0.52
1:D:1386:UNK:O	1:D:1395:UNK:N	2.42	0.52
1:D:3761:GLN:NE2	1:D:3762:ARG:HG2	2.24	0.52
1:D:3808:GLY:O	1:D:3813:GLN:NE2	2.43	0.52
1:B:1783:VAL:O	1:B:1783:VAL:HG12	2.09	0.52
1:B:2124:LEU:HD11	1:B:2128:TYR:CZ	2.45	0.52
1:B:3808:GLY:O	1:B:3813:GLN:NE2	2.43	0.52
1:B:4864:ASN:OD1	1:B:4875:LYS:NZ	2.39	0.52
1:A:1122:TYR:CZ	1:A:1182:ILE:HD11	2.45	0.52
1:A:3808:GLY:O	1:A:3813:GLN:NE2	2.43	0.52
1:C:2356:LEU:HA	1:C:2359:ARG:HG2	1.91	0.52
1:C:4984:ASN:O	1:C:4985:LEU:HG	2.10	0.52
1:D:1078:GLU:HB2	1:D:1081:TYR:HD2	1.75	0.52
1:C:3761:GLN:NE2	1:C:3762:ARG:HG2	2.24	0.52
1:C:3808:GLY:O	1:C:3813:GLN:NE2	2.43	0.52
1:B:350:HIS:HE1	1:B:352:ALA:HB3	1.73	0.52
1:B:2695:UNK:H	1:B:2761:TYR:HH	1.52	0.52
1:A:1577:ALA:HB1	1:A:1584:ARG:HA	1.91	0.52
1:C:714:TYR:HB3	1:C:768:PHE:CE2	2.45	0.52
1:C:3985:LEU:HD21	1:C:4026:MET:HE1	1.90	0.52
1:D:2356:LEU:HA	1:D:2359:ARG:HG2	1.91	0.52
1:A:2124:LEU:HD11	1:A:2128:TYR:CZ	2.44	0.51
1:C:3944:GLU:HG2	1:C:3947:GLY:H	1.75	0.51
1:D:2162:ILE:HG23	1:D:2178:MET:HE1	1.92	0.51
1:D:3446:UNK:O	1:D:3451:UNK:N	2.42	0.51
1:D:4567:LEU:HA	1:D:4816:ILE:HG12	1.92	0.51
1:B:1680:ARG:HB2	1:B:1796:ALA:HB3	1.87	0.51
1:B:2580:UNK:HA	1:B:2900:GLY:HA2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2695:UNK:H	1:A:2761:TYR:HH	1.53	0.51
1:D:266:ARG:O	1:D:270:SER:OG	2.27	0.51
1:D:1580:PHE:HE2	1:D:1592:PRO:HG2	1.76	0.51
1:B:275:ARG:H	1:B:278:GLN:HE22	1.58	0.51
1:B:714:TYR:HB3	1:B:768:PHE:CE2	2.45	0.51
1:C:4567:LEU:HA	1:C:4816:ILE:HG12	1.93	0.51
1:D:4583:SER:HG	1:D:4630:TYR:HE1	1.57	0.51
1:A:2645:UNK:C	1:A:2874:MET:HE1	2.41	0.51
1:A:4251:ILE:O	1:A:4251:ILE:HG13	2.11	0.51
1:C:1122:TYR:CZ	1:C:1182:ILE:HD11	2.45	0.51
1:C:1153:ILE:HG22	1:C:1160:ILE:HG23	1.91	0.51
1:D:793:LEU:CD1	1:D:821:LEU:HD21	2.38	0.51
1:D:1933:GLU:HA	1:D:1936:LYS:HD3	1.93	0.51
1:D:4251:ILE:HG13	1:D:4251:ILE:O	2.11	0.51
1:B:4152:GLU:OE1	1:B:4194:TYR:OH	2.26	0.51
1:B:4858:PHE:HE2	5:B:5106:POV:C33	2.12	0.51
1:A:3761:GLN:NE2	1:A:3762:ARG:HG2	2.24	0.51
1:A:3767:GLN:O	1:A:3772:THR:OG1	2.27	0.51
1:B:682:LEU:HD22	1:B:738:LEU:HG	1.91	0.51
1:A:224:HIS:NE2	1:A:385:ASP:O	2.43	0.51
1:A:1580:PHE:HE2	1:A:1592:PRO:HG2	1.76	0.51
1:A:2867:LEU:O	1:A:2868:SER:C	2.53	0.51
1:C:667:MET:SD	1:C:743:VAL:HG12	2.51	0.51
1:C:2124:LEU:HD11	1:C:2128:TYR:CZ	2.46	0.51
1:C:4684:ASP:N	1:C:4684:ASP:OD1	2.44	0.51
1:B:963:ASN:ND2	1:B:965:TYR:O	2.43	0.51
1:B:4567:LEU:HA	1:B:4816:ILE:HG12	1.93	0.51
1:A:2921:GLU:O	1:A:2924:GLN:NE2	2.41	0.51
1:C:578:ILE:HD12	1:C:583:ILE:HD11	1.93	0.51
1:D:667:MET:SD	1:D:743:VAL:HG12	2.51	0.51
1:D:963:ASN:ND2	1:D:965:TYR:O	2.43	0.51
1:B:3985:LEU:HD21	1:B:4026:MET:HE1	1.91	0.51
1:C:143:GLY:HA3	1:C:147:TRP:HE1	1.76	0.51
1:D:2580:UNK:HA	1:D:2900:GLY:HA2	1.92	0.51
1:B:4251:ILE:HG13	1:B:4251:ILE:O	2.11	0.51
1:A:143:GLY:HA3	1:A:147:TRP:HE1	1.76	0.51
1:A:274:LEU:HB3	1:A:339:ILE:HD12	1.92	0.51
1:C:758:ARG:HH12	1:C:764:VAL:H	1.57	0.51
1:C:1617:THR:HA	1:C:1627:ALA:O	2.11	0.51
1:D:249:GLY:HA2	1:D:372:LEU:HD23	1.91	0.51
1:D:2680:UNK:O	1:D:2741:GLU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1712:TYR:OH	1:B:1814:MET:SD	2.69	0.51
1:B:3944:GLU:HG2	1:B:3947:GLY:H	1.75	0.51
1:A:1087:ARG:HG3	1:A:1223:PHE:HA	1.94	0.50
1:A:2680:UNK:O	1:A:2741:GLU:N	2.45	0.50
1:A:4794:TRP:HA	1:A:4797:VAL:HG12	1.92	0.50
1:C:275:ARG:H	1:C:278:GLN:HE22	1.57	0.50
1:C:1087:ARG:HG3	1:C:1223:PHE:HA	1.94	0.50
1:D:215:THR:OG1	1:D:271:GLY:O	2.28	0.50
1:D:4851:TYR:CE1	5:D:5105:POV:H312	2.42	0.50
1:B:274:LEU:HB3	1:B:339:ILE:HD12	1.92	0.50
1:B:1786:LEU:CD1	1:B:1786:LEU:N	2.74	0.50
1:B:2198:MET:HE2	1:B:2198:MET:N	2.26	0.50
1:C:4251:ILE:O	1:C:4251:ILE:HG13	2.11	0.50
1:C:4864:ASN:OD1	1:C:4875:LYS:NZ	2.38	0.50
1:D:143:GLY:HA3	1:D:147:TRP:HE1	1.77	0.50
1:D:275:ARG:H	1:D:278:GLN:HE22	1.57	0.50
1:D:714:TYR:HB3	1:D:768:PHE:CE2	2.45	0.50
1:D:2198:MET:HE2	1:D:2198:MET:N	2.26	0.50
1:A:661:LYS:HE2	1:A:808:TYR:CE2	2.47	0.50
1:A:4567:LEU:HA	1:A:4816:ILE:HG12	1.92	0.50
1:C:2680:UNK:O	1:C:2741:GLU:N	2.44	0.50
1:D:1087:ARG:HG3	1:D:1223:PHE:HA	1.93	0.50
1:D:2099:SER:HB2	1:D:2128:TYR:HE1	1.75	0.50
1:A:27:THR:OG1	1:A:29:LEU:O	2.30	0.50
1:A:921:ASN:O	1:A:924:MET:HG3	2.12	0.50
1:C:2198:MET:N	1:C:2198:MET:HE2	2.26	0.50
1:D:921:ASN:O	1:D:924:MET:HG3	2.12	0.50
1:D:2102:VAL:HG11	1:D:2124:LEU:HB2	1.94	0.50
1:B:2102:VAL:HG11	1:B:2124:LEU:HB2	1.94	0.50
1:A:221:ARG:NH1	1:A:253:CYS:O	2.45	0.50
1:D:626:LEU:HD23	1:D:628:GLY:H	1.76	0.50
1:D:2626:UNK:H	1:D:2892:GLN:NE2	2.10	0.50
1:B:667:MET:SD	1:B:743:VAL:HG12	2.51	0.50
1:B:921:ASN:O	1:B:924:MET:HG3	2.12	0.50
1:B:1078:GLU:HB2	1:B:1081:TYR:HD2	1.75	0.50
1:C:266:ARG:O	1:C:270:SER:OG	2.27	0.50
1:D:2128:TYR:HB3	1:D:3669:PHE:HZ	1.76	0.50
1:B:2680:UNK:O	1:B:2741:GLU:N	2.45	0.50
1:B:3890:LEU:HD12	1:B:3893:GLU:HB2	1.94	0.50
1:A:2626:UNK:H	1:A:2892:GLN:NE2	2.10	0.50
1:C:3561:UNK:O	1:C:3563:UNK:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:LEU:HD23	1:D:525:LEU:HD13	1.94	0.50
1:D:3561:UNK:O	1:D:3563:UNK:N	2.45	0.50
1:B:27:THR:OG1	1:B:29:LEU:O	2.29	0.50
1:B:661:LYS:HE2	1:B:808:TYR:CE2	2.47	0.50
1:B:2291:GLN:NE2	1:B:2292:GLU:H	2.09	0.50
1:A:210:GLU:OE2	1:A:273:HIS:NE2	2.45	0.50
1:C:921:ASN:O	1:C:924:MET:HG3	2.11	0.50
1:C:1712:TYR:OH	1:C:1814:MET:SD	2.69	0.50
1:D:758:ARG:HH12	1:D:764:VAL:H	1.57	0.50
1:D:2877:GLN:NE2	1:D:2877:GLN:O	2.45	0.50
1:B:867:LEU:HD22	1:B:933:LEU:HD21	1.94	0.50
1:B:1933:GLU:HA	1:B:1936:LYS:HD3	1.93	0.50
1:C:2102:VAL:HG11	1:C:2124:LEU:HB2	1.94	0.50
1:C:2626:UNK:H	1:C:2892:GLN:NE2	2.10	0.50
1:C:4861:LYS:HG2	1:C:4862:PHE:N	2.27	0.50
1:D:867:LEU:HD22	1:D:933:LEU:HD21	1.94	0.50
1:B:215:THR:OG1	1:B:271:GLY:O	2.29	0.50
1:B:1087:ARG:HG3	1:B:1223:PHE:HA	1.94	0.50
1:A:2291:GLN:NE2	1:A:2292:GLU:H	2.09	0.49
1:C:2291:GLN:NE2	1:C:2292:GLU:H	2.09	0.49
1:C:3117:UNK:O	1:C:3121:UNK:N	2.45	0.49
1:C:3670:GLU:OE2	1:C:3731:LYS:HG3	2.12	0.49
1:C:3890:LEU:HD12	1:C:3893:GLU:HB2	1.94	0.49
1:C:4915:VAL:O	1:C:4919:THR:HG22	2.12	0.49
1:D:210:GLU:OE2	1:D:273:HIS:NE2	2.45	0.49
1:B:1580:PHE:HE2	1:B:1592:PRO:HG2	1.77	0.49
1:B:2868:SER:N	1:B:2872:GLN:HE22	2.10	0.49
1:B:3561:UNK:O	1:B:3563:UNK:N	2.45	0.49
1:B:4858:PHE:CD2	5:B:5106:POV:H33	2.46	0.49
1:A:2198:MET:HE2	1:A:2198:MET:N	2.26	0.49
1:A:2679:UNK:HA	1:A:2741:GLU:HA	1.94	0.49
1:C:215:THR:OG1	1:C:271:GLY:O	2.28	0.49
1:C:661:LYS:HE2	1:C:808:TYR:CE2	2.47	0.49
1:D:761:GLY:C	1:D:763:PRO:HD3	2.37	0.49
1:B:143:GLY:HA3	1:B:147:TRP:HE1	1.77	0.49
1:B:626:LEU:HD23	1:B:628:GLY:H	1.76	0.49
1:A:144:GLU:O	1:A:175:SER:OG	2.24	0.49
1:A:2812:SER:O	1:A:2882:TYR:OH	2.28	0.49
1:A:3117:UNK:O	1:A:3121:UNK:N	2.46	0.49
1:A:3561:UNK:O	1:A:3563:UNK:N	2.45	0.49
1:A:4059:LEU:HD13	1:A:4167:ALA:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4579:PHE:HD2	1:A:4639:MET:SD	2.34	0.49
1:A:4849:TYR:HD2	1:A:4850:LEU:HD23	1.78	0.49
1:C:867:LEU:HD22	1:C:933:LEU:HD21	1.95	0.49
1:C:1580:PHE:HE2	1:C:1592:PRO:HG2	1.78	0.49
1:C:1738:LEU:HB2	1:C:2146:PRO:HD3	1.94	0.49
1:B:1797:ARG:O	1:B:1798:LEU:C	2.51	0.49
1:A:1742:THR:OG1	1:A:1769:THR:OG1	2.24	0.49
1:C:703:GLY:N	1:C:1647:CYS:SG	2.86	0.49
1:C:761:GLY:C	1:C:763:PRO:HD3	2.38	0.49
1:D:1738:LEU:HB2	1:D:2146:PRO:HD3	1.94	0.49
1:D:3890:LEU:HD12	1:D:3893:GLU:HB2	1.94	0.49
1:B:3117:UNK:O	1:B:3121:UNK:N	2.45	0.49
1:A:2102:VAL:HG11	1:A:2124:LEU:HB2	1.94	0.49
1:A:4880:MET:HE3	1:B:4579:PHE:HA	1.93	0.49
1:C:27:THR:OG1	1:C:29:LEU:O	2.29	0.49
1:C:1991:THR:O	1:C:1995:THR:HG23	2.13	0.49
1:C:2679:UNK:HA	1:C:2741:GLU:HA	1.94	0.49
1:C:4121:GLU:HG3	1:C:4122:MET:H	1.78	0.49
1:D:647:ASN:OD1	1:D:821:LEU:HD12	2.13	0.49
1:B:1127:HIS:ND1	1:B:1128:ARG:HG3	2.27	0.49
1:B:4684:ASP:OD1	1:B:4684:ASP:N	2.44	0.49
1:B:4871:GLU:N	1:B:4872:PRO:HD3	2.28	0.49
1:A:626:LEU:HD23	1:A:628:GLY:H	1.77	0.49
1:A:2105:TRP:HE3	1:A:2120:MET:HE2	1.78	0.49
1:A:2580:UNK:HA	1:A:2900:GLY:HA2	1.94	0.49
1:C:18:ASP:OD1	1:C:18:ASP:N	2.41	0.49
1:C:3767:GLN:O	1:C:3772:THR:OG1	2.26	0.49
1:D:4121:GLU:HG3	1:D:4122:MET:H	1.78	0.49
1:D:4871:GLU:N	1:D:4872:PRO:HD3	2.28	0.49
1:B:266:ARG:O	1:B:270:SER:OG	2.26	0.49
1:A:233:ILE:HG22	1:A:242:ARG:HG2	1.94	0.49
1:A:2642:UNK:N	1:A:2876:GLU:OE1	2.45	0.49
1:A:3890:LEU:HD12	1:A:3893:GLU:HB2	1.94	0.49
1:A:4068:LEU:HA	1:A:4071:ILE:HG22	1.95	0.49
1:A:4871:GLU:N	1:A:4872:PRO:HD3	2.28	0.49
1:C:2105:TRP:HE3	1:C:2120:MET:HE2	1.78	0.49
1:C:4871:GLU:N	1:C:4872:PRO:HD3	2.28	0.49
1:D:1991:THR:O	1:D:1995:THR:HG23	2.13	0.49
1:D:4198:SER:OG	1:D:4201:ASN:ND2	2.46	0.49
1:B:2626:UNK:H	1:B:2892:GLN:NE2	2.10	0.49
1:A:2359:ARG:NH2	1:D:179:TYR:OH	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4858:PHE:HE2	5:A:5106:POV:C33	2.11	0.49
1:C:2627:UNK:H	1:C:2889:LYS:HZ3	1.59	0.49
1:D:233:ILE:HG22	1:D:242:ARG:HG2	1.94	0.49
1:D:2105:TRP:HE3	1:D:2120:MET:HE2	1.78	0.49
1:D:3500:UNK:O	1:D:3504:UNK:N	2.46	0.49
1:D:3767:GLN:O	1:D:3772:THR:OG1	2.28	0.49
1:B:233:ILE:HG22	1:B:242:ARG:HG2	1.94	0.49
1:B:404:ILE:HG23	1:B:483:MET:HE2	1.94	0.49
1:B:1616:GLU:O	1:B:1628:VAL:HA	2.12	0.49
1:B:3676:ASP:HA	1:B:3679:LYS:HB2	1.95	0.49
1:A:761:GLY:C	1:A:763:PRO:HD3	2.37	0.49
1:A:867:LEU:HD22	1:A:933:LEU:HD21	1.95	0.49
1:A:4851:TYR:CE1	5:A:5106:POV:H312	2.45	0.49
1:C:1742:THR:OG1	1:C:1769:THR:OG1	2.24	0.49
1:C:2642:UNK:C	1:C:2875:ALA:HB3	2.43	0.49
1:D:661:LYS:HE2	1:D:808:TYR:CE2	2.47	0.49
1:D:3117:UNK:O	1:D:3121:UNK:N	2.45	0.49
1:B:445:LEU:HD23	1:B:525:LEU:HD13	1.95	0.49
1:B:1738:LEU:HB2	1:B:2146:PRO:HD3	1.94	0.49
1:B:2105:TRP:HE3	1:B:2120:MET:HE2	1.78	0.49
1:A:1679:ASN:O	1:A:1797:ARG:NH2	2.46	0.49
1:D:1742:THR:O	1:D:1745:ILE:HG22	2.13	0.49
1:D:2291:GLN:NE2	1:D:2292:GLU:H	2.10	0.49
1:B:761:GLY:C	1:B:763:PRO:HD3	2.37	0.49
1:B:4953:ASP:HA	1:B:4956:THR:HG22	1.95	0.49
1:A:445:LEU:HD23	1:A:525:LEU:HD13	1.94	0.48
1:C:233:ILE:HG22	1:C:242:ARG:HG2	1.94	0.48
1:C:2128:TYR:HB3	1:C:3669:PHE:HZ	1.77	0.48
1:D:221:ARG:NH1	1:D:253:CYS:O	2.46	0.48
1:D:2642:UNK:C	1:D:2875:ALA:HB3	2.43	0.48
1:D:2667:UNK:HA	1:D:2809:ILE:HD11	1.95	0.48
1:B:134:ASP:N	1:B:134:ASP:OD1	2.45	0.48
1:B:1786:LEU:HD13	1:B:1786:LEU:N	2.28	0.48
1:B:1991:THR:O	1:B:1995:THR:HG23	2.13	0.48
1:A:1742:THR:O	1:A:1745:ILE:HG22	2.13	0.48
1:A:2128:TYR:HB3	1:A:3669:PHE:CZ	2.48	0.48
1:A:3500:UNK:O	1:A:3504:UNK:N	2.46	0.48
1:A:4177:TYR:CE1	1:A:4199:GLU:HB3	2.48	0.48
1:C:134:ASP:OD1	1:C:134:ASP:N	2.45	0.48
1:B:1742:THR:OG1	1:B:1769:THR:OG1	2.24	0.48
1:B:2667:UNK:HA	1:B:2809:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:GLY:N	1:A:1647:CYS:SG	2.86	0.48
1:A:3722:TYR:CD1	1:A:3782:MET:HE2	2.48	0.48
1:C:221:ARG:NH1	1:C:253:CYS:O	2.46	0.48
1:D:404:ILE:HG23	1:D:483:MET:HE2	1.95	0.48
1:B:4152:GLU:OE2	1:B:4180:ARG:NH1	2.47	0.48
1:A:1991:THR:O	1:A:1995:THR:HG23	2.13	0.48
1:C:4954:MET:HE2	1:C:4954:MET:HA	1.95	0.48
1:D:505:GLU:HG2	1:D:512:ALA:HB2	1.95	0.48
1:D:4865:LYS:HG2	1:D:4875:LYS:CE	2.44	0.48
1:B:4851:TYR:CE1	5:B:5106:POV:H312	2.40	0.48
1:A:293:LEU:HD11	1:A:297:GLN:N	2.24	0.48
1:A:2667:UNK:HA	1:A:2809:ILE:HD11	1.95	0.48
1:C:682:LEU:HD22	1:C:738:LEU:HG	1.95	0.48
1:C:2667:UNK:HA	1:C:2809:ILE:HD11	1.96	0.48
1:D:682:LEU:HD22	1:D:738:LEU:HG	1.95	0.48
1:B:1742:THR:O	1:B:1745:ILE:HG22	2.13	0.48
1:A:1618:ARG:O	1:A:1626:TRP:CA	2.62	0.48
1:C:1698:LEU:HB3	1:C:1814:MET:HE1	1.95	0.48
1:C:1932:PRO:HD2	1:C:1935:VAL:HG12	1.95	0.48
1:C:4880:MET:HE3	1:D:4579:PHE:HA	1.95	0.48
1:D:134:ASP:N	1:D:134:ASP:OD1	2.45	0.48
1:D:1130:GLN:OE1	1:D:1136:SER:OG	2.32	0.48
1:D:4858:PHE:CD2	5:D:5105:POV:H33	2.46	0.48
1:B:1618:ARG:O	1:B:1627:ALA:N	2.47	0.48
1:B:2679:UNK:HA	1:B:2741:GLU:HA	1.95	0.48
1:A:4684:ASP:OD1	1:A:4684:ASP:N	2.44	0.48
1:C:1742:THR:O	1:C:1745:ILE:HG22	2.13	0.48
1:C:3500:UNK:O	1:C:3504:UNK:N	2.46	0.48
1:D:27:THR:OG1	1:D:29:LEU:O	2.32	0.48
1:A:61:ASP:OD1	1:A:61:ASP:N	2.47	0.48
1:A:505:GLU:HG2	1:A:512:ALA:HB2	1.96	0.48
1:C:626:LEU:HD23	1:C:628:GLY:H	1.78	0.48
1:C:1156:THR:OG1	1:C:1157:GLU:OE1	2.32	0.48
1:D:4900:GLU:N	1:D:4900:GLU:OE2	2.47	0.48
1:B:210:GLU:OE2	1:B:273:HIS:NE2	2.47	0.48
1:B:3986:TRP:HD1	1:B:4047:MET:HG3	1.78	0.48
1:C:61:ASP:OD1	1:C:61:ASP:N	2.47	0.48
1:C:249:GLY:HA2	1:C:372:LEU:HD23	1.94	0.48
1:C:675:LEU:HG	1:C:676:THR:H	1.79	0.48
1:A:1932:PRO:HD2	1:A:1935:VAL:HG12	1.95	0.48
1:A:4242:ILE:HD12	1:A:4993:MET:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4863:TYR:HA	1:A:4901:ILE:HG23	1.96	0.48
1:A:4912:TYR:HD2	5:A:5106:POV:H34	1.79	0.48
1:C:1154:ASP:OD2	1:C:1156:THR:OG1	2.32	0.48
1:C:2580:UNK:HA	1:C:2900:GLY:HA2	1.94	0.48
1:D:4175:ARG:HG2	1:D:4175:ARG:HH11	1.79	0.48
1:B:3451:UNK:O	1:B:3455:UNK:N	2.47	0.48
1:B:3500:UNK:O	1:B:3504:UNK:N	2.46	0.48
1:B:3767:GLN:O	1:B:3772:THR:OG1	2.28	0.48
1:A:2877:GLN:O	1:A:2877:GLN:NE2	2.47	0.47
1:A:3451:UNK:O	1:A:3455:UNK:N	2.47	0.47
1:C:404:ILE:HG23	1:C:483:MET:HE2	1.95	0.47
1:C:505:GLU:HG2	1:C:512:ALA:HB2	1.95	0.47
1:C:2642:UNK:N	1:C:2872:GLN:HB2	2.28	0.47
1:D:1927:LEU:HD21	1:D:1939:MET:HE2	1.95	0.47
1:D:4580:TYR:OH	1:D:4629:TYR:HB3	2.14	0.47
1:B:675:LEU:HG	1:B:676:THR:H	1.79	0.47
1:B:3699:HIS:HD2	1:B:3771:HIS:HD2	1.61	0.47
1:A:134:ASP:OD1	1:A:134:ASP:N	2.45	0.47
1:A:758:ARG:NH2	1:A:763:PRO:HD2	2.29	0.47
1:A:1738:LEU:HB2	1:A:2146:PRO:HD3	1.94	0.47
1:A:3986:TRP:HD1	1:A:4047:MET:HG3	1.79	0.47
1:A:4567:LEU:HG	1:A:4816:ILE:HG13	1.96	0.47
1:C:238:SER:OG	1:C:240:ASP:OD1	2.30	0.47
1:C:1749:PRO:HG3	1:C:1760:HIS:CE1	2.49	0.47
1:C:3980:LEU:HD21	1:C:3985:LEU:HD22	1.96	0.47
1:C:4152:GLU:OE2	1:C:4180:ARG:NH1	2.47	0.47
1:D:675:LEU:HG	1:D:676:THR:H	1.79	0.47
1:D:758:ARG:NH2	1:D:763:PRO:HD2	2.29	0.47
1:B:1927:LEU:HD21	1:B:1939:MET:HE2	1.96	0.47
1:B:2606:UNK:O	1:B:2650:UNK:HA	2.14	0.47
1:B:2641:UNK:HA	1:B:2872:GLN:HG3	1.97	0.47
1:C:262:LEU:HB2	1:C:280:LEU:HD13	1.96	0.47
1:C:2644:UNK:O	1:C:2873:ALA:N	2.41	0.47
1:D:3451:UNK:O	1:D:3455:UNK:N	2.47	0.47
1:D:4579:PHE:HD2	1:D:4639:MET:SD	2.36	0.47
1:B:505:GLU:HG2	1:B:512:ALA:HB2	1.96	0.47
1:B:3980:LEU:HD21	1:B:3985:LEU:HD22	1.97	0.47
1:B:4121:GLU:HG3	1:B:4122:MET:H	1.78	0.47
1:B:4579:PHE:HD2	1:B:4639:MET:SD	2.37	0.47
1:A:2644:UNK:CB	1:A:2874:MET:H	2.27	0.47
1:A:3661:TRP:HE3	1:A:3663:LEU:HD22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:GLU:OE2	1:C:273:HIS:NE2	2.47	0.47
1:C:4924:VAL:O	1:C:4928:LEU:HB2	2.14	0.47
1:D:2679:UNK:HA	1:D:2741:GLU:HA	1.94	0.47
1:D:3772:THR:HG22	1:D:3815:LYS:HD2	1.96	0.47
1:D:3980:LEU:HD21	1:D:3985:LEU:HD22	1.97	0.47
1:D:3986:TRP:HD1	1:D:4047:MET:HG3	1.79	0.47
1:D:4152:GLU:OE2	1:D:4180:ARG:NH1	2.47	0.47
1:B:1130:GLN:OE1	1:B:1136:SER:OG	2.31	0.47
1:B:1749:PRO:HG3	1:B:1760:HIS:CE1	2.49	0.47
1:B:4579:PHE:HB2	1:B:4639:MET:SD	2.55	0.47
1:A:3980:LEU:HD21	1:A:3985:LEU:HD22	1.96	0.47
1:C:2128:TYR:HB3	1:C:3669:PHE:CZ	2.49	0.47
1:C:2877:GLN:O	1:C:2877:GLN:NE2	2.45	0.47
1:D:4684:ASP:OD1	1:D:4684:ASP:N	2.45	0.47
1:A:3497:UNK:O	1:A:3502:UNK:N	2.48	0.47
1:A:4152:GLU:OE2	1:A:4180:ARG:NH1	2.47	0.47
1:D:2641:UNK:HA	1:D:2872:GLN:HG3	1.96	0.47
1:D:4580:TYR:HH	1:D:4629:TYR:HD1	1.59	0.47
1:B:262:LEU:HB2	1:B:280:LEU:HD13	1.97	0.47
1:B:3497:UNK:O	1:B:3502:UNK:N	2.48	0.47
1:A:262:LEU:HB2	1:A:280:LEU:HD13	1.97	0.47
1:A:266:ARG:O	1:A:270:SER:OG	2.26	0.47
1:A:375:LYS:HD3	1:A:377:ILE:HD11	1.96	0.47
1:A:404:ILE:HG23	1:A:483:MET:HE2	1.95	0.47
1:A:1156:THR:OG1	1:A:1157:GLU:OE1	2.32	0.47
1:A:3699:HIS:HD2	1:A:3771:HIS:HD2	1.61	0.47
1:A:4858:PHE:CD2	5:A:5106:POV:H33	2.46	0.47
1:C:1176:GLU:H	1:C:1176:GLU:CD	2.23	0.47
1:C:2099:SER:HB2	1:C:2128:TYR:HE1	1.79	0.47
1:C:2644:UNK:CB	1:C:2874:MET:H	2.28	0.47
1:C:4059:LEU:HD13	1:C:4167:ALA:HB2	1.96	0.47
1:C:4112:LEU:O	1:C:4115:SER:OG	2.32	0.47
1:C:4239:GLU:CD	1:C:4679:ARG:HH22	2.22	0.47
1:B:221:ARG:NH1	1:B:253:CYS:O	2.48	0.47
1:B:1237:TRP:CH2	1:B:1652:GLU:HG2	2.49	0.47
1:B:1698:LEU:HB3	1:B:1814:MET:HE1	1.96	0.47
1:B:2297:LYS:O	1:B:2300:SER:OG	2.33	0.47
1:A:714:TYR:HB3	1:A:768:PHE:CE2	2.49	0.47
1:A:1618:ARG:O	1:A:1626:TRP:HA	2.15	0.47
1:A:1749:PRO:HG3	1:A:1760:HIS:CE1	2.49	0.47
1:C:3451:UNK:O	1:C:3455:UNK:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3986:TRP:HD1	1:C:4047:MET:HG3	1.79	0.47
1:C:4865:LYS:HG2	1:C:4875:LYS:CE	2.44	0.47
1:D:2644:UNK:CB	1:D:2874:MET:H	2.28	0.47
1:B:4175:ARG:HG2	1:B:4175:ARG:HH11	1.79	0.47
1:A:310:LYS:HE3	1:A:352:ALA:HB2	1.97	0.47
1:A:4175:ARG:HG2	1:A:4175:ARG:HH11	1.79	0.47
1:C:758:ARG:NH2	1:C:763:PRO:HD2	2.30	0.47
1:C:955:LEU:O	1:C:966:LYS:NZ	2.48	0.47
1:C:3661:TRP:HE3	1:C:3663:LEU:HD22	1.80	0.47
1:D:1237:TRP:CH2	1:D:1652:GLU:HG2	2.49	0.47
1:D:1683:HIS:CE1	1:D:1780:PRO:HA	2.49	0.47
1:D:2642:UNK:N	1:D:2872:GLN:HB2	2.28	0.47
1:D:3497:UNK:O	1:D:3502:UNK:N	2.48	0.47
1:D:4156:HIS:NE2	1:D:5036:LEU:HD11	2.30	0.47
1:B:2099:SER:HB2	1:B:2128:TYR:HE1	1.80	0.47
1:B:2627:UNK:H	1:B:2889:LYS:HZ3	1.61	0.47
1:B:4177:TYR:CE1	1:B:4199:GLU:HB3	2.50	0.47
1:D:238:SER:OG	1:D:240:ASP:OD1	2.29	0.47
1:D:375:LYS:HD3	1:D:377:ILE:HD11	1.97	0.47
1:D:1156:THR:OG1	1:D:1157:GLU:OE1	2.32	0.47
1:D:3670:GLU:OE1	1:D:3731:LYS:HE3	2.14	0.47
1:B:4156:HIS:NE2	1:B:5036:LEU:HD11	2.30	0.47
1:B:4892:ARG:C	1:B:4894:GLY:H	2.23	0.47
1:A:1969:LEU:HD13	1:A:2009:LEU:HD11	1.97	0.46
1:A:4764:LEU:O	1:A:4765:LEU:HG	2.15	0.46
1:C:4156:HIS:NE2	1:C:5036:LEU:HD11	2.30	0.46
1:C:4175:ARG:HG2	1:C:4175:ARG:HH11	1.79	0.46
1:B:2648:UNK:HA	1:B:2869:ARG:CZ	2.45	0.46
1:B:3818:ASP:OD1	1:B:3819:TYR:N	2.49	0.46
1:B:5004:THR:HG22	1:B:5005:GLY:N	2.30	0.46
1:A:877:ASN:O	1:A:880:GLU:HG3	2.16	0.46
1:A:1130:GLN:OE1	1:A:1136:SER:OG	2.33	0.46
1:A:2802:LYS:HA	1:A:2806:ARG:HB2	1.97	0.46
1:C:445:LEU:HD23	1:C:525:LEU:HD13	1.96	0.46
1:D:61:ASP:OD1	1:D:61:ASP:N	2.47	0.46
1:D:262:LEU:HB2	1:D:280:LEU:HD13	1.97	0.46
1:D:1749:PRO:HG3	1:D:1760:HIS:CE1	2.49	0.46
1:B:1618:ARG:O	1:B:1626:TRP:C	2.57	0.46
1:B:4567:LEU:HG	1:B:4816:ILE:HG13	1.98	0.46
1:A:3535:UNK:O	1:A:3537:UNK:N	2.49	0.46
1:C:375:LYS:HD3	1:C:377:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2641:UNK:HA	1:C:2872:GLN:HG3	1.96	0.46
1:C:3497:UNK:O	1:C:3502:UNK:N	2.48	0.46
1:D:293:LEU:HD11	1:D:297:GLN:N	2.24	0.46
1:D:3489:UNK:O	1:D:3491:UNK:N	2.49	0.46
1:D:4219:PHE:HD1	1:D:4950:VAL:HG11	1.80	0.46
1:D:4239:GLU:CD	1:D:4679:ARG:HH22	2.22	0.46
1:D:4874:MET:HE2	1:D:4874:MET:HA	1.97	0.46
1:B:758:ARG:NH2	1:B:763:PRO:HD2	2.29	0.46
1:B:3772:THR:HG22	1:B:3815:LYS:HD2	1.97	0.46
1:B:3773:ARG:HD3	1:B:3773:ARG:H	1.79	0.46
1:A:294:THR:HG23	1:A:295:GLU:N	2.31	0.46
1:A:675:LEU:HG	1:A:676:THR:H	1.80	0.46
1:A:2882:TYR:O	1:A:2886:TRP:HD1	1.99	0.46
1:C:310:LYS:HE3	1:C:352:ALA:HB2	1.97	0.46
1:C:3489:UNK:O	1:C:3491:UNK:N	2.48	0.46
1:D:4249:ALA:O	1:D:4252:SER:OG	2.32	0.46
1:B:747:CYS:SG	1:B:756:SER:HB3	2.56	0.46
1:B:1176:GLU:CD	1:B:1176:GLU:H	2.23	0.46
1:B:1969:LEU:HD13	1:B:2009:LEU:HD11	1.97	0.46
1:B:4059:LEU:HD13	1:B:4167:ALA:HB2	1.96	0.46
1:A:5004:THR:HG22	1:A:5005:GLY:N	2.31	0.46
1:C:2875:ALA:HB1	1:C:2939:ARG:HD3	1.98	0.46
1:D:877:ASN:O	1:D:880:GLU:HG3	2.16	0.46
1:D:955:LEU:O	1:D:966:LYS:NZ	2.48	0.46
1:D:1969:LEU:HD13	1:D:2009:LEU:HD11	1.97	0.46
1:D:2802:LYS:HA	1:D:2806:ARG:HB2	1.97	0.46
1:D:3749:VAL:O	1:D:3751:VAL:HG23	2.16	0.46
1:D:4059:LEU:HD13	1:D:4167:ALA:HB2	1.95	0.46
1:B:3670:GLU:OE1	1:B:3731:LYS:HE3	2.15	0.46
1:A:2644:UNK:O	1:A:2873:ALA:N	2.43	0.46
1:A:3749:VAL:O	1:A:3751:VAL:HG23	2.16	0.46
1:A:4044:MET:HE3	1:A:4044:MET:HB2	1.87	0.46
1:C:877:ASN:O	1:C:880:GLU:HG3	2.16	0.46
1:C:1087:ARG:HB2	1:C:1223:PHE:CE2	2.51	0.46
1:C:1929:MET:HE2	1:C:1929:MET:HB3	1.84	0.46
1:C:3773:ARG:H	1:C:3773:ARG:HD3	1.79	0.46
1:D:2867:LEU:N	1:D:2872:GLN:NE2	2.64	0.46
1:B:375:LYS:HD3	1:B:377:ILE:HD11	1.96	0.46
1:B:3535:UNK:O	1:B:3537:UNK:N	2.49	0.46
1:A:1078:GLU:HB2	1:A:1081:TYR:CD2	2.50	0.46
1:A:1087:ARG:HB2	1:A:1223:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2924:GLN:NE2	1:A:2925:GLU:HG3	2.31	0.46
1:A:3454:UNK:O	1:A:3458:UNK:N	2.49	0.46
1:A:4156:HIS:NE2	1:A:5036:LEU:HD11	2.30	0.46
1:C:747:CYS:SG	1:C:756:SER:HB3	2.56	0.46
1:C:2880:GLU:HA	1:C:2883:HIS:CE1	2.51	0.46
1:D:310:LYS:HE3	1:D:352:ALA:HB2	1.97	0.46
1:D:747:CYS:SG	1:D:756:SER:HB3	2.56	0.46
1:D:1618:ARG:O	1:D:1626:TRP:N	2.48	0.46
1:D:2644:UNK:H	1:D:2872:GLN:HA	1.81	0.46
1:D:3454:UNK:O	1:D:3458:UNK:N	2.49	0.46
1:B:3454:UNK:O	1:B:3458:UNK:N	2.49	0.46
1:B:3722:TYR:CD2	1:B:3782:MET:CE	2.99	0.46
1:A:3818:ASP:OD1	1:A:3819:TYR:N	2.49	0.46
1:C:1969:LEU:HD13	1:C:2009:LEU:HD11	1.97	0.46
1:C:4764:LEU:O	1:C:4765:LEU:HG	2.16	0.46
1:D:219:VAL:HG12	1:D:261:ARG:HB2	1.98	0.46
1:D:1176:GLU:H	1:D:1176:GLU:CD	2.23	0.46
1:B:3749:VAL:O	1:B:3751:VAL:HG23	2.16	0.46
1:B:3983:SER:OG	1:B:3984:ARG:N	2.49	0.46
1:A:1176:GLU:H	1:A:1176:GLU:CD	2.23	0.46
1:A:3773:ARG:HD3	1:A:3773:ARG:H	1.79	0.46
1:A:4802:GLY:O	1:A:4805:ASN:HB3	2.16	0.46
1:D:618:GLN:OE1	1:D:1678:ASN:ND2	2.38	0.46
1:D:1742:THR:OG1	1:D:1769:THR:OG1	2.24	0.46
1:D:2627:UNK:H	1:D:2889:LYS:HZ3	1.62	0.46
1:D:3818:ASP:OD1	1:D:3819:TYR:N	2.49	0.46
1:D:4567:LEU:HG	1:D:4816:ILE:HG13	1.98	0.46
1:B:1156:THR:OG1	1:B:1157:GLU:OE1	2.32	0.46
1:B:4892:ARG:C	1:B:4894:GLY:N	2.74	0.46
1:A:955:LEU:O	1:A:966:LYS:NZ	2.49	0.46
1:C:4880:MET:HE2	1:C:4880:MET:N	2.31	0.46
1:D:320:LYS:HA	1:D:356:TRP:CH2	2.51	0.46
1:D:2880:GLU:HA	1:D:2883:HIS:CE1	2.51	0.46
1:D:4764:LEU:O	1:D:4765:LEU:HG	2.15	0.46
1:B:294:THR:HG23	1:B:295:GLU:N	2.31	0.46
1:B:955:LEU:O	1:B:966:LYS:NZ	2.48	0.46
1:A:445:LEU:HB3	1:A:521:LEU:CD2	2.46	0.45
1:A:2880:GLU:HA	1:A:2883:HIS:CE1	2.51	0.45
1:C:294:THR:HG23	1:C:295:GLU:N	2.31	0.45
1:C:1130:GLN:OE1	1:C:1136:SER:OG	2.33	0.45
1:C:2924:GLN:NE2	1:C:2925:GLU:HG3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2875:ALA:HB1	1:D:2939:ARG:HD3	1.98	0.45
1:B:1087:ARG:HB2	1:B:1223:PHE:CE2	2.51	0.45
1:B:4764:LEU:O	1:B:4765:LEU:HG	2.15	0.45
1:A:773:LEU:HD23	1:A:773:LEU:H	1.82	0.45
1:A:998:ARG:HA	1:A:1002:ALA:HB3	1.98	0.45
1:A:3489:UNK:O	1:A:3491:UNK:N	2.48	0.45
1:A:3749:VAL:O	1:A:3750:GLU:HG2	2.16	0.45
1:A:3772:THR:HG22	1:A:3815:LYS:HD2	1.97	0.45
1:A:5027:CYS:O	1:A:5028:PHE:HB3	2.16	0.45
1:C:3749:VAL:O	1:C:3751:VAL:HG23	2.16	0.45
1:D:3856:LEU:HD23	1:D:3856:LEU:H	1.82	0.45
1:D:5004:THR:HG22	1:D:5005:GLY:N	2.30	0.45
1:D:5027:CYS:O	1:D:5028:PHE:HB3	2.16	0.45
1:B:3794:VAL:HG11	1:B:3835:LEU:HD11	1.98	0.45
1:A:597:HIS:HB2	1:A:1665:HIS:ND1	2.32	0.45
1:A:4865:LYS:NZ	1:A:4875:LYS:HE3	2.31	0.45
1:C:3454:UNK:O	1:C:3458:UNK:N	2.49	0.45
1:C:3749:VAL:O	1:C:3750:GLU:HG2	2.17	0.45
1:C:3818:ASP:OD1	1:C:3819:TYR:N	2.48	0.45
1:C:5027:CYS:O	1:C:5028:PHE:HB3	2.16	0.45
1:D:2606:UNK:O	1:D:2650:UNK:HA	2.17	0.45
1:D:3535:UNK:O	1:D:3537:UNK:N	2.49	0.45
1:D:3773:ARG:HD3	1:D:3773:ARG:H	1.79	0.45
1:D:4044:MET:HE3	1:D:4044:MET:HB2	1.87	0.45
1:D:4198:SER:OG	1:D:4198:SER:O	2.30	0.45
1:D:4579:PHE:HB2	1:D:4639:MET:SD	2.57	0.45
1:B:5027:CYS:O	1:B:5028:PHE:HB3	2.16	0.45
1:A:629:ARG:HB3	1:A:634:GLN:CD	2.41	0.45
1:A:4219:PHE:HD1	1:A:4950:VAL:HG11	1.80	0.45
1:C:320:LYS:HA	1:C:356:TRP:CH2	2.51	0.45
1:C:773:LEU:HD23	1:C:773:LEU:H	1.81	0.45
1:C:2644:UNK:H	1:C:2872:GLN:HA	1.81	0.45
1:C:2882:TYR:O	1:C:2886:TRP:HD1	2.00	0.45
1:C:3535:UNK:O	1:C:3537:UNK:N	2.49	0.45
1:D:3749:VAL:O	1:D:3750:GLU:HG2	2.17	0.45
1:B:2203:MET:HE2	1:B:2203:MET:HB3	1.80	0.45
1:B:2288:LEU:O	1:B:3849:ARG:NH1	2.50	0.45
1:B:2882:TYR:O	1:B:2886:TRP:HD1	2.00	0.45
1:B:3489:UNK:O	1:B:3491:UNK:N	2.48	0.45
1:B:3749:VAL:O	1:B:3750:GLU:HG2	2.17	0.45
1:A:747:CYS:SG	1:A:756:SER:HB3	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3856:LEU:H	1:A:3856:LEU:HD23	1.82	0.45
1:C:1155:LEU:HD13	1:C:1184:ILE:HG23	1.98	0.45
1:D:1155:LEU:HD13	1:D:1184:ILE:HG23	1.98	0.45
1:D:2882:TYR:O	1:D:2886:TRP:HD1	2.00	0.45
1:D:2932:MET:N	1:D:2932:MET:SD	2.90	0.45
1:D:4849:TYR:HD2	1:D:4850:LEU:HD23	1.82	0.45
1:B:2924:GLN:NE2	1:B:2925:GLU:HG3	2.31	0.45
1:A:1207:ASP:OD1	1:A:1207:ASP:N	2.48	0.45
1:A:4112:LEU:O	1:A:4115:SER:OG	2.32	0.45
1:C:534:ARG:HH11	1:C:534:ARG:HG2	1.82	0.45
1:C:809:ALA:N	1:C:810:PRO:HD3	2.32	0.45
1:C:4219:PHE:HD1	1:C:4950:VAL:HG11	1.81	0.45
1:C:5004:THR:HG22	1:C:5005:GLY:N	2.30	0.45
1:D:1087:ARG:HB2	1:D:1223:PHE:CE2	2.51	0.45
1:D:1618:ARG:O	1:D:1626:TRP:C	2.55	0.45
1:D:1651:LEU:HD13	1:D:1702:HIS:NE2	2.32	0.45
1:D:1783:VAL:O	1:D:1783:VAL:HG12	2.17	0.45
1:D:2924:GLN:NE2	1:D:2925:GLU:HG3	2.31	0.45
1:B:310:LYS:HE3	1:B:352:ALA:HB2	1.97	0.45
1:B:629:ARG:HB3	1:B:634:GLN:CD	2.42	0.45
1:B:1680:ARG:CB	1:B:1796:ALA:HB1	2.44	0.45
1:B:2802:LYS:HA	1:B:2806:ARG:HB2	1.97	0.45
1:B:2932:MET:N	1:B:2932:MET:SD	2.90	0.45
1:B:4039:MET:HB3	1:B:4042:ARG:HH21	1.82	0.45
1:B:4112:LEU:O	1:B:4115:SER:OG	2.33	0.45
1:C:2802:LYS:HA	1:C:2806:ARG:HB2	1.97	0.45
1:C:3856:LEU:HD23	1:C:3856:LEU:H	1.82	0.45
1:C:4857:ASN:ND2	5:C:5107:POV:H34	2.32	0.45
1:D:445:LEU:HB3	1:D:521:LEU:CD2	2.47	0.45
1:D:652:ARG:HH21	1:D:773:LEU:HD13	1.82	0.45
1:D:998:ARG:HA	1:D:1002:ALA:HB3	1.98	0.45
1:B:773:LEU:HD23	1:B:773:LEU:H	1.81	0.45
1:A:1111:PRO:HD3	1:A:1605:TRP:NE1	2.32	0.45
1:A:4239:GLU:CD	1:A:4679:ARG:HH22	2.22	0.45
1:C:219:VAL:HG12	1:C:261:ARG:HB2	1.98	0.45
1:C:1111:PRO:HD3	1:C:1605:TRP:NE1	2.32	0.45
1:C:2203:MET:HE2	1:C:2203:MET:HB3	1.80	0.45
1:C:4733:GLY:HA3	1:C:4736:ARG:HG3	1.99	0.45
1:D:629:ARG:HB3	1:D:634:GLN:CD	2.41	0.45
1:D:809:ALA:N	1:D:810:PRO:HD3	2.32	0.45
1:D:1111:PRO:HD3	1:D:1605:TRP:NE1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:877:ASN:O	1:B:880:GLU:HG3	2.16	0.45
1:B:960:MET:O	1:B:960:MET:HE3	2.17	0.45
1:B:3856:LEU:HD23	1:B:3856:LEU:H	1.82	0.45
1:B:3946:GLN:OE1	1:B:3949:ARG:NH2	2.50	0.45
1:A:1580:PHE:CE2	1:A:1592:PRO:HG2	2.52	0.45
1:A:2336:ARG:HG3	1:A:2435:ARG:HD2	1.99	0.45
1:A:2867:LEU:N	1:A:2872:GLN:NE2	2.65	0.45
1:A:3699:HIS:HD2	1:A:3771:HIS:CD2	2.35	0.45
1:C:293:LEU:HD11	1:C:297:GLN:N	2.24	0.45
1:C:3772:THR:HG22	1:C:3815:LYS:HD2	1.98	0.45
1:D:960:MET:O	1:D:960:MET:HE3	2.17	0.45
1:D:2288:LEU:O	1:D:3849:ARG:NH1	2.50	0.45
1:D:2665:UNK:O	1:D:2922:LYS:NZ	2.50	0.45
1:D:4112:LEU:O	1:D:4115:SER:OG	2.34	0.45
1:D:4910:GLU:C	1:D:4912:TYR:H	2.24	0.45
1:B:703:GLY:N	1:B:1647:CYS:SG	2.90	0.45
1:B:1683:HIS:CE1	1:B:1780:PRO:HA	2.52	0.45
1:B:2336:ARG:HG3	1:B:2435:ARG:HD2	1.99	0.45
1:B:2930:LEU:HD23	1:B:2930:LEU:HA	1.88	0.45
1:A:2665:UNK:O	1:A:2922:LYS:NZ	2.50	0.45
1:A:4851:TYR:OH	1:A:4919:THR:HG23	2.16	0.45
1:C:4567:LEU:HG	1:C:4816:ILE:HG13	1.98	0.45
1:B:219:VAL:HG12	1:B:261:ARG:HB2	1.97	0.45
1:B:1680:ARG:HB2	1:B:1796:ALA:HB1	1.91	0.45
1:B:2880:GLU:HA	1:B:2883:HIS:CE1	2.52	0.45
1:B:3297:UNK:HA	1:B:3302:UNK:HA	1.99	0.45
1:A:875:ALA:HA	1:A:878:ILE:HG12	1.99	0.44
1:A:960:MET:O	1:A:960:MET:HE3	2.17	0.44
1:A:4910:GLU:C	1:A:4912:TYR:H	2.25	0.44
1:C:998:ARG:HA	1:C:1002:ALA:HB3	1.98	0.44
1:C:2932:MET:N	1:C:2932:MET:SD	2.90	0.44
1:D:2895:GLU:OE2	1:D:2902:HIS:NE2	2.50	0.44
1:D:4733:GLY:HA3	1:D:4736:ARG:HG3	1.99	0.44
1:B:809:ALA:N	1:B:810:PRO:HD3	2.32	0.44
1:B:2128:TYR:HB3	1:B:3669:PHE:CZ	2.51	0.44
1:A:219:VAL:HG12	1:A:261:ARG:HB2	1.99	0.44
1:C:2606:UNK:O	1:C:2650:UNK:HA	2.17	0.44
1:D:703:GLY:N	1:D:1647:CYS:SG	2.90	0.44
1:D:821:LEU:HG	1:D:821:LEU:O	2.17	0.44
1:D:1932:PRO:HD2	1:D:1935:VAL:HG12	1.99	0.44
1:B:626:LEU:HD23	1:B:628:GLY:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:875:ALA:HA	1:B:878:ILE:HG12	1.99	0.44
1:B:1651:LEU:HD13	1:B:1702:HIS:NE2	2.32	0.44
1:B:1932:PRO:HD2	1:B:1935:VAL:HG12	1.99	0.44
1:B:2665:UNK:O	1:B:2922:LYS:NZ	2.50	0.44
1:C:2645:UNK:O	1:C:2874:MET:HE1	2.18	0.44
1:D:1580:PHE:CE2	1:D:1592:PRO:HG2	2.52	0.44
1:D:2128:TYR:HB3	1:D:3669:PHE:CZ	2.52	0.44
1:D:2336:ARG:HG3	1:D:2435:ARG:HD2	2.00	0.44
1:D:3794:VAL:HG11	1:D:3835:LEU:HD11	1.98	0.44
1:D:4912:TYR:HD2	5:D:5105:POV:H34	1.80	0.44
1:A:320:LYS:HA	1:A:356:TRP:CH2	2.51	0.44
1:A:2142:TYR:CG	1:A:2197:LEU:HD13	2.53	0.44
1:C:960:MET:HE3	1:C:960:MET:O	2.17	0.44
1:C:1966:VAL:HG21	1:C:3649:ALA:HB1	1.99	0.44
1:C:2142:TYR:CG	1:C:2197:LEU:HD13	2.53	0.44
1:C:2336:ARG:HG3	1:C:2435:ARG:HD2	1.99	0.44
1:C:2911:LEU:HD11	1:C:2914:LYS:HG3	1.99	0.44
1:C:2930:LEU:HD23	1:C:2930:LEU:HA	1.88	0.44
1:C:4039:MET:HB3	1:C:4042:ARG:HH21	1.82	0.44
1:C:4958:CYS:O	4:C:5104:ACP:C2	2.66	0.44
1:D:2142:TYR:CG	1:D:2197:LEU:HD13	2.53	0.44
1:D:2911:LEU:HD11	1:D:2914:LYS:HG3	1.99	0.44
1:D:3297:UNK:HA	1:D:3302:UNK:HA	1.99	0.44
1:B:2911:LEU:HD11	1:B:2914:LYS:HG3	1.99	0.44
1:B:4793:GLY:O	1:B:4797:VAL:HG23	2.17	0.44
1:A:3946:GLN:OE1	1:A:3949:ARG:NH2	2.50	0.44
1:A:4039:MET:HB3	1:A:4042:ARG:HH21	1.82	0.44
1:A:4583:SER:HG	1:A:4630:TYR:HE1	1.62	0.44
1:C:875:ALA:HA	1:C:878:ILE:HG12	1.99	0.44
1:C:3790:THR:HG22	1:C:3835:LEU:HG	1.99	0.44
1:D:1805:GLU:HA	1:D:1808:ARG:NE	2.33	0.44
1:D:2239:PHE:O	1:D:2242:ILE:HG22	2.18	0.44
1:D:2645:UNK:O	1:D:2874:MET:HE1	2.18	0.44
1:B:445:LEU:HB3	1:B:521:LEU:CD2	2.47	0.44
1:B:1111:PRO:HD3	1:B:1605:TRP:NE1	2.32	0.44
1:B:4583:SER:HG	1:B:4630:TYR:HE1	1.66	0.44
1:A:2911:LEU:HD11	1:A:2914:LYS:HG3	2.00	0.44
1:A:2932:MET:SD	1:A:2932:MET:N	2.90	0.44
1:C:805:PRO:HB2	1:C:808:TYR:CD2	2.53	0.44
1:C:1969:LEU:HD23	1:C:1969:LEU:HA	1.87	0.44
1:C:3946:GLN:OE1	1:C:3949:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:THR:HG23	1:D:295:GLU:N	2.31	0.44
1:B:652:ARG:HH21	1:B:773:LEU:HD13	1.83	0.44
1:B:2646:UNK:CB	1:B:2874:MET:HE3	2.48	0.44
1:B:4733:GLY:HA3	1:B:4736:ARG:HG3	1.99	0.44
1:B:4910:GLU:C	1:B:4912:TYR:H	2.24	0.44
1:B:4912:TYR:HD2	5:B:5106:POV:H34	1.80	0.44
1:B:4984:ASN:C	1:B:4986:ALA:H	2.26	0.44
1:A:1966:VAL:HG21	1:A:3649:ALA:HB1	1.99	0.44
1:A:2288:LEU:O	1:A:3849:ARG:NH1	2.50	0.44
1:A:3794:VAL:HG11	1:A:3835:LEU:HD11	1.99	0.44
1:A:4733:GLY:HA3	1:A:4736:ARG:HG3	1.99	0.44
1:C:1237:TRP:CH2	1:C:1652:GLU:HG2	2.53	0.44
1:C:3297:UNK:HA	1:C:3302:UNK:HA	1.99	0.44
1:C:4849:TYR:HD2	1:C:4850:LEU:HD23	1.83	0.44
1:D:597:HIS:HB2	1:D:1665:HIS:ND1	2.32	0.44
1:D:879:HIS:CG	1:D:921:ASN:HD22	2.36	0.44
1:D:3661:TRP:CE2	1:D:3662:ILE:HG22	2.53	0.44
1:D:4793:GLY:O	1:D:4797:VAL:HG23	2.18	0.44
1:B:998:ARG:HA	1:B:1002:ALA:HB3	1.98	0.44
1:B:1735:ILE:HD11	1:B:2201:LEU:HD11	1.99	0.44
1:B:2095:GLN:HA	1:B:2127:GLN:OE1	2.18	0.44
1:B:4198:SER:OG	1:B:4198:SER:O	2.31	0.44
1:A:796:ARG:HH21	1:A:820:ARG:HH22	1.66	0.44
1:A:831:ARG:HE	1:A:840:VAL:HG11	1.83	0.44
1:A:1155:LEU:HD13	1:A:1184:ILE:HG23	1.98	0.44
1:A:2606:UNK:O	1:A:2650:UNK:HA	2.18	0.44
1:A:3835:LEU:HD21	1:A:3880:PHE:CZ	2.52	0.44
1:C:445:LEU:HB3	1:C:521:LEU:CD2	2.47	0.44
1:C:2288:LEU:O	1:C:3849:ARG:NH1	2.50	0.44
1:C:3338:UNK:O	1:C:3342:UNK:N	2.51	0.44
1:C:3794:VAL:HG11	1:C:3835:LEU:HD11	1.99	0.44
1:D:3946:GLN:OE1	1:D:3949:ARG:NH2	2.51	0.44
1:D:4844:LEU:O	1:D:4848:VAL:HG23	2.18	0.44
1:B:805:PRO:HB2	1:B:808:TYR:CD2	2.53	0.44
1:B:2924:GLN:O	1:B:2928:LYS:NZ	2.35	0.44
1:B:3661:TRP:CE2	1:B:3662:ILE:HG22	2.53	0.44
1:B:4913:ARG:HG2	1:B:4913:ARG:HH11	1.82	0.44
1:A:661:LYS:HD2	1:A:748:LEU:O	2.18	0.44
1:C:629:ARG:HB3	1:C:634:GLN:CD	2.42	0.44
1:C:2239:PHE:O	1:C:2242:ILE:HG22	2.18	0.44
1:C:4580:TYR:OH	1:C:4629:TYR:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:HIS:CE1	1:D:352:ALA:HB3	2.53	0.44
1:D:773:LEU:HD23	1:D:773:LEU:H	1.81	0.44
1:D:1639:LEU:HD23	1:D:1640:HIS:N	2.33	0.44
1:D:4177:TYR:CE1	1:D:4199:GLU:HB3	2.52	0.44
1:B:2877:GLN:O	1:B:2877:GLN:NE2	2.44	0.44
1:B:3790:THR:HG22	1:B:3835:LEU:HG	1.99	0.44
1:A:809:ALA:N	1:A:810:PRO:HD3	2.32	0.43
1:A:3297:UNK:HA	1:A:3302:UNK:HA	1.99	0.43
1:C:661:LYS:HD2	1:C:748:LEU:O	2.18	0.43
1:C:879:HIS:CG	1:C:921:ASN:HD22	2.36	0.43
1:B:2895:GLU:OE2	1:B:2902:HIS:NE2	2.50	0.43
1:C:1078:GLU:HB2	1:C:1081:TYR:CD2	2.50	0.43
1:C:2891:LYS:O	1:C:2894:LEU:HD23	2.19	0.43
1:C:4071:ILE:HD11	1:C:4102:GLN:HE21	1.83	0.43
1:C:4981:GLU:HB2	1:C:4982:GLU:OE2	2.19	0.43
1:D:928:THR:HA	1:D:931:THR:HG22	2.01	0.43
1:B:758:ARG:NH1	1:B:762:CYS:HA	2.33	0.43
1:B:1155:LEU:HD13	1:B:1184:ILE:HG23	1.99	0.43
1:B:2643:UNK:HA	1:B:2871:LEU:O	2.18	0.43
1:A:2297:LYS:O	1:A:2300:SER:OG	2.34	0.43
1:C:597:HIS:HB2	1:C:1665:HIS:ND1	2.32	0.43
1:C:652:ARG:HH21	1:C:773:LEU:HD13	1.83	0.43
1:C:758:ARG:NH1	1:C:762:CYS:HA	2.34	0.43
1:C:4044:MET:HE3	1:C:4044:MET:HB2	1.84	0.43
1:C:4921:PHE:CE2	1:D:4892:ARG:HB2	2.52	0.43
1:D:805:PRO:HB2	1:D:808:TYR:CD2	2.53	0.43
1:D:1735:ILE:HD11	1:D:2201:LEU:HD11	2.00	0.43
1:B:320:LYS:HA	1:B:356:TRP:CH2	2.52	0.43
1:B:4880:MET:N	1:B:4880:MET:HE2	2.33	0.43
1:B:4981:GLU:HB2	1:B:4982:GLU:OE2	2.18	0.43
1:A:350:HIS:CE1	1:A:352:ALA:HB3	2.53	0.43
1:A:652:ARG:HH21	1:A:773:LEU:HD13	1.83	0.43
1:A:758:ARG:NH1	1:A:762:CYS:HA	2.33	0.43
1:A:2203:MET:HE2	1:A:2203:MET:HB3	1.79	0.43
1:A:2239:PHE:O	1:A:2242:ILE:HG22	2.18	0.43
1:A:2930:LEU:HD23	1:A:2930:LEU:HA	1.88	0.43
1:A:3338:UNK:O	1:A:3342:UNK:N	2.51	0.43
1:A:4880:MET:HE2	1:A:4880:MET:N	2.32	0.43
1:C:928:THR:HA	1:C:931:THR:HG22	2.01	0.43
1:C:2895:GLU:OE2	1:C:2902:HIS:NE2	2.51	0.43
1:C:3835:LEU:HD21	1:C:3880:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:875:ALA:HA	1:D:878:ILE:HG12	1.99	0.43
1:D:2912:THR:OG1	1:D:2914:LYS:NZ	2.39	0.43
1:D:3338:UNK:O	1:D:3342:UNK:N	2.51	0.43
1:D:3713:LYS:HE2	1:D:3713:LYS:HB3	1.86	0.43
1:D:4039:MET:HB3	1:D:4042:ARG:HH21	1.82	0.43
1:B:2239:PHE:O	1:B:2242:ILE:HG22	2.18	0.43
1:A:1313:UNK:O	1:A:1315:UNK:N	2.51	0.43
1:A:2895:GLU:OE2	1:A:2902:HIS:NE2	2.51	0.43
1:A:4892:ARG:O	1:A:4893:ALA:C	2.61	0.43
1:C:402:ARG:HA	1:C:402:ARG:HD2	1.87	0.43
1:C:1683:HIS:CE1	1:C:1780:PRO:HA	2.52	0.43
1:D:157:ARG:CZ	1:D:164:ARG:HH22	2.32	0.43
1:D:831:ARG:HE	1:D:840:VAL:HG11	1.84	0.43
1:D:1087:ARG:HB2	1:D:1223:PHE:CD2	2.54	0.43
1:D:2433:LEU:HD22	1:D:2457:LEU:HD21	2.00	0.43
1:D:3835:LEU:HD21	1:D:3880:PHE:CZ	2.53	0.43
1:D:5004:THR:HG22	1:D:5005:GLY:H	1.83	0.43
1:B:597:HIS:HB2	1:B:1665:HIS:ND1	2.32	0.43
1:B:2142:TYR:CG	1:B:2197:LEU:HD13	2.53	0.43
1:B:3338:UNK:O	1:B:3342:UNK:N	2.51	0.43
1:B:4580:TYR:OH	1:B:4629:TYR:HB3	2.18	0.43
1:A:805:PRO:HB2	1:A:808:TYR:CD2	2.53	0.43
1:A:1307:UNK:O	1:A:1309:UNK:N	2.51	0.43
1:C:1204:LEU:HD12	1:C:1226:PHE:HB3	2.01	0.43
1:C:1307:UNK:O	1:C:1309:UNK:N	2.51	0.43
1:C:1313:UNK:O	1:C:1315:UNK:N	2.51	0.43
1:D:626:LEU:HD23	1:D:628:GLY:N	2.32	0.43
1:B:27:THR:OG1	1:B:31:GLU:O	2.28	0.43
1:B:61:ASP:OD1	1:B:61:ASP:N	2.47	0.43
1:B:157:ARG:CZ	1:B:164:ARG:HH22	2.31	0.43
1:B:293:LEU:HD11	1:B:297:GLN:N	2.24	0.43
1:B:831:ARG:HE	1:B:840:VAL:HG11	1.83	0.43
1:B:1969:LEU:HD23	1:B:1969:LEU:HA	1.87	0.43
1:B:4242:ILE:HD12	1:B:4993:MET:HG2	1.99	0.43
1:A:660:GLY:HA3	1:A:750:LEU:HD21	2.00	0.43
1:A:928:THR:HA	1:A:931:THR:HG22	2.01	0.43
1:A:3790:THR:HG22	1:A:3835:LEU:HG	1.99	0.43
1:D:2891:LYS:O	1:D:2894:LEU:HD23	2.19	0.43
1:D:3790:THR:HG22	1:D:3835:LEU:HG	1.99	0.43
1:D:4011:GLU:O	1:D:4015:GLU:HG3	2.18	0.43
1:B:4071:ILE:HD11	1:B:4102:GLN:HE21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4851:TYR:CE1	5:B:5106:POV:H31E	2.54	0.43
1:B:4874:MET:HE2	1:B:4874:MET:HA	2.00	0.43
1:B:4995:LEU:HD23	1:B:4995:LEU:HA	1.90	0.43
1:A:1237:TRP:CH2	1:A:1652:GLU:HG2	2.53	0.43
1:A:1680:ARG:HH12	1:A:1786:LEU:HD12	1.84	0.43
1:A:1771:LEU:C	1:A:1772:ARG:HD2	2.44	0.43
1:D:647:ASN:OD1	1:D:821:LEU:C	2.62	0.43
1:D:661:LYS:HD2	1:D:748:LEU:O	2.19	0.43
1:D:758:ARG:NH1	1:D:762:CYS:HA	2.34	0.43
1:D:1154:ASP:OD2	1:D:1156:THR:OG1	2.32	0.43
1:D:1307:UNK:O	1:D:1309:UNK:N	2.51	0.43
1:B:1580:PHE:CE2	1:B:1592:PRO:HG2	2.54	0.43
1:B:3835:LEU:HD21	1:B:3880:PHE:CZ	2.53	0.43
1:B:4865:LYS:HG2	1:B:4875:LYS:CE	2.49	0.43
1:A:879:HIS:CG	1:A:921:ASN:HD22	2.36	0.43
1:A:1735:ILE:HD11	1:A:2201:LEU:HD11	1.99	0.43
1:C:626:LEU:HD23	1:C:628:GLY:N	2.34	0.43
1:C:660:GLY:HA3	1:C:750:LEU:HD21	2.01	0.43
1:C:831:ARG:HE	1:C:840:VAL:HG11	1.84	0.43
1:C:1087:ARG:HB2	1:C:1223:PHE:CD2	2.54	0.43
1:C:1651:LEU:HD13	1:C:1702:HIS:NE2	2.34	0.43
1:D:2095:GLN:HA	1:D:2127:GLN:OE1	2.18	0.43
1:D:2867:LEU:C	1:D:2872:GLN:NE2	2.77	0.43
1:D:3723:MET:HE2	1:D:3723:MET:HB2	1.96	0.43
1:B:661:LYS:HD2	1:B:748:LEU:O	2.19	0.43
1:B:1307:UNK:O	1:B:1309:UNK:N	2.51	0.43
1:A:1087:ARG:HB2	1:A:1223:PHE:CD2	2.54	0.43
1:A:2648:UNK:HA	1:A:2869:ARG:CZ	2.49	0.43
1:A:2867:LEU:C	1:A:2868:SER:O	2.61	0.43
1:A:2912:THR:OG1	1:A:2914:LYS:NZ	2.38	0.43
1:A:3891:LEU:HD23	1:A:3891:LEU:HA	1.91	0.43
1:A:5004:THR:HG22	1:A:5005:GLY:H	1.84	0.43
1:C:1580:PHE:CE2	1:C:1592:PRO:HG2	2.54	0.43
1:C:3798:LEU:HD23	1:C:3798:LEU:HA	1.85	0.43
1:D:2930:LEU:HD23	1:D:2930:LEU:HA	1.88	0.43
1:B:1207:ASP:OD1	1:B:1207:ASP:N	2.48	0.43
1:A:2356:LEU:HA	1:A:2359:ARG:HG2	2.00	0.42
1:A:2891:LYS:O	1:A:2894:LEU:HD23	2.18	0.42
1:A:4874:MET:HE2	1:A:4874:MET:HA	2.01	0.42
1:C:707:VAL:HG13	1:C:713:SER:HB3	2.01	0.42
1:C:1735:ILE:HD11	1:C:2201:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3661:TRP:CG	1:B:3662:ILE:H	2.37	0.42
1:A:758:ARG:CZ	1:A:762:CYS:H	2.33	0.42
1:A:765:GLN:HG3	1:A:1387:UNK:C	2.50	0.42
1:A:2880:GLU:OE1	1:A:2883:HIS:NE2	2.42	0.42
1:C:4874:MET:HA	1:C:4874:MET:HE2	2.01	0.42
1:C:4910:GLU:C	1:C:4912:TYR:H	2.27	0.42
1:C:5004:THR:HG22	1:C:5005:GLY:H	1.84	0.42
1:D:4851:TYR:OH	1:D:4919:THR:HG23	2.19	0.42
1:D:4984:ASN:C	1:D:4986:ALA:H	2.26	0.42
1:B:1313:UNK:O	1:B:1315:UNK:N	2.51	0.42
1:B:1966:VAL:HG21	1:B:3649:ALA:HB1	2.00	0.42
1:A:157:ARG:CZ	1:A:164:ARG:HH22	2.32	0.42
1:A:1204:LEU:HD12	1:A:1226:PHE:HB3	2.01	0.42
1:A:1651:LEU:HD13	1:A:1702:HIS:NE2	2.34	0.42
1:A:2182:ILE:O	1:A:2185:ILE:HG22	2.19	0.42
1:A:4981:GLU:HB2	1:A:4982:GLU:OE2	2.19	0.42
1:C:1771:LEU:C	1:C:1772:ARG:HD2	2.44	0.42
1:D:707:VAL:HG13	1:D:713:SER:HB3	2.01	0.42
1:D:3969:ILE:HG23	1:D:3977:GLN:HG2	2.01	0.42
1:B:758:ARG:CZ	1:B:762:CYS:H	2.33	0.42
1:B:2891:LYS:O	1:B:2894:LEU:HD23	2.19	0.42
1:B:2912:THR:OG1	1:B:2914:LYS:NZ	2.39	0.42
1:B:4849:TYR:HD2	1:B:4850:LEU:HD23	1.84	0.42
1:A:238:SER:OG	1:A:240:ASP:OD1	2.30	0.42
1:A:1639:LEU:HD23	1:A:1640:HIS:N	2.34	0.42
1:C:4583:SER:HG	1:C:4630:TYR:HE1	1.65	0.42
1:C:4913:ARG:HG3	1:C:4913:ARG:HH11	1.84	0.42
1:D:1771:LEU:C	1:D:1772:ARG:HD2	2.44	0.42
1:D:1798:LEU:N	1:D:1798:LEU:CD2	2.81	0.42
1:B:660:GLY:HA3	1:B:750:LEU:HD21	2.01	0.42
1:A:626:LEU:HD23	1:A:628:GLY:N	2.33	0.42
1:C:1639:LEU:HD23	1:C:1640:HIS:N	2.34	0.42
1:D:4071:ILE:HD11	1:D:4102:GLN:HE21	1.84	0.42
1:B:2873:ALA:CB	1:B:2874:MET:HE2	2.46	0.42
1:B:4044:MET:HE3	1:B:4044:MET:HB2	1.84	0.42
1:B:4239:GLU:CD	1:B:4679:ARG:HH22	2.23	0.42
1:B:4851:TYR:CD1	1:B:4916:PHE:HE1	2.37	0.42
1:B:4893:ALA:O	1:B:4894:GLY:C	2.63	0.42
1:A:801:LYS:HE2	1:A:801:LYS:HB3	1.93	0.42
1:A:2643:UNK:HA	1:A:2871:LEU:O	2.19	0.42
1:A:4745:LEU:HD23	1:A:4745:LEU:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:TYR:HA	1:B:696:PRO:HD3	1.95	0.42
1:B:879:HIS:CG	1:B:921:ASN:HD22	2.37	0.42
1:B:1771:LEU:C	1:B:1772:ARG:HD2	2.44	0.42
1:C:796:ARG:HH21	1:C:820:ARG:HH22	1.66	0.42
1:C:2463:LEU:HD23	1:C:2464:ASP:N	2.35	0.42
1:C:2665:UNK:O	1:C:2922:LYS:NZ	2.50	0.42
1:C:4921:PHE:CD2	1:D:4892:ARG:HD2	2.54	0.42
1:D:659:TYR:CG	1:D:810:PRO:HG2	2.55	0.42
1:B:5004:THR:HG22	1:B:5005:GLY:H	1.84	0.42
1:A:2463:LEU:HD23	1:A:2464:ASP:N	2.35	0.42
1:A:4864:ASN:HA	1:A:4875:LYS:HE2	2.00	0.42
1:C:659:TYR:CG	1:C:810:PRO:HG2	2.55	0.42
1:C:2626:UNK:H	1:C:2892:GLN:HE21	1.68	0.42
1:D:54:ASN:HB2	1:D:57:ASN:HB2	2.01	0.42
1:D:758:ARG:CZ	1:D:762:CYS:H	2.32	0.42
1:D:1204:LEU:HD12	1:D:1226:PHE:HB3	2.02	0.42
1:B:932:LEU:HD12	1:B:933:LEU:HD22	2.02	0.42
1:B:1078:GLU:HB2	1:B:1081:TYR:CD2	2.53	0.42
1:A:2433:LEU:HD23	1:A:2433:LEU:HA	1.87	0.42
1:A:3969:ILE:HG23	1:A:3977:GLN:HG2	2.02	0.42
1:C:54:ASN:HB2	1:C:57:ASN:HB2	2.01	0.42
1:C:350:HIS:CE1	1:C:352:ALA:HB3	2.53	0.42
1:C:722:TRP:CD1	1:C:727:ALA:HA	2.55	0.42
1:D:660:GLY:HA3	1:D:750:LEU:HD21	2.01	0.42
1:D:765:GLN:N	1:D:765:GLN:OE1	2.53	0.42
1:D:1313:UNK:O	1:D:1315:UNK:N	2.51	0.42
1:B:350:HIS:CE1	1:B:352:ALA:HB3	2.53	0.42
1:B:765:GLN:OE1	1:B:765:GLN:N	2.53	0.42
1:B:3751:VAL:HG12	1:B:3756:LYS:HB2	2.02	0.42
1:A:659:TYR:CG	1:A:810:PRO:HG2	2.55	0.42
1:A:1974:ARG:HH21	1:A:3642:TYR:HB2	1.85	0.42
1:A:2368:LEU:HD13	1:A:2376:LEU:HD11	2.02	0.42
1:A:2579:UNK:N	1:A:2902:HIS:O	2.53	0.42
1:C:1648:MET:HE3	1:C:1648:MET:HB2	1.88	0.42
1:C:2182:ILE:O	1:C:2185:ILE:HG22	2.20	0.42
1:C:2250:MET:HE3	1:C:2250:MET:O	2.20	0.42
1:D:181:HIS:ND1	1:D:198:THR:OG1	2.53	0.42
1:D:214:VAL:HG22	1:D:341:TYR:CE1	2.55	0.42
1:D:765:GLN:HG3	1:D:1387:UNK:C	2.50	0.42
1:D:2626:UNK:H	1:D:2892:GLN:HE21	1.68	0.42
1:D:4851:TYR:CD1	1:D:4916:PHE:HE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:VAL:HG22	1:B:341:TYR:CE1	2.55	0.42
1:B:796:ARG:HH21	1:B:820:ARG:HH22	1.67	0.42
1:A:1929:MET:HE2	1:A:1929:MET:HB3	1.84	0.41
1:A:2627:UNK:H	1:A:2889:LYS:HZ3	1.66	0.41
1:A:5027:CYS:C	1:A:5029:ARG:H	2.28	0.41
1:C:1077:ALA:HB2	1:C:1190:PRO:HG2	2.02	0.41
1:C:1974:ARG:HH21	1:C:3642:TYR:HB2	1.85	0.41
1:C:4793:GLY:O	1:C:4797:VAL:HG23	2.19	0.41
1:D:3751:VAL:HG12	1:D:3756:LYS:HB2	2.02	0.41
1:D:3798:LEU:HD23	1:D:3798:LEU:HA	1.85	0.41
1:D:4745:LEU:HD23	1:D:4745:LEU:HA	1.92	0.41
1:C:526:LEU:O	1:C:530:ILE:HD12	2.20	0.41
1:C:758:ARG:CZ	1:C:762:CYS:H	2.33	0.41
1:C:765:GLN:OE1	1:C:765:GLN:N	2.53	0.41
1:C:4851:TYR:O	1:C:4855:ALA:N	2.48	0.41
1:C:4861:LYS:C	1:C:4863:TYR:H	2.29	0.41
1:D:526:LEU:O	1:D:530:ILE:HD12	2.20	0.41
1:D:722:TRP:CD1	1:D:727:ALA:HA	2.55	0.41
1:D:1966:VAL:HG21	1:D:3649:ALA:HB1	2.01	0.41
1:D:3661:TRP:CG	1:D:3662:ILE:H	2.37	0.41
5:D:5105:POV:O12	5:D:5105:POV:C15	2.68	0.41
1:B:526:LEU:O	1:B:530:ILE:HD12	2.20	0.41
1:B:765:GLN:HG3	1:B:1387:UNK:C	2.50	0.41
1:B:1087:ARG:HB2	1:B:1223:PHE:CD2	2.54	0.41
1:B:2463:LEU:HD23	1:B:2464:ASP:N	2.35	0.41
1:A:222:LEU:HD23	1:A:222:LEU:H	1.85	0.41
1:A:1154:ASP:OD2	1:A:1156:THR:OG1	2.32	0.41
1:C:4861:LYS:O	1:C:4863:TYR:N	2.54	0.41
1:D:1974:ARG:HH21	1:D:3642:TYR:HB2	1.85	0.41
1:D:2182:ILE:O	1:D:2185:ILE:HG22	2.21	0.41
1:D:2299:VAL:HG11	1:D:2356:LEU:CD2	2.51	0.41
1:D:3778:MET:O	1:D:3782:MET:HG2	2.20	0.41
1:B:54:ASN:HB2	1:B:57:ASN:HB2	2.01	0.41
1:B:479:GLN:HG3	1:B:536:ASN:OD1	2.20	0.41
1:B:659:TYR:CG	1:B:810:PRO:HG2	2.55	0.41
1:B:3713:LYS:HE2	1:B:3713:LYS:HB3	1.86	0.41
1:A:683:ARG:HE	1:A:717:ASP:HB2	1.85	0.41
1:C:445:LEU:HB3	1:C:521:LEU:HD21	2.03	0.41
1:C:4027:LEU:HD23	1:C:4027:LEU:HA	1.92	0.41
1:C:5027:CYS:C	1:C:5029:ARG:H	2.28	0.41
1:D:2297:LYS:O	1:D:2300:SER:OG	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2463:LEU:HD23	1:D:2464:ASP:N	2.35	0.41
1:B:1639:LEU:HD23	1:B:1640:HIS:N	2.34	0.41
1:B:2250:MET:O	1:B:2250:MET:HE3	2.20	0.41
1:B:2868:SER:C	1:B:2872:GLN:HE22	2.25	0.41
1:A:526:LEU:O	1:A:530:ILE:HD12	2.20	0.41
1:A:3661:TRP:CE2	1:A:3662:ILE:HG22	2.56	0.41
1:A:3798:LEU:HD23	1:A:3798:LEU:HA	1.85	0.41
1:C:479:GLN:HG3	1:C:536:ASN:OD1	2.21	0.41
1:C:3661:TRP:CE2	1:C:3662:ILE:HG22	2.56	0.41
1:D:5027:CYS:C	1:D:5029:ARG:H	2.28	0.41
1:B:222:LEU:HD23	1:B:222:LEU:H	1.85	0.41
1:B:1204:LEU:HD12	1:B:1226:PHE:HB3	2.02	0.41
1:A:687:ALA:HB3	1:A:778:PHE:CZ	2.55	0.41
1:A:2250:MET:O	1:A:2250:MET:HE3	2.20	0.41
1:A:4580:TYR:OH	1:A:4629:TYR:HB3	2.21	0.41
1:C:1617:THR:CB	1:C:1628:VAL:HG22	2.49	0.41
1:C:3723:MET:HE2	1:C:3723:MET:HB2	1.96	0.41
1:C:4865:LYS:H	1:C:4875:LYS:CE	2.29	0.41
5:C:5106:POV:C13	1:D:4629:TYR:CE2	3.02	0.41
1:D:4030:LEU:HD23	1:D:4030:LEU:HA	1.88	0.41
1:A:765:GLN:OE1	1:A:765:GLN:N	2.53	0.41
1:A:4865:LYS:HG2	1:A:4875:LYS:CE	2.50	0.41
1:C:765:GLN:HG3	1:C:1387:UNK:C	2.50	0.41
1:D:978:THR:HA	1:D:979:PRO:HD3	1.95	0.41
1:D:2250:MET:O	1:D:2250:MET:HE3	2.20	0.41
1:D:3906:GLN:OE1	1:D:3906:GLN:N	2.54	0.41
1:D:4079:ASP:OD1	1:D:4080:TYR:N	2.54	0.41
1:B:975:VAL:HG11	1:B:1048:GLY:HA2	2.03	0.41
1:B:2323:TRP:CD1	1:B:2323:TRP:H	2.39	0.41
1:B:3780:LEU:HD23	1:B:3780:LEU:HA	1.86	0.41
1:B:3962:PHE:O	1:B:3966:THR:HG23	2.20	0.41
1:B:4999:ASP:HB3	1:B:5002:GLU:HG2	2.03	0.41
1:B:5027:CYS:C	1:B:5029:ARG:H	2.28	0.41
5:B:5106:POV:O12	5:B:5106:POV:C15	2.69	0.41
1:A:224:HIS:O	1:A:229:GLU:HB2	2.20	0.41
1:A:4876:CYS:HB2	1:A:4882:CYS:HB2	1.51	0.41
1:A:4892:ARG:O	1:A:4894:GLY:N	2.53	0.41
1:C:2368:LEU:HD13	1:C:2376:LEU:HD11	2.03	0.41
1:B:1974:ARG:HH21	1:B:3642:TYR:HB2	1.85	0.41
1:B:4907:ASP:N	1:B:4907:ASP:OD1	2.53	0.41
1:A:54:ASN:HB2	1:A:57:ASN:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:VAL:HG11	1:A:1048:GLY:HA2	2.03	0.41
1:A:4079:ASP:OD1	1:A:4080:TYR:N	2.54	0.41
5:A:5106:POV:O12	5:A:5106:POV:C15	2.69	0.41
1:C:631:LEU:HD12	1:C:631:LEU:HA	1.96	0.41
1:C:1225:PRO:HG2	1:C:1228:ILE:HD13	2.03	0.41
1:C:3751:VAL:HG12	1:C:3756:LYS:HB2	2.02	0.41
1:C:3962:PHE:O	1:C:3966:THR:HG23	2.21	0.41
1:C:3969:ILE:HG23	1:C:3977:GLN:HG2	2.02	0.41
1:C:4205:TRP:HH2	1:C:4214:LYS:HD3	1.86	0.41
1:C:4921:PHE:HD2	1:D:4892:ARG:HD2	1.86	0.41
1:D:13:PHE:HE1	1:D:164:ARG:HD2	1.86	0.41
1:D:222:LEU:HD23	1:D:222:LEU:H	1.85	0.41
1:D:975:VAL:HG11	1:D:1048:GLY:HA2	2.03	0.41
1:D:4792:LEU:HD23	1:D:4792:LEU:HA	1.86	0.41
1:B:722:TRP:CD1	1:B:727:ALA:HA	2.55	0.41
1:B:1639:LEU:N	1:B:1648:MET:O	2.54	0.41
1:B:1815:LEU:HD13	1:B:1845:VAL:HG21	2.03	0.41
1:B:2875:ALA:HB1	1:B:2939:ARG:HD3	2.03	0.41
1:B:3782:MET:HE1	1:B:3793:MET:HE3	2.02	0.41
1:B:3969:ILE:HG23	1:B:3977:GLN:HG2	2.02	0.41
1:A:3906:GLN:OE1	1:A:3906:GLN:N	2.54	0.41
1:A:3962:PHE:O	1:A:3966:THR:HG23	2.21	0.41
1:A:4984:ASN:C	1:A:4986:ALA:H	2.28	0.41
1:C:224:HIS:O	1:C:229:GLU:HB2	2.21	0.41
1:C:4177:TYR:CE1	1:C:4199:GLU:HB3	2.56	0.41
1:C:4907:ASP:N	1:C:4907:ASP:OD1	2.54	0.41
1:D:1078:GLU:HB2	1:D:1081:TYR:CD2	2.53	0.41
1:D:2579:UNK:N	1:D:2902:HIS:O	2.54	0.41
1:D:3962:PHE:O	1:D:3966:THR:HG23	2.20	0.41
1:D:4154:VAL:O	1:D:4154:VAL:HG13	2.21	0.41
1:D:4907:ASP:OD1	1:D:4907:ASP:N	2.53	0.41
1:D:4999:ASP:HB3	1:D:5002:GLU:HG2	2.03	0.41
1:B:445:LEU:HB3	1:B:521:LEU:HD21	2.03	0.41
1:B:928:THR:HA	1:B:931:THR:HG22	2.02	0.41
1:B:2299:VAL:HG11	1:B:2356:LEU:CD2	2.51	0.41
1:B:4736:ARG:O	1:B:4739:GLU:HG3	2.21	0.41
1:A:220:LEU:HD23	1:A:260:TRP:O	2.21	0.40
1:A:1077:ALA:HB2	1:A:1190:PRO:HG2	2.02	0.40
1:A:2323:TRP:CD1	1:A:2323:TRP:H	2.39	0.40
1:A:4156:HIS:N	1:A:4161:ARG:HH12	2.19	0.40
1:A:4907:ASP:N	1:A:4907:ASP:OD1	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2579:UNK:N	1:C:2902:HIS:O	2.53	0.40
1:C:3827:GLY:HA2	1:C:3830:GLN:HG2	2.03	0.40
1:C:3906:GLN:OE1	1:C:3906:GLN:N	2.54	0.40
1:C:4154:VAL:HG13	1:C:4154:VAL:O	2.21	0.40
1:B:661:LYS:HE3	1:B:747:CYS:HB2	2.03	0.40
1:B:1617:THR:HA	1:B:1628:VAL:HG22	2.01	0.40
1:B:2182:ILE:O	1:B:2185:ILE:HG22	2.21	0.40
1:B:2626:UNK:H	1:B:2892:GLN:HE21	1.68	0.40
1:A:412:ASN:HA	1:A:415:ILE:HG22	2.03	0.40
1:A:618:GLN:OE1	1:A:1678:ASN:ND2	2.40	0.40
1:A:3751:VAL:HG12	1:A:3756:LYS:HB2	2.02	0.40
1:A:4060:LYS:O	1:A:4064:MET:HG3	2.22	0.40
1:A:4094:GLN:HG3	1:A:4108:ILE:HG21	2.03	0.40
1:C:157:ARG:CZ	1:C:164:ARG:HH22	2.34	0.40
1:C:214:VAL:HG22	1:C:341:TYR:CE1	2.55	0.40
1:C:220:LEU:HD23	1:C:260:TRP:O	2.22	0.40
1:C:222:LEU:HD23	1:C:222:LEU:H	1.85	0.40
1:C:975:VAL:HG11	1:C:1048:GLY:HA2	2.03	0.40
1:C:2323:TRP:H	1:C:2323:TRP:CD1	2.39	0.40
1:C:2380:ILE:O	1:C:2384:ILE:HG12	2.22	0.40
5:C:5106:POV:O12	5:C:5106:POV:C15	2.69	0.40
1:D:224:HIS:O	1:D:229:GLU:HB2	2.20	0.40
1:D:308:HIS:C	1:D:310:LYS:H	2.29	0.40
1:D:553:ARG:CZ	1:D:1593:PRO:HG3	2.51	0.40
1:D:1639:LEU:N	1:D:1648:MET:O	2.55	0.40
1:D:1819:VAL:HG12	1:D:1926:LEU:HD13	2.03	0.40
1:D:3827:GLY:HA2	1:D:3830:GLN:HG2	2.03	0.40
1:D:3937:TYR:OH	1:D:3944:GLU:OE2	2.31	0.40
1:D:4027:LEU:HD23	1:D:4027:LEU:HA	1.92	0.40
1:B:139:GLU:OE2	1:B:139:GLU:N	2.52	0.40
1:B:238:SER:OG	1:B:240:ASP:OD1	2.34	0.40
1:B:412:ASN:HA	1:B:415:ILE:HG22	2.03	0.40
1:A:214:VAL:HG22	1:A:341:TYR:CE1	2.55	0.40
1:A:553:ARG:CZ	1:A:1593:PRO:HG3	2.51	0.40
1:A:2114:PRO:HA	1:A:2117:VAL:HG12	2.03	0.40
1:C:4867:GLU:OE1	1:C:4875:LYS:NZ	2.39	0.40
1:D:2285:GLU:OE1	1:D:2285:GLU:N	2.55	0.40
1:D:4876:CYS:HB2	1:D:4882:CYS:HB2	1.51	0.40
1:B:2380:ILE:O	1:B:2384:ILE:HG12	2.22	0.40
1:B:4156:HIS:N	1:B:4161:ARG:HH12	2.20	0.40
1:B:4983:HIS:O	1:B:4983:HIS:ND1	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4984:ASN:O	1:B:4985:LEU:HG	2.22	0.40
1:A:2626:UNK:H	1:A:2892:GLN:HE21	1.68	0.40
1:A:4242:ILE:HD12	1:A:4993:MET:SD	2.61	0.40
1:D:103:TYR:CE2	1:D:163:VAL:HG12	2.56	0.40
1:D:479:GLN:HG3	1:D:536:ASN:OD1	2.21	0.40
1:D:805:PRO:HB2	1:D:808:TYR:CE2	2.56	0.40
1:D:2323:TRP:H	1:D:2323:TRP:CD1	2.39	0.40
1:D:2644:UNK:O	1:D:2873:ALA:N	2.41	0.40
1:B:213:TYR:CD1	1:B:337:PRO:HB2	2.56	0.40
1:B:220:LEU:HD23	1:B:260:TRP:O	2.22	0.40
1:B:4154:VAL:HG13	1:B:4154:VAL:O	2.22	0.40
1:B:4745:LEU:HD23	1:B:4745:LEU:HA	1.92	0.40
1:A:213:TYR:CD1	1:A:337:PRO:HB2	2.57	0.40
1:A:1225:PRO:HG2	1:A:1228:ILE:HD13	2.04	0.40
1:A:2868:SER:OG	1:A:2869:ARG:N	2.55	0.40
1:A:4154:VAL:O	1:A:4154:VAL:HG13	2.22	0.40
1:C:687:ALA:HB3	1:C:778:PHE:CZ	2.57	0.40
1:C:920:TYR:O	1:C:923:GLN:HG2	2.22	0.40
1:C:2297:LYS:O	1:C:2300:SER:OG	2.34	0.40
1:C:4030:LEU:HD23	1:C:4030:LEU:HA	1.88	0.40
1:C:4249:ALA:O	1:C:4252:SER:OG	2.31	0.40
1:C:4999:ASP:HB3	1:C:5002:GLU:HG2	2.03	0.40
1:D:27:THR:OG1	1:D:31:GLU:O	2.29	0.40
1:D:758:ARG:NE	1:D:762:CYS:H	2.20	0.40
1:B:103:TYR:CE2	1:B:163:VAL:HG12	2.57	0.40
1:B:805:PRO:HB2	1:B:808:TYR:CE2	2.56	0.40
1:B:2579:UNK:N	1:B:2902:HIS:O	2.54	0.40
1:B:3906:GLN:N	1:B:3906:GLN:OE1	2.54	0.40
1:B:4876:CYS:HB2	1:B:4882:CYS:HB2	1.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3203/5037 (64%)	2993 (93%)	207 (6%)	3 (0%)	48	79
1	B	3203/5037 (64%)	2988 (93%)	215 (7%)	0	100	100
1	C	3203/5037 (64%)	2989 (93%)	212 (7%)	2 (0%)	48	79
1	D	3203/5037 (64%)	2994 (94%)	207 (6%)	2 (0%)	48	79
All	All	12812/20148 (64%)	11964 (93%)	841 (7%)	7 (0%)	49	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1797	ARG
1	A	2868	SER
1	C	1796	ALA
1	D	2868	SER
1	C	1797	ARG
1	A	1781	CYS
1	D	1795	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	2512/3264 (77%)	2505 (100%)	7 (0%)	86	84
1	B	2512/3264 (77%)	2505 (100%)	7 (0%)	86	84
1	C	2512/3264 (77%)	2504 (100%)	8 (0%)	86	84
1	D	2508/3264 (77%)	2502 (100%)	6 (0%)	87	87
All	All	10044/13056 (77%)	10016 (100%)	28 (0%)	84	84

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4628	VAL
1	A	4631	PHE
1	A	4632	LEU
1	A	4850	LEU

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Mol	Chain	Res	Type
1	A	4853	VAL
1	A	4891	VAL
1	A	4892	ARG
1	C	1786	LEU
1	C	4628	VAL
1	C	4631	PHE
1	C	4632	LEU
1	C	4850	LEU
1	C	4853	VAL
1	C	4859	PHE
1	C	4861	LYS
1	D	4628	VAL
1	D	4631	PHE
1	D	4632	LEU
1	D	4850	LEU
1	D	4853	VAL
1	D	4891	VAL
1	B	1786	LEU
1	B	3781	GLN
1	B	4628	VAL
1	B	4631	PHE
1	B	4632	LEU
1	B	4853	VAL
1	B	4891	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (119) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	105	HIS
1	A	113	HIS
1	A	151	HIS
1	A	278	GLN
1	A	379	HIS
1	A	380	GLN
1	A	383	HIS
1	A	473	ASN
1	A	593	HIS
1	A	634	GLN
1	A	658	GLN
1	A	735	GLN
1	A	877	ASN

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Mol	Chain	Res	Type
1	A	921	ASN
1	A	1206	GLN
1	A	1645	ASN
1	A	2032	GLN
1	A	2127	GLN
1	A	2291	GLN
1	A	3699	HIS
1	A	3771	HIS
1	A	3806	ASN
1	A	3813	GLN
1	A	3895	HIS
1	A	4043	GLN
1	A	4201	ASN
1	A	4714	ASN
1	A	4806	ASN
1	A	4997	ASN
1	C	44	ASN
1	C	105	HIS
1	C	113	HIS
1	C	278	GLN
1	C	379	HIS
1	C	380	GLN
1	C	383	HIS
1	C	473	ASN
1	C	475	GLN
1	C	634	GLN
1	C	735	GLN
1	C	921	ASN
1	C	1206	GLN
1	C	1645	ASN
1	C	2032	GLN
1	C	2127	GLN
1	C	2194	HIS
1	C	2291	GLN
1	C	2872	GLN
1	C	3781	GLN
1	C	3806	ASN
1	C	3813	GLN
1	C	3895	HIS
1	C	4043	GLN
1	C	4102	GLN
1	C	4201	ASN

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Mol	Chain	Res	Type
1	C	4209	GLN
1	C	4558	ASN
1	C	4714	ASN
1	C	4857	ASN
1	C	4997	ASN
1	D	44	ASN
1	D	113	HIS
1	D	278	GLN
1	D	379	HIS
1	D	380	GLN
1	D	383	HIS
1	D	473	ASN
1	D	634	GLN
1	D	735	GLN
1	D	877	ASN
1	D	921	ASN
1	D	1206	GLN
1	D	1952	GLN
1	D	2032	GLN
1	D	2194	HIS
1	D	2291	GLN
1	D	2872	GLN
1	D	3699	HIS
1	D	3806	ASN
1	D	3813	GLN
1	D	3895	HIS
1	D	3994	HIS
1	D	4043	GLN
1	D	4102	GLN
1	D	4201	ASN
1	D	4558	ASN
1	D	4700	GLN
1	D	4714	ASN
1	D	4857	ASN
1	D	4997	ASN
1	B	44	ASN
1	B	113	HIS
1	B	278	GLN
1	B	379	HIS
1	B	380	GLN
1	B	383	HIS
1	B	473	ASN

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Mol	Chain	Res	Type
1	B	634	GLN
1	B	735	GLN
1	B	877	ASN
1	B	921	ASN
1	B	1206	GLN
1	B	1683	HIS
1	B	1693	GLN
1	B	2032	GLN
1	B	2291	GLN
1	B	2872	GLN
1	B	3699	HIS
1	B	3806	ASN
1	B	3813	GLN
1	B	3830	GLN
1	B	3895	HIS
1	B	3994	HIS
1	B	4043	GLN
1	B	4102	GLN
1	B	4201	ASN
1	B	4558	ASN
1	B	4714	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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
4	ACP	D	5104	-	31,33,33	1.60	10 (32%)	47,52,52	1.96	14 (29%)
5	POV	B	5106	-	44,44,51	0.94	0	50,52,59	0.77	2 (4%)
5	POV	C	5107	-	14,14,51	55.82	5 (35%)	12,12,59	3.98	1 (8%)
5	POV	C	5105	-	14,14,51	55.82	5 (35%)	12,12,59	3.98	1 (8%)
5	POV	A	5105	-	14,14,51	55.82	5 (35%)	12,12,59	3.98	1 (8%)
4	ACP	C	5104	-	31,33,33	1.64	10 (32%)	47,52,52	1.98	14 (29%)
5	POV	A	5106	-	44,44,51	0.94	0	50,52,59	0.78	2 (4%)
5	POV	D	5105	-	44,44,51	0.94	0	50,52,59	0.78	2 (4%)
4	ACP	B	5104	-	31,33,33	1.64	10 (32%)	47,52,52	1.99	14 (29%)
5	POV	B	5105	-	14,14,51	55.82	5 (35%)	12,12,59	3.98	1 (8%)
5	POV	C	5106	-	44,44,51	0.94	0	50,52,59	0.77	2 (4%)
4	ACP	A	5104	-	31,33,33	1.64	10 (32%)	47,52,52	1.99	14 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACP	D	5104	-	-	6/19/38/38	0/3/3/3
5	POV	B	5106	-	-	20/48/48/55	-
5	POV	C	5107	-	-	2/11/11/55	-
5	POV	C	5105	-	-	2/11/11/55	-
5	POV	A	5105	-	-	2/11/11/55	-
4	ACP	C	5104	-	-	6/19/38/38	0/3/3/3
5	POV	A	5106	-	-	20/48/48/55	-
5	POV	D	5105	-	-	20/48/48/55	-
4	ACP	B	5104	-	-	6/19/38/38	0/3/3/3
5	POV	B	5105	-	-	2/11/11/55	-
5	POV	C	5106	-	-	20/48/48/55	-
4	ACP	A	5104	-	-	6/19/38/38	0/3/3/3

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5105	POV	C314-C313	208.78	16.36	1.50
5	C	5107	POV	C314-C313	208.78	16.36	1.50
5	C	5105	POV	C314-C313	208.77	16.36	1.50
5	B	5105	POV	C314-C313	208.77	16.36	1.50
5	A	5105	POV	C32-C33	-4.09	1.26	1.51
5	B	5105	POV	C32-C33	-4.09	1.26	1.51
5	C	5105	POV	C32-C33	-4.09	1.26	1.51
5	C	5107	POV	C32-C33	-4.08	1.26	1.51
4	A	5104	ACP	C5-C4	4.00	1.46	1.39
4	B	5104	ACP	C5-C4	3.98	1.46	1.39
4	C	5104	ACP	C5-C4	3.96	1.46	1.39
4	D	5104	ACP	C5-C4	3.89	1.46	1.39
4	A	5104	ACP	O4'-C4'	-3.07	1.38	1.45
4	C	5104	ACP	O4'-C4'	-3.04	1.38	1.45
4	B	5104	ACP	O4'-C4'	-3.04	1.38	1.45
4	A	5104	ACP	PG-O2G	2.87	1.61	1.55
4	D	5104	ACP	PG-O2G	2.86	1.61	1.55
4	C	5104	ACP	PG-O2G	2.84	1.61	1.55
4	B	5104	ACP	PG-O2G	2.83	1.61	1.55
4	C	5104	ACP	PG-O3G	2.80	1.61	1.55
4	A	5104	ACP	PG-O3G	2.79	1.61	1.55
4	D	5104	ACP	PG-O3G	2.79	1.61	1.55
4	B	5104	ACP	PG-O3G	2.78	1.61	1.55
4	B	5104	ACP	C5-N7	-2.66	1.34	1.39
4	D	5104	ACP	C5-N7	-2.65	1.34	1.39
4	C	5104	ACP	C5-N7	-2.62	1.34	1.39
4	A	5104	ACP	C5-N7	-2.61	1.34	1.39
4	C	5104	ACP	C4-N9	-2.47	1.32	1.37
4	A	5104	ACP	C4-N9	-2.46	1.32	1.37
4	D	5104	ACP	C4-N9	-2.46	1.32	1.37
4	B	5104	ACP	C4-N9	-2.45	1.32	1.37
4	D	5104	ACP	O4'-C4'	-2.44	1.39	1.45
4	A	5104	ACP	PB-O3A	2.40	1.61	1.58
4	D	5104	ACP	PB-O3A	2.37	1.61	1.58
4	C	5104	ACP	PB-O3A	2.37	1.61	1.58
4	B	5104	ACP	PB-O3A	2.35	1.61	1.58
4	B	5104	ACP	C8-N7	2.25	1.36	1.31
5	B	5105	POV	C38-C37	-2.25	1.40	1.51
5	A	5105	POV	C38-C37	-2.25	1.40	1.51
5	C	5107	POV	C38-C37	-2.23	1.40	1.51
4	D	5104	ACP	C8-N7	2.23	1.36	1.31
4	C	5104	ACP	C8-N7	2.23	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	5105	POV	C38-C37	-2.22	1.40	1.51
4	B	5104	ACP	C5-C6	2.22	1.47	1.41
4	A	5104	ACP	C5-C6	2.21	1.47	1.41
4	C	5104	ACP	C5-C6	2.20	1.47	1.41
4	A	5104	ACP	C8-N7	2.19	1.35	1.31
4	D	5104	ACP	C5-C6	2.18	1.47	1.41
5	A	5105	POV	C39-C38	-2.13	1.41	1.51
5	C	5107	POV	C39-C38	-2.13	1.41	1.51
5	C	5105	POV	C39-C38	-2.12	1.41	1.51
5	B	5105	POV	C39-C38	-2.12	1.41	1.51
4	B	5104	ACP	PB-O2B	2.08	1.61	1.56
5	C	5105	POV	C37-C36	-2.07	1.41	1.51
4	C	5104	ACP	PB-O2B	2.07	1.61	1.56
5	A	5105	POV	C37-C36	-2.07	1.41	1.51
5	B	5105	POV	C37-C36	-2.07	1.41	1.51
5	C	5107	POV	C37-C36	-2.07	1.41	1.51
4	D	5104	ACP	PB-O2B	2.06	1.61	1.56
4	A	5104	ACP	PB-O2B	2.05	1.61	1.56

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5105	POV	C314-C313-C312	-13.41	22.80	113.36
5	B	5105	POV	C314-C313-C312	-13.41	22.82	113.36
5	C	5107	POV	C314-C313-C312	-13.41	22.84	113.36
5	A	5105	POV	C314-C313-C312	-13.41	22.85	113.36
4	A	5104	ACP	C5-C4-N3	-5.00	119.84	126.72
4	C	5104	ACP	C5-C4-N3	-4.98	119.86	126.72
4	B	5104	ACP	C5-C4-N3	-4.98	119.86	126.72
4	D	5104	ACP	C5-C4-N3	-4.97	119.87	126.72
4	C	5104	ACP	PB-O3A-PA	-4.58	117.42	132.37
4	A	5104	ACP	PB-O3A-PA	-4.58	117.43	132.37
4	B	5104	ACP	PB-O3A-PA	-4.57	117.45	132.37
4	D	5104	ACP	PB-O3A-PA	-4.57	117.45	132.37
4	A	5104	ACP	N3-C4-N9	4.05	134.06	127.17
4	B	5104	ACP	N3-C4-N9	4.04	134.04	127.17
4	C	5104	ACP	N3-C4-N9	4.04	134.04	127.17
4	D	5104	ACP	N3-C4-N9	3.98	133.94	127.17
4	B	5104	ACP	N3-C2-N1	-3.90	122.67	128.58
4	C	5104	ACP	N3-C2-N1	-3.89	122.69	128.58
4	D	5104	ACP	N3-C2-N1	-3.89	122.70	128.58
4	A	5104	ACP	N3-C2-N1	-3.87	122.73	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5104	ACP	C2-N3-C4	3.62	120.68	111.83
4	C	5104	ACP	C2-N3-C4	3.61	120.66	111.83
4	D	5104	ACP	C2-N3-C4	3.61	120.66	111.83
4	B	5104	ACP	C2-N3-C4	3.61	120.65	111.83
4	C	5104	ACP	C4-N9-C8	3.28	109.18	105.74
4	B	5104	ACP	C4-N9-C8	3.27	109.18	105.74
4	A	5104	ACP	C4-N9-C8	3.26	109.16	105.74
4	D	5104	ACP	C4-N9-C8	3.20	109.09	105.74
4	A	5104	ACP	C4-C5-N7	-3.13	107.01	110.58
4	C	5104	ACP	C4-C5-N7	-3.11	107.02	110.58
4	D	5104	ACP	C4-C5-N7	-3.11	107.03	110.58
4	B	5104	ACP	C4-C5-N7	-3.11	107.03	110.58
4	C	5104	ACP	C2'-C1'-N9	-2.99	105.87	113.30
4	B	5104	ACP	C2'-C1'-N9	-2.99	105.88	113.30
4	A	5104	ACP	C2'-C1'-N9	-2.99	105.89	113.30
4	D	5104	ACP	C2'-C1'-N9	-2.98	105.91	113.30
4	A	5104	ACP	O4'-C1'-N9	2.79	113.45	108.09
4	C	5104	ACP	O4'-C1'-N9	2.76	113.40	108.09
4	D	5104	ACP	O4'-C1'-N9	2.75	113.37	108.09
4	B	5104	ACP	O4'-C1'-N9	2.75	113.37	108.09
4	D	5104	ACP	N9-C8-N7	-2.60	110.25	113.94
5	D	5105	POV	O13-P-O12	-2.58	95.85	107.57
5	B	5106	POV	O13-P-O12	-2.58	95.86	107.57
4	B	5104	ACP	N9-C8-N7	-2.58	110.27	113.94
5	A	5106	POV	O13-P-O12	-2.58	95.88	107.57
5	C	5106	POV	O13-P-O12	-2.57	95.90	107.57
4	C	5104	ACP	N9-C8-N7	-2.57	110.29	113.94
4	A	5104	ACP	N9-C8-N7	-2.57	110.29	113.94
4	D	5104	ACP	C5-N7-C8	2.54	107.44	103.45
4	A	5104	ACP	C5-N7-C8	2.53	107.43	103.45
4	B	5104	ACP	C5-N7-C8	2.53	107.43	103.45
4	C	5104	ACP	C5-N7-C8	2.52	107.40	103.45
4	A	5104	ACP	C6-C5-N7	2.28	136.49	132.09
4	C	5104	ACP	C6-C5-N7	2.28	136.48	132.09
4	B	5104	ACP	C6-C5-N7	2.27	136.47	132.09
4	D	5104	ACP	C6-C5-N7	2.25	136.43	132.09
4	B	5104	ACP	C2-N1-C6	2.22	122.37	118.73
4	C	5104	ACP	C2-N1-C6	2.18	122.31	118.73
4	A	5104	ACP	C2-N1-C6	2.18	122.31	118.73
4	D	5104	ACP	C2-N1-C6	2.15	122.26	118.73
4	D	5104	ACP	C3'-C2'-C1'	2.12	105.47	101.46
4	B	5104	ACP	C3'-C2'-C1'	2.12	105.47	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	5104	ACP	C3'-C2'-C1'	2.10	105.44	101.46
4	A	5104	ACP	C3'-C2'-C1'	2.10	105.43	101.46
5	D	5105	POV	O11-P-O14	2.03	116.96	108.94
5	A	5106	POV	O11-P-O14	2.02	116.93	108.94
5	C	5106	POV	O11-P-O14	2.02	116.93	108.94
5	B	5106	POV	O11-P-O14	2.01	116.92	108.94

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5104	ACP	PB-C3B-PG-O1G
4	A	5104	ACP	PB-C3B-PG-O2G
4	A	5104	ACP	PB-C3B-PG-O3G
4	A	5104	ACP	PG-C3B-PB-O1B
4	A	5104	ACP	PG-C3B-PB-O3A
4	C	5104	ACP	PB-C3B-PG-O1G
4	C	5104	ACP	PB-C3B-PG-O2G
4	C	5104	ACP	PB-C3B-PG-O3G
4	C	5104	ACP	PG-C3B-PB-O1B
4	C	5104	ACP	PG-C3B-PB-O3A
4	D	5104	ACP	PB-C3B-PG-O1G
4	D	5104	ACP	PB-C3B-PG-O2G
4	D	5104	ACP	PB-C3B-PG-O3G
4	D	5104	ACP	PG-C3B-PB-O1B
4	D	5104	ACP	PG-C3B-PB-O3A
4	B	5104	ACP	PB-C3B-PG-O1G
4	B	5104	ACP	PB-C3B-PG-O2G
4	B	5104	ACP	PB-C3B-PG-O3G
4	B	5104	ACP	PG-C3B-PB-O1B
4	B	5104	ACP	PG-C3B-PB-O3A
5	A	5106	POV	C1-O11-P-O12
5	A	5106	POV	C11-O12-P-O14
5	C	5106	POV	C1-O11-P-O12
5	C	5106	POV	C11-O12-P-O14
5	D	5105	POV	C1-O11-P-O12
5	D	5105	POV	C11-O12-P-O14
5	B	5106	POV	C1-O11-P-O12
5	B	5106	POV	C11-O12-P-O14
5	A	5106	POV	O21-C2-C3-O31
5	C	5106	POV	O21-C2-C3-O31
5	D	5105	POV	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
5	B	5106	POV	O21-C2-C3-O31
5	C	5106	POV	C31-C32-C33-C34
5	D	5105	POV	C31-C32-C33-C34
5	B	5106	POV	C31-C32-C33-C34
5	A	5106	POV	C31-C32-C33-C34
5	A	5106	POV	C311-C312-C313-C314
5	D	5105	POV	C311-C312-C313-C314
5	C	5106	POV	C311-C312-C313-C314
5	B	5106	POV	C311-C312-C313-C314
5	A	5106	POV	C26-C27-C28-C29
5	C	5106	POV	C26-C27-C28-C29
5	D	5105	POV	C26-C27-C28-C29
5	B	5106	POV	C26-C27-C28-C29
5	A	5105	POV	C311-C310-C39-C38
5	C	5107	POV	C311-C310-C39-C38
5	B	5105	POV	C311-C310-C39-C38
5	A	5106	POV	O11-C1-C2-O21
5	C	5106	POV	O11-C1-C2-O21
5	D	5105	POV	O11-C1-C2-O21
5	B	5106	POV	O11-C1-C2-O21
5	C	5105	POV	C311-C310-C39-C38
5	B	5106	POV	C37-C38-C39-C310
5	A	5106	POV	C37-C38-C39-C310
5	C	5106	POV	C37-C38-C39-C310
5	D	5105	POV	C37-C38-C39-C310
5	A	5106	POV	C1-C2-C3-O31
5	C	5106	POV	C1-C2-C3-O31
5	D	5105	POV	C1-C2-C3-O31
5	B	5106	POV	C1-C2-C3-O31
5	C	5106	POV	C22-C23-C24-C25
5	D	5105	POV	C22-C23-C24-C25
5	A	5106	POV	C22-C23-C24-C25
5	B	5106	POV	C22-C23-C24-C25
5	C	5105	POV	C311-C312-C313-C314
5	C	5107	POV	C311-C312-C313-C314
5	B	5105	POV	C311-C312-C313-C314
5	D	5105	POV	C34-C35-C36-C37
5	A	5105	POV	C311-C312-C313-C314
5	A	5106	POV	C34-C35-C36-C37
5	C	5106	POV	C34-C35-C36-C37
5	B	5106	POV	C311-C310-C39-C38
5	B	5106	POV	C34-C35-C36-C37

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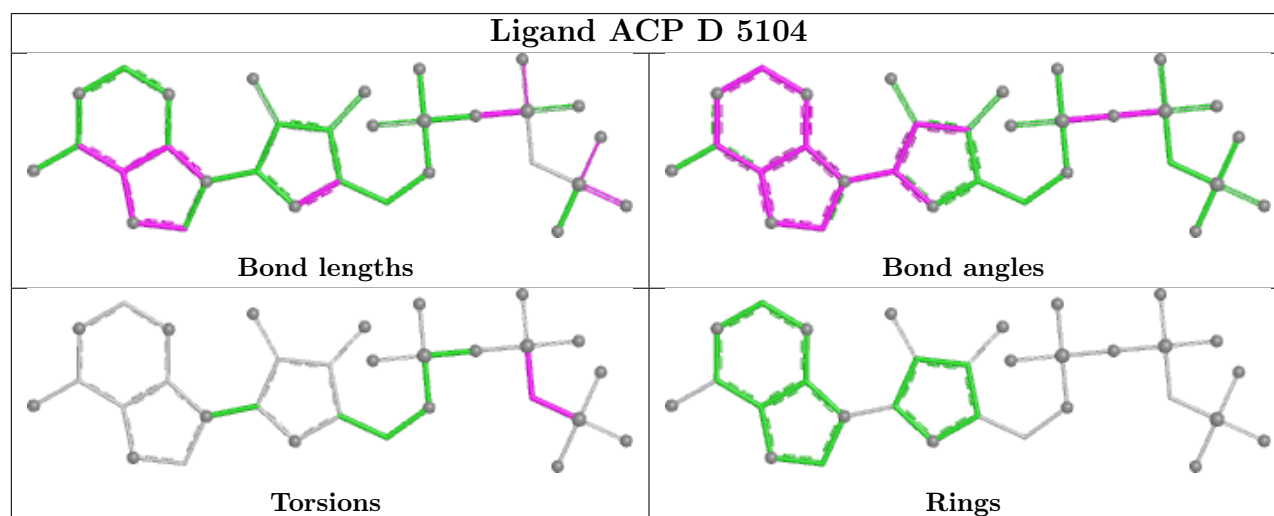
Mol	Chain	Res	Type	Atoms
5	A	5106	POV	C311-C310-C39-C38
5	D	5105	POV	C311-C310-C39-C38
5	C	5106	POV	C311-C310-C39-C38
5	C	5106	POV	C33-C34-C35-C36
5	A	5106	POV	C33-C34-C35-C36
5	D	5105	POV	C33-C34-C35-C36
5	B	5106	POV	C33-C34-C35-C36
4	A	5104	ACP	PG-C3B-PB-O2B
4	C	5104	ACP	PG-C3B-PB-O2B
4	D	5104	ACP	PG-C3B-PB-O2B
4	B	5104	ACP	PG-C3B-PB-O2B
5	A	5106	POV	C1-O11-P-O14
5	A	5106	POV	C11-O12-P-O11
5	C	5106	POV	C1-O11-P-O14
5	C	5106	POV	C11-O12-P-O11
5	D	5105	POV	C1-O11-P-O14
5	D	5105	POV	C11-O12-P-O11
5	B	5106	POV	C1-O11-P-O14
5	B	5106	POV	C11-O12-P-O11
5	A	5106	POV	C3-C2-O21-C21
5	C	5106	POV	C3-C2-O21-C21
5	D	5105	POV	C3-C2-O21-C21
5	B	5106	POV	C3-C2-O21-C21
5	A	5106	POV	O11-C1-C2-C3
5	C	5106	POV	O11-C1-C2-C3
5	D	5105	POV	O11-C1-C2-C3
5	B	5106	POV	O11-C1-C2-C3
5	C	5106	POV	C27-C28-C29-C210
5	B	5106	POV	C27-C28-C29-C210
5	A	5106	POV	C27-C28-C29-C210
5	D	5105	POV	C27-C28-C29-C210
5	B	5106	POV	C32-C33-C34-C35
5	C	5106	POV	C32-C33-C34-C35
5	D	5105	POV	C32-C33-C34-C35
5	A	5106	POV	C32-C33-C34-C35
5	A	5106	POV	O31-C31-C32-C33
5	C	5106	POV	O31-C31-C32-C33
5	D	5105	POV	O31-C31-C32-C33
5	B	5106	POV	O31-C31-C32-C33

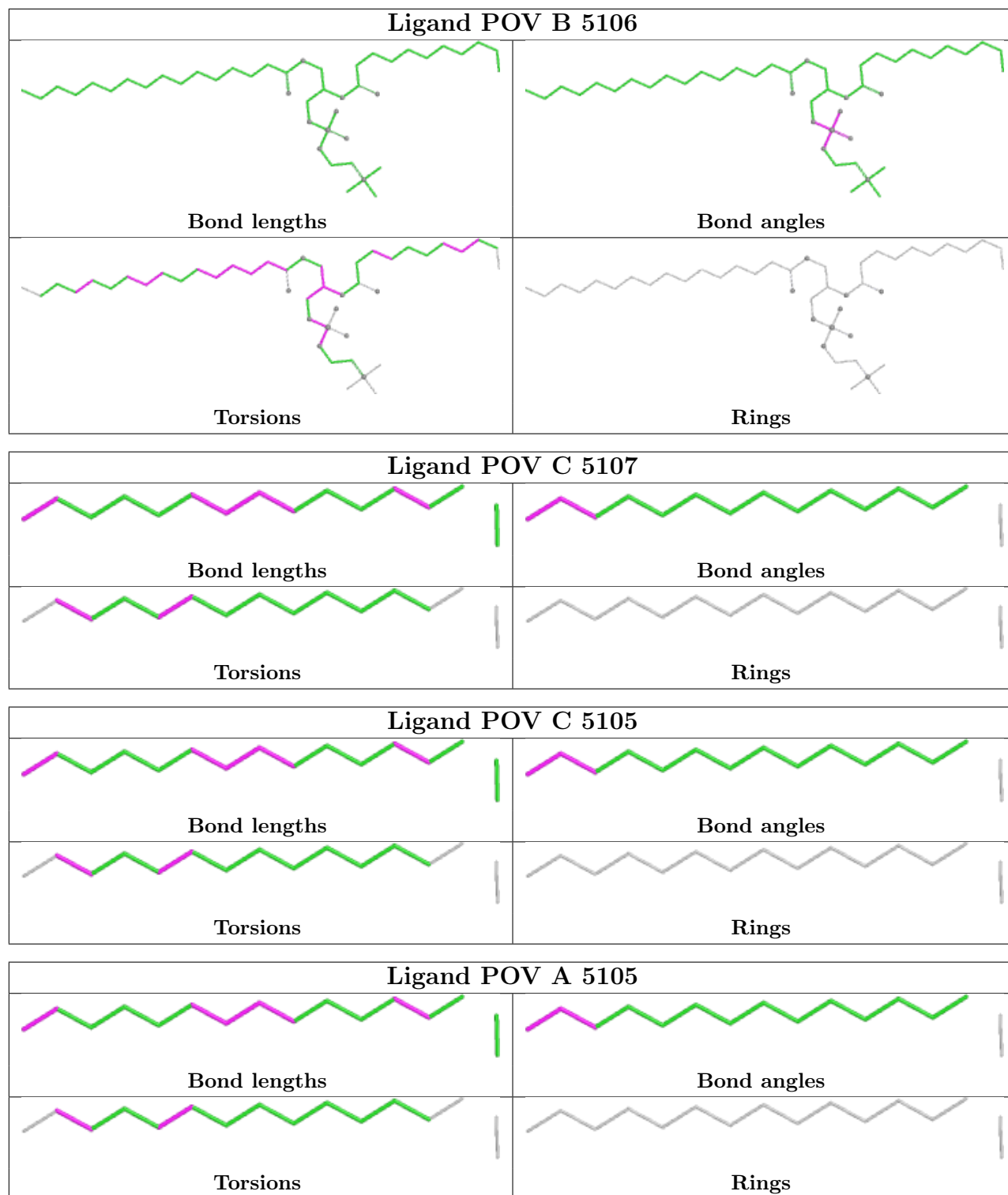
There are no ring outliers.

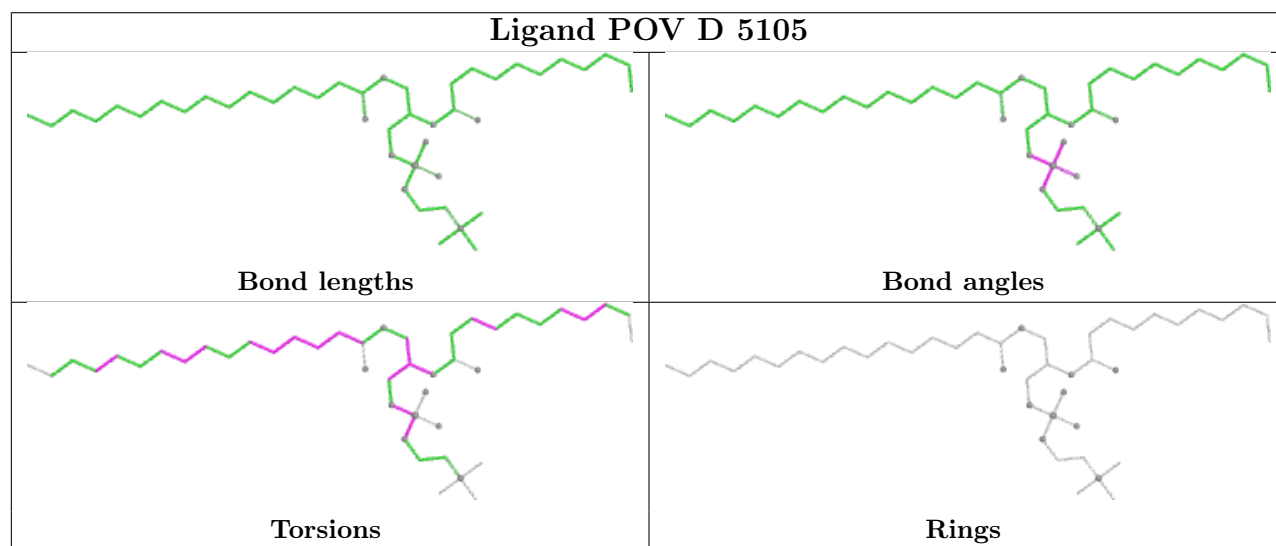
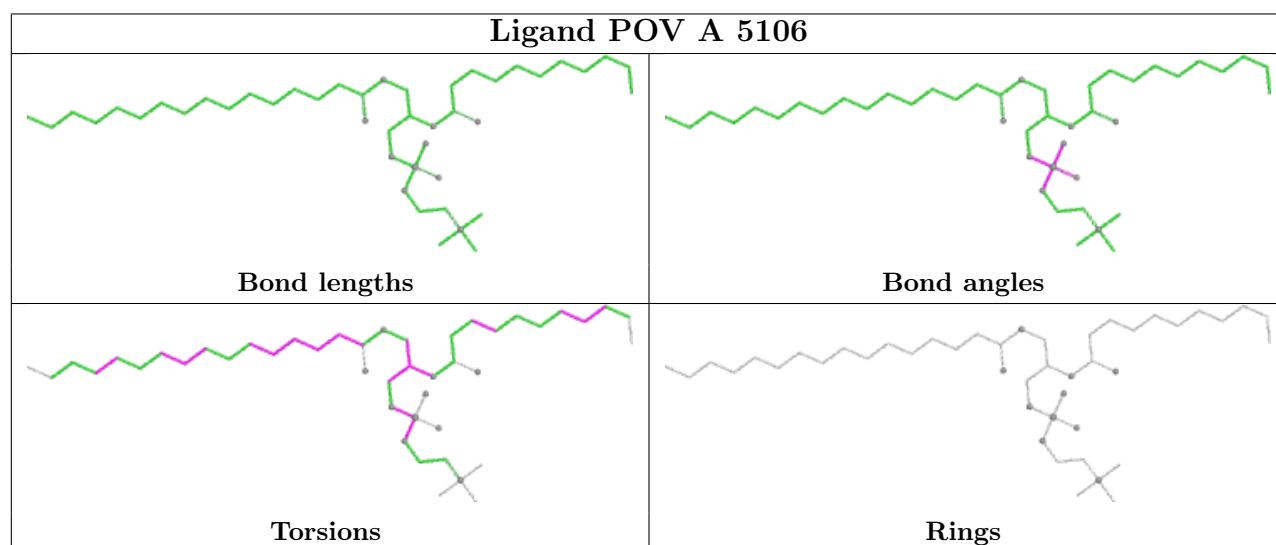
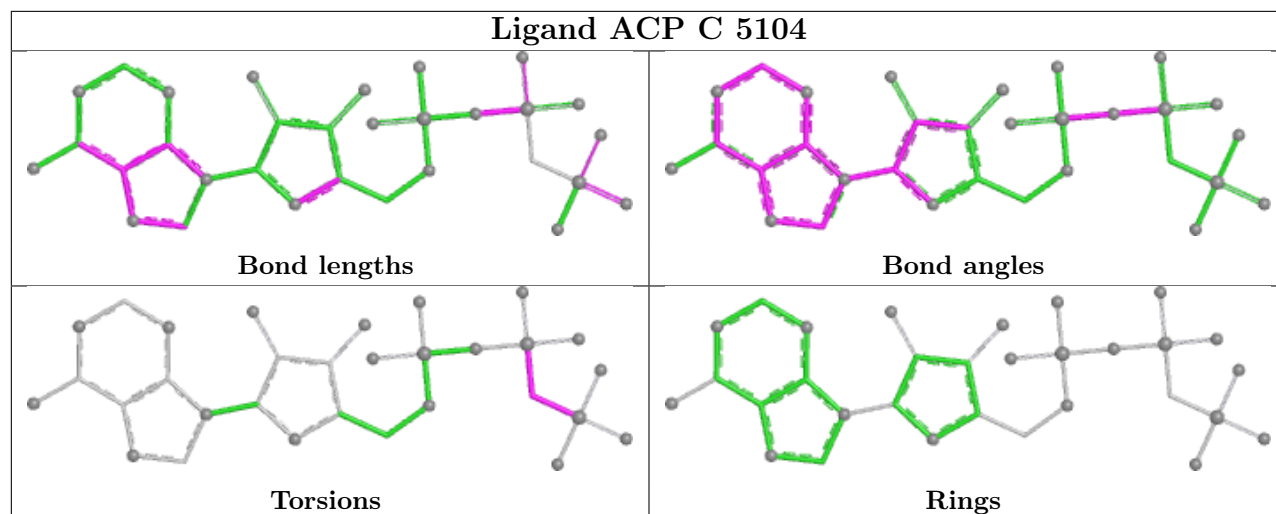
12 monomers are involved in 75 short contacts:

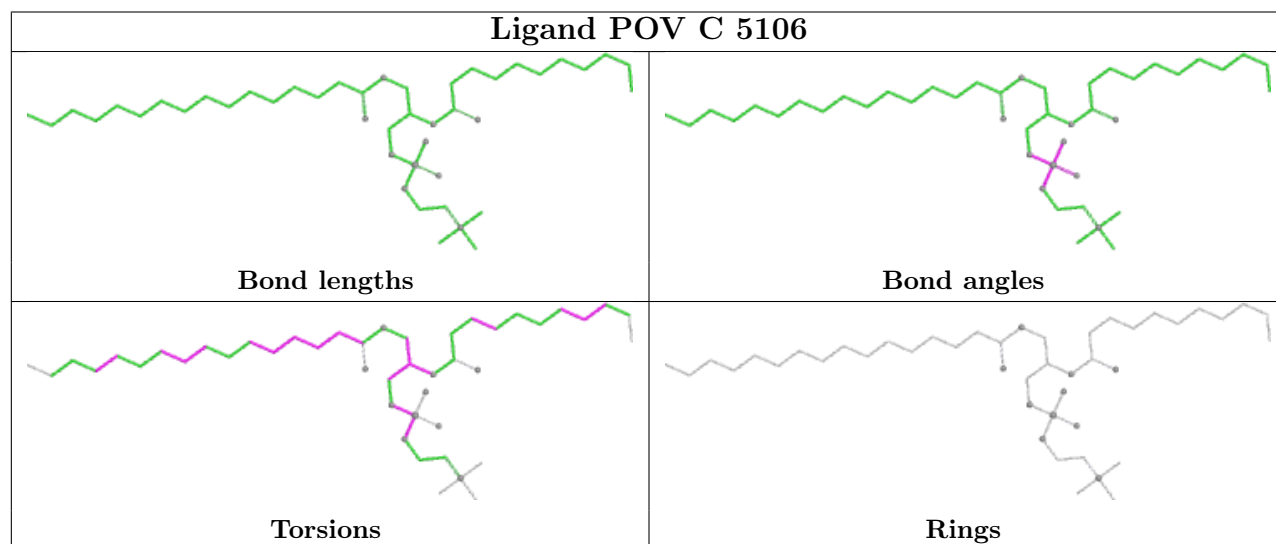
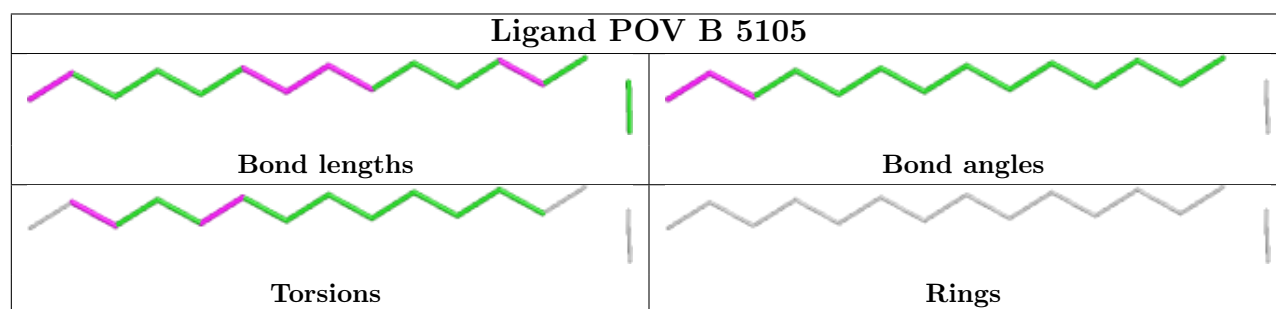
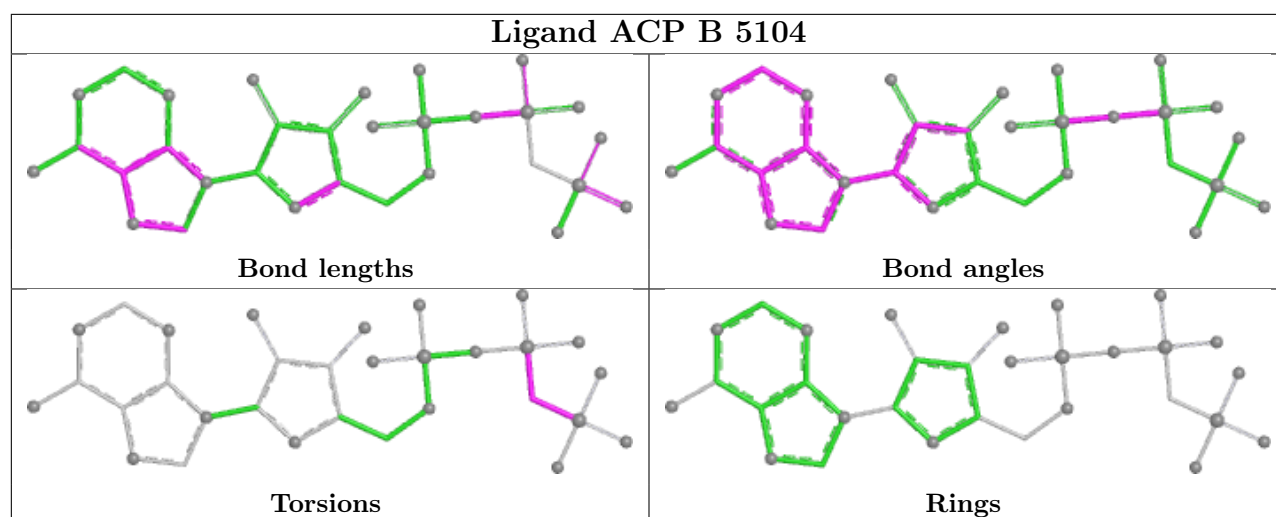
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5104	ACP	1	0
5	B	5106	POV	17	0
5	C	5107	POV	4	0
5	C	5105	POV	2	0
5	A	5105	POV	2	0
4	C	5104	ACP	2	0
5	A	5106	POV	16	0
5	D	5105	POV	16	0
4	B	5104	ACP	1	0
5	B	5105	POV	2	0
5	C	5106	POV	11	0
4	A	5104	ACP	1	0

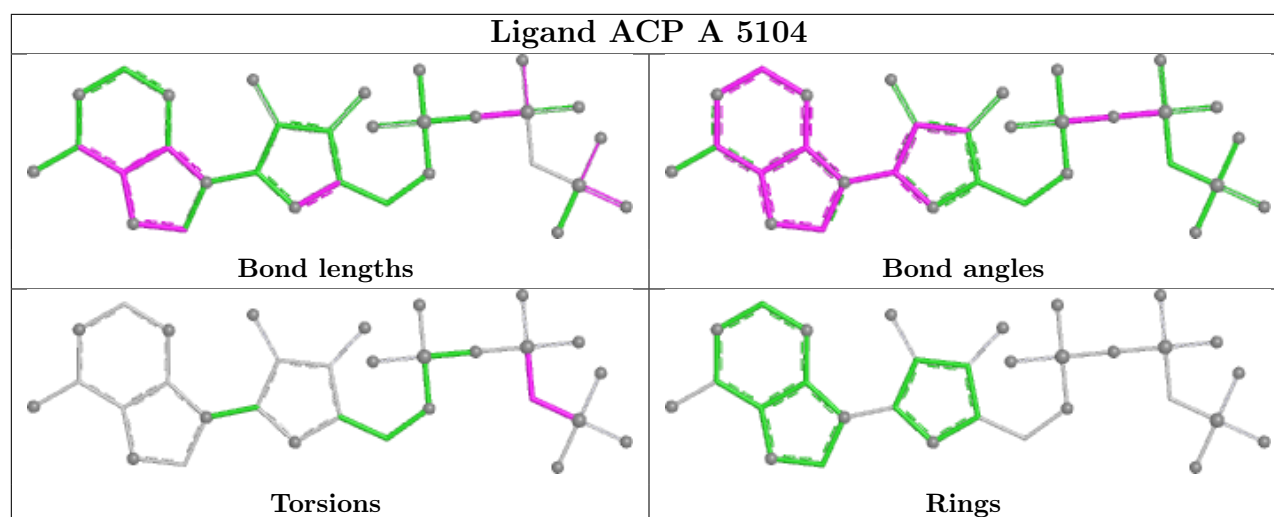
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	7
1	D	7
1	B	7
1	A	7

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	3122:UNK	C	3123:UNK	N	14.33
1	D	3122:UNK	C	3123:UNK	N	14.33
1	B	3122:UNK	C	3123:UNK	N	14.33
1	A	3122:UNK	C	3123:UNK	N	14.32
1	A	3221:UNK	C	3222:UNK	N	13.70
1	C	3221:UNK	C	3222:UNK	N	13.70
1	D	3221:UNK	C	3222:UNK	N	13.70
1	B	3221:UNK	C	3222:UNK	N	13.70
1	C	3510:UNK	C	3511:UNK	N	13.52
1	D	3510:UNK	C	3511:UNK	N	13.52
1	B	3510:UNK	C	3511:UNK	N	13.52
1	A	3510:UNK	C	3511:UNK	N	13.51
1	B	3288:UNK	C	3289:UNK	N	13.29

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3288:UNK	C	3289:UNK	N	13.28
1	C	3288:UNK	C	3289:UNK	N	13.28
1	D	3288:UNK	C	3289:UNK	N	13.28
1	A	3191:UNK	C	3192:UNK	N	8.26
1	C	3191:UNK	C	3192:UNK	N	8.26
1	B	3191:UNK	C	3192:UNK	N	8.26
1	D	3191:UNK	C	3192:UNK	N	8.25
1	C	3302:UNK	C	3303:UNK	N	8.15
1	D	3302:UNK	C	3303:UNK	N	8.15
1	A	3302:UNK	C	3303:UNK	N	8.14
1	B	3302:UNK	C	3303:UNK	N	8.14
1	A	1297:UNK	C	1298:UNK	N	7.59
1	C	1297:UNK	C	1298:UNK	N	7.59
1	D	1297:UNK	C	1298:UNK	N	7.59
1	B	1297:UNK	C	1298:UNK	N	7.59

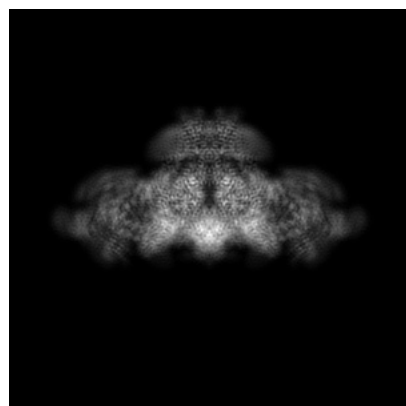
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25828. These allow visual inspection of the internal detail of the map and identification of artifacts.

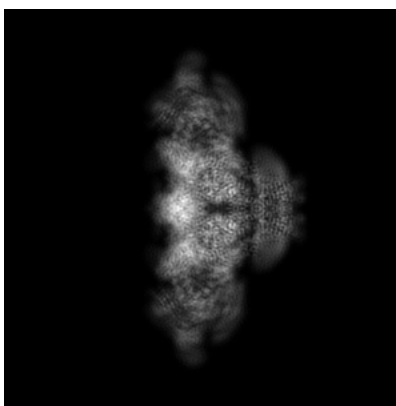
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

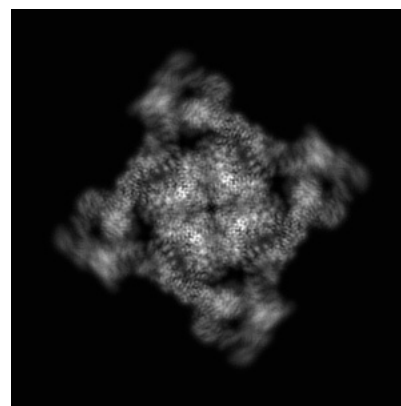
6.1.1 Primary map



X

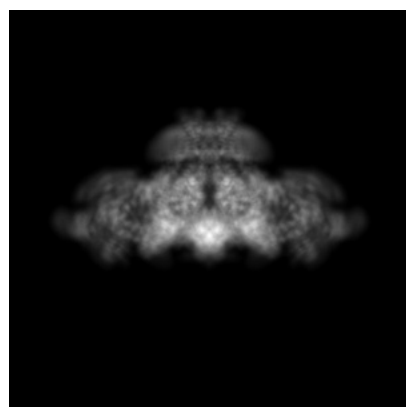


Y

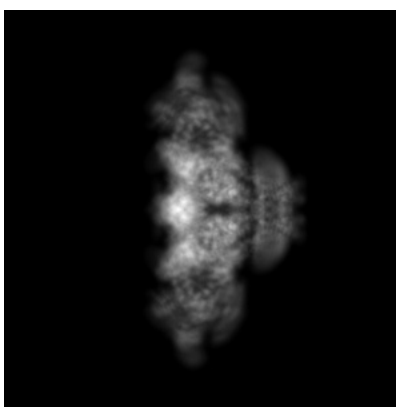


Z

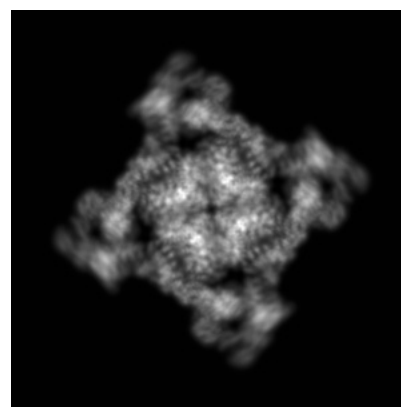
6.1.2 Raw map



X



Y

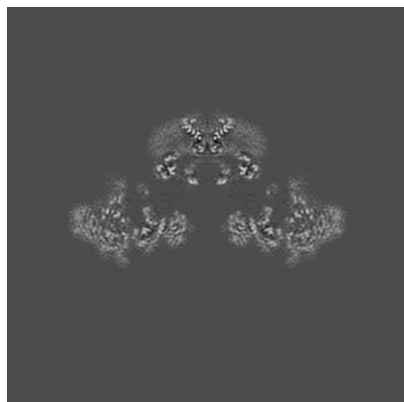


Z

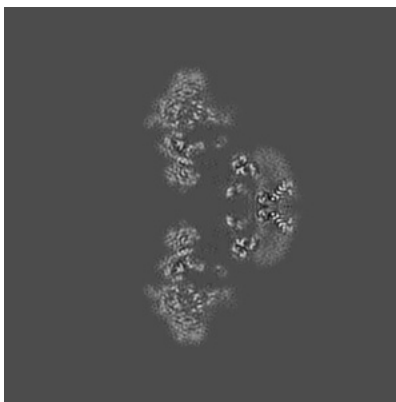
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

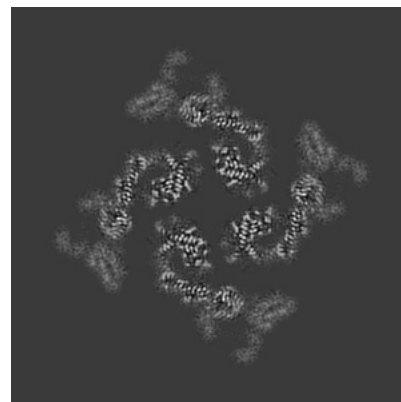
6.2.1 Primary map



X Index: 216

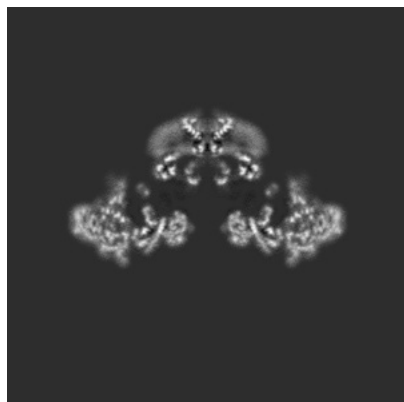


Y Index: 216

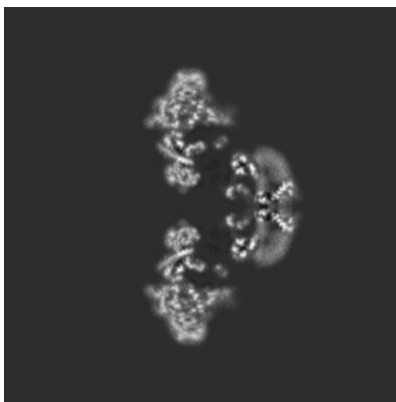


Z Index: 216

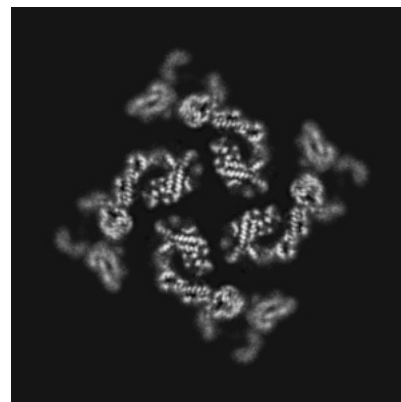
6.2.2 Raw map



X Index: 216



Y Index: 216

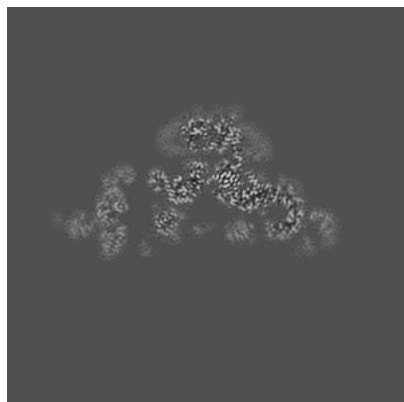


Z Index: 216

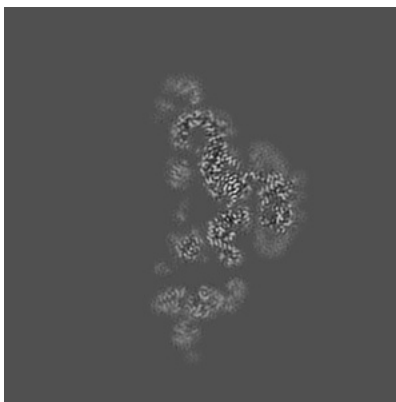
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

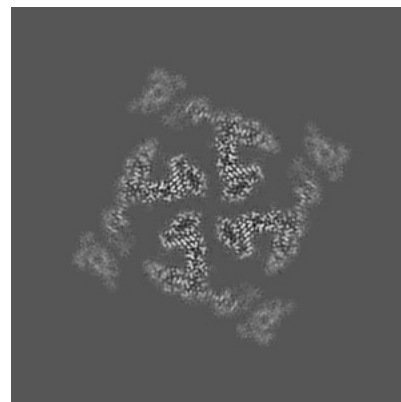
6.3.1 Primary map



X Index: 233

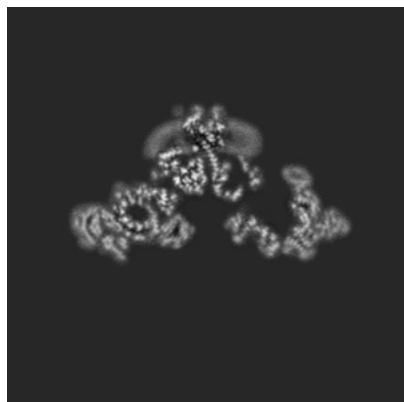


Y Index: 199

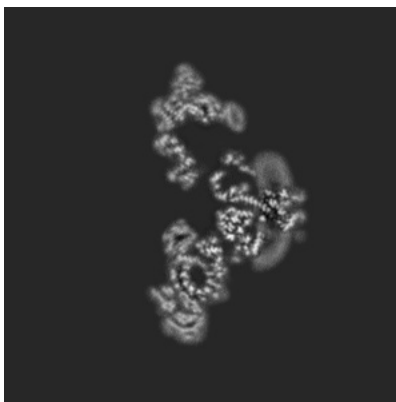


Z Index: 228

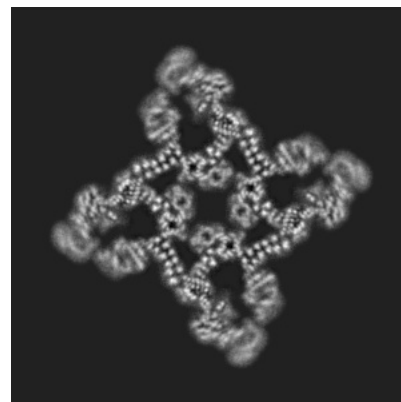
6.3.2 Raw map



X Index: 207



Y Index: 225

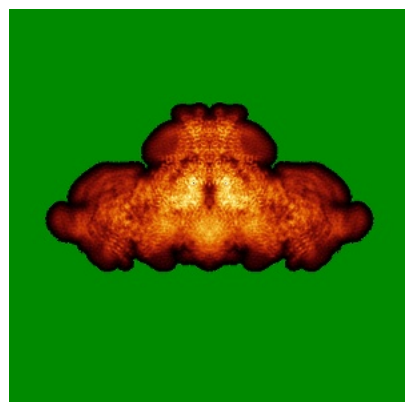


Z Index: 198

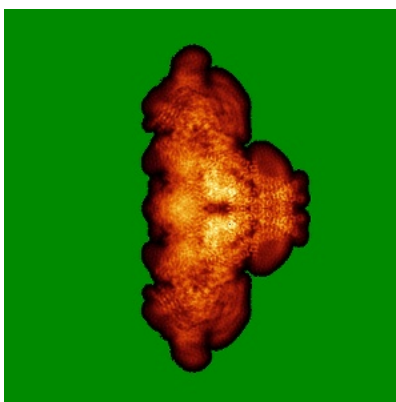
The images above show the largest variance slices of the map in three orthogonal directions.

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

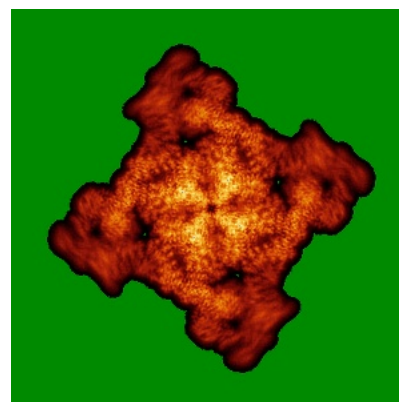
6.4.1 Primary map



X

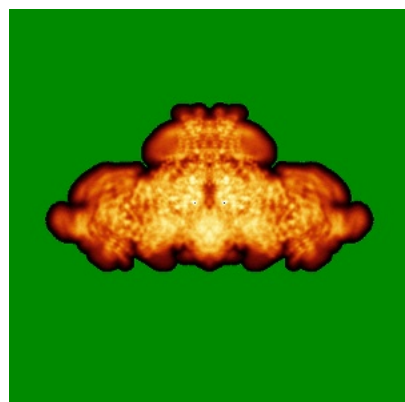


Y

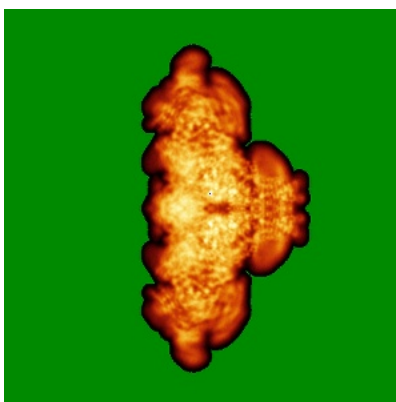


Z

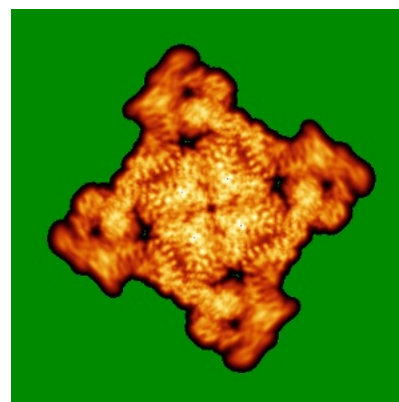
6.4.2 Raw map



X



Y

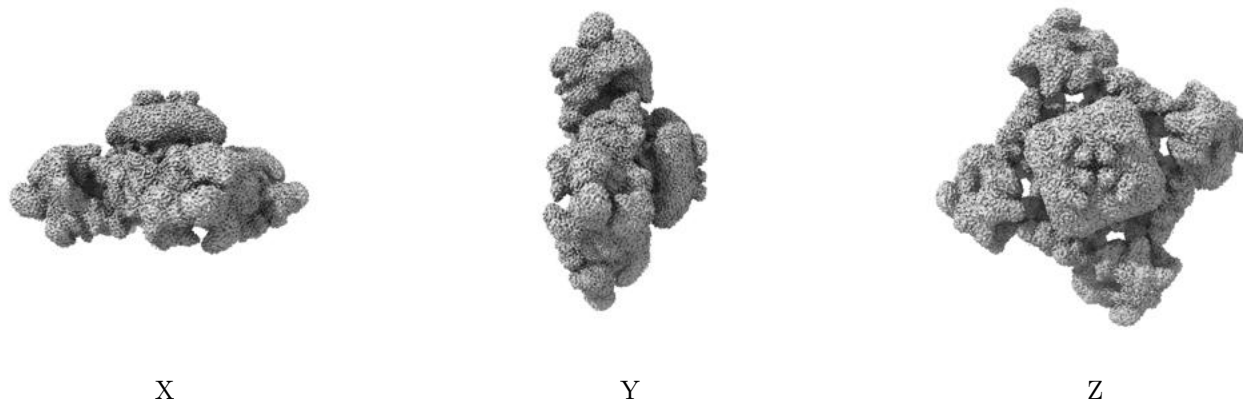


Z

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.

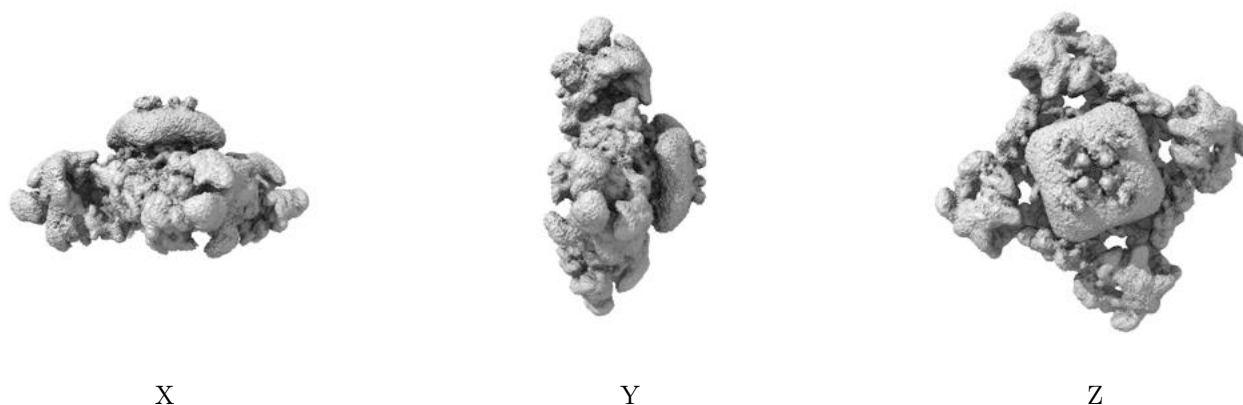
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

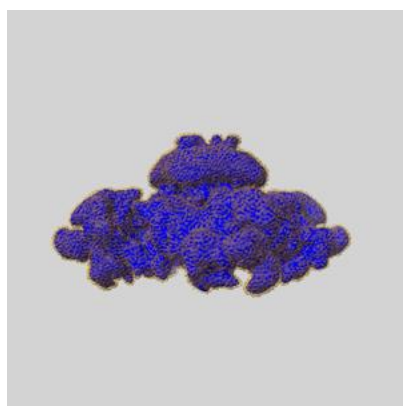
6.6 Mask visualisation [i](#)

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

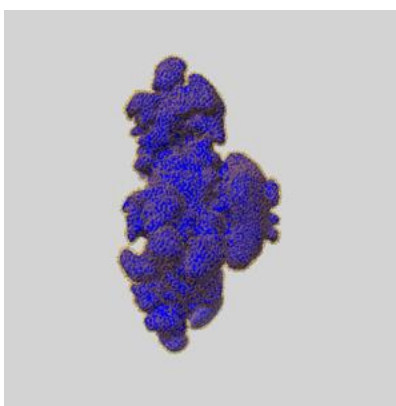
A mask typically either:

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

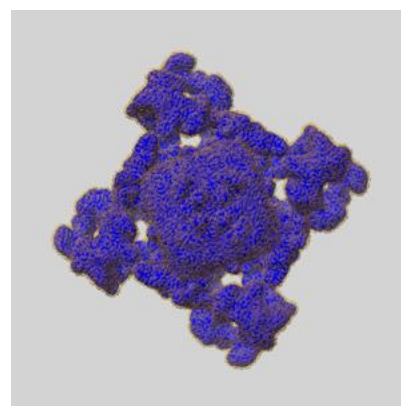
6.6.1 emd_25828_msk_1.map [i](#)



X



Y

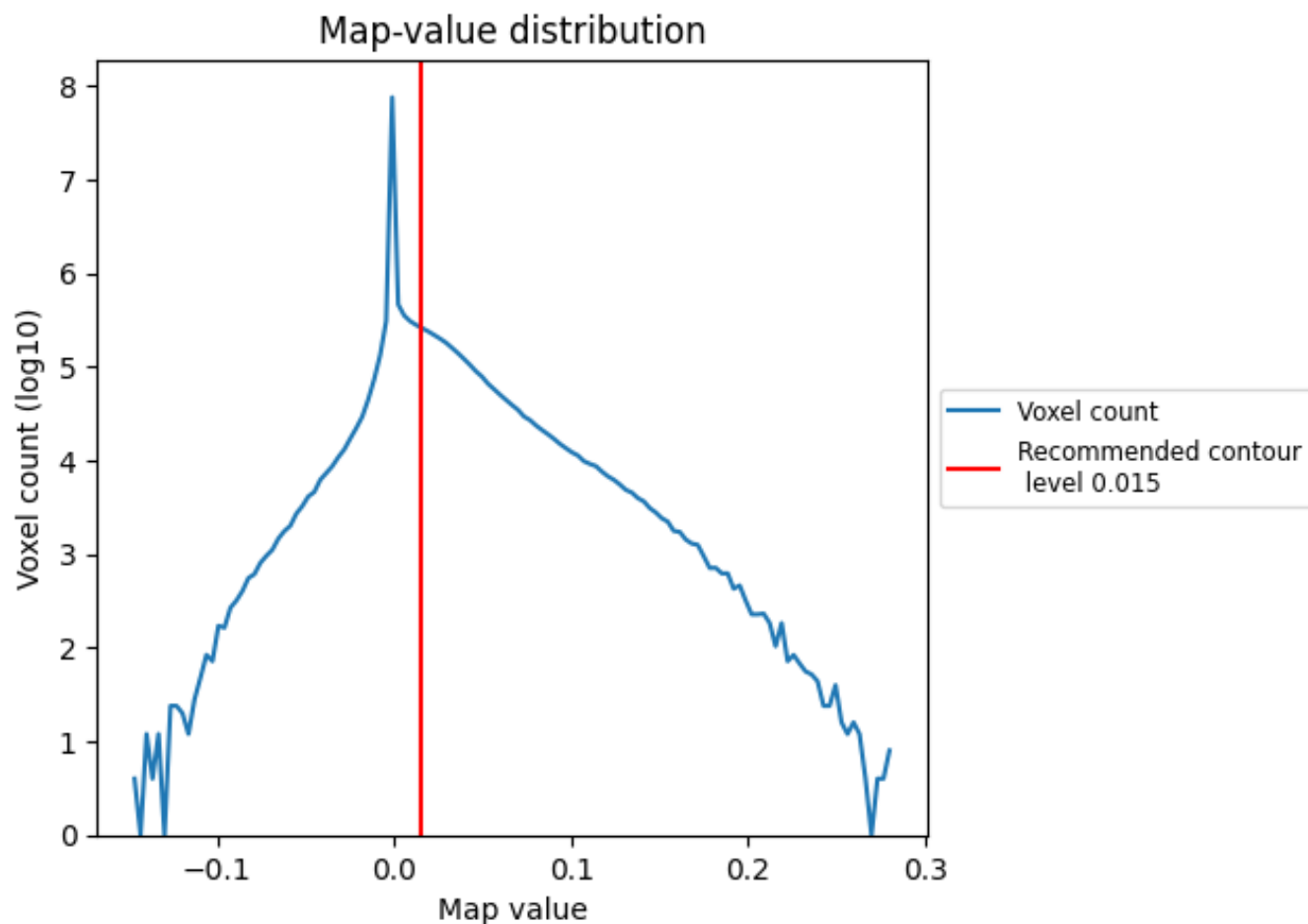


Z

7 Map analysis [i](#)

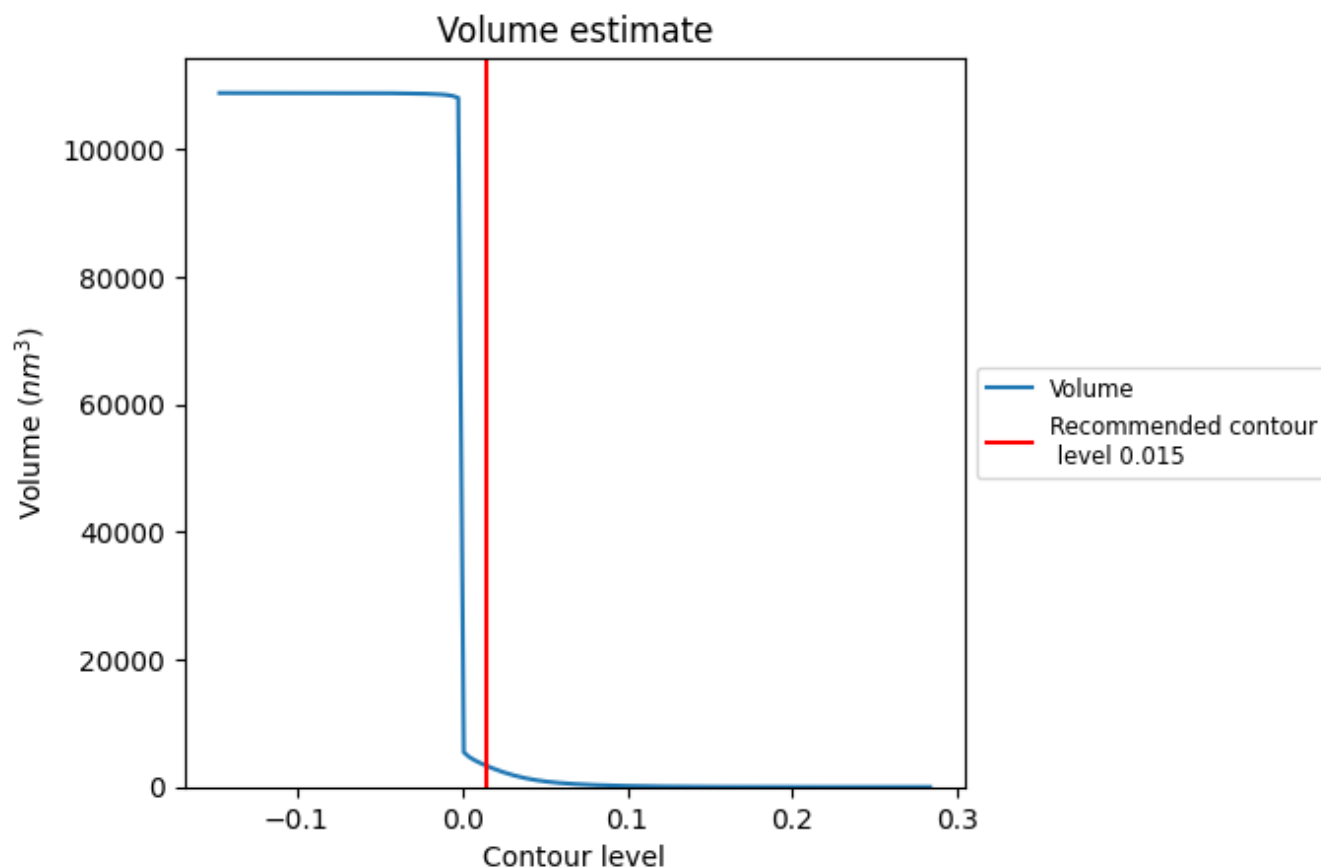
This section contains the results of statistical analysis of the map.

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.

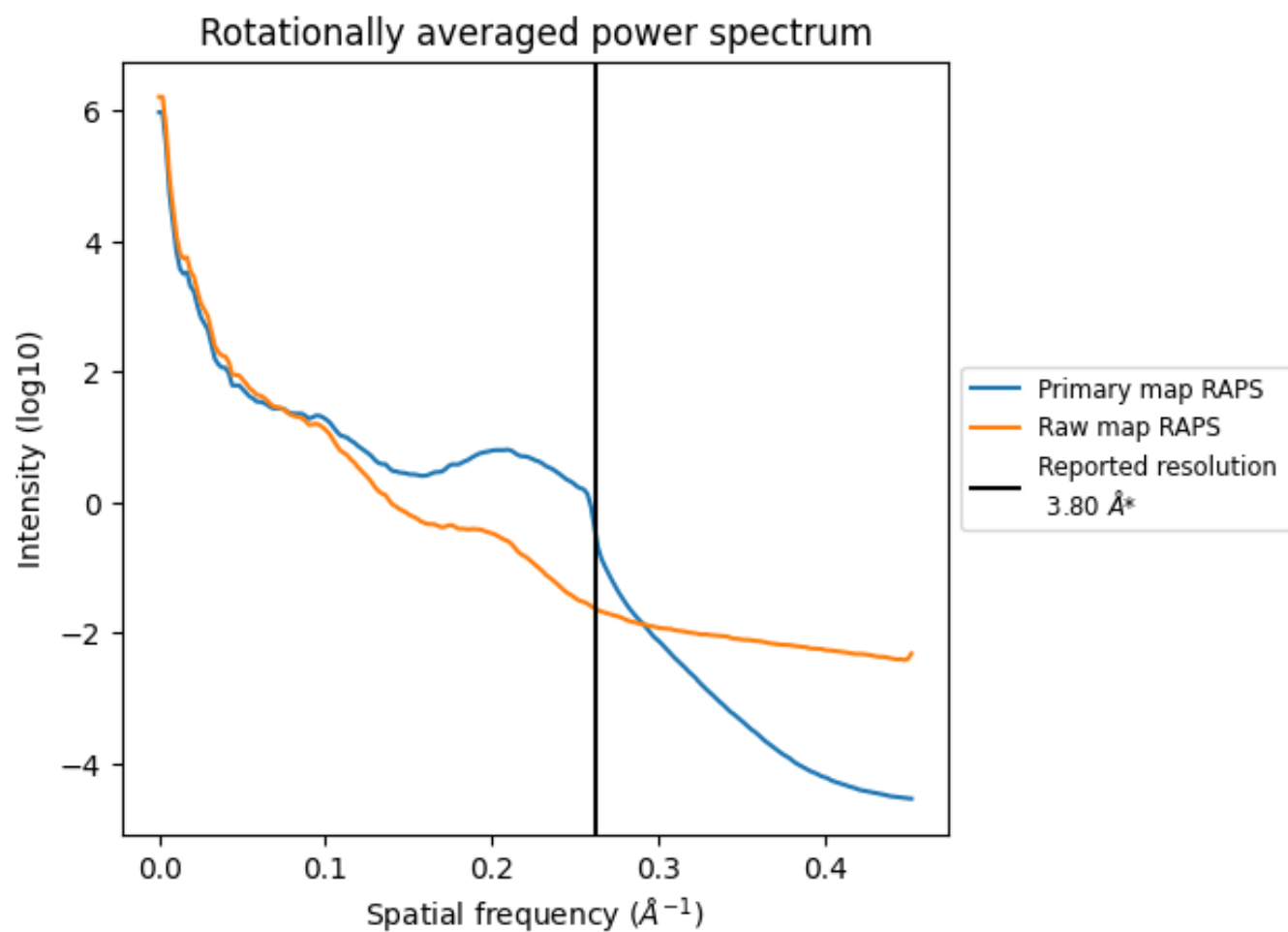
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3290 nm³; this corresponds to an approximate mass of 2972 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

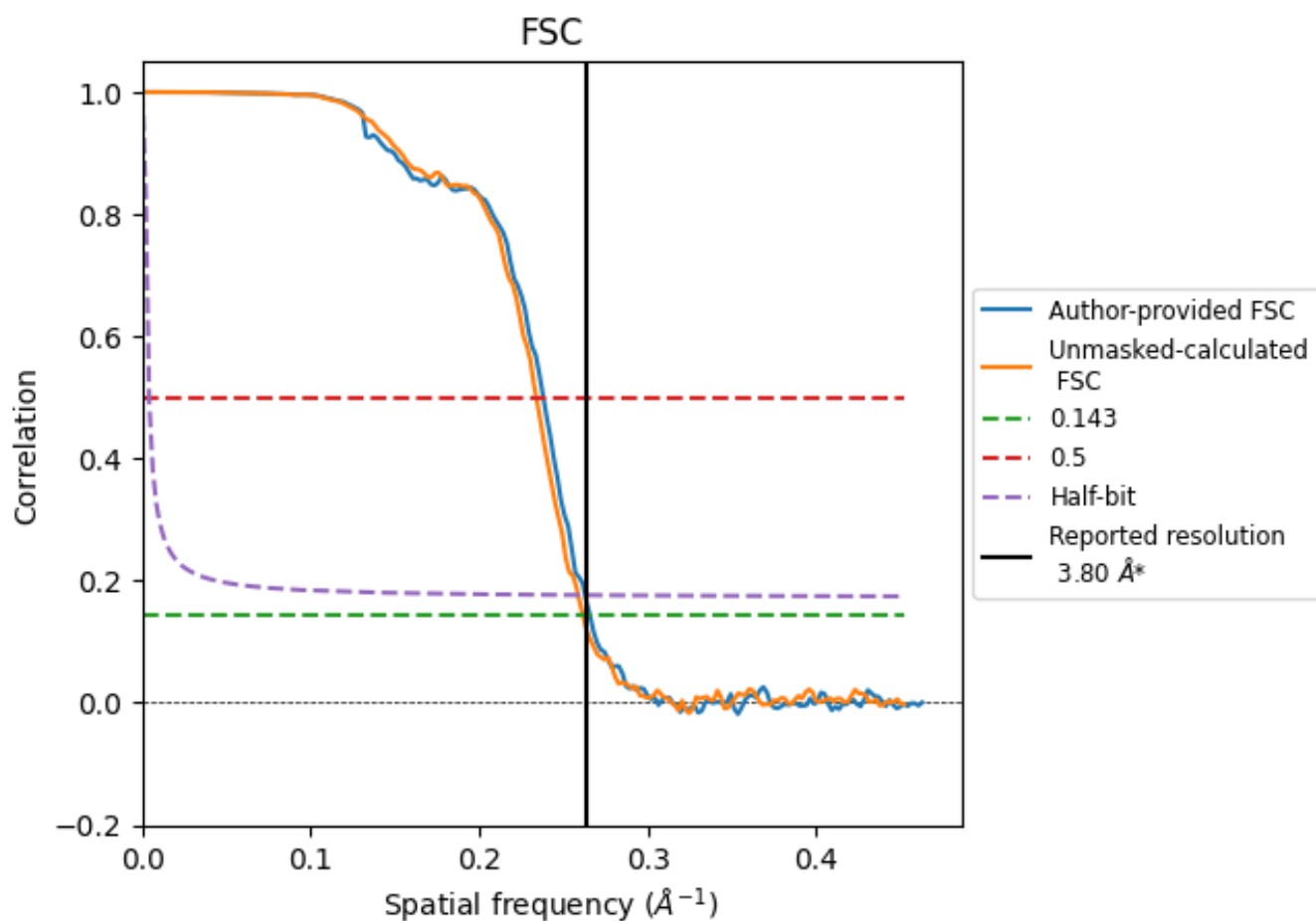


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

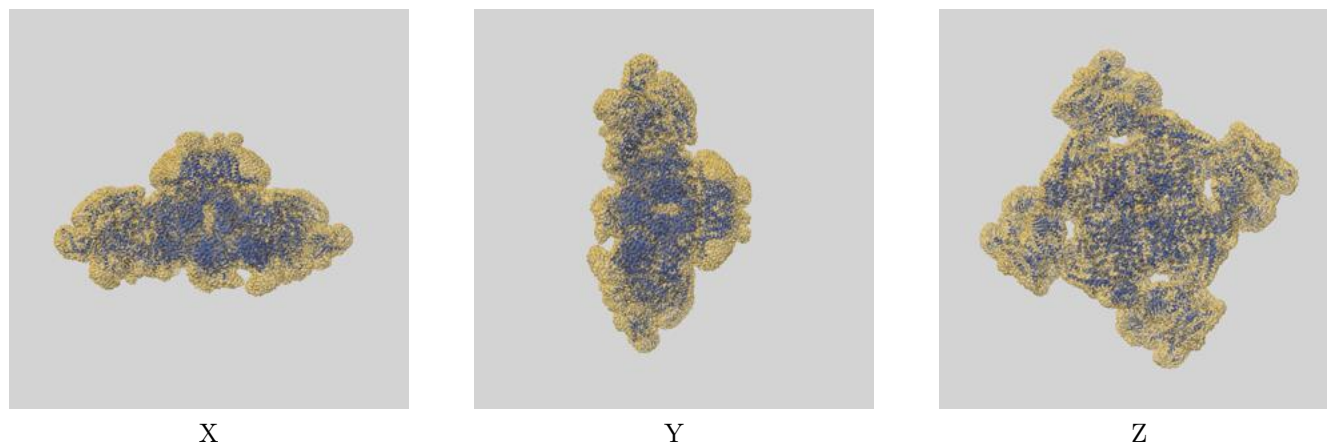
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.76	4.20	3.80
Unmasked-calculated*	3.82	4.28	3.87

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

9 Map-model fit [i](#)

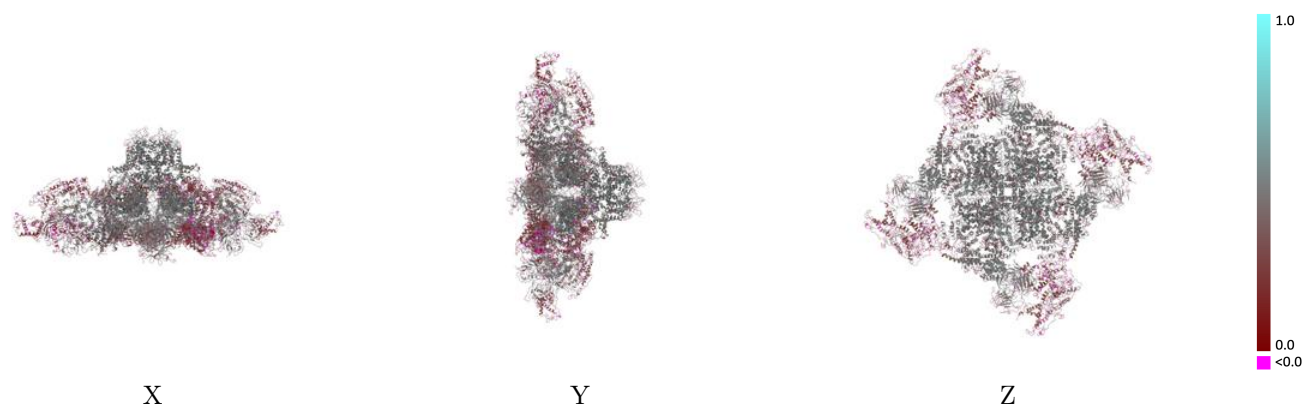
This section contains information regarding the fit between EMDB map EMD-25828 and PDB model 7TDG. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



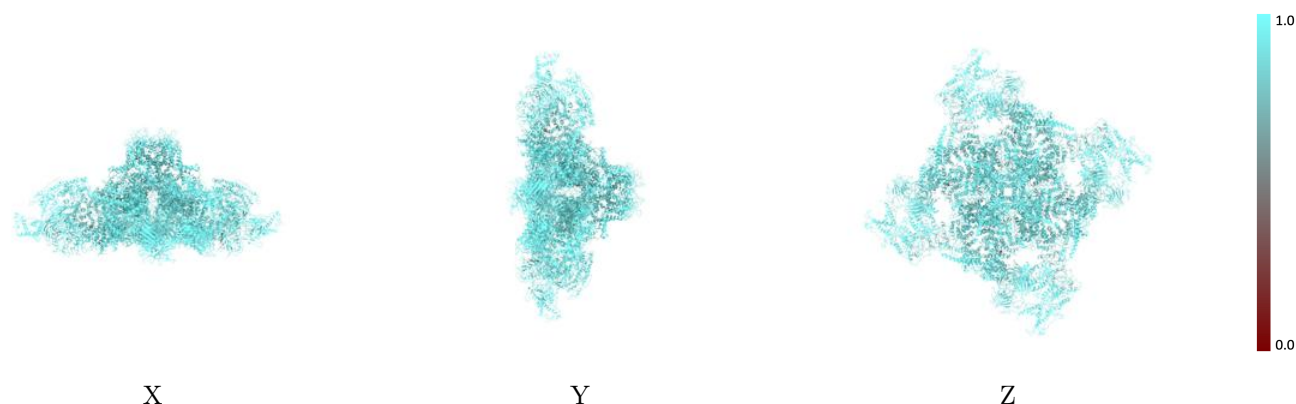
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



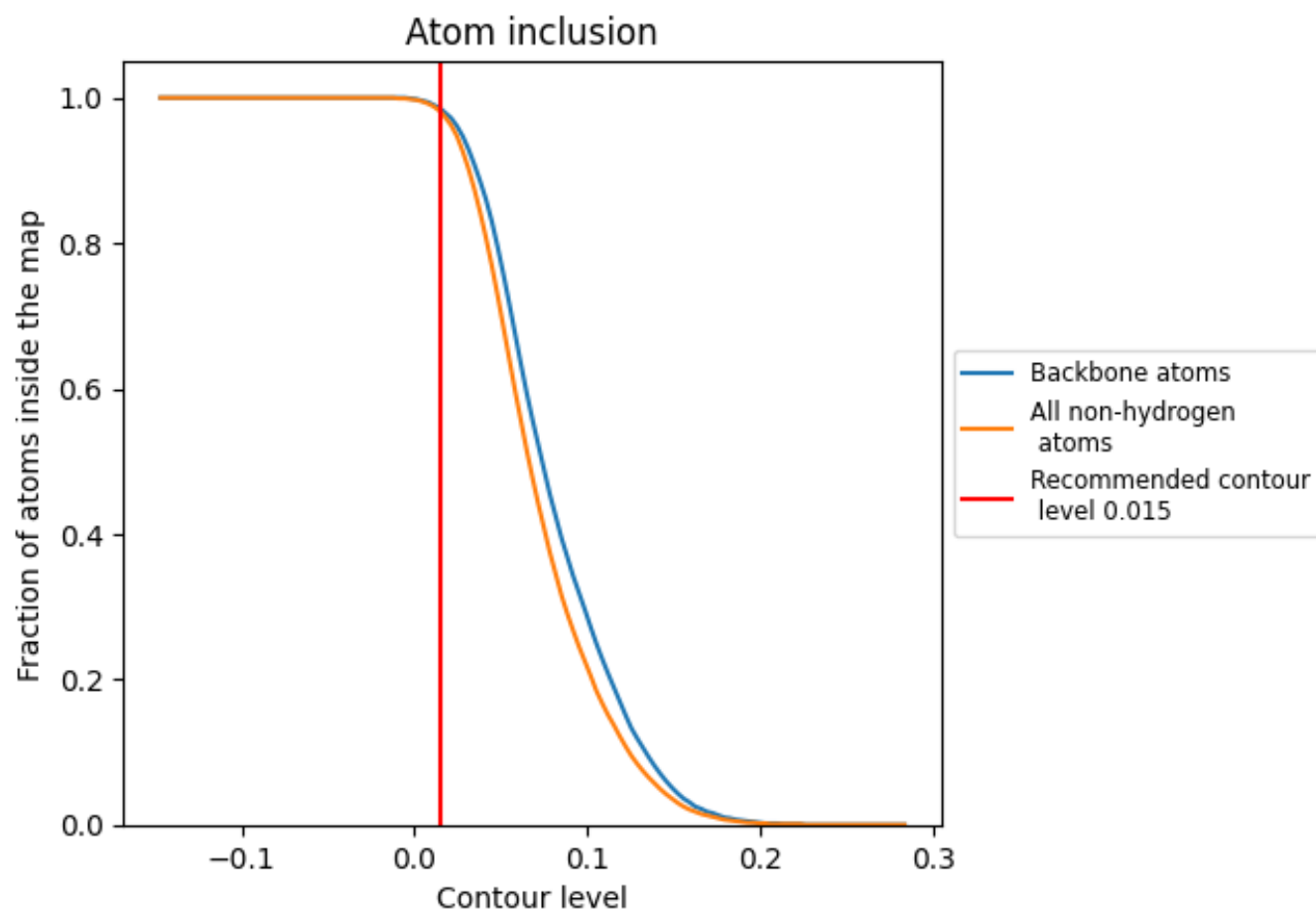
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9810	0.3860
A	0.9810	0.3860
B	0.9810	0.3860
C	0.9810	0.3860
D	0.9810	0.3850

