



## Full wwPDB EM Validation Report ⓘ

Sep 29, 2025 – 11:59 AM EDT

PDB ID : 9NMQ / pdb\_00009nmq  
EMDB ID : EMD-49537  
Title : Structure of mouse RyR1 with simvastatin (Ca<sup>2+</sup>/CFF/ATP dataset; closed pore)  
Authors : Weninger, G.; Marks, A.R.  
Deposited on : 2025-03-04  
Resolution : 2.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

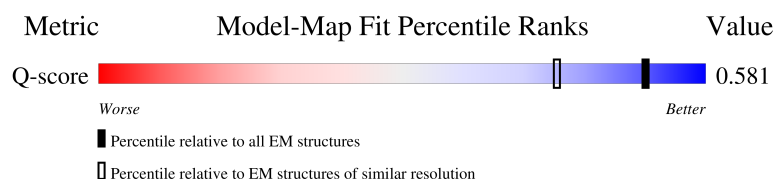
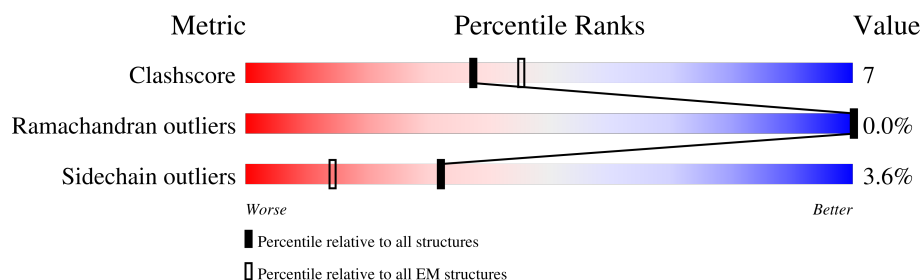
EMDB validation analysis : 0.0.1.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB 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) : 2.46

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.60 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	8728 ( 2.10 - 3.10 )

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

Mol	Chain	Length	Quality of chain
1	A	5035	<div> <div>8%</div> <div>75%</div> <div>10%</div> <div>13%</div> </div>
1	B	5035	<div> <div>8%</div> <div>75%</div> <div>11%</div> <div>13%</div> </div>
1	C	5035	<div> <div>8%</div> <div>75%</div> <div>10%</div> <div>13%</div> </div>
1	D	5035	<div> <div>8%</div> <div>75%</div> <div>10%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	108	 92% 7% •
2	F	108	 92% 7% •
2	G	108	 92% 7% •
2	H	108	 92% 7% •

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 143492 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		
1	B	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		
1	C	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		
1	D	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		

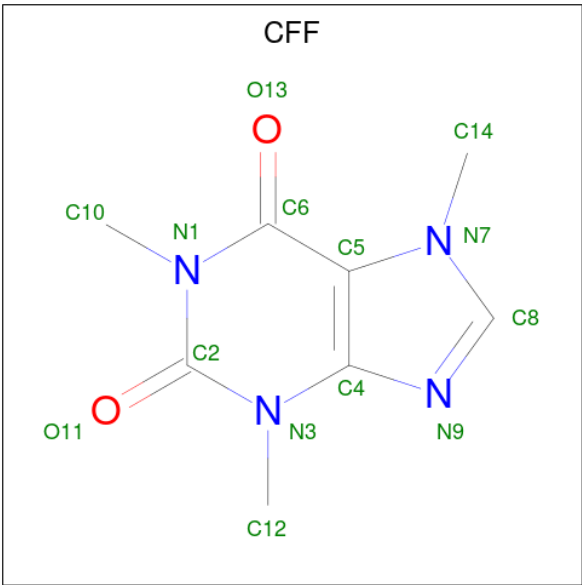
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			830	526	146	155	3		
2	F	107	Total	C	N	O	S	0	0
			830	526	146	155	3		
2	G	107	Total	C	N	O	S	0	0
			830	526	146	155	3		
2	H	107	Total	C	N	O	S	0	0
			830	526	146	155	3		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

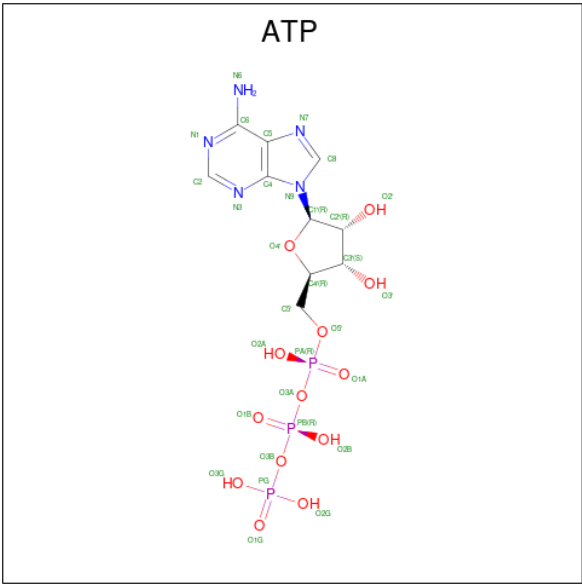
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	4	2	
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	C	1	Total	C	N	O	0
			14	8	4	2	
4	D	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

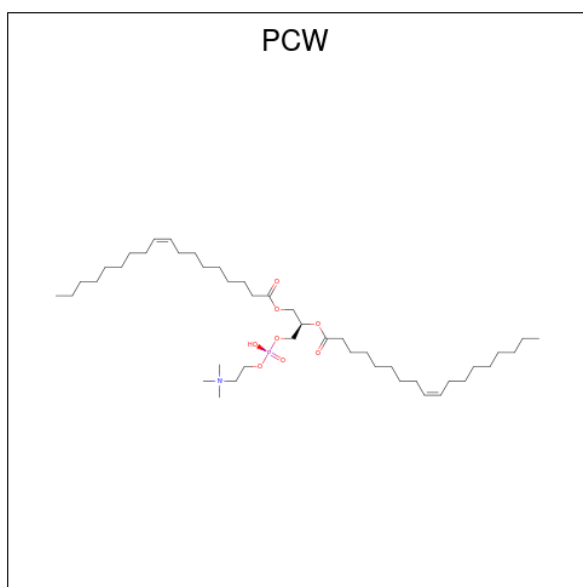


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

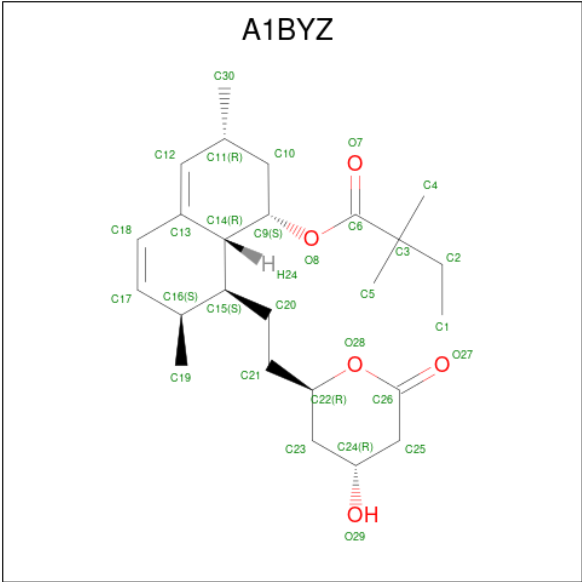
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	
6	D	1	Total	Ca	0
			1	1	

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C<sub>44</sub>H<sub>85</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	D	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 8 is (1S,3R,7S,8S,8aR)-8-{2-[(2R,4R)-4-hydroxy-6-oxooxan-2-yl]ethyl}-3,7-dimethyl-1,2,3,7,8,8a-hexahydronaphthalen-1-yl 2,2-dimethylbutanoate (CCD ID: A1BYZ) (formula: C<sub>25</sub>H<sub>38</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).

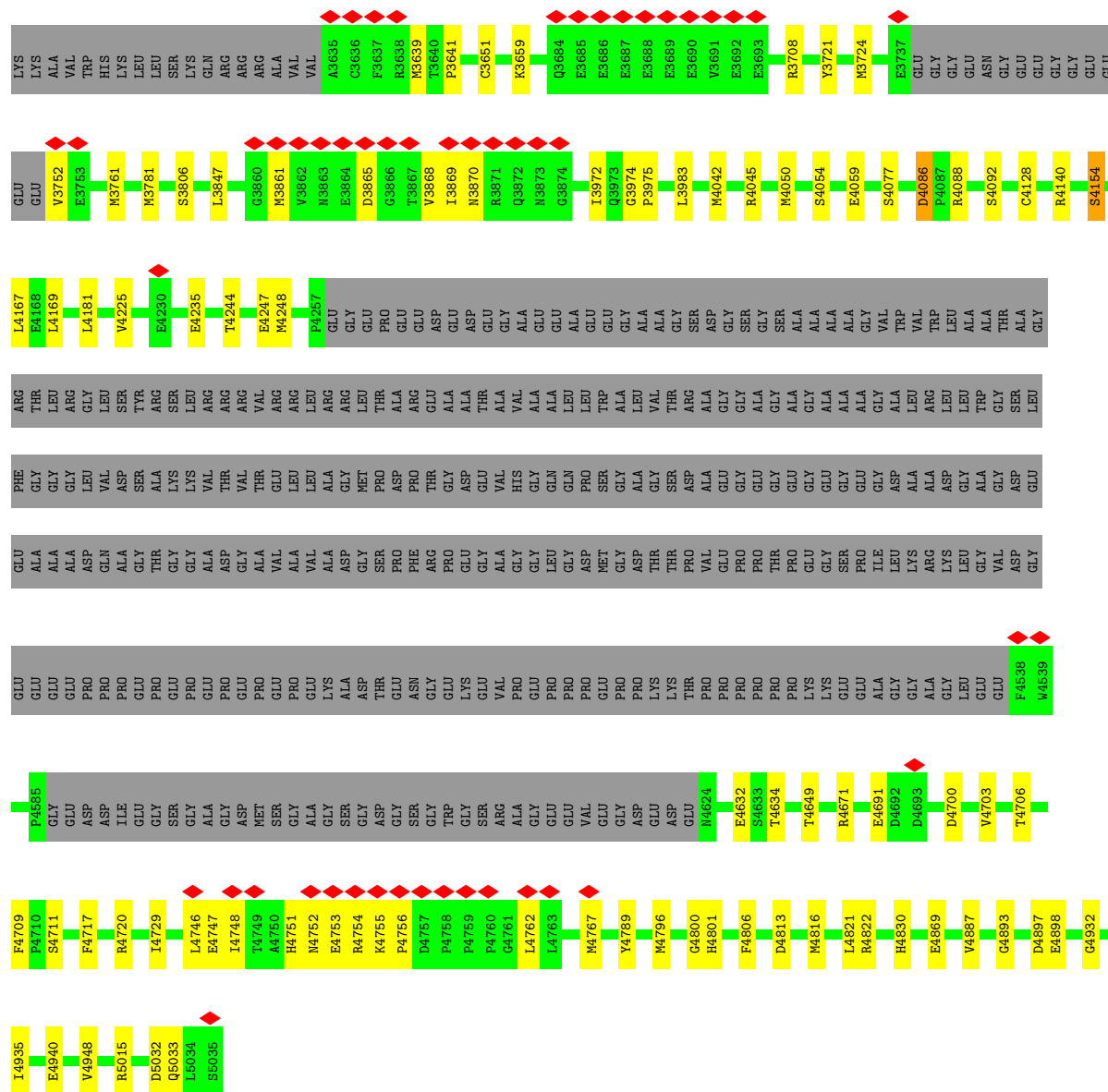


Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			30	25	5	
8	A	1	Total	C	O	0
			30	25	5	
8	B	1	Total	C	O	0
			30	25	5	
8	B	1	Total	C	O	0
			30	25	5	
8	C	1	Total	C	O	0
			30	25	5	
8	C	1	Total	C	O	0
			30	25	5	
8	D	1	Total	C	O	0
			30	25	5	
8	D	1	Total	C	O	0
			30	25	5	

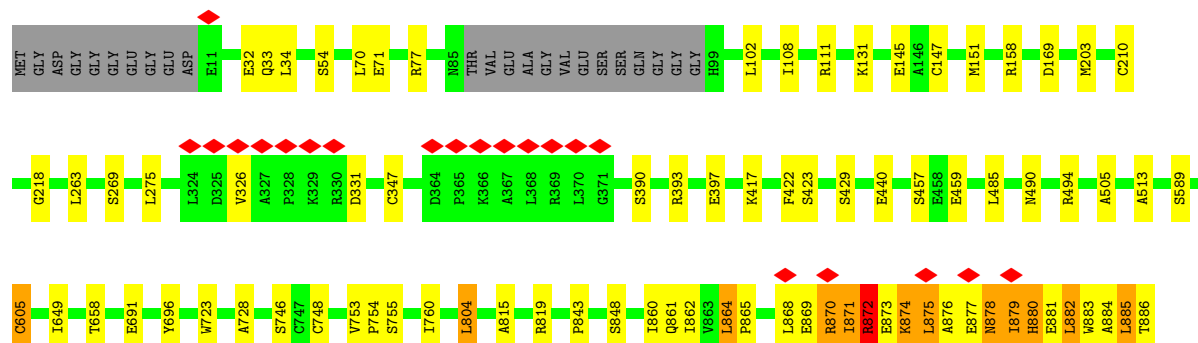
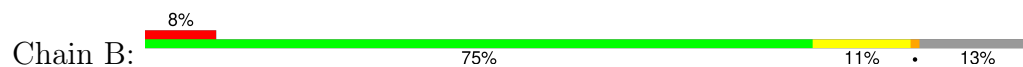


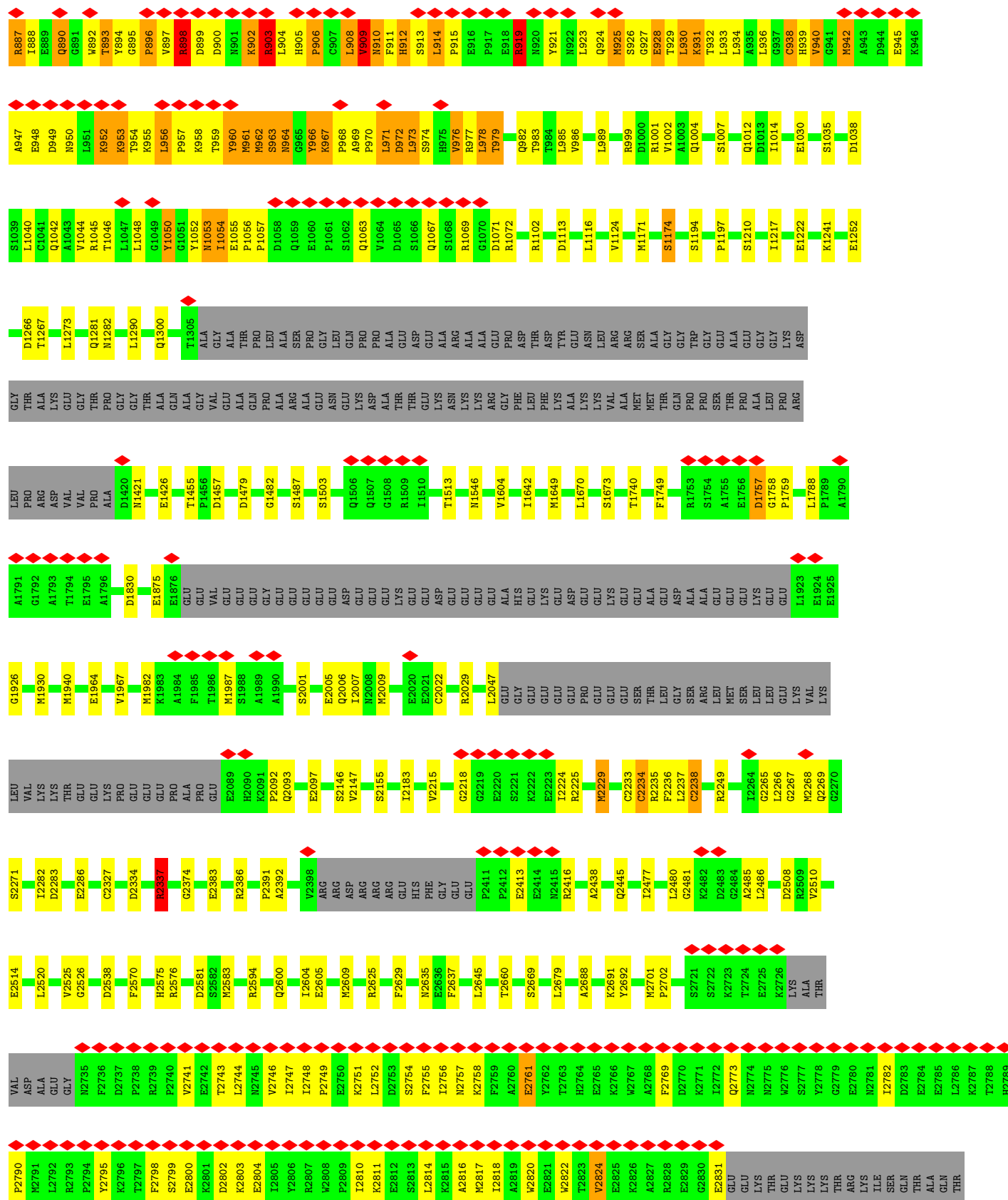




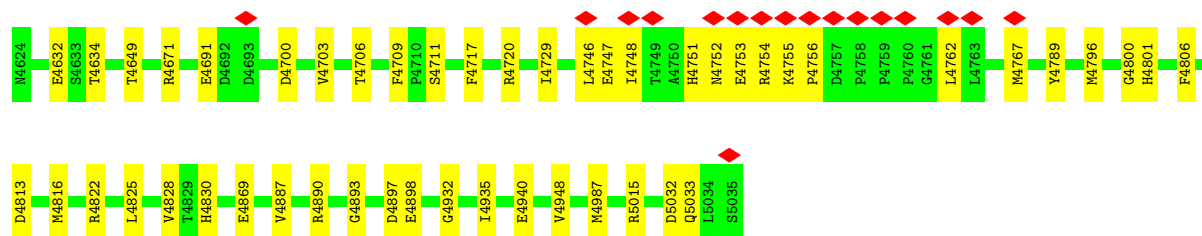


• Molecule 1: Ryanodine receptor 1

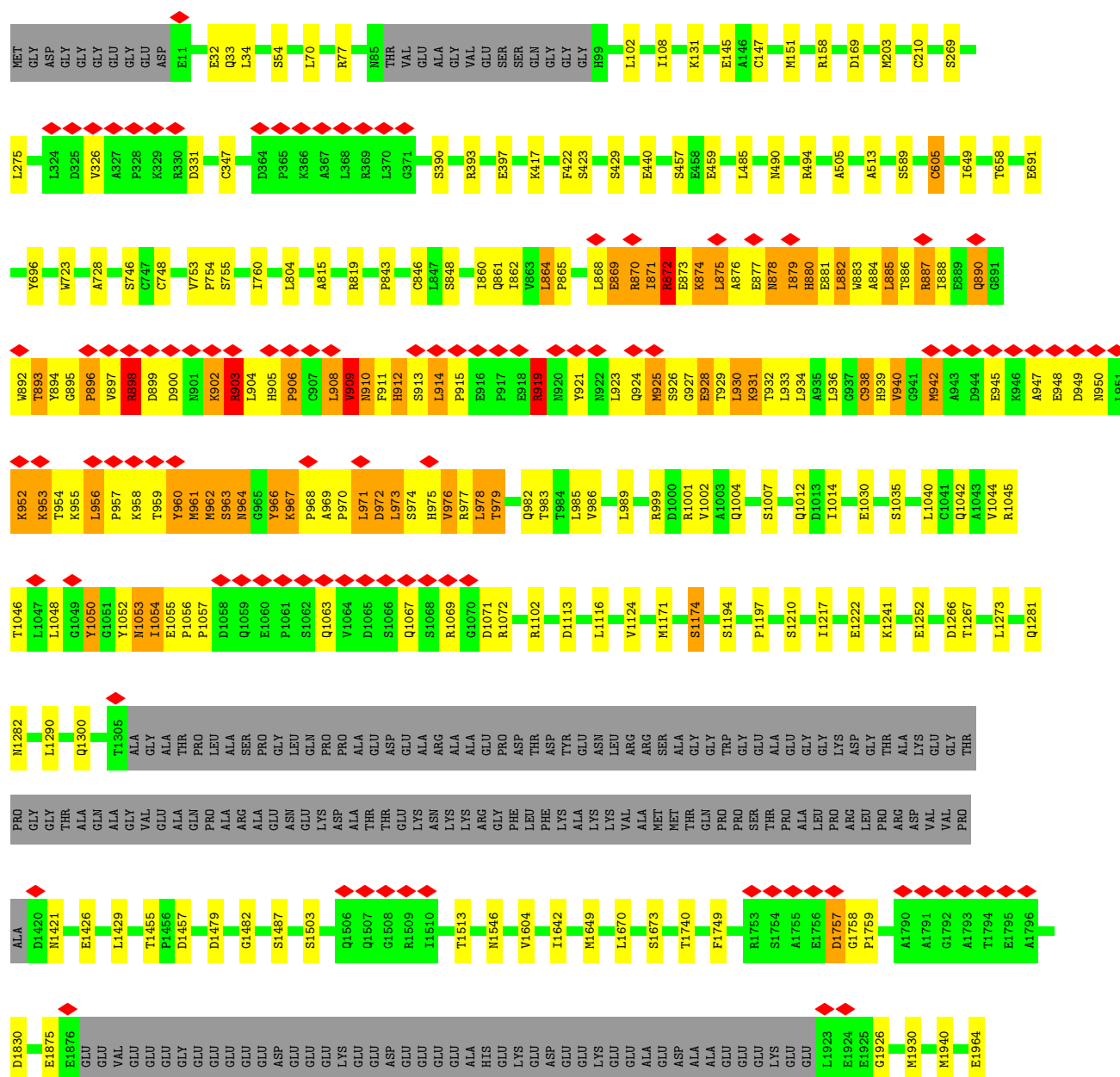
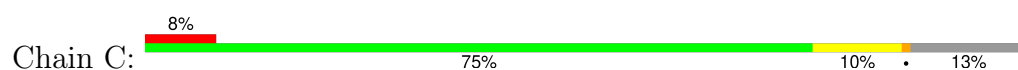




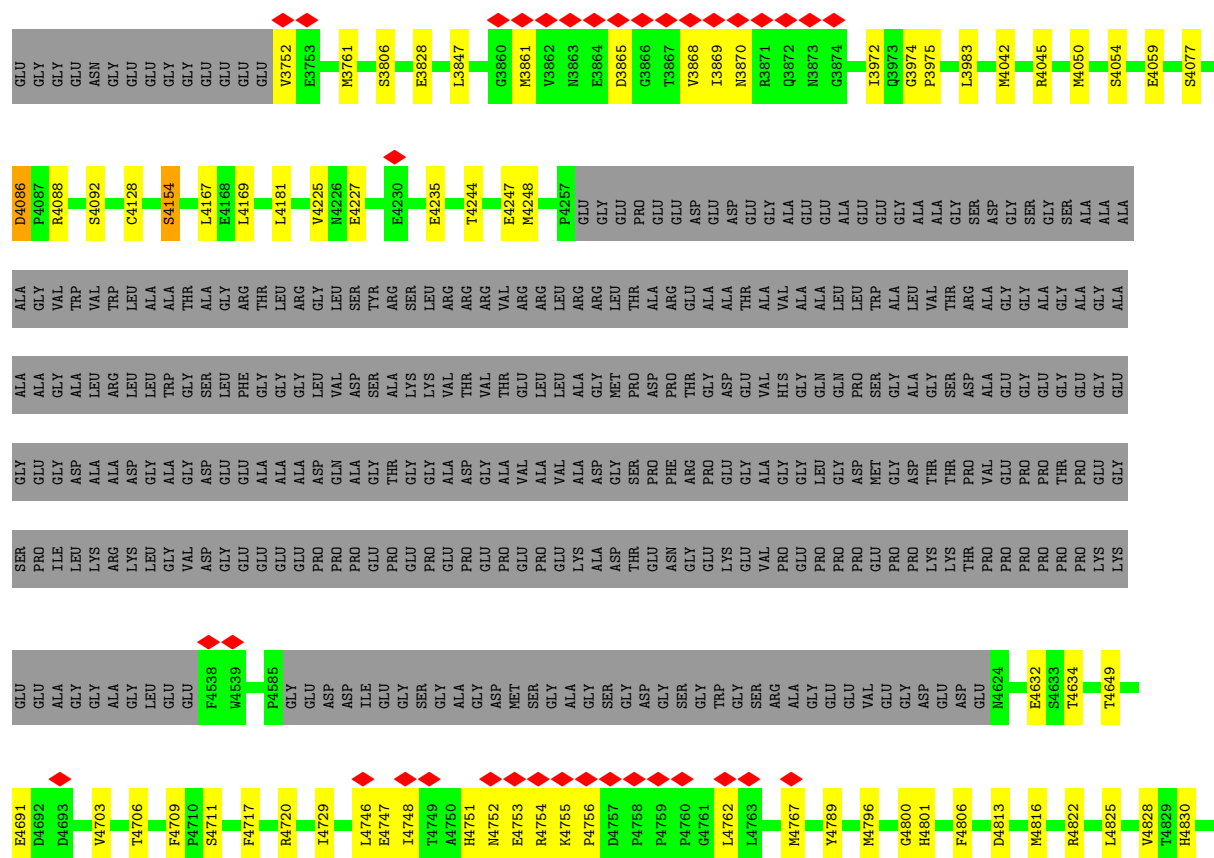




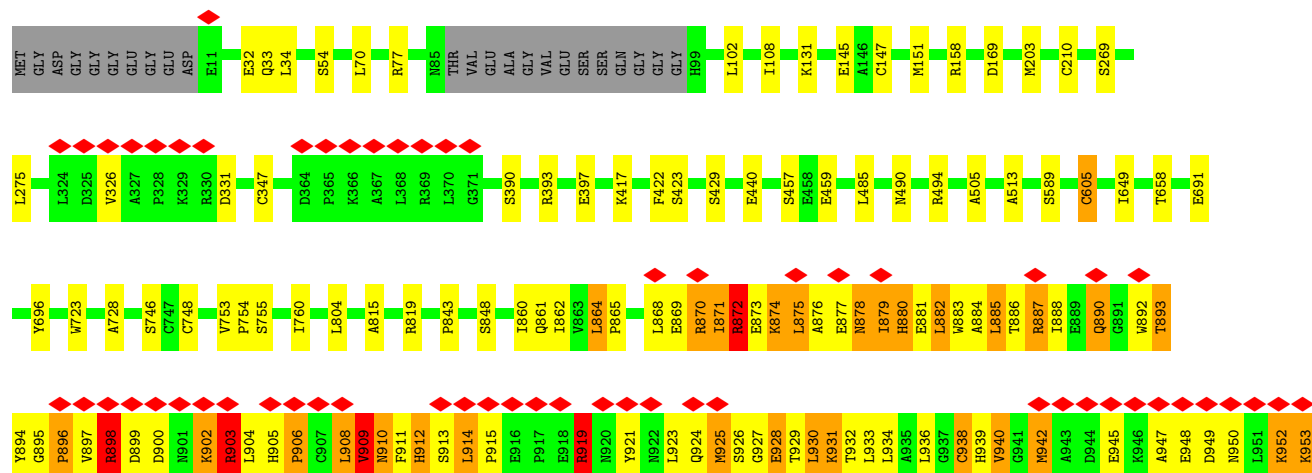
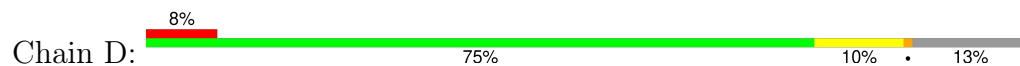
• Molecule 1: Ryanodine receptor 1





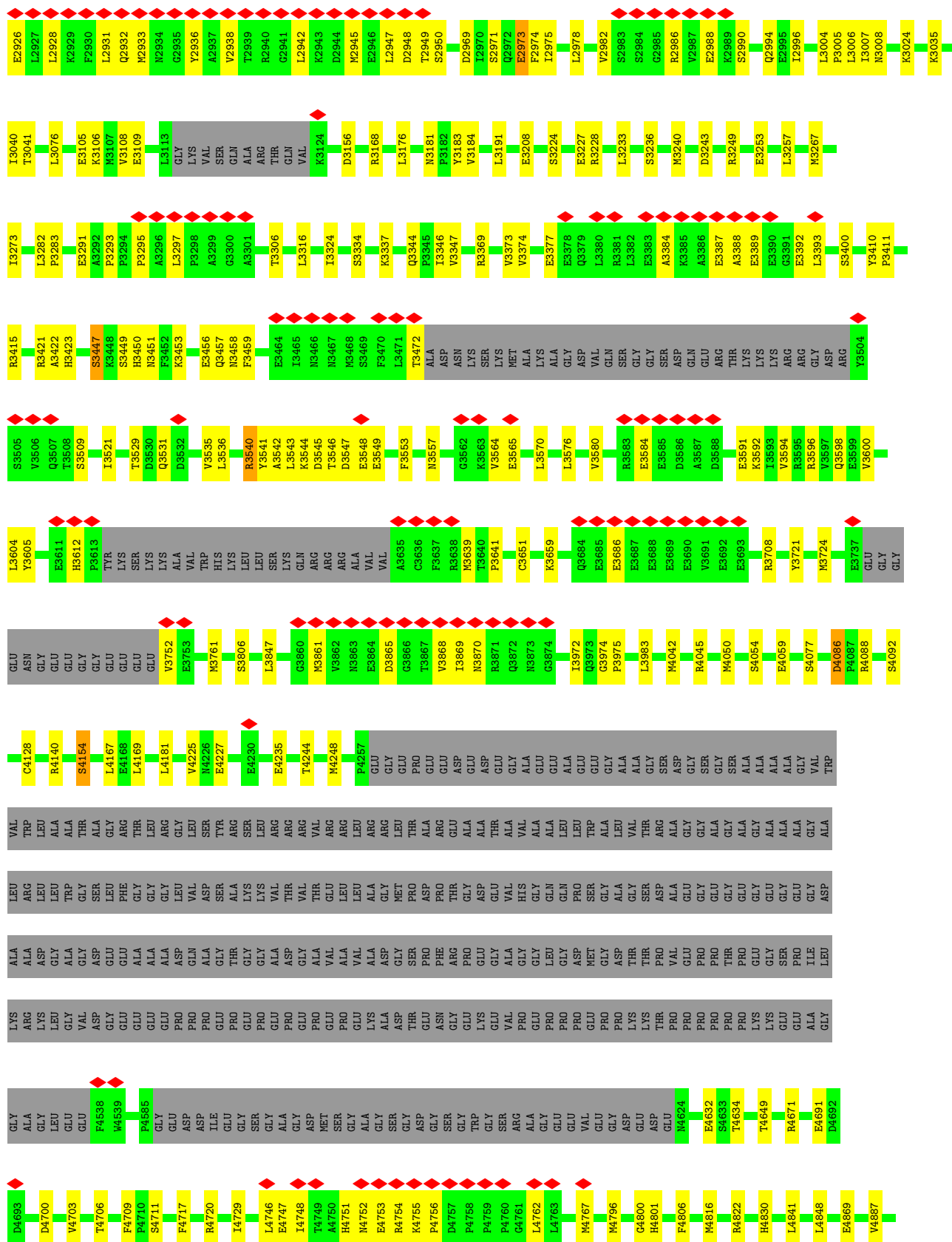


• Molecule 1: Ryanodine receptor 1











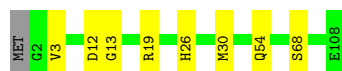
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain E: 92% 7%



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F: 92% 7%



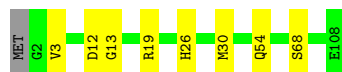
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain G: 92% 7%



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain H: 92% 7%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65309	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.747	Depositor
Minimum map value	0.000	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	424.448, 424.448, 424.448	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, PCW, ZN, CA, A1BYZ, CFF

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	0.28	1/35586 (0.0%)	0.43	10/48203 (0.0%)
1	B	0.28	1/35586 (0.0%)	0.44	10/48203 (0.0%)
1	C	0.28	1/35586 (0.0%)	0.44	10/48203 (0.0%)
1	D	0.28	1/35586 (0.0%)	0.44	10/48203 (0.0%)
2	E	0.20	0/848	0.32	0/1143
2	F	0.20	0/848	0.33	0/1143
2	G	0.20	0/848	0.32	0/1143
2	H	0.20	0/848	0.33	0/1143
All	All	0.28	4/145736 (0.0%)	0.43	40/197384 (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	A	0	7
1	B	0	7
1	C	0	7
1	D	0	7
All	All	0	28

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2238	CYS	CB-SG	5.43	1.99	1.81
1	C	2238	CYS	CB-SG	5.43	1.99	1.81
1	D	2238	CYS	CB-SG	5.43	1.99	1.81
1	B	2238	CYS	CB-SG	5.42	1.99	1.81

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	896	PRO	N-CA-C	-8.38	101.88	113.53
1	A	896	PRO	N-CA-C	-8.37	101.89	113.53
1	B	896	PRO	N-CA-C	-8.37	101.89	113.53
1	D	896	PRO	N-CA-C	-8.37	101.89	113.53
1	B	1050	TYR	N-CA-C	-6.62	104.06	111.28
1	D	2234	CYS	N-CA-CB	6.60	121.64	110.49
1	B	2234	CYS	N-CA-CB	6.60	121.64	110.49
1	A	2234	CYS	N-CA-CB	6.60	121.64	110.49
1	A	1050	TYR	N-CA-C	-6.59	104.09	111.28
1	C	1050	TYR	N-CA-C	-6.58	104.10	111.28
1	C	2234	CYS	N-CA-CB	6.58	121.61	110.49
1	D	1050	TYR	N-CA-C	-6.57	104.12	111.28
1	B	2233	CYS	CA-C-N	-6.37	109.38	121.54
1	B	2233	CYS	C-N-CA	-6.37	109.38	121.54
1	C	2233	CYS	CA-C-N	-6.37	109.38	121.54
1	C	2233	CYS	C-N-CA	-6.37	109.38	121.54
1	A	2233	CYS	CA-C-N	-6.36	109.40	121.54
1	A	2233	CYS	C-N-CA	-6.36	109.40	121.54
1	D	2233	CYS	CA-C-N	-6.36	109.40	121.54
1	D	2233	CYS	C-N-CA	-6.36	109.40	121.54
1	D	3540	ARG	CG-CD-NE	6.33	125.94	112.00
1	C	3540	ARG	CG-CD-NE	6.33	125.92	112.00
1	A	3540	ARG	CG-CD-NE	6.32	125.90	112.00
1	B	3540	ARG	CG-CD-NE	6.30	125.87	112.00
1	D	903	ARG	N-CA-C	-6.24	104.26	112.24
1	C	903	ARG	N-CA-C	-6.21	104.29	112.24
1	A	903	ARG	N-CA-C	-6.20	104.31	112.24
1	B	903	ARG	N-CA-C	-6.19	104.32	112.24
1	B	906	PRO	N-CA-C	-5.58	105.77	113.53
1	D	906	PRO	N-CA-C	-5.58	105.77	113.53
1	C	2234	CYS	CA-CB-SG	5.57	127.21	114.40
1	A	906	PRO	N-CA-C	-5.57	105.79	113.53
1	A	2234	CYS	CA-CB-SG	5.56	127.20	114.40
1	D	2234	CYS	CA-CB-SG	5.56	127.19	114.40
1	B	2234	CYS	CA-CB-SG	5.55	127.16	114.40
1	C	906	PRO	N-CA-C	-5.54	105.82	113.53
1	C	890	GLN	N-CA-C	-5.40	106.65	113.18
1	D	890	GLN	N-CA-C	-5.40	106.65	113.18
1	A	890	GLN	N-CA-C	-5.38	106.67	113.18
1	B	890	GLN	N-CA-C	-5.35	106.70	113.18

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2337	ARG	Sidechain
1	A	605	CYS	Peptide
1	A	872	ARG	Sidechain
1	A	887	ARG	Sidechain
1	A	898	ARG	Sidechain
1	A	903	ARG	Sidechain
1	A	919	ARG	Sidechain
1	B	2337	ARG	Sidechain
1	B	605	CYS	Peptide
1	B	872	ARG	Sidechain
1	B	887	ARG	Sidechain
1	B	898	ARG	Sidechain
1	B	903	ARG	Sidechain
1	B	919	ARG	Sidechain
1	C	2337	ARG	Sidechain
1	C	605	CYS	Peptide
1	C	872	ARG	Sidechain
1	C	887	ARG	Sidechain
1	C	898	ARG	Sidechain
1	C	903	ARG	Sidechain
1	C	919	ARG	Sidechain
1	D	2337	ARG	Sidechain
1	D	605	CYS	Peptide
1	D	872	ARG	Sidechain
1	D	887	ARG	Sidechain
1	D	898	ARG	Sidechain
1	D	903	ARG	Sidechain
1	D	919	ARG	Sidechain

## 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	34797	0	34382	513	0
1	B	34797	0	34382	529	0
1	C	34797	0	34382	518	0
1	D	34797	0	34382	521	0
2	E	830	0	828	5	0
2	F	830	0	828	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	830	0	828	5	0
2	H	830	0	828	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	14	0	10	0	0
4	B	14	0	10	0	0
4	C	14	0	10	0	0
4	D	14	0	10	0	0
5	A	62	0	24	0	0
5	B	62	0	24	0	0
5	C	62	0	24	0	0
5	D	62	0	24	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	108	0	168	5	0
7	B	108	0	168	7	0
7	C	108	0	168	6	0
7	D	108	0	168	6	0
8	A	60	0	0	2	0
8	B	60	0	0	2	0
8	C	60	0	0	2	0
8	D	60	0	0	2	0
All	All	143492	0	141648	2082	0

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

All (2082) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:888:ILE:HG12	1:D:960:TYR:HA	1.14	1.14
1:C:888:ILE:HG12	1:C:960:TYR:HA	1.14	1.12
1:B:888:ILE:HG12	1:B:960:TYR:HA	1.14	1.10
1:A:884:ALA:HB3	1:A:968:PRO:HB3	1.34	1.10
1:A:888:ILE:HG12	1:A:960:TYR:HA	1.14	1.09
1:B:884:ALA:HB3	1:B:968:PRO:HB3	1.34	1.09
1:C:884:ALA:HB3	1:C:968:PRO:HB3	1.34	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:884:ALA:HB3	1:D:968:PRO:HB3	1.34	1.07
1:B:953:LYS:HE3	1:B:969:ALA:HB1	1.42	1.01
1:B:605:CYS:SG	1:B:1673:SER:OG	2.20	1.00
1:A:953:LYS:HE3	1:A:969:ALA:HB1	1.42	1.00
1:A:605:CYS:SG	1:A:1673:SER:OG	2.20	1.00
1:C:953:LYS:HE3	1:C:969:ALA:HB1	1.42	0.98
1:C:605:CYS:SG	1:C:1673:SER:OG	2.20	0.98
1:D:605:CYS:SG	1:D:1673:SER:OG	2.20	0.98
1:D:953:LYS:HE3	1:D:969:ALA:HB1	1.42	0.97
1:D:899:ASP:HB3	1:D:902:LYS:HB2	1.47	0.96
1:B:899:ASP:HB3	1:B:902:LYS:HB2	1.47	0.94
1:A:899:ASP:HB3	1:A:902:LYS:HB2	1.47	0.94
1:C:899:ASP:HB3	1:C:902:LYS:HB2	1.47	0.94
1:C:986:VAL:HG22	1:C:1044:VAL:HG21	1.52	0.92
1:B:986:VAL:HG22	1:B:1044:VAL:HG21	1.52	0.91
1:D:986:VAL:HG22	1:D:1044:VAL:HG21	1.52	0.91
1:A:986:VAL:HG22	1:A:1044:VAL:HG21	1.52	0.90
1:C:868:LEU:HD13	1:C:930:LEU:HB3	1.55	0.89
1:B:1281:GLN:O	1:B:1282:ASN:ND2	2.06	0.89
1:B:868:LEU:HD13	1:B:930:LEU:HB3	1.55	0.89
1:A:868:LEU:HD13	1:A:930:LEU:HB3	1.55	0.88
1:A:1281:GLN:O	1:A:1282:ASN:ND2	2.06	0.88
1:C:871:ILE:HA	1:C:874:LYS:HD3	1.55	0.88
1:A:871:ILE:HA	1:A:874:LYS:HD3	1.55	0.88
1:D:1281:GLN:O	1:D:1282:ASN:ND2	2.06	0.88
1:C:1281:GLN:O	1:C:1282:ASN:ND2	2.06	0.88
1:D:868:LEU:HD22	1:D:930:LEU:HG	1.56	0.88
1:D:871:ILE:HA	1:D:874:LYS:HD3	1.55	0.87
1:D:868:LEU:HD13	1:D:930:LEU:HB3	1.55	0.87
1:B:871:ILE:HA	1:B:874:LYS:HD3	1.55	0.87
1:C:864:LEU:HD11	1:C:930:LEU:HB2	1.57	0.86
1:A:868:LEU:HD22	1:A:930:LEU:HG	1.56	0.86
1:C:868:LEU:HD22	1:C:930:LEU:HG	1.56	0.86
1:B:868:LEU:HD22	1:B:930:LEU:HG	1.56	0.85
1:D:864:LEU:HD11	1:D:930:LEU:HB2	1.57	0.85
1:B:864:LEU:HD11	1:B:930:LEU:HB2	1.57	0.85
1:C:956:LEU:HD22	1:C:957:PRO:HD2	1.59	0.84
1:A:2234:CYS:O	1:A:2235:ARG:C	2.20	0.84
1:B:956:LEU:HD22	1:B:957:PRO:HD2	1.59	0.84
1:A:864:LEU:HD11	1:A:930:LEU:HB2	1.57	0.83
1:D:2234:CYS:O	1:D:2235:ARG:C	2.20	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:879:ILE:HD12	1:B:882:LEU:HD11	1.61	0.83
1:B:956:LEU:HD21	1:B:968:PRO:HG2	1.60	0.83
1:D:956:LEU:HD22	1:D:957:PRO:HD2	1.59	0.82
1:D:879:ILE:HD12	1:D:882:LEU:HD11	1.61	0.82
1:C:108:ILE:HG23	1:C:151:MET:HE2	1.62	0.82
1:A:956:LEU:HD22	1:A:957:PRO:HD2	1.59	0.82
1:A:1067:GLN:OE1	1:A:1069:ARG:NH2	2.13	0.82
1:C:1067:GLN:OE1	1:C:1069:ARG:NH2	2.13	0.82
1:A:956:LEU:HD21	1:A:968:PRO:HG2	1.60	0.82
1:B:108:ILE:HG23	1:B:151:MET:HE2	1.62	0.82
1:C:4816:MET:O	1:C:4822:ARG:NH1	2.13	0.82
1:D:4816:MET:O	1:D:4822:ARG:NH1	2.13	0.82
1:D:1067:GLN:OE1	1:D:1069:ARG:NH2	2.13	0.82
1:C:879:ILE:HD12	1:C:882:LEU:HD11	1.61	0.82
1:A:108:ILE:HG23	1:A:151:MET:HE2	1.62	0.81
1:A:879:ILE:HD12	1:A:882:LEU:HD11	1.61	0.81
1:C:956:LEU:HD21	1:C:968:PRO:HG2	1.60	0.81
1:C:2234:CYS:O	1:C:2235:ARG:C	2.20	0.81
1:A:4816:MET:O	1:A:4822:ARG:NH1	2.13	0.81
1:B:4816:MET:O	1:B:4822:ARG:NH1	2.13	0.81
1:D:956:LEU:HD21	1:D:968:PRO:HG2	1.60	0.81
1:B:2234:CYS:O	1:B:2235:ARG:C	2.20	0.81
1:D:108:ILE:HG23	1:D:151:MET:HE2	1.62	0.81
1:B:888:ILE:HG12	1:B:960:TYR:CA	2.06	0.81
1:A:2383:GLU:OE1	1:A:2386:ARG:NH1	2.14	0.81
1:B:2383:GLU:OE1	1:B:2386:ARG:NH1	2.14	0.80
1:C:3540:ARG:O	1:C:3543:LEU:N	2.15	0.80
1:A:3540:ARG:O	1:A:3543:LEU:N	2.15	0.80
1:C:2383:GLU:OE1	1:C:2386:ARG:NH1	2.14	0.80
1:B:1067:GLN:OE1	1:B:1069:ARG:NH2	2.13	0.80
1:B:3540:ARG:O	1:B:3543:LEU:N	2.15	0.80
1:D:2268:MET:HA	1:D:2268:MET:HE2	1.64	0.80
1:D:3540:ARG:O	1:D:3543:LEU:N	2.15	0.80
1:D:2383:GLU:OE1	1:D:2386:ARG:NH1	2.14	0.80
1:C:2268:MET:HE2	1:C:2268:MET:HA	1.64	0.79
2:F:12:ASP:OD2	2:F:13:GLY:N	2.15	0.79
1:A:2268:MET:HE2	1:A:2268:MET:HA	1.64	0.79
2:G:12:ASP:OD2	2:G:13:GLY:N	2.15	0.79
2:H:12:ASP:OD2	2:H:13:GLY:N	2.15	0.79
1:B:2268:MET:HE2	1:B:2268:MET:HA	1.64	0.79
1:A:888:ILE:HG12	1:A:960:TYR:CA	2.06	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:884:ALA:CB	1:D:968:PRO:HB3	2.13	0.79
2:E:12:ASP:OD2	2:E:13:GLY:N	2.15	0.78
1:C:884:ALA:CB	1:C:968:PRO:HB3	2.13	0.78
1:A:884:ALA:CB	1:A:968:PRO:HB3	2.13	0.77
1:B:1982:MET:HE2	1:B:1982:MET:HA	1.66	0.77
1:D:888:ILE:HG12	1:D:960:TYR:CA	2.06	0.77
1:B:2538:ASP:O	1:B:2594:ARG:NH1	2.19	0.77
1:C:1982:MET:HE2	1:C:1982:MET:HA	1.66	0.77
1:A:2973:GLU:OE2	1:A:2973:GLU:N	2.19	0.76
1:B:2973:GLU:N	1:B:2973:GLU:OE2	2.19	0.76
1:C:2538:ASP:O	1:C:2594:ARG:NH1	2.18	0.76
1:A:1982:MET:HE2	1:A:1982:MET:HA	1.66	0.76
1:D:2973:GLU:N	1:D:2973:GLU:OE2	2.19	0.76
1:A:2538:ASP:O	1:A:2594:ARG:NH1	2.19	0.76
1:C:888:ILE:HG12	1:C:960:TYR:CA	2.06	0.76
1:C:2973:GLU:N	1:C:2973:GLU:OE2	2.19	0.76
1:C:2982:VAL:O	1:C:2986:ARG:NH1	2.19	0.76
1:A:3176:LEU:O	1:A:3176:LEU:HD23	1.87	0.75
1:D:1982:MET:HA	1:D:1982:MET:HE2	1.66	0.75
1:B:3176:LEU:O	1:B:3176:LEU:HD23	1.87	0.75
1:D:4755:LYS:NZ	1:D:4756:PRO:O	2.19	0.75
1:A:2234:CYS:O	1:A:2236:PHE:N	2.20	0.75
1:D:883:TRP:HH2	1:D:908:LEU:HA	1.51	0.75
1:D:2538:ASP:O	1:D:2594:ARG:NH1	2.19	0.75
1:D:2982:VAL:O	1:D:2986:ARG:NH1	2.19	0.75
1:D:940:VAL:HG23	1:D:1052:TYR:HB3	1.69	0.75
1:A:883:TRP:HH2	1:A:908:LEU:HA	1.51	0.75
1:A:2982:VAL:O	1:A:2986:ARG:NH1	2.19	0.75
1:C:940:VAL:HG23	1:C:1052:TYR:HB3	1.68	0.75
1:C:3176:LEU:HD23	1:C:3176:LEU:O	1.87	0.75
1:B:884:ALA:CB	1:B:968:PRO:HB3	2.13	0.74
1:B:2982:VAL:O	1:B:2986:ARG:NH1	2.19	0.74
1:C:2234:CYS:O	1:C:2236:PHE:N	2.20	0.74
1:D:2234:CYS:O	1:D:2236:PHE:N	2.20	0.74
1:B:2234:CYS:O	1:B:2236:PHE:N	2.20	0.74
1:D:3176:LEU:O	1:D:3176:LEU:HD23	1.87	0.74
2:F:54:GLN:N	2:F:54:GLN:OE1	2.20	0.74
1:B:940:VAL:HG23	1:B:1052:TYR:HB3	1.69	0.74
1:B:3181:ASN:OD1	1:B:3183:TYR:N	2.20	0.74
2:G:54:GLN:OE1	2:G:54:GLN:N	2.21	0.74
1:A:2858:PRO:O	1:A:2859:GLN:NE2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:54:GLN:OE1	2:H:54:GLN:N	2.20	0.73
1:C:2858:PRO:O	1:C:2859:GLN:NE2	2.21	0.73
1:D:2858:PRO:O	1:D:2859:GLN:NE2	2.21	0.73
1:C:883:TRP:HH2	1:C:908:LEU:HA	1.51	0.73
1:A:3181:ASN:OD1	1:A:3183:TYR:N	2.20	0.73
1:A:4755:LYS:NZ	1:A:4756:PRO:O	2.19	0.73
1:A:940:VAL:HG23	1:A:1052:TYR:HB3	1.69	0.73
1:B:883:TRP:HH2	1:B:908:LEU:HA	1.51	0.73
1:B:2858:PRO:O	1:B:2859:GLN:NE2	2.21	0.73
1:D:3861:MET:SD	1:D:3868:VAL:HG21	2.29	0.73
1:D:3181:ASN:OD1	1:D:3183:TYR:N	2.21	0.73
1:D:957:PRO:HG2	1:D:960:TYR:HB2	1.71	0.73
1:C:3181:ASN:OD1	1:C:3183:TYR:N	2.20	0.72
1:C:3861:MET:SD	1:C:3868:VAL:HG21	2.29	0.72
1:D:3540:ARG:NH2	1:D:3549:GLU:O	2.23	0.72
1:B:885:LEU:HD22	1:B:970:PRO:HG3	1.72	0.72
1:B:3540:ARG:NH2	1:B:3549:GLU:O	2.23	0.72
1:A:957:PRO:HG2	1:A:960:TYR:HB2	1.71	0.72
1:B:3861:MET:SD	1:B:3868:VAL:HG21	2.29	0.72
1:C:957:PRO:HG2	1:C:960:TYR:HB2	1.71	0.72
1:C:3540:ARG:NH2	1:C:3549:GLU:O	2.23	0.72
1:A:885:LEU:HD22	1:A:970:PRO:HG3	1.72	0.72
1:A:985:LEU:HD22	1:A:1056:PRO:HA	1.72	0.71
1:D:985:LEU:HD22	1:D:1056:PRO:HA	1.72	0.71
1:D:942:MET:HA	1:D:1052:TYR:HA	1.72	0.71
1:B:942:MET:HA	1:B:1052:TYR:HA	1.72	0.71
1:A:3861:MET:SD	1:A:3868:VAL:HG21	2.29	0.71
1:D:2817:MET:SD	1:D:2938:VAL:HG21	2.31	0.71
1:A:2752:LEU:HD21	1:A:2824:VAL:HG11	1.73	0.71
1:B:2817:MET:SD	1:B:2938:VAL:HG21	2.31	0.71
1:C:885:LEU:HD22	1:C:970:PRO:HG3	1.72	0.71
1:D:973:LEU:HD21	1:D:1046:THR:HG22	1.71	0.71
1:B:957:PRO:HG2	1:B:960:TYR:HB2	1.71	0.71
1:B:2752:LEU:HD21	1:B:2824:VAL:HG11	1.73	0.71
1:C:942:MET:HA	1:C:1052:TYR:HA	1.72	0.71
1:C:973:LEU:HD21	1:C:1046:THR:HG22	1.71	0.71
1:A:3540:ARG:NH2	1:A:3549:GLU:O	2.23	0.71
1:B:976:VAL:HB	1:B:1045:ARG:HD2	1.72	0.71
1:A:976:VAL:HB	1:A:1045:ARG:HD2	1.72	0.70
1:B:3249:ARG:NH2	1:B:3253:GLU:OE2	2.24	0.70
1:C:967:LYS:HE2	1:C:969:ALA:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2752:LEU:HD21	1:C:2824:VAL:HG11	1.73	0.70
1:A:2817:MET:SD	1:A:2938:VAL:HG21	2.31	0.70
1:B:985:LEU:HD22	1:B:1056:PRO:HA	1.72	0.70
1:C:940:VAL:HA	1:C:1053:ASN:O	1.92	0.70
1:C:2817:MET:SD	1:C:2938:VAL:HG21	2.31	0.70
1:B:940:VAL:HA	1:B:1053:ASN:O	1.92	0.70
1:D:3249:ARG:NH2	1:D:3253:GLU:OE2	2.24	0.70
1:A:973:LEU:HD21	1:A:1046:THR:HG22	1.71	0.70
1:A:3249:ARG:NH2	1:A:3253:GLU:OE2	2.24	0.70
1:A:888:ILE:HB	1:A:962:MET:HE1	1.74	0.70
1:A:942:MET:HA	1:A:1052:TYR:HA	1.72	0.70
1:B:973:LEU:HD21	1:B:1046:THR:HG22	1.71	0.70
1:C:3249:ARG:NH2	1:C:3253:GLU:OE2	2.24	0.70
1:D:885:LEU:HD22	1:D:970:PRO:HG3	1.72	0.70
1:D:940:VAL:HA	1:D:1053:ASN:O	1.92	0.70
1:A:940:VAL:HA	1:A:1053:ASN:O	1.92	0.70
1:C:985:LEU:HD22	1:C:1056:PRO:HA	1.72	0.70
1:D:2752:LEU:HD21	1:D:2824:VAL:HG11	1.73	0.70
1:B:967:LYS:HE2	1:B:969:ALA:HB2	1.73	0.69
1:B:4755:LYS:NZ	1:B:4756:PRO:O	2.19	0.69
1:C:888:ILE:HB	1:C:962:MET:HE1	1.74	0.69
1:D:967:LYS:HE2	1:D:969:ALA:HB2	1.74	0.69
1:C:976:VAL:HB	1:C:1045:ARG:HD2	1.72	0.69
1:D:860:ILE:HD12	1:D:861:GLN:N	2.08	0.69
1:D:976:VAL:HB	1:D:1045:ARG:HD2	1.72	0.69
1:A:865:PRO:HD2	1:A:868:LEU:HB2	1.75	0.69
2:E:54:GLN:OE1	2:E:54:GLN:N	2.26	0.69
1:B:865:PRO:HD2	1:B:868:LEU:HB2	1.75	0.69
1:C:4748:ILE:HG22	1:C:4754:ARG:NH2	2.08	0.69
1:D:888:ILE:HB	1:D:962:MET:HE1	1.74	0.69
1:D:2755:PHE:HD2	1:D:2814:LEU:HD11	1.58	0.69
1:C:2755:PHE:HD2	1:C:2814:LEU:HD11	1.58	0.69
1:A:967:LYS:HE2	1:A:969:ALA:HB2	1.74	0.69
1:B:888:ILE:HB	1:B:962:MET:HE1	1.74	0.69
1:C:953:LYS:HB3	1:C:971:LEU:HA	1.75	0.69
1:C:956:LEU:CD1	1:C:960:TYR:HB3	2.23	0.69
1:A:956:LEU:CD1	1:A:960:TYR:HB3	2.23	0.68
1:A:2743:THR:OG1	1:A:2816:ALA:N	2.27	0.68
1:B:956:LEU:CD1	1:B:960:TYR:HB3	2.23	0.68
1:C:4755:LYS:NZ	1:C:4756:PRO:O	2.19	0.68
1:A:4748:ILE:HG22	1:A:4754:ARG:NH2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4086:ASP:OD2	1:B:4088:ARG:N	2.26	0.68
1:C:860:ILE:HD12	1:C:861:GLN:N	2.08	0.68
1:D:4086:ASP:OD2	1:D:4088:ARG:N	2.26	0.68
1:A:881:GLU:HB3	1:A:969:ALA:C	2.18	0.68
1:B:881:GLU:HB3	1:B:969:ALA:C	2.18	0.68
1:B:2743:THR:OG1	1:B:2816:ALA:N	2.27	0.68
1:B:2755:PHE:HD2	1:B:2814:LEU:HD11	1.58	0.68
1:B:860:ILE:HD12	1:B:861:GLN:N	2.08	0.68
1:D:953:LYS:HB3	1:D:971:LEU:HA	1.75	0.68
1:D:4748:ILE:HG22	1:D:4754:ARG:NH2	2.08	0.68
1:A:860:ILE:HD12	1:A:861:GLN:N	2.08	0.68
1:A:2755:PHE:HD2	1:A:2814:LEU:HD11	1.58	0.68
1:C:4086:ASP:OD2	1:C:4088:ARG:N	2.26	0.68
1:A:967:LYS:CE	1:A:969:ALA:HB2	2.24	0.68
1:B:4748:ILE:HG22	1:B:4754:ARG:NH2	2.08	0.68
1:D:956:LEU:CD1	1:D:960:TYR:HB3	2.23	0.68
1:A:4086:ASP:OD2	1:A:4088:ARG:N	2.26	0.67
1:D:2743:THR:OG1	1:D:2816:ALA:N	2.27	0.67
1:B:953:LYS:HB3	1:B:971:LEU:HA	1.75	0.67
1:C:2234:CYS:O	1:C:2237:LEU:N	2.28	0.67
1:A:953:LYS:HB3	1:A:971:LEU:HA	1.75	0.67
1:C:865:PRO:HD2	1:C:868:LEU:HB2	1.75	0.67
1:D:865:PRO:HD2	1:D:868:LEU:HB2	1.75	0.67
1:D:868:LEU:HD23	1:D:871:ILE:HD12	1.75	0.67
1:B:2234:CYS:O	1:B:2237:LEU:N	2.28	0.67
1:B:864:LEU:HD11	1:B:930:LEU:CB	2.25	0.67
1:C:881:GLU:HB3	1:C:969:ALA:C	2.18	0.67
1:D:930:LEU:HA	1:D:933:LEU:HD12	1.76	0.67
1:A:864:LEU:HD11	1:A:930:LEU:CB	2.25	0.67
1:C:2743:THR:OG1	1:C:2816:ALA:N	2.27	0.67
1:D:881:GLU:HB3	1:D:969:ALA:C	2.19	0.67
1:A:868:LEU:HD23	1:A:871:ILE:HD12	1.75	0.67
1:D:967:LYS:CE	1:D:969:ALA:HB2	2.25	0.67
1:B:868:LEU:HD23	1:B:871:ILE:HD12	1.75	0.67
1:B:967:LYS:CE	1:B:969:ALA:HB2	2.25	0.67
1:D:3541:TYR:HB3	1:D:3605:TYR:CD2	2.30	0.67
1:C:903:ARG:HH21	1:C:903:ARG:HA	1.61	0.66
1:C:930:LEU:HA	1:C:933:LEU:HD12	1.76	0.66
1:B:903:ARG:HA	1:B:903:ARG:HH21	1.60	0.66
1:B:3565:GLU:N	1:B:3565:GLU:OE1	2.29	0.66
1:D:903:ARG:HA	1:D:903:ARG:HH21	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2234:CYS:O	1:D:2237:LEU:N	2.28	0.66
1:A:2234:CYS:O	1:A:2237:LEU:N	2.28	0.66
1:A:3541:TYR:HB3	1:A:3605:TYR:CD2	2.30	0.66
1:B:3541:TYR:HB3	1:B:3605:TYR:CD2	2.31	0.66
1:C:868:LEU:HD23	1:C:871:ILE:HD12	1.75	0.66
1:C:3565:GLU:OE1	1:C:3565:GLU:N	2.29	0.66
1:B:3531:GLN:O	1:B:3535:VAL:HG23	1.96	0.66
1:C:1048:LEU:HD21	1:C:1054:ILE:HG13	1.78	0.66
1:B:3972:ILE:HG21	1:B:3983:LEU:HD12	1.78	0.66
1:C:864:LEU:HD11	1:C:930:LEU:CB	2.25	0.66
1:D:864:LEU:HD11	1:D:930:LEU:CB	2.25	0.66
1:D:872:ARG:HG3	1:D:927:GLY:HA2	1.78	0.66
1:D:3565:GLU:OE1	1:D:3565:GLU:N	2.29	0.66
1:C:872:ARG:HG3	1:C:927:GLY:HA2	1.78	0.66
1:C:967:LYS:CE	1:C:969:ALA:HB2	2.25	0.66
1:C:102:LEU:HB3	1:C:151:MET:HE1	1.78	0.65
1:C:3972:ILE:HG21	1:C:3983:LEU:HD12	1.78	0.65
1:A:3531:GLN:O	1:A:3535:VAL:HG23	1.96	0.65
1:C:3541:TYR:HB3	1:C:3605:TYR:CD2	2.30	0.65
1:D:1048:LEU:HD21	1:D:1054:ILE:HG13	1.78	0.65
1:A:872:ARG:HG3	1:A:927:GLY:HA2	1.78	0.65
1:A:930:LEU:HA	1:A:933:LEU:HD12	1.76	0.65
1:A:3972:ILE:HG21	1:A:3983:LEU:HD12	1.78	0.65
1:B:1048:LEU:HD21	1:B:1054:ILE:HG13	1.78	0.65
1:D:102:LEU:HB3	1:D:151:MET:HE1	1.78	0.65
1:D:914:LEU:HD12	1:D:915:PRO:HD2	1.79	0.65
1:D:2988:GLU:N	1:D:2988:GLU:OE1	2.30	0.65
1:A:914:LEU:HD12	1:A:915:PRO:HD2	1.79	0.65
1:C:914:LEU:HD12	1:C:915:PRO:HD2	1.79	0.65
1:C:3531:GLN:O	1:C:3535:VAL:HG23	1.96	0.65
1:A:887:ARG:HG3	1:A:892:TRP:CB	2.27	0.65
1:A:3565:GLU:OE1	1:A:3565:GLU:N	2.29	0.65
1:C:876:ALA:CB	1:C:923:LEU:HA	2.27	0.65
1:D:887:ARG:HG3	1:D:892:TRP:CB	2.27	0.65
1:B:872:ARG:HG3	1:B:927:GLY:HA2	1.78	0.65
1:B:914:LEU:HD12	1:B:915:PRO:HD2	1.79	0.65
1:A:903:ARG:HH21	1:A:903:ARG:HA	1.61	0.65
1:A:879:ILE:HA	1:A:882:LEU:HD11	1.79	0.65
1:B:102:LEU:HB3	1:B:151:MET:HE1	1.79	0.65
1:B:876:ALA:CB	1:B:923:LEU:HA	2.27	0.65
1:B:930:LEU:HA	1:B:933:LEU:HD12	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2988:GLU:OE1	1:C:2988:GLU:N	2.30	0.65
1:A:102:LEU:HB3	1:A:151:MET:HE1	1.78	0.64
1:A:2988:GLU:N	1:A:2988:GLU:OE1	2.30	0.64
1:B:2988:GLU:OE1	1:B:2988:GLU:N	2.30	0.64
1:C:887:ARG:HG3	1:C:892:TRP:HB2	1.79	0.64
1:A:887:ARG:HG3	1:A:892:TRP:HB2	1.79	0.64
1:B:2741:VAL:HG11	1:B:2820:TRP:NE1	2.12	0.64
1:D:3531:GLN:O	1:D:3535:VAL:HG23	1.96	0.64
1:A:1048:LEU:HD21	1:A:1054:ILE:HG13	1.78	0.64
1:B:887:ARG:HG3	1:B:892:TRP:HB2	1.79	0.64
1:D:872:ARG:HH21	1:D:873:GLU:HA	1.62	0.64
1:D:887:ARG:HG3	1:D:892:TRP:HB2	1.79	0.64
1:D:2635:ASN:OD1	1:D:2637:PHE:N	2.31	0.64
1:A:876:ALA:CB	1:A:923:LEU:HA	2.27	0.64
1:B:879:ILE:HA	1:B:882:LEU:HD11	1.79	0.64
1:C:2741:VAL:HG11	1:C:2820:TRP:NE1	2.12	0.64
1:A:2741:VAL:HG11	1:A:2820:TRP:NE1	2.12	0.64
1:B:3546:THR:OG1	1:B:3548:GLU:OE2	2.15	0.64
1:C:2756:ILE:HG13	1:C:2814:LEU:HD12	1.80	0.64
1:D:2741:VAL:HG11	1:D:2820:TRP:NE1	2.12	0.64
1:D:3972:ILE:HG21	1:D:3983:LEU:HD12	1.78	0.64
1:B:887:ARG:HG3	1:B:892:TRP:CB	2.27	0.64
1:C:887:ARG:HG3	1:C:892:TRP:CB	2.27	0.64
1:C:902:LYS:HB3	1:C:904:LEU:HG	1.80	0.64
1:A:872:ARG:HH21	1:A:873:GLU:HA	1.62	0.64
1:C:868:LEU:HD23	1:C:871:ILE:CD1	2.28	0.64
1:D:879:ILE:HA	1:D:882:LEU:HD11	1.79	0.64
1:C:2249:ARG:NH2	1:C:2286:GLU:OE2	2.31	0.64
1:C:4042:MET:SD	1:C:4045:ARG:NH1	2.71	0.64
1:D:876:ALA:CB	1:D:923:LEU:HA	2.27	0.64
1:A:865:PRO:HD2	1:A:868:LEU:CB	2.28	0.64
1:A:2249:ARG:NH2	1:A:2286:GLU:OE2	2.31	0.64
1:A:4154:SER:HB2	1:A:4167:LEU:HD11	1.79	0.64
1:C:872:ARG:HH21	1:C:873:GLU:HA	1.62	0.64
1:D:909:VAL:HB	1:D:913:SER:HB3	1.80	0.64
1:D:902:LYS:HB3	1:D:904:LEU:HG	1.80	0.64
1:D:2688:ALA:O	1:D:2994:GLN:NE2	2.31	0.64
1:D:4748:ILE:O	1:D:4754:ARG:NH1	2.27	0.64
1:A:868:LEU:HD23	1:A:871:ILE:CD1	2.28	0.63
1:B:902:LYS:HB3	1:B:904:LEU:HG	1.79	0.63
1:B:2756:ILE:HG13	1:B:2814:LEU:HD12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:865:PRO:HD2	1:C:868:LEU:HD12	1.80	0.63
1:C:2688:ALA:O	1:C:2994:GLN:NE2	2.31	0.63
1:C:4767:MET:HE2	1:C:4767:MET:HA	1.80	0.63
1:D:865:PRO:HD2	1:D:868:LEU:HD12	1.80	0.63
1:B:4154:SER:HB2	1:B:4167:LEU:HD11	1.79	0.63
1:A:902:LYS:HB3	1:A:904:LEU:HG	1.80	0.63
1:B:872:ARG:HH21	1:B:873:GLU:HA	1.62	0.63
1:D:865:PRO:HD2	1:D:868:LEU:CB	2.28	0.63
1:D:2249:ARG:NH2	1:D:2286:GLU:OE2	2.31	0.63
1:D:4767:MET:HA	1:D:4767:MET:HE2	1.80	0.63
1:A:865:PRO:HD2	1:A:868:LEU:HD12	1.80	0.63
1:B:2799:SER:N	1:B:2802:ASP:OD2	2.32	0.63
1:D:2756:ILE:HG13	1:D:2814:LEU:HD12	1.80	0.63
1:D:2799:SER:N	1:D:2802:ASP:OD2	2.32	0.63
1:A:875:LEU:HB3	1:A:926:SER:HB2	1.81	0.63
1:B:2863:LEU:HD12	1:B:2926:GLU:OE1	1.98	0.63
1:C:2635:ASN:OD1	1:C:2637:PHE:N	2.31	0.63
1:C:2863:LEU:HD12	1:C:2926:GLU:OE1	1.98	0.63
1:D:883:TRP:CH2	1:D:908:LEU:HA	2.33	0.63
1:D:4042:MET:SD	1:D:4045:ARG:NH1	2.71	0.63
1:A:875:LEU:HA	1:A:878:ASN:HD22	1.64	0.63
1:A:909:VAL:HB	1:A:913:SER:HB3	1.80	0.63
1:A:2756:ILE:HG13	1:A:2814:LEU:HD12	1.80	0.63
1:B:865:PRO:HD2	1:B:868:LEU:CB	2.28	0.63
1:B:865:PRO:HD2	1:B:868:LEU:HD12	1.80	0.63
1:B:868:LEU:HD23	1:B:871:ILE:CD1	2.28	0.63
1:C:909:VAL:HB	1:C:913:SER:HB3	1.80	0.63
1:D:875:LEU:HA	1:D:878:ASN:HD22	1.64	0.63
1:B:875:LEU:HB3	1:B:926:SER:HB2	1.81	0.63
1:B:4042:MET:SD	1:B:4045:ARG:NH1	2.71	0.63
1:B:4767:MET:HE2	1:B:4767:MET:HA	1.80	0.63
1:C:875:LEU:HB3	1:C:926:SER:HB2	1.81	0.63
1:A:2863:LEU:HD12	1:A:2926:GLU:OE1	1.98	0.63
1:B:893:THR:HG22	1:B:904:LEU:HD22	1.80	0.63
1:D:875:LEU:HB3	1:D:926:SER:HB2	1.81	0.63
1:D:2863:LEU:HD12	1:D:2926:GLU:OE1	1.98	0.63
1:A:893:THR:HG22	1:A:904:LEU:HD22	1.81	0.63
1:C:883:TRP:CH2	1:C:908:LEU:HA	2.33	0.63
1:A:2799:SER:N	1:A:2802:ASP:OD2	2.32	0.62
1:A:4748:ILE:O	1:A:4754:ARG:NH1	2.27	0.62
1:C:879:ILE:HA	1:C:882:LEU:HD11	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4154:SER:HB2	1:C:4167:LEU:HD11	1.79	0.62
1:D:4154:SER:HB2	1:D:4167:LEU:HD11	1.79	0.62
1:A:1421:ASN:O	1:A:1421:ASN:ND2	2.33	0.62
1:A:4042:MET:SD	1:A:4045:ARG:NH1	2.71	0.62
1:B:909:VAL:HB	1:B:913:SER:HB3	1.80	0.62
1:C:1421:ASN:ND2	1:C:1421:ASN:O	2.33	0.62
1:A:2635:ASN:OD1	1:A:2637:PHE:N	2.31	0.62
1:A:5032:ASP:OD2	1:A:5033:GLN:N	2.33	0.62
1:B:883:TRP:CH2	1:B:908:LEU:HA	2.33	0.62
1:B:5032:ASP:OD2	1:B:5033:GLN:N	2.33	0.62
1:C:875:LEU:HA	1:C:878:ASN:HD22	1.64	0.62
1:C:5032:ASP:OD2	1:C:5033:GLN:N	2.33	0.62
1:B:2249:ARG:NH2	1:B:2286:GLU:OE2	2.31	0.62
1:B:2635:ASN:OD1	1:B:2637:PHE:N	2.31	0.62
1:B:3176:LEU:HD21	1:B:3184:VAL:HG13	1.82	0.62
1:C:865:PRO:HD2	1:C:868:LEU:CB	2.28	0.62
1:A:872:ARG:HH12	1:A:923:LEU:HB3	1.65	0.62
1:A:883:TRP:CH2	1:A:908:LEU:HA	2.33	0.62
1:B:875:LEU:HA	1:B:878:ASN:HD22	1.64	0.62
1:C:956:LEU:CB	1:C:967:LYS:HB2	2.29	0.62
1:C:2799:SER:N	1:C:2802:ASP:OD2	2.31	0.62
1:D:956:LEU:CB	1:D:967:LYS:HB2	2.29	0.62
1:D:5032:ASP:OD2	1:D:5033:GLN:N	2.33	0.62
1:A:3176:LEU:HD21	1:A:3184:VAL:HG13	1.82	0.62
1:B:956:LEU:CB	1:B:967:LYS:HB2	2.29	0.62
1:B:2688:ALA:O	1:B:2994:GLN:NE2	2.31	0.62
1:D:868:LEU:HD23	1:D:871:ILE:CD1	2.28	0.62
1:A:956:LEU:CB	1:A:967:LYS:HB2	2.29	0.62
1:A:4767:MET:HA	1:A:4767:MET:HE2	1.80	0.61
1:A:2877:GLU:OE1	1:A:2921:ARG:NE	2.33	0.61
1:B:2942:LEU:O	1:B:2945:MET:HE1	2.00	0.61
1:B:4748:ILE:O	1:B:4754:ARG:NH1	2.27	0.61
1:C:2877:GLU:OE1	1:C:2921:ARG:NE	2.33	0.61
1:D:928:GLU:HA	1:D:931:LYS:HG3	1.83	0.61
1:D:2877:GLU:OE1	1:D:2921:ARG:NE	2.33	0.61
1:A:3546:THR:OG1	1:A:3548:GLU:OE2	2.15	0.61
1:C:2942:LEU:O	1:C:2945:MET:HE1	2.00	0.61
1:A:2688:ALA:O	1:A:2994:GLN:NE2	2.31	0.61
1:D:893:THR:HG22	1:D:904:LEU:HD22	1.81	0.61
1:C:864:LEU:HD21	1:C:930:LEU:HD23	1.83	0.61
1:A:928:GLU:HA	1:A:931:LYS:HG3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:LEU:HD21	1:A:930:LEU:HD23	1.83	0.61
1:D:872:ARG:HH12	1:D:923:LEU:HB3	1.65	0.61
1:D:1421:ASN:O	1:D:1421:ASN:ND2	2.33	0.61
1:B:872:ARG:HH12	1:B:923:LEU:HB3	1.65	0.61
1:B:1421:ASN:O	1:B:1421:ASN:ND2	2.33	0.61
1:D:3176:LEU:HD21	1:D:3184:VAL:HG13	1.82	0.61
1:A:2942:LEU:O	1:A:2945:MET:HE1	2.00	0.61
1:B:4632:GLU:OE2	1:B:4634:THR:OG1	2.17	0.61
1:D:2942:LEU:O	1:D:2945:MET:HE1	2.00	0.60
1:C:1987:MET:N	1:C:1987:MET:SD	2.74	0.60
1:B:892:TRP:HB3	1:B:908:LEU:HD11	1.84	0.60
1:C:893:THR:HG22	1:C:904:LEU:HD22	1.81	0.60
1:C:3176:LEU:HD21	1:C:3184:VAL:HG13	1.82	0.60
1:B:892:TRP:HA	1:B:903:ARG:O	2.02	0.60
1:B:914:LEU:HD11	1:B:919:ARG:N	2.16	0.60
1:C:914:LEU:HD11	1:C:919:ARG:N	2.16	0.60
1:A:3421:ARG:HG2	1:A:3521:ILE:HD11	1.84	0.60
1:B:956:LEU:HD13	1:B:960:TYR:HB3	1.84	0.60
1:C:928:GLU:HA	1:C:931:LYS:HG3	1.82	0.60
1:C:4748:ILE:O	1:C:4754:ARG:NH1	2.27	0.60
1:A:892:TRP:HA	1:A:903:ARG:O	2.02	0.60
1:A:914:LEU:HD11	1:A:919:ARG:N	2.16	0.60
1:B:108:ILE:CG2	1:B:151:MET:HE2	2.31	0.60
1:C:108:ILE:CG2	1:C:151:MET:HE2	2.31	0.60
1:C:872:ARG:HH12	1:C:923:LEU:HB3	1.65	0.60
1:A:956:LEU:HD13	1:A:960:TYR:HB3	1.84	0.60
1:B:864:LEU:HD21	1:B:930:LEU:HD23	1.83	0.60
1:B:2877:GLU:OE1	1:B:2921:ARG:NE	2.33	0.60
1:C:4720:ARG:HH21	1:C:4746:LEU:HD13	1.66	0.60
1:A:2749:PRO:HD2	1:A:2752:LEU:HD12	1.84	0.60
1:A:892:TRP:HB3	1:A:908:LEU:HD11	1.84	0.60
1:D:914:LEU:HD11	1:D:919:ARG:N	2.16	0.60
1:D:892:TRP:HB3	1:D:908:LEU:HD11	1.84	0.60
1:D:892:TRP:HA	1:D:903:ARG:O	2.02	0.60
1:D:1987:MET:N	1:D:1987:MET:SD	2.74	0.60
1:B:956:LEU:HD21	1:B:960:TYR:HD2	1.67	0.59
1:C:892:TRP:HA	1:C:903:ARG:O	2.02	0.59
1:C:956:LEU:HD21	1:C:960:TYR:HD2	1.67	0.59
1:D:3421:ARG:HG2	1:D:3521:ILE:HD11	1.84	0.59
1:D:864:LEU:HD21	1:D:930:LEU:HD23	1.83	0.59
1:D:3536:LEU:HD23	1:D:3553:PHE:HZ	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:956:LEU:HD21	1:A:960:TYR:HD2	1.67	0.59
1:B:928:GLU:HA	1:B:931:LYS:HG3	1.83	0.59
1:B:3421:ARG:HG2	1:B:3521:ILE:HD11	1.84	0.59
1:C:1300:GLN:OE1	1:C:1546:ASN:ND2	2.35	0.59
1:A:894:TYR:OH	1:A:896:PRO:HA	2.03	0.59
1:A:4720:ARG:HH21	1:A:4746:LEU:HD13	1.66	0.59
1:C:2477:ILE:HD12	1:C:2477:ILE:O	2.02	0.59
1:A:108:ILE:CG2	1:A:151:MET:HE2	2.31	0.59
1:A:2912:LEU:O	1:A:2917:LYS:NZ	2.32	0.59
1:C:892:TRP:HB3	1:C:908:LEU:HD11	1.84	0.59
1:C:4632:GLU:OE2	1:C:4634:THR:OG1	2.17	0.59
1:D:894:TYR:OH	1:D:896:PRO:HA	2.03	0.59
1:D:4747:GLU:O	1:D:4751:HIS:ND1	2.36	0.59
1:B:2749:PRO:HD2	1:B:2752:LEU:HD12	1.84	0.59
1:C:32:GLU:OE1	1:C:32:GLU:HA	2.03	0.59
1:C:4747:GLU:O	1:C:4751:HIS:ND1	2.36	0.59
1:D:2477:ILE:HD12	1:D:2477:ILE:O	2.02	0.59
1:A:3536:LEU:HD23	1:A:3553:PHE:HZ	1.67	0.59
1:B:459:GLU:N	1:B:459:GLU:OE2	2.36	0.59
1:B:2477:ILE:O	1:B:2477:ILE:HD12	2.02	0.59
1:B:3536:LEU:HD23	1:B:3553:PHE:HZ	1.67	0.59
1:C:956:LEU:HD13	1:C:960:TYR:HB3	1.84	0.59
1:C:1426:GLU:OE1	1:C:1426:GLU:N	2.34	0.59
1:C:3421:ARG:HG2	1:C:3521:ILE:HD11	1.84	0.59
1:D:956:LEU:HD21	1:D:960:TYR:HD2	1.67	0.59
1:D:1300:GLN:OE1	1:D:1546:ASN:ND2	2.35	0.59
1:D:3257:LEU:HD23	1:D:3267:MET:HE3	1.85	0.59
1:B:1300:GLN:OE1	1:B:1546:ASN:ND2	2.35	0.59
1:C:2749:PRO:HD2	1:C:2752:LEU:HD12	1.84	0.59
1:C:3377:GLU:OE2	1:C:3451:ASN:ND2	2.33	0.59
1:A:2477:ILE:HD12	1:A:2477:ILE:O	2.02	0.58
1:D:875:LEU:HD23	1:D:930:LEU:HD21	1.85	0.58
1:D:956:LEU:HD13	1:D:960:TYR:HB3	1.84	0.58
1:A:875:LEU:HD23	1:A:930:LEU:HD21	1.85	0.58
1:A:4747:GLU:O	1:A:4751:HIS:ND1	2.36	0.58
1:B:32:GLU:OE1	1:B:32:GLU:HA	2.03	0.58
1:B:4720:ARG:HH21	1:B:4746:LEU:HD13	1.66	0.58
1:D:4720:ARG:HH21	1:D:4746:LEU:HD13	1.66	0.58
1:C:3536:LEU:HD23	1:C:3553:PHE:HZ	1.67	0.58
1:A:32:GLU:OE1	1:A:32:GLU:HA	2.03	0.58
1:A:911:PHE:HA	1:A:914:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3257:LEU:HD23	1:A:3267:MET:HE3	1.85	0.58
1:C:459:GLU:N	1:C:459:GLU:OE2	2.36	0.58
1:A:2876:ALA:HB3	1:A:2921:ARG:NH1	2.19	0.58
1:B:875:LEU:HD23	1:B:930:LEU:HD21	1.85	0.58
1:B:1987:MET:N	1:B:1987:MET:SD	2.74	0.58
1:B:3334:SER:O	1:B:3337:LYS:NZ	2.36	0.58
1:C:3257:LEU:HD23	1:C:3267:MET:HE3	1.85	0.58
1:B:956:LEU:CD2	1:B:968:PRO:HG2	2.33	0.58
1:B:4747:GLU:O	1:B:4751:HIS:ND1	2.36	0.58
1:D:32:GLU:OE1	1:D:32:GLU:HA	2.03	0.58
1:D:459:GLU:N	1:D:459:GLU:OE2	2.36	0.58
1:D:2749:PRO:HD2	1:D:2752:LEU:HD12	1.84	0.58
1:D:2876:ALA:HB3	1:D:2921:ARG:NH1	2.19	0.58
1:A:914:LEU:HD21	1:A:919:ARG:HB2	1.86	0.58
1:A:1426:GLU:OE1	1:A:1426:GLU:N	2.34	0.58
1:B:894:TYR:OH	1:B:896:PRO:HA	2.03	0.58
1:B:2876:ALA:HB3	1:B:2921:ARG:NH1	2.19	0.58
1:B:4752:ASN:O	1:B:4754:ARG:NH1	2.37	0.58
1:C:876:ALA:HB1	1:C:923:LEU:HA	1.85	0.58
1:B:958:LYS:HA	1:B:961:MET:CE	2.34	0.58
1:C:894:TYR:OH	1:C:896:PRO:HA	2.03	0.58
1:C:2876:ALA:HB3	1:C:2921:ARG:NH1	2.19	0.58
1:C:4752:ASN:O	1:C:4754:ARG:NH1	2.37	0.58
1:D:2822:TRP:CE3	1:D:2875:MET:HE2	2.39	0.58
1:D:4752:ASN:O	1:D:4754:ARG:NH1	2.37	0.58
1:C:877:GLU:HG3	1:C:911:PHE:CG	2.39	0.58
1:C:911:PHE:HA	1:C:914:LEU:HD23	1.86	0.58
1:D:958:LYS:HA	1:D:961:MET:CE	2.34	0.58
1:B:914:LEU:HD21	1:B:919:ARG:HB2	1.86	0.58
1:B:956:LEU:HD11	1:B:968:PRO:HD2	1.86	0.58
1:C:875:LEU:HD23	1:C:930:LEU:HD21	1.85	0.58
1:D:108:ILE:CG2	1:D:151:MET:HE2	2.31	0.58
1:D:3334:SER:O	1:D:3337:LYS:NZ	2.36	0.58
1:A:459:GLU:OE2	1:A:459:GLU:N	2.36	0.57
1:A:1300:GLN:OE1	1:A:1546:ASN:ND2	2.35	0.57
1:C:2691:LYS:NZ	1:C:2692:TYR:O	2.37	0.57
1:C:3369:ARG:O	1:C:3373:VAL:HG23	2.04	0.57
1:D:914:LEU:HD21	1:D:919:ARG:HB2	1.86	0.57
1:D:956:LEU:CG	1:D:967:LYS:HB2	2.34	0.57
1:A:876:ALA:HB1	1:A:923:LEU:HA	1.85	0.57
1:A:958:LYS:HA	1:A:961:MET:CE	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:956:LEU:CG	1:B:967:LYS:HB2	2.34	0.57
1:C:914:LEU:HD21	1:C:919:ARG:HB2	1.86	0.57
1:C:3334:SER:O	1:C:3337:LYS:NZ	2.36	0.57
1:D:3369:ARG:O	1:D:3373:VAL:HG23	2.04	0.57
1:A:877:GLU:HG3	1:A:911:PHE:CG	2.39	0.57
1:A:3334:SER:O	1:A:3337:LYS:NZ	2.36	0.57
1:A:3369:ARG:O	1:A:3373:VAL:HG23	2.04	0.57
1:A:4752:ASN:O	1:A:4754:ARG:NH1	2.37	0.57
1:B:903:ARG:HA	1:B:903:ARG:NH2	2.19	0.57
1:B:3257:LEU:HD23	1:B:3267:MET:HE3	1.85	0.57
1:C:956:LEU:CG	1:C:967:LYS:HB2	2.34	0.57
1:A:956:LEU:CD2	1:A:968:PRO:HG2	2.33	0.57
1:A:2822:TRP:CE3	1:A:2875:MET:HE2	2.39	0.57
1:D:921:TYR:O	1:D:924:GLN:HG3	2.04	0.57
1:A:921:TYR:O	1:A:924:GLN:HG3	2.04	0.57
1:A:1987:MET:N	1:A:1987:MET:SD	2.74	0.57
1:A:2625:ARG:NH1	1:A:2907:VAL:HG21	2.20	0.57
1:A:2691:LYS:NZ	1:A:2692:TYR:O	2.37	0.57
1:B:877:GLU:HG3	1:B:911:PHE:CG	2.39	0.57
1:D:1426:GLU:OE1	1:D:1426:GLU:N	2.34	0.57
1:A:903:ARG:HA	1:A:903:ARG:NH2	2.19	0.57
1:A:956:LEU:HD11	1:A:968:PRO:HD2	1.86	0.57
1:B:2691:LYS:NZ	1:B:2692:TYR:O	2.37	0.57
1:B:876:ALA:HB1	1:B:923:LEU:HA	1.85	0.57
1:B:3377:GLU:OE2	1:B:3451:ASN:ND2	2.33	0.57
1:A:956:LEU:CG	1:A:967:LYS:HB2	2.34	0.57
1:A:3472:THR:HG23	1:B:1171:MET:HE3	1.86	0.57
1:B:911:PHE:HA	1:B:914:LEU:HD23	1.85	0.57
1:B:1116:LEU:HD12	1:B:1194:SER:HB2	1.86	0.57
1:B:2625:ARG:NH1	1:B:2907:VAL:HG21	2.20	0.57
1:C:958:LYS:HA	1:C:961:MET:CE	2.34	0.57
1:D:2691:LYS:NZ	1:D:2692:TYR:O	2.37	0.57
1:A:908:LEU:HD22	1:A:962:MET:HG3	1.87	0.57
1:B:921:TYR:O	1:B:924:GLN:HG3	2.04	0.57
1:C:908:LEU:HD22	1:C:962:MET:HG3	1.87	0.57
1:C:921:TYR:O	1:C:924:GLN:HG3	2.04	0.57
1:C:2001:SER:O	1:C:2006:GLN:NE2	2.37	0.57
1:C:2822:TRP:CE3	1:C:2875:MET:HE2	2.39	0.57
1:D:876:ALA:HB1	1:D:923:LEU:HA	1.85	0.57
1:A:1116:LEU:HD12	1:A:1194:SER:HB2	1.86	0.56
1:A:3570:LEU:H	1:A:3570:LEU:HD22	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2822:TRP:CE3	1:B:2875:MET:HE2	2.39	0.56
1:C:1116:LEU:HD12	1:C:1194:SER:HB2	1.86	0.56
1:D:877:GLU:HG3	1:D:911:PHE:CG	2.39	0.56
1:A:882:LEU:CA	1:A:970:PRO:HB3	2.36	0.56
1:A:3377:GLU:OE2	1:A:3451:ASN:ND2	2.33	0.56
1:B:1426:GLU:OE1	1:B:1426:GLU:N	2.34	0.56
1:B:3570:LEU:H	1:B:3570:LEU:HD22	1.71	0.56
1:C:956:LEU:HD11	1:C:968:PRO:HD2	1.86	0.56
1:D:911:PHE:HA	1:D:914:LEU:HD23	1.85	0.56
1:B:3369:ARG:O	1:B:3373:VAL:HG23	2.04	0.56
1:C:903:ARG:HA	1:C:903:ARG:NH2	2.19	0.56
1:C:2625:ARG:NH1	1:C:2907:VAL:HG21	2.20	0.56
1:C:2748:ILE:HA	1:C:2818:ILE:HD13	1.88	0.56
1:C:2752:LEU:HD12	1:C:2818:ILE:HD11	1.87	0.56
1:C:2755:PHE:CD2	1:C:2814:LEU:HD11	2.40	0.56
1:C:4753:GLU:C	1:C:4754:ARG:HD2	2.31	0.56
1:D:872:ARG:HH22	1:D:923:LEU:HD23	1.71	0.56
1:D:2625:ARG:NH1	1:D:2907:VAL:HG21	2.20	0.56
1:D:2752:LEU:HD12	1:D:2818:ILE:HD11	1.87	0.56
1:A:2022:CYS:O	1:A:2029:ARG:NH2	2.38	0.56
1:B:862:ILE:HG21	1:B:931:LYS:HA	1.88	0.56
1:C:956:LEU:CD2	1:C:968:PRO:HG2	2.33	0.56
1:D:956:LEU:HD11	1:D:968:PRO:HD2	1.86	0.56
1:A:872:ARG:HH22	1:A:923:LEU:HD23	1.71	0.56
1:A:942:MET:CE	1:A:945:GLU:HG3	2.35	0.56
1:A:4753:GLU:C	1:A:4754:ARG:HD2	2.31	0.56
1:C:2266:LEU:HD21	1:C:2327:CYS:HB2	1.88	0.56
1:C:3570:LEU:HD22	1:C:3570:LEU:H	1.71	0.56
1:A:2266:LEU:HD21	1:A:2327:CYS:HB2	1.88	0.56
1:C:942:MET:CE	1:C:945:GLU:HG3	2.35	0.56
8:C:8009:A1BYZ:C5	8:C:8009:A1BYZ:C9	2.84	0.56
1:D:2266:LEU:HD21	1:D:2327:CYS:HB2	1.88	0.56
1:D:4753:GLU:C	1:D:4754:ARG:HD2	2.31	0.56
1:D:871:ILE:HA	1:D:874:LYS:CD	2.33	0.56
1:D:2912:LEU:O	1:D:2917:LYS:NZ	2.32	0.56
1:D:3570:LEU:H	1:D:3570:LEU:HD22	1.71	0.56
1:B:2266:LEU:HD21	1:B:2327:CYS:HB2	1.88	0.56
1:B:4753:GLU:C	1:B:4754:ARG:HD2	2.31	0.56
8:B:8009:A1BYZ:C5	8:B:8009:A1BYZ:C9	2.84	0.56
1:C:882:LEU:CA	1:C:970:PRO:HB3	2.36	0.56
1:D:877:GLU:HG3	1:D:911:PHE:CB	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:882:LEU:CA	1:D:970:PRO:HB3	2.36	0.56
1:D:908:LEU:HD22	1:D:962:MET:HG3	1.87	0.56
1:D:1116:LEU:HD12	1:D:1194:SER:HB2	1.86	0.56
1:A:2743:THR:HG23	1:A:2744:LEU:N	2.21	0.56
1:A:2748:ILE:HA	1:A:2818:ILE:HD13	1.88	0.56
1:A:3422:ALA:HB1	1:B:1217:ILE:HD13	1.88	0.56
1:B:882:LEU:CA	1:B:970:PRO:HB3	2.36	0.56
1:B:908:LEU:HD22	1:B:962:MET:HG3	1.86	0.56
1:C:2743:THR:HG23	1:C:2744:LEU:N	2.21	0.56
1:D:903:ARG:HA	1:D:903:ARG:NH2	2.19	0.56
1:D:2022:CYS:O	1:D:2029:ARG:NH2	2.38	0.56
1:B:2755:PHE:CD2	1:B:2814:LEU:HD11	2.40	0.56
1:C:862:ILE:HG21	1:C:931:LYS:HA	1.88	0.56
1:C:871:ILE:HA	1:C:874:LYS:CD	2.33	0.56
1:D:942:MET:CE	1:D:945:GLU:HG3	2.35	0.56
1:A:877:GLU:HG3	1:A:911:PHE:CB	2.36	0.55
1:B:942:MET:CE	1:B:945:GLU:HG3	2.35	0.55
1:D:2743:THR:HG23	1:D:2744:LEU:N	2.21	0.55
1:A:4632:GLU:OE2	1:A:4634:THR:OG1	2.17	0.55
1:A:2752:LEU:HD12	1:A:2818:ILE:HD11	1.87	0.55
1:B:2748:ILE:HA	1:B:2818:ILE:HD13	1.88	0.55
1:D:2755:PHE:CD2	1:D:2814:LEU:HD11	2.40	0.55
1:A:2873:GLN:O	1:A:2877:GLU:HG2	2.07	0.55
1:B:1014:ILE:H	1:B:1014:ILE:HD12	1.72	0.55
1:D:862:ILE:HG21	1:D:931:LYS:HA	1.88	0.55
1:B:2743:THR:HG23	1:B:2744:LEU:N	2.21	0.55
1:D:908:LEU:HD22	1:D:962:MET:CG	2.37	0.55
1:D:3344:GLN:O	1:D:3347:VAL:HG12	2.07	0.55
1:D:4887:VAL:HG12	1:D:4898:GLU:HG3	1.89	0.55
1:A:3576:LEU:O	1:A:3580:VAL:HG23	2.07	0.55
1:A:4887:VAL:HG12	1:A:4898:GLU:HG3	1.89	0.55
1:B:2752:LEU:HD12	1:B:2818:ILE:HD11	1.87	0.55
1:C:908:LEU:HD22	1:C:962:MET:CG	2.37	0.55
1:C:2022:CYS:O	1:C:2029:ARG:NH2	2.38	0.55
1:D:2748:ILE:HA	1:D:2818:ILE:HD13	1.88	0.55
1:D:3576:LEU:O	1:D:3580:VAL:HG23	2.07	0.55
1:A:1014:ILE:H	1:A:1014:ILE:HD12	1.72	0.55
1:A:3847:LEU:HD13	1:B:77:ARG:NH1	2.22	0.55
1:B:2022:CYS:O	1:B:2029:ARG:NH2	2.38	0.55
8:D:8009:A1BYZ:C5	8:D:8009:A1BYZ:C9	2.84	0.55
8:A:8009:A1BYZ:C5	8:A:8009:A1BYZ:C9	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3576:LEU:O	1:B:3580:VAL:HG23	2.07	0.55
1:B:4887:VAL:HG12	1:B:4898:GLU:HG3	1.89	0.55
1:C:2873:GLN:O	1:C:2877:GLU:HG2	2.07	0.55
1:D:2520:LEU:HD13	1:D:2576:ARG:HG3	1.89	0.55
1:D:3450:HIS:O	1:D:3450:HIS:ND1	2.35	0.55
1:B:2873:GLN:O	1:B:2877:GLU:HG2	2.07	0.55
1:C:2520:LEU:HD13	1:C:2576:ARG:HG3	1.89	0.55
1:D:1014:ILE:H	1:D:1014:ILE:HD12	1.72	0.55
1:D:2873:GLN:O	1:D:2877:GLU:HG2	2.07	0.55
1:A:2755:PHE:CD2	1:A:2814:LEU:HD11	2.40	0.54
1:B:605:CYS:SG	1:B:1670:LEU:HD12	2.47	0.54
1:B:3536:LEU:HD23	1:B:3553:PHE:CZ	2.42	0.54
1:B:3861:MET:HE1	1:B:3870:ASN:HA	1.89	0.54
1:A:862:ILE:HG21	1:A:931:LYS:HA	1.88	0.54
1:B:908:LEU:HD22	1:B:962:MET:CG	2.37	0.54
1:C:877:GLU:HG3	1:C:911:PHE:CB	2.36	0.54
1:D:885:LEU:CD2	1:D:970:PRO:HG3	2.37	0.54
1:B:877:GLU:HG3	1:B:911:PHE:CB	2.36	0.54
1:C:872:ARG:HH22	1:C:923:LEU:HD23	1.71	0.54
1:C:1014:ILE:H	1:C:1014:ILE:HD12	1.72	0.54
1:D:605:CYS:SG	1:D:1670:LEU:HD12	2.47	0.54
1:A:3344:GLN:O	1:A:3347:VAL:HG12	2.07	0.54
1:B:872:ARG:HH22	1:B:923:LEU:HD23	1.71	0.54
1:B:2570:PHE:CE1	1:B:2583:MET:HE1	2.43	0.54
1:C:605:CYS:SG	1:C:1670:LEU:HD12	2.47	0.54
1:C:3344:GLN:O	1:C:3347:VAL:HG12	2.07	0.54
1:D:976:VAL:HG11	1:D:1045:ARG:O	2.08	0.54
1:D:2001:SER:O	1:D:2006:GLN:NE2	2.37	0.54
1:A:605:CYS:SG	1:A:1670:LEU:HD12	2.47	0.54
1:A:908:LEU:HD22	1:A:962:MET:CG	2.37	0.54
1:A:976:VAL:HG11	1:A:1045:ARG:O	2.08	0.54
1:B:2758:LYS:NZ	1:B:2831:GLU:O	2.24	0.54
1:B:3344:GLN:O	1:B:3347:VAL:HG12	2.07	0.54
1:C:2912:LEU:O	1:C:2917:LYS:NZ	2.32	0.54
1:A:2570:PHE:CE1	1:A:2583:MET:HE1	2.43	0.54
1:A:3456:GLU:OE2	1:A:3457:GLN:N	2.41	0.54
1:A:3536:LEU:HD23	1:A:3553:PHE:CZ	2.42	0.54
1:A:3861:MET:HE1	1:A:3870:ASN:HA	1.89	0.54
1:D:865:PRO:CD	1:D:868:LEU:HD12	2.38	0.54
1:B:942:MET:SD	1:B:945:GLU:HA	2.48	0.54
1:C:3576:LEU:O	1:C:3580:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4887:VAL:HG12	1:C:4898:GLU:HG3	1.89	0.54
8:C:8009:A1BYZ:C9	8:C:8009:A1BYZ:C4	2.86	0.54
8:B:8009:A1BYZ:C9	8:B:8009:A1BYZ:C4	2.86	0.54
1:C:976:VAL:HG11	1:C:1045:ARG:O	2.08	0.54
1:C:2570:PHE:CE1	1:C:2583:MET:HE1	2.43	0.54
1:C:3861:MET:HE1	1:C:3870:ASN:HA	1.89	0.54
1:B:976:VAL:HG11	1:B:1045:ARG:O	2.08	0.54
1:B:3456:GLU:OE2	1:B:3457:GLN:N	2.41	0.54
1:C:961:MET:HG3	1:C:967:LYS:HB3	1.90	0.54
1:D:2570:PHE:CE1	1:D:2583:MET:HE1	2.43	0.54
1:A:942:MET:SD	1:A:945:GLU:HA	2.48	0.54
1:B:894:TYR:H	1:B:962:MET:HB3	1.72	0.54
1:B:2520:LEU:HD13	1:B:2576:ARG:HG3	1.89	0.54
1:C:942:MET:SD	1:C:945:GLU:HA	2.48	0.54
1:D:875:LEU:HA	1:D:878:ASN:ND2	2.23	0.54
1:A:875:LEU:HA	1:A:878:ASN:ND2	2.23	0.53
1:B:2005:GLU:OE2	1:B:2005:GLU:HA	2.08	0.53
1:C:865:PRO:CD	1:C:868:LEU:HD12	2.38	0.53
1:C:894:TYR:H	1:C:962:MET:HB3	1.72	0.53
1:C:3536:LEU:HD23	1:C:3553:PHE:CZ	2.43	0.53
1:D:2758:LYS:NZ	1:D:2831:GLU:O	2.24	0.53
1:D:3536:LEU:HD23	1:D:3553:PHE:CZ	2.42	0.53
8:D:8009:A1BYZ:C9	8:D:8009:A1BYZ:C4	2.86	0.53
1:D:956:LEU:CD2	1:D:968:PRO:HG2	2.33	0.53
1:D:2005:GLU:HA	1:D:2005:GLU:OE2	2.08	0.53
1:D:3456:GLU:OE2	1:D:3457:GLN:N	2.41	0.53
1:A:914:LEU:HD21	1:A:919:ARG:HA	1.90	0.53
1:A:2005:GLU:HA	1:A:2005:GLU:OE2	2.08	0.53
1:C:658:THR:HG22	1:C:1002:VAL:CG2	2.39	0.53
1:C:3208:GLU:OE2	1:C:3306:THR:OG1	2.15	0.53
1:A:2520:LEU:HD13	1:A:2576:ARG:HG3	1.89	0.53
1:B:885:LEU:CD2	1:B:970:PRO:HG3	2.38	0.53
1:B:957:PRO:CG	1:B:960:TYR:HB2	2.38	0.53
1:C:2758:LYS:NZ	1:C:2831:GLU:O	2.24	0.53
1:A:908:LEU:O	1:A:909:VAL:HG13	2.09	0.53
1:A:956:LEU:HD11	1:A:960:TYR:HB3	1.90	0.53
1:A:961:MET:HG3	1:A:967:LYS:HB3	1.90	0.53
1:B:4935:ILE:HG12	1:C:4932:GLY:HA2	1.91	0.53
1:C:898:ARG:HB2	1:C:906:PRO:CD	2.39	0.53
1:C:908:LEU:O	1:C:909:VAL:HG13	2.09	0.53
1:D:894:TYR:H	1:D:962:MET:HB3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:914:LEU:HD21	1:D:919:ARG:HA	1.90	0.53
1:D:961:MET:HG3	1:D:967:LYS:HB3	1.90	0.53
1:B:882:LEU:HA	1:B:885:LEU:HD23	1.91	0.53
1:B:961:MET:HG3	1:B:967:LYS:HB3	1.90	0.53
1:D:658:THR:HG22	1:D:1002:VAL:CG2	2.39	0.53
1:D:3861:MET:HE1	1:D:3870:ASN:HA	1.89	0.53
1:A:865:PRO:CD	1:A:868:LEU:HD12	2.38	0.53
8:A:8009:A1BYZ:C9	8:A:8009:A1BYZ:C4	2.86	0.53
1:B:871:ILE:HA	1:B:874:LYS:CD	2.33	0.53
1:C:2480:LEU:HD13	1:C:2486:LEU:HD12	1.91	0.53
1:C:3546:THR:OG1	1:C:3548:GLU:OE2	2.15	0.53
1:D:898:ARG:HB2	1:D:906:PRO:CD	2.39	0.53
1:D:942:MET:SD	1:D:945:GLU:HA	2.48	0.53
1:A:894:TYR:H	1:A:962:MET:HB3	1.72	0.53
1:A:2756:ILE:CG1	1:A:2814:LEU:HD12	2.39	0.53
1:B:914:LEU:HD21	1:B:919:ARG:HA	1.90	0.53
1:C:956:LEU:CD2	1:C:960:TYR:HD2	2.22	0.53
1:A:885:LEU:CD2	1:A:970:PRO:HG3	2.37	0.53
1:A:956:LEU:HB2	1:A:967:LYS:HD2	1.91	0.53
1:B:956:LEU:HD11	1:B:960:TYR:HB3	1.90	0.53
1:C:914:LEU:HD21	1:C:919:ARG:HA	1.90	0.53
1:C:3847:LEU:HD13	1:D:77:ARG:NH1	2.24	0.53
1:A:882:LEU:HA	1:A:885:LEU:HD23	1.91	0.53
1:A:1171:MET:HE3	1:D:3472:THR:HG23	1.91	0.53
1:A:2758:LYS:NZ	1:A:2831:GLU:O	2.24	0.53
1:C:3456:GLU:OE2	1:C:3457:GLN:N	2.41	0.53
1:C:4935:ILE:HG12	1:D:4932:GLY:HA2	1.91	0.53
1:D:3377:GLU:OE2	1:D:3451:ASN:ND2	2.33	0.53
1:A:2265:GLY:O	1:A:2267:GLY:N	2.42	0.52
1:B:2822:TRP:CZ3	1:B:2875:MET:HE2	2.45	0.52
1:C:911:PHE:CE2	1:C:923:LEU:HG	2.44	0.52
1:C:2822:TRP:CZ3	1:C:2875:MET:HE2	2.45	0.52
1:D:908:LEU:O	1:D:909:VAL:HG13	2.09	0.52
1:A:871:ILE:HA	1:A:874:LYS:CD	2.33	0.52
1:A:2822:TRP:CZ3	1:A:2875:MET:HE2	2.45	0.52
1:A:4225:VAL:HG11	1:A:4948:VAL:HA	1.91	0.52
1:B:2756:ILE:CG1	1:B:2814:LEU:HD12	2.39	0.52
1:C:875:LEU:HA	1:C:878:ASN:ND2	2.23	0.52
1:D:956:LEU:HD11	1:D:960:TYR:HB3	1.90	0.52
1:D:2756:ILE:CG1	1:D:2814:LEU:HD12	2.39	0.52
1:D:2822:TRP:CZ3	1:D:2875:MET:HE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:ARG:CZ	1:A:870:ARG:HB3	2.39	0.52
1:A:892:TRP:CE2	1:A:903:ARG:HD3	2.44	0.52
1:B:865:PRO:CD	1:B:868:LEU:HD12	2.38	0.52
1:B:658:THR:HG22	1:B:1002:VAL:CG2	2.39	0.52
1:B:875:LEU:HA	1:B:878:ASN:ND2	2.23	0.52
1:C:882:LEU:HA	1:C:885:LEU:HD23	1.91	0.52
1:C:956:LEU:HB2	1:C:967:LYS:HD2	1.91	0.52
1:C:2005:GLU:HA	1:C:2005:GLU:OE2	2.08	0.52
1:D:885:LEU:HG	1:D:886:THR:N	2.25	0.52
1:B:908:LEU:O	1:B:909:VAL:HG13	2.09	0.52
1:B:3472:THR:HG23	1:C:1171:MET:HE3	1.90	0.52
1:B:3847:LEU:HD13	1:C:77:ARG:NH1	2.24	0.52
1:D:2480:LEU:HD13	1:D:2486:LEU:HD12	1.91	0.52
1:A:649:ILE:HG23	1:A:815:ALA:HB3	1.91	0.52
1:A:658:THR:HG22	1:A:1002:VAL:CG2	2.39	0.52
1:A:2001:SER:O	1:A:2006:GLN:NE2	2.38	0.52
1:A:2884:HIS:CE1	1:A:2912:LEU:HD11	2.45	0.52
1:B:956:LEU:CD2	1:B:960:TYR:HD2	2.22	0.52
1:B:956:LEU:HB2	1:B:967:LYS:HD2	1.91	0.52
1:B:2884:HIS:CE1	1:B:2912:LEU:HD11	2.45	0.52
1:B:4225:VAL:HG11	1:B:4948:VAL:HA	1.91	0.52
1:D:892:TRP:CE2	1:D:903:ARG:HD3	2.44	0.52
1:D:911:PHE:CE2	1:D:923:LEU:HG	2.44	0.52
1:B:892:TRP:CE2	1:B:903:ARG:HD3	2.44	0.52
1:B:4649:THR:OG1	1:B:4801:HIS:NE2	2.39	0.52
1:C:892:TRP:CE2	1:C:903:ARG:HD3	2.44	0.52
1:C:2265:GLY:O	1:C:2267:GLY:N	2.42	0.52
1:C:2884:HIS:CE1	1:C:2912:LEU:HD11	2.45	0.52
1:C:3472:THR:HG23	1:D:1171:MET:HE3	1.90	0.52
1:C:4244:THR:HG22	1:C:4248:MET:HE3	1.92	0.52
1:D:979:THR:H	1:D:982:GLN:HB2	1.75	0.52
1:D:2265:GLY:O	1:D:2267:GLY:N	2.42	0.52
1:A:956:LEU:CD2	1:A:960:TYR:HD2	2.22	0.52
1:A:2480:LEU:HD13	1:A:2486:LEU:HD12	1.91	0.52
1:B:911:PHE:CE2	1:B:923:LEU:HG	2.44	0.52
1:C:979:THR:H	1:C:982:GLN:HB2	1.75	0.52
1:A:3384:ALA:N	1:A:3387:GLU:OE1	2.41	0.52
1:B:898:ARG:HB2	1:B:906:PRO:CD	2.39	0.52
1:B:4244:THR:HG22	1:B:4248:MET:HE3	1.92	0.52
1:D:882:LEU:HA	1:D:885:LEU:HD23	1.91	0.52
1:D:956:LEU:CD2	1:D:960:TYR:HD2	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1758:GLY:N	1:D:1759:PRO:CD	2.73	0.52
1:A:911:PHE:CE2	1:A:923:LEU:HG	2.44	0.52
1:B:331:ASP:OD1	1:B:331:ASP:C	2.53	0.52
1:C:870:ARG:HB3	1:C:870:ARG:CZ	2.39	0.52
1:C:1455:THR:OG1	1:C:1457:ASP:OD1	2.27	0.52
1:C:1758:GLY:N	1:C:1759:PRO:CD	2.73	0.52
1:B:2001:SER:O	1:B:2006:GLN:NE2	2.37	0.51
1:B:2265:GLY:O	1:B:2267:GLY:N	2.42	0.51
1:C:894:TYR:CB	1:C:962:MET:HB3	2.40	0.51
1:D:870:ARG:CZ	1:D:870:ARG:HB3	2.39	0.51
1:D:1455:THR:OG1	1:D:1457:ASP:OD1	2.28	0.51
1:A:898:ARG:HB2	1:A:906:PRO:CD	2.39	0.51
1:A:1455:THR:OG1	1:A:1457:ASP:OD1	2.27	0.51
1:A:4244:THR:HG22	1:A:4248:MET:HE3	1.92	0.51
1:B:649:ILE:HG23	1:B:815:ALA:HB3	1.92	0.51
1:B:893:THR:HA	1:B:962:MET:SD	2.51	0.51
1:B:942:MET:HE3	1:B:945:GLU:HG3	1.92	0.51
1:D:2751:LYS:O	1:D:2754:SER:OG	2.26	0.51
1:D:4086:ASP:OD1	1:D:4088:ARG:NH2	2.43	0.51
1:D:4244:THR:HG22	1:D:4248:MET:HE3	1.92	0.51
1:A:942:MET:HE3	1:A:945:GLU:HG3	1.92	0.51
1:A:957:PRO:CG	1:A:960:TYR:HB2	2.38	0.51
1:A:3541:TYR:HB3	1:A:3605:TYR:HD2	1.75	0.51
1:A:4893:GLY:N	1:A:4897:ASP:OD1	2.41	0.51
1:B:881:GLU:HB3	1:B:970:PRO:N	2.25	0.51
1:C:2756:ILE:CG1	1:C:2814:LEU:HD12	2.39	0.51
1:D:894:TYR:CB	1:D:962:MET:HB3	2.40	0.51
1:B:870:ARG:HB3	1:B:870:ARG:CZ	2.39	0.51
1:C:331:ASP:C	1:C:331:ASP:OD1	2.53	0.51
1:D:957:PRO:CG	1:D:960:TYR:HB2	2.38	0.51
1:A:894:TYR:CB	1:A:962:MET:HB3	2.40	0.51
1:A:2751:LYS:O	1:A:2754:SER:OG	2.26	0.51
1:B:1455:THR:OG1	1:B:1457:ASP:OD1	2.27	0.51
1:B:2948:ASP:OD1	1:B:2948:ASP:N	2.44	0.51
1:C:893:THR:HA	1:C:962:MET:SD	2.51	0.51
1:C:956:LEU:HD11	1:C:960:TYR:HB3	1.90	0.51
1:C:1222:GLU:OE1	1:C:1222:GLU:N	2.40	0.51
1:D:2884:HIS:CE1	1:D:2912:LEU:HD11	2.45	0.51
1:D:4225:VAL:HG11	1:D:4948:VAL:HA	1.91	0.51
1:A:1222:GLU:OE1	1:A:1222:GLU:N	2.40	0.51
1:A:1758:GLY:N	1:A:1759:PRO:CD	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:881:GLU:HB3	1:C:970:PRO:N	2.25	0.51
1:C:885:LEU:CD2	1:C:970:PRO:HG3	2.37	0.51
1:C:1113:ASP:OD1	1:C:1113:ASP:N	2.41	0.51
1:C:3447:SER:O	1:C:3453:LYS:NZ	2.40	0.51
1:D:956:LEU:HB2	1:D:967:LYS:HD2	1.91	0.51
1:D:4649:THR:OG1	1:D:4801:HIS:NE2	2.39	0.51
1:A:876:ALA:HB2	1:A:923:LEU:HA	1.92	0.51
1:A:885:LEU:HG	1:A:886:THR:N	2.25	0.51
1:A:911:PHE:CZ	1:A:923:LEU:HG	2.46	0.51
1:A:3105:GLU:O	1:A:3108:VAL:HG12	2.11	0.51
1:B:1758:GLY:N	1:B:1759:PRO:CD	2.73	0.51
1:B:4086:ASP:OD1	1:B:4088:ARG:NH2	2.43	0.51
1:C:2215:VAL:HG11	1:C:2229:MET:HE2	1.93	0.51
1:D:2215:VAL:HG11	1:D:2229:MET:HE2	1.93	0.51
1:D:3388:ALA:O	1:D:3392:GLU:N	2.39	0.51
1:A:4649:THR:OG1	1:A:4801:HIS:NE2	2.39	0.51
1:B:894:TYR:CB	1:B:962:MET:HB3	2.40	0.51
1:B:952:LYS:O	1:B:972:ASP:HB3	2.11	0.51
1:B:2215:VAL:HG11	1:B:2229:MET:HE2	1.93	0.51
1:B:4893:GLY:N	1:B:4897:ASP:OD1	2.41	0.51
1:A:2215:VAL:HG11	1:A:2229:MET:HE2	1.93	0.51
1:A:4800:GLY:HA2	1:A:4806:PHE:HB2	1.93	0.51
1:B:885:LEU:HG	1:B:886:THR:N	2.25	0.51
1:B:979:THR:H	1:B:982:GLN:HB2	1.75	0.51
1:B:1222:GLU:OE1	1:B:1222:GLU:N	2.40	0.51
1:C:912:HIS:HA	1:C:919:ARG:NH1	2.26	0.51
1:D:3347:VAL:HG11	1:D:3415:ARG:HB2	1.93	0.51
1:D:4800:GLY:HA2	1:D:4806:PHE:HB2	1.93	0.51
1:A:331:ASP:C	1:A:331:ASP:OD1	2.53	0.51
1:A:893:THR:HA	1:A:962:MET:SD	2.51	0.51
1:B:911:PHE:CZ	1:B:923:LEU:HG	2.46	0.51
1:C:862:ILE:HB	1:C:931:LYS:HE2	1.93	0.51
1:D:876:ALA:HB2	1:D:923:LEU:HA	1.92	0.51
1:D:3384:ALA:N	1:D:3387:GLU:OE1	2.41	0.51
1:A:952:LYS:O	1:A:972:ASP:HB3	2.11	0.50
1:A:3472:THR:HG23	1:B:1171:MET:CE	2.42	0.50
1:B:2480:LEU:HD13	1:B:2486:LEU:HD12	1.91	0.50
1:C:876:ALA:HB2	1:C:923:LEU:HA	1.92	0.50
1:C:952:LYS:O	1:C:972:ASP:HB3	2.11	0.50
1:D:649:ILE:HG23	1:D:815:ALA:HB3	1.92	0.50
1:D:881:GLU:HB3	1:D:970:PRO:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:952:LYS:O	1:D:972:ASP:HB3	2.11	0.50
1:A:1048:LEU:HD21	1:A:1054:ILE:CG1	2.42	0.50
1:A:1300:GLN:O	1:A:1300:GLN:NE2	2.41	0.50
1:B:876:ALA:HB2	1:B:923:LEU:HA	1.92	0.50
1:C:4086:ASP:OD1	1:C:4088:ARG:NH2	2.43	0.50
1:C:4225:VAL:HG11	1:C:4948:VAL:HA	1.91	0.50
1:D:942:MET:HE3	1:D:945:GLU:HG3	1.92	0.50
1:B:658:THR:HG22	1:B:1002:VAL:HG21	1.94	0.50
1:B:912:HIS:HA	1:B:919:ARG:NH1	2.26	0.50
1:B:2912:LEU:O	1:B:2917:LYS:NZ	2.32	0.50
1:C:649:ILE:HG23	1:C:815:ALA:HB3	1.92	0.50
1:C:911:PHE:CZ	1:C:923:LEU:HG	2.46	0.50
1:A:979:THR:H	1:A:982:GLN:HB2	1.75	0.50
1:B:964:ASN:OD1	1:B:966:TYR:HB3	2.11	0.50
1:B:2234:CYS:C	1:B:2236:PHE:N	2.70	0.50
1:B:3105:GLU:O	1:B:3108:VAL:HG12	2.11	0.50
1:C:3541:TYR:HB3	1:C:3605:TYR:HD2	1.75	0.50
1:C:3542:ALA:O	1:C:3544:LYS:HE3	2.11	0.50
1:A:862:ILE:HB	1:A:931:LYS:HE2	1.93	0.50
1:A:2218:GLY:O	1:A:2225:ARG:NH1	2.38	0.50
1:A:3542:ALA:O	1:A:3544:LYS:HE3	2.11	0.50
1:C:942:MET:HE3	1:C:945:GLU:HG3	1.91	0.50
1:D:331:ASP:C	1:D:331:ASP:OD1	2.53	0.50
1:D:893:THR:HA	1:D:962:MET:SD	2.51	0.50
1:D:1300:GLN:O	1:D:1300:GLN:NE2	2.41	0.50
1:D:2218:GLY:O	1:D:2225:ARG:NH1	2.38	0.50
1:A:912:HIS:HA	1:A:919:ARG:NH1	2.26	0.50
1:A:2948:ASP:N	1:A:2948:ASP:OD1	2.44	0.50
1:A:3347:VAL:HG11	1:A:3415:ARG:HB2	1.93	0.50
1:C:4800:GLY:HA2	1:C:4806:PHE:HB2	1.93	0.50
1:D:911:PHE:CZ	1:D:923:LEU:HG	2.46	0.50
1:D:3105:GLU:O	1:D:3108:VAL:HG12	2.11	0.50
1:A:658:THR:HG22	1:A:1002:VAL:HG21	1.94	0.50
1:A:3584:GLU:OE1	1:A:3584:GLU:N	2.42	0.50
1:B:3459:PHE:C	1:B:3459:PHE:CD2	2.90	0.50
1:B:3541:TYR:HB3	1:B:3605:TYR:HD2	1.75	0.50
1:B:3542:ALA:O	1:B:3544:LYS:HE3	2.11	0.50
1:C:964:ASN:OD1	1:C:966:TYR:HB3	2.11	0.50
1:D:2971:SER:HA	1:D:2974:PHE:CE2	2.47	0.50
1:D:3584:GLU:OE1	1:D:3584:GLU:N	2.42	0.50
1:B:862:ILE:HB	1:B:931:LYS:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2948:ASP:OD1	1:C:2948:ASP:N	2.44	0.50
1:C:3105:GLU:O	1:C:3108:VAL:HG12	2.11	0.50
1:C:957:PRO:CG	1:C:960:TYR:HB2	2.38	0.50
1:C:2910:ASP:OD1	1:C:2911:THR:N	2.45	0.50
1:A:881:GLU:HB3	1:A:970:PRO:N	2.25	0.49
1:A:2872:LEU:O	1:A:2875:MET:HB3	2.12	0.49
1:A:2971:SER:HA	1:A:2974:PHE:CE2	2.47	0.49
1:B:4800:GLY:HA2	1:B:4806:PHE:HB2	1.93	0.49
1:C:1048:LEU:HD21	1:C:1054:ILE:CG1	2.42	0.49
1:C:2971:SER:HA	1:C:2974:PHE:CE2	2.47	0.49
1:D:912:HIS:HA	1:D:919:ARG:NH1	2.26	0.49
1:D:2949:THR:OG1	1:D:2950:SER:N	2.46	0.49
1:D:3347:VAL:HG11	1:D:3415:ARG:CB	2.42	0.49
1:D:3459:PHE:C	1:D:3459:PHE:CD2	2.90	0.49
1:A:3347:VAL:HG11	1:A:3415:ARG:CB	2.42	0.49
1:C:658:THR:HG22	1:C:1002:VAL:HG21	1.94	0.49
1:D:3541:TYR:HB3	1:D:3605:TYR:HD2	1.75	0.49
1:B:953:LYS:HA	1:B:971:LEU:HA	1.94	0.49
1:B:3347:VAL:HG11	1:B:3415:ARG:HB2	1.93	0.49
1:C:953:LYS:HA	1:C:971:LEU:HA	1.94	0.49
1:D:2234:CYS:C	1:D:2236:PHE:N	2.70	0.49
1:D:2948:ASP:N	1:D:2948:ASP:OD1	2.44	0.49
1:A:3459:PHE:C	1:A:3459:PHE:CD2	2.90	0.49
1:B:2438:ALA:HB2	1:B:2510:VAL:HG22	1.95	0.49
1:B:3347:VAL:HG11	1:B:3415:ARG:CB	2.42	0.49
1:B:3422:ALA:HB1	1:C:1217:ILE:HD13	1.94	0.49
1:C:885:LEU:HG	1:C:886:THR:N	2.25	0.49
1:C:956:LEU:HD22	1:C:957:PRO:CD	2.39	0.49
1:D:658:THR:HG22	1:D:1002:VAL:HG21	1.94	0.49
1:D:953:LYS:HA	1:D:971:LEU:HA	1.94	0.49
1:D:956:LEU:HB2	1:D:967:LYS:NZ	2.28	0.49
1:A:926:SER:O	1:A:930:LEU:HD22	2.13	0.49
1:A:982:GLN:HG2	1:A:1054:ILE:HD11	1.95	0.49
1:B:2872:LEU:O	1:B:2875:MET:HB3	2.12	0.49
1:C:2928:LEU:O	1:C:2928:LEU:HD13	2.13	0.49
1:D:964:ASN:OD1	1:D:966:TYR:HB3	2.11	0.49
1:D:4632:GLU:OE2	1:D:4634:THR:OG1	2.17	0.49
1:B:884:ALA:O	1:B:888:ILE:HG22	2.13	0.49
1:B:3384:ALA:N	1:B:3387:GLU:OE1	2.41	0.49
1:C:3347:VAL:HG11	1:C:3415:ARG:CB	2.42	0.49
1:C:3347:VAL:HG11	1:C:3415:ARG:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:910:ASN:H	1:D:913:SER:HB3	1.78	0.49
1:D:2928:LEU:O	1:D:2928:LEU:HD13	2.13	0.49
1:A:884:ALA:O	1:A:888:ILE:HG22	2.13	0.49
1:A:910:ASN:H	1:A:913:SER:HB3	1.78	0.49
1:A:2438:ALA:HB2	1:A:2510:VAL:HG22	1.95	0.49
1:B:870:ARG:HH21	1:B:871:ILE:HG23	1.78	0.49
1:C:926:SER:O	1:C:930:LEU:HD22	2.13	0.49
1:C:956:LEU:HB2	1:C:967:LYS:NZ	2.28	0.49
1:C:3388:ALA:O	1:C:3392:GLU:N	2.39	0.49
1:D:870:ARG:HH21	1:D:871:ILE:HG23	1.78	0.49
1:D:2872:LEU:O	1:D:2875:MET:HB3	2.12	0.49
1:D:3208:GLU:OE2	1:D:3306:THR:OG1	2.15	0.49
1:A:890:GLN:HB2	1:A:892:TRP:HD1	1.78	0.49
1:A:953:LYS:HA	1:A:971:LEU:HA	1.94	0.49
1:C:903:ARG:C	1:C:904:LEU:HD23	2.38	0.49
1:D:862:ILE:HB	1:D:931:LYS:HE2	1.93	0.49
1:D:1048:LEU:HD21	1:D:1054:ILE:CG1	2.42	0.49
1:A:964:ASN:OD1	1:A:966:TYR:HB3	2.11	0.49
1:A:3447:SER:O	1:A:3453:LYS:NZ	2.40	0.49
1:A:4935:ILE:HG12	1:B:4932:GLY:HA2	1.95	0.49
1:C:878:ASN:O	1:C:881:GLU:HB2	2.13	0.49
1:C:890:GLN:HB2	1:C:892:TRP:HD1	1.78	0.49
1:D:890:GLN:HB2	1:D:892:TRP:HD1	1.78	0.49
1:D:899:ASP:CB	1:D:902:LYS:HB2	2.33	0.49
1:D:3542:ALA:O	1:D:3544:LYS:HE3	2.11	0.49
1:B:956:LEU:HD22	1:B:957:PRO:CD	2.39	0.49
1:C:2949:THR:OG1	1:C:2950:SER:N	2.46	0.49
1:C:3422:ALA:HB1	1:D:1217:ILE:HD13	1.94	0.49
1:C:3459:PHE:C	1:C:3459:PHE:CD2	2.90	0.49
1:D:903:ARG:C	1:D:904:LEU:HD23	2.38	0.49
1:D:956:LEU:HB3	1:D:967:LYS:HB2	1.94	0.49
1:D:1758:GLY:N	1:D:1759:PRO:HD2	2.28	0.49
1:A:956:LEU:HB3	1:A:967:LYS:HB2	1.94	0.48
1:A:2234:CYS:C	1:A:2236:PHE:N	2.70	0.48
1:A:2910:ASP:OD1	1:A:2911:THR:N	2.45	0.48
1:A:2949:THR:OG1	1:A:2950:SER:N	2.45	0.48
1:A:4086:ASP:OD1	1:A:4088:ARG:NH2	2.43	0.48
1:B:870:ARG:NH2	1:B:871:ILE:HG23	2.28	0.48
1:B:895:GLY:O	1:B:906:PRO:HA	2.13	0.48
1:B:910:ASN:H	1:B:913:SER:HB3	1.78	0.48
1:B:926:SER:O	1:B:930:LEU:HD22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2910:ASP:OD1	1:B:2911:THR:N	2.45	0.48
1:B:2928:LEU:HD13	1:B:2928:LEU:O	2.13	0.48
1:B:2969:ASP:O	1:B:2973:GLU:OE2	2.31	0.48
1:C:1758:GLY:N	1:C:1759:PRO:HD2	2.28	0.48
1:C:2872:LEU:O	1:C:2875:MET:HB3	2.12	0.48
1:D:884:ALA:O	1:D:888:ILE:HG22	2.13	0.48
1:D:926:SER:O	1:D:930:LEU:HD22	2.13	0.48
1:A:3243:ASP:N	1:A:3243:ASP:OD1	2.46	0.48
1:B:1048:LEU:HD21	1:B:1054:ILE:CG1	2.42	0.48
1:B:1758:GLY:N	1:B:1759:PRO:HD2	2.28	0.48
1:B:3450:HIS:O	1:B:3450:HIS:ND1	2.35	0.48
1:C:884:ALA:O	1:C:888:ILE:HG22	2.13	0.48
1:C:956:LEU:HB3	1:C:967:LYS:HB2	1.94	0.48
1:C:2761:GLU:OE2	1:C:2795:TYR:CG	2.66	0.48
1:B:890:GLN:HB2	1:B:892:TRP:HD1	1.78	0.48
1:C:2751:LYS:O	1:C:2754:SER:OG	2.26	0.48
1:D:982:GLN:HG2	1:D:1054:ILE:HD11	1.95	0.48
1:D:2438:ALA:HB2	1:D:2510:VAL:HG22	1.95	0.48
1:D:2761:GLU:OE2	1:D:2795:TYR:CG	2.67	0.48
1:D:2802:ASP:OD1	1:D:2803:LYS:N	2.46	0.48
1:A:895:GLY:O	1:A:906:PRO:HA	2.13	0.48
1:A:956:LEU:HB2	1:A:967:LYS:NZ	2.27	0.48
1:A:2928:LEU:O	1:A:2928:LEU:HD13	2.13	0.48
1:B:2971:SER:HA	1:B:2974:PHE:CE2	2.47	0.48
1:D:1222:GLU:OE1	1:D:1222:GLU:N	2.40	0.48
1:D:2969:ASP:O	1:D:2973:GLU:OE2	2.31	0.48
1:A:870:ARG:HH21	1:A:871:ILE:HG23	1.78	0.48
1:A:870:ARG:NH2	1:A:871:ILE:HG23	2.28	0.48
1:A:888:ILE:HG21	1:A:960:TYR:CG	2.49	0.48
1:A:1102:ARG:NH1	1:A:1116:LEU:O	2.44	0.48
1:A:1758:GLY:N	1:A:1759:PRO:HD2	2.28	0.48
1:A:2743:THR:HG23	1:A:2744:LEU:H	1.77	0.48
1:B:878:ASN:O	1:B:881:GLU:HB2	2.13	0.48
1:B:888:ILE:HG21	1:B:960:TYR:CG	2.49	0.48
1:C:870:ARG:HH21	1:C:871:ILE:HG23	1.78	0.48
1:C:895:GLY:O	1:C:906:PRO:HA	2.13	0.48
1:C:989:LEU:HB3	1:C:1040:LEU:HD12	1.95	0.48
1:D:956:LEU:HD22	1:D:957:PRO:CD	2.39	0.48
1:A:2761:GLU:OE2	1:A:2795:TYR:CG	2.66	0.48
1:B:903:ARG:C	1:B:904:LEU:HD23	2.38	0.48
1:B:956:LEU:HB2	1:B:967:LYS:NZ	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2761:GLU:OE2	1:B:2795:TYR:CG	2.67	0.48
1:C:942:MET:HE2	1:C:1052:TYR:CE2	2.49	0.48
1:C:1102:ARG:NH1	1:C:1116:LEU:O	2.45	0.48
1:C:2802:ASP:OD1	1:C:2803:LYS:N	2.46	0.48
1:C:2969:ASP:O	1:C:2973:GLU:OE2	2.31	0.48
1:C:4235:GLU:OE2	1:C:5015:ARG:NH2	2.47	0.48
1:D:1266:ASP:OD1	1:D:1266:ASP:N	2.47	0.48
1:D:2910:ASP:OD1	1:D:2911:THR:N	2.45	0.48
1:B:2751:LYS:O	1:B:2754:SER:OG	2.26	0.48
1:B:3540:ARG:HD2	1:B:3545:ASP:OD2	2.14	0.48
1:C:888:ILE:HG21	1:C:960:TYR:CG	2.49	0.48
1:D:868:LEU:HA	1:D:871:ILE:CD1	2.44	0.48
1:D:878:ASN:O	1:D:881:GLU:HB2	2.13	0.48
1:D:932:THR:O	1:D:936:LEU:HG	2.14	0.48
1:A:868:LEU:HA	1:A:871:ILE:CD1	2.44	0.48
1:A:932:THR:O	1:A:936:LEU:HG	2.14	0.48
1:A:989:LEU:HB3	1:A:1040:LEU:HD12	1.95	0.48
1:B:2802:ASP:OD1	1:B:2803:LYS:N	2.46	0.48
1:C:870:ARG:NH2	1:C:871:ILE:HG23	2.28	0.48
1:C:902:LYS:HD2	1:C:902:LYS:HA	1.41	0.48
1:C:2438:ALA:HB2	1:C:2510:VAL:HG22	1.95	0.48
1:D:3243:ASP:N	1:D:3243:ASP:OD1	2.46	0.48
1:D:3540:ARG:HD2	1:D:3545:ASP:OD2	2.14	0.48
1:A:942:MET:HE2	1:A:1052:TYR:CE2	2.49	0.48
1:A:3540:ARG:O	1:A:3541:TYR:C	2.57	0.48
1:A:3540:ARG:HD2	1:A:3545:ASP:OD2	2.14	0.48
1:B:3388:ALA:O	1:B:3392:GLU:N	2.39	0.48
1:C:3243:ASP:OD1	1:C:3243:ASP:N	2.46	0.48
1:D:875:LEU:CB	1:D:926:SER:HB2	2.43	0.48
1:D:888:ILE:HG21	1:D:960:TYR:CG	2.49	0.48
1:D:895:GLY:O	1:D:906:PRO:HA	2.13	0.48
1:A:2969:ASP:O	1:A:2973:GLU:OE2	2.31	0.48
1:B:932:THR:O	1:B:936:LEU:HG	2.14	0.48
1:B:3584:GLU:OE1	1:B:3584:GLU:N	2.43	0.48
1:C:868:LEU:HA	1:C:871:ILE:CD1	2.44	0.48
1:C:914:LEU:CD2	1:C:919:ARG:HB2	2.44	0.48
1:C:932:THR:O	1:C:936:LEU:HG	2.14	0.48
1:D:871:ILE:H	1:D:871:ILE:HG13	1.40	0.48
1:D:2947:LEU:O	1:D:2950:SER:OG	2.26	0.48
1:D:4893:GLY:N	1:D:4897:ASP:OD1	2.41	0.48
1:B:868:LEU:HA	1:B:871:ILE:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:942:MET:HE2	1:B:1052:TYR:CE2	2.49	0.47
1:B:989:LEU:HB3	1:B:1040:LEU:HD12	1.95	0.47
1:C:885:LEU:HD12	1:C:960:TYR:HE2	1.79	0.47
1:C:910:ASN:H	1:C:913:SER:HB3	1.78	0.47
1:C:911:PHE:O	1:C:914:LEU:HD23	2.14	0.47
1:C:919:ARG:HG3	1:C:923:LEU:CD1	2.44	0.47
1:C:1300:GLN:O	1:C:1300:GLN:NE2	2.41	0.47
1:C:2234:CYS:C	1:C:2236:PHE:N	2.70	0.47
1:D:898:ARG:HB2	1:D:906:PRO:HD3	1.96	0.47
1:D:911:PHE:O	1:D:914:LEU:HD23	2.14	0.47
1:D:942:MET:HE2	1:D:1052:TYR:CE2	2.49	0.47
1:A:903:ARG:HA	1:A:903:ARG:NE	2.29	0.47
1:A:911:PHE:O	1:A:914:LEU:HD23	2.14	0.47
1:A:1072:ARG:HA	1:A:1072:ARG:HE	1.79	0.47
1:A:2802:ASP:OD1	1:A:2803:LYS:N	2.46	0.47
2:H:12:ASP:OD2	2:H:12:ASP:C	2.57	0.47
1:B:911:PHE:O	1:B:914:LEU:HD23	2.14	0.47
1:B:914:LEU:CD2	1:B:919:ARG:HB2	2.44	0.47
1:B:919:ARG:HG3	1:B:923:LEU:CD1	2.44	0.47
1:B:4235:GLU:OE2	1:B:5015:ARG:NH2	2.47	0.47
1:D:870:ARG:NH2	1:D:871:ILE:HG23	2.28	0.47
1:D:903:ARG:HA	1:D:903:ARG:NE	2.29	0.47
1:D:4235:GLU:OE2	1:D:5015:ARG:NH2	2.47	0.47
1:A:985:LEU:HD13	1:A:1057:PRO:HD2	1.96	0.47
1:B:956:LEU:HB3	1:B:967:LYS:HB2	1.94	0.47
1:B:2391:PRO:O	1:B:2392:ALA:HB3	2.15	0.47
1:B:2949:THR:OG1	1:B:2950:SER:N	2.45	0.47
1:C:898:ARG:HB2	1:C:906:PRO:HD3	1.96	0.47
1:D:914:LEU:CD2	1:D:919:ARG:HB2	2.44	0.47
1:A:875:LEU:CB	1:A:926:SER:HB2	2.44	0.47
1:B:885:LEU:HD12	1:B:960:TYR:HE2	1.79	0.47
1:C:982:GLN:HG2	1:C:1054:ILE:HD11	1.95	0.47
1:C:4830:HIS:NE2	1:C:4940:GLU:OE1	2.48	0.47
1:D:985:LEU:HD13	1:D:1057:PRO:HD2	1.96	0.47
1:A:878:ASN:O	1:A:881:GLU:HB2	2.13	0.47
1:A:914:LEU:CD2	1:A:919:ARG:HB2	2.44	0.47
1:A:3468:MET:SD	1:B:1174:SER:O	2.72	0.47
1:A:4235:GLU:OE2	1:A:5015:ARG:NH2	2.47	0.47
2:G:12:ASP:OD2	2:G:12:ASP:C	2.57	0.47
1:B:982:GLN:HG2	1:B:1054:ILE:HD11	1.95	0.47
1:B:3389:GLU:O	1:B:3393:LEU:HD23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4830:HIS:NE2	1:B:4940:GLU:OE1	2.48	0.47
1:C:2234:CYS:O	1:C:2236:PHE:C	2.58	0.47
1:C:2743:THR:HG23	1:C:2744:LEU:H	1.77	0.47
1:D:885:LEU:HD12	1:D:960:TYR:HE2	1.79	0.47
1:D:905:HIS:O	1:D:908:LEU:HB2	2.15	0.47
1:D:1072:ARG:HA	1:D:1072:ARG:HE	1.79	0.47
1:A:903:ARG:C	1:A:904:LEU:HD23	2.38	0.47
1:A:1266:ASP:N	1:A:1266:ASP:OD1	2.47	0.47
1:A:2391:PRO:O	1:A:2392:ALA:HB3	2.15	0.47
2:F:12:ASP:OD2	2:F:12:ASP:C	2.57	0.47
1:B:877:GLU:HA	1:B:911:PHE:CD1	2.49	0.47
1:B:903:ARG:HA	1:B:903:ARG:NE	2.29	0.47
1:B:1300:GLN:O	1:B:1300:GLN:NE2	2.41	0.47
1:A:877:GLU:HA	1:A:911:PHE:CD1	2.49	0.47
1:A:885:LEU:HD12	1:A:960:TYR:HE2	1.79	0.47
1:A:956:LEU:HD22	1:A:957:PRO:CD	2.39	0.47
2:E:12:ASP:OD2	2:E:12:ASP:C	2.57	0.47
1:B:440:GLU:CD	1:B:440:GLU:H	2.22	0.47
1:B:905:HIS:O	1:B:908:LEU:HB2	2.15	0.47
1:B:978:LEU:HD22	1:B:982:GLN:OE1	2.15	0.47
1:B:986:VAL:HA	1:B:989:LEU:HD12	1.97	0.47
1:B:1102:ARG:NH1	1:B:1116:LEU:O	2.45	0.47
1:B:2218:GLY:O	1:B:2225:ARG:NH1	2.38	0.47
1:B:2234:CYS:O	1:B:2236:PHE:C	2.58	0.47
1:B:2743:THR:HG23	1:B:2744:LEU:H	1.77	0.47
1:B:4789:TYR:OH	1:B:4813:ASP:OD1	2.28	0.47
1:C:877:GLU:HA	1:C:911:PHE:CD1	2.49	0.47
1:C:899:ASP:CB	1:C:902:LYS:HB2	2.33	0.47
1:C:903:ARG:HA	1:C:903:ARG:NE	2.29	0.47
1:C:905:HIS:O	1:C:908:LEU:HB2	2.15	0.47
1:C:1266:ASP:OD1	1:C:1266:ASP:N	2.47	0.47
1:C:2926:GLU:OE1	1:C:2926:GLU:HA	2.15	0.47
1:C:2947:LEU:O	1:C:2950:SER:OG	2.26	0.47
1:C:3389:GLU:O	1:C:3393:LEU:HD23	2.15	0.47
1:D:440:GLU:H	1:D:440:GLU:CD	2.22	0.47
1:D:989:LEU:HB3	1:D:1040:LEU:HD12	1.95	0.47
1:A:77:ARG:NH1	1:D:3847:LEU:HD13	2.29	0.47
1:A:894:TYR:HB3	1:A:964:ASN:H	1.80	0.47
1:A:905:HIS:O	1:A:908:LEU:HB2	2.15	0.47
1:A:2876:ALA:HB3	1:A:2921:ARG:HH12	1.79	0.47
1:A:3389:GLU:O	1:A:3393:LEU:HD23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:19:ARG:HB3	2:E:19:ARG:NH1	2.30	0.47
1:C:875:LEU:CB	1:C:926:SER:HB2	2.44	0.47
1:C:978:LEU:HD22	1:C:982:GLN:OE1	2.15	0.47
1:C:2391:PRO:O	1:C:2392:ALA:HB3	2.15	0.47
1:D:1102:ARG:NH1	1:D:1116:LEU:O	2.45	0.47
1:D:2746:VAL:HG22	1:D:2747:ILE:N	2.30	0.47
1:D:2926:GLU:OE1	1:D:2926:GLU:HA	2.15	0.47
1:A:898:ARG:HB2	1:A:906:PRO:HD3	1.97	0.47
1:B:893:THR:O	1:B:904:LEU:HA	2.15	0.47
1:C:985:LEU:HD13	1:C:1057:PRO:HD2	1.96	0.47
1:D:2234:CYS:O	1:D:2236:PHE:C	2.58	0.47
1:A:440:GLU:H	1:A:440:GLU:CD	2.22	0.47
1:B:1072:ARG:HA	1:B:1072:ARG:HE	1.79	0.47
1:B:4796:MET:HE1	7:B:8006:PCW:H212	1.97	0.47
1:C:605:CYS:CB	1:C:1673:SER:OG	2.63	0.47
1:C:986:VAL:HA	1:C:989:LEU:HD12	1.97	0.47
1:C:2746:VAL:HG22	1:C:2747:ILE:N	2.30	0.47
1:C:4796:MET:HE1	7:C:8006:PCW:H212	1.97	0.47
1:D:877:GLU:HA	1:D:911:PHE:CD1	2.49	0.47
1:D:919:ARG:HG3	1:D:923:LEU:CD1	2.44	0.47
1:D:3389:GLU:O	1:D:3393:LEU:HD23	2.15	0.47
1:D:4709:PHE:CD1	1:D:4709:PHE:C	2.93	0.47
1:A:2481:GLY:O	1:A:2485:ALA:HB3	2.16	0.46
1:B:605:CYS:CB	1:B:1673:SER:OG	2.63	0.46
1:B:872:ARG:NH2	1:B:873:GLU:HA	2.30	0.46
1:B:898:ARG:HB2	1:B:906:PRO:HD3	1.97	0.46
1:B:902:LYS:HA	1:B:902:LYS:HD2	1.42	0.46
1:B:985:LEU:HD13	1:B:1057:PRO:HD2	1.96	0.46
1:B:2481:GLY:O	1:B:2485:ALA:HB3	2.15	0.46
1:B:3472:THR:HG23	1:C:1171:MET:CE	2.45	0.46
1:C:3024:LYS:NZ	1:C:3024:LYS:HB3	2.30	0.46
1:C:3384:ALA:N	1:C:3387:GLU:OE1	2.41	0.46
1:C:3540:ARG:HD2	1:C:3545:ASP:OD2	2.14	0.46
1:D:887:ARG:HG3	1:D:908:LEU:HD11	1.98	0.46
1:D:3605:TYR:CD1	1:D:3605:TYR:C	2.92	0.46
1:A:887:ARG:HG3	1:A:908:LEU:HD11	1.98	0.46
1:A:893:THR:O	1:A:904:LEU:HA	2.15	0.46
1:A:919:ARG:HG3	1:A:923:LEU:CD1	2.44	0.46
1:A:986:VAL:HA	1:A:989:LEU:HD12	1.97	0.46
1:A:3605:TYR:CD1	1:A:3605:TYR:C	2.92	0.46
1:B:875:LEU:CB	1:B:926:SER:HB2	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2481:GLY:O	1:C:2485:ALA:HB3	2.15	0.46
1:A:899:ASP:CB	1:A:902:LYS:HB2	2.33	0.46
1:A:978:LEU:HD22	1:A:982:GLN:OE1	2.15	0.46
1:A:2374:GLY:O	1:B:131:LYS:NZ	2.48	0.46
1:B:819:ARG:NH2	1:B:1030:GLU:OE1	2.49	0.46
1:B:879:ILE:HA	1:B:882:LEU:CD1	2.45	0.46
1:B:2974:PHE:C	1:B:2974:PHE:CD1	2.93	0.46
1:C:1072:ARG:HA	1:C:1072:ARG:HE	1.80	0.46
1:C:4709:PHE:CD1	1:C:4709:PHE:C	2.93	0.46
1:D:978:LEU:HD12	1:D:983:THR:HG22	1.98	0.46
1:A:819:ARG:NH2	1:A:1030:GLU:OE1	2.49	0.46
1:A:3024:LYS:HB3	1:A:3024:LYS:NZ	2.30	0.46
1:A:4709:PHE:CD1	1:A:4709:PHE:C	2.93	0.46
1:B:887:ARG:HG3	1:B:908:LEU:HD11	1.98	0.46
1:B:2215:VAL:HG21	1:B:2229:MET:CE	2.46	0.46
1:B:2374:GLY:O	1:C:131:LYS:NZ	2.49	0.46
1:B:4703:VAL:O	1:B:4706:THR:OG1	2.34	0.46
1:C:894:TYR:HB3	1:C:962:MET:HB3	1.98	0.46
1:C:961:MET:CG	1:C:967:LYS:HB3	2.45	0.46
1:D:961:MET:CG	1:D:967:LYS:HB3	2.45	0.46
1:D:1113:ASP:OD1	1:D:1113:ASP:N	2.41	0.46
1:D:2747:ILE:N	1:D:2747:ILE:HD12	2.31	0.46
1:D:3024:LYS:HB3	1:D:3024:LYS:NZ	2.30	0.46
1:A:4729:ILE:HD12	1:A:4729:ILE:N	2.30	0.46
2:H:19:ARG:HB3	2:H:19:ARG:NH1	2.30	0.46
1:B:2746:VAL:HG22	1:B:2747:ILE:N	2.30	0.46
1:C:819:ARG:NH2	1:C:1030:GLU:OE1	2.49	0.46
1:C:978:LEU:HD12	1:C:983:THR:HG22	1.98	0.46
1:C:2215:VAL:HG21	1:C:2229:MET:CE	2.46	0.46
1:C:2876:ALA:HB3	1:C:2921:ARG:HH12	1.79	0.46
1:C:4703:VAL:O	1:C:4706:THR:OG1	2.34	0.46
1:D:893:THR:HG22	1:D:904:LEU:HD13	1.98	0.46
1:D:3540:ARG:O	1:D:3541:TYR:C	2.57	0.46
1:A:605:CYS:CB	1:A:1673:SER:OG	2.63	0.46
1:A:872:ARG:NH2	1:A:873:GLU:HA	2.30	0.46
1:A:961:MET:CG	1:A:967:LYS:HB3	2.46	0.46
1:A:2747:ILE:HD12	1:A:2747:ILE:N	2.31	0.46
2:G:19:ARG:NH1	2:G:19:ARG:HB3	2.30	0.46
1:B:2926:GLU:OE1	1:B:2926:GLU:HA	2.15	0.46
1:B:3024:LYS:NZ	1:B:3024:LYS:HB3	2.30	0.46
1:B:3243:ASP:OD1	1:B:3243:ASP:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1252:GLU:N	1:C:1252:GLU:OE2	2.48	0.46
1:C:2374:GLY:O	1:D:131:LYS:NZ	2.49	0.46
1:D:819:ARG:NH2	1:D:1030:GLU:OE1	2.49	0.46
1:D:2974:PHE:CD1	1:D:2974:PHE:C	2.93	0.46
1:A:723:TRP:CZ2	1:A:728:ALA:HB2	2.51	0.46
1:A:2215:VAL:HG21	1:A:2229:MET:CE	2.46	0.46
1:A:2746:VAL:HG22	1:A:2747:ILE:N	2.30	0.46
1:A:4796:MET:HE1	7:A:8006:PCW:H20	1.98	0.46
1:A:4830:HIS:NE2	1:A:4940:GLU:OE1	2.48	0.46
1:B:1266:ASP:OD1	1:B:1266:ASP:N	2.46	0.46
1:B:3447:SER:O	1:B:3453:LYS:NZ	2.40	0.46
1:B:4796:MET:HE1	7:B:8006:PCW:H20	1.98	0.46
1:C:440:GLU:H	1:C:440:GLU:CD	2.22	0.46
1:C:3605:TYR:CD1	1:C:3605:TYR:C	2.92	0.46
1:D:1252:GLU:N	1:D:1252:GLU:OE2	2.48	0.46
1:D:2391:PRO:O	1:D:2392:ALA:HB3	2.15	0.46
1:D:2481:GLY:O	1:D:2485:ALA:HB3	2.16	0.46
1:B:961:MET:CG	1:B:967:LYS:HB3	2.45	0.46
1:C:887:ARG:HG3	1:C:908:LEU:HD11	1.98	0.46
1:C:2974:PHE:CD1	1:C:2974:PHE:C	2.93	0.46
1:C:4729:ILE:HD12	1:C:4729:ILE:N	2.30	0.46
1:D:893:THR:O	1:D:904:LEU:HA	2.15	0.46
1:D:2743:THR:HG23	1:D:2744:LEU:H	1.77	0.46
1:A:883:TRP:HE1	1:A:887:ARG:HH11	1.64	0.46
1:A:2926:GLU:OE1	1:A:2926:GLU:HA	2.15	0.46
1:A:2974:PHE:CD1	1:A:2974:PHE:C	2.93	0.46
2:F:19:ARG:HB3	2:F:19:ARG:NH1	2.30	0.46
1:B:3384:ALA:O	1:B:3388:ALA:HB2	2.16	0.46
1:C:723:TRP:CZ2	1:C:728:ALA:HB2	2.51	0.46
1:C:3472:THR:HG23	1:D:1171:MET:CE	2.46	0.46
1:D:605:CYS:CB	1:D:1673:SER:OG	2.63	0.46
1:D:978:LEU:HD22	1:D:982:GLN:OE1	2.15	0.46
1:D:986:VAL:HA	1:D:989:LEU:HD12	1.97	0.46
1:D:3546:THR:OG1	1:D:3548:GLU:OE2	2.15	0.46
1:A:893:THR:HG22	1:A:904:LEU:HD13	1.98	0.46
1:B:894:TYR:HB3	1:B:962:MET:HB3	1.98	0.46
1:B:894:TYR:HB3	1:B:964:ASN:H	1.80	0.46
1:B:957:PRO:HG2	1:B:960:TYR:CB	2.44	0.46
1:B:3108:VAL:HG23	1:B:3176:LEU:CD1	2.47	0.46
1:B:3282:LEU:HD12	1:B:3316:LEU:HD22	1.98	0.46
1:C:953:LYS:CB	1:C:971:LEU:HA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1001:ARG:NH2	1:C:1004:GLN:OE1	2.49	0.46
1:C:3600:VAL:HG12	1:C:3604:LEU:CD1	2.46	0.46
1:D:894:TYR:HB3	1:D:964:ASN:H	1.80	0.46
1:D:957:PRO:HG2	1:D:960:TYR:CB	2.44	0.46
1:D:1001:ARG:NH2	1:D:1004:GLN:OE1	2.49	0.46
1:D:2215:VAL:HG21	1:D:2229:MET:CE	2.46	0.46
1:A:894:TYR:HB3	1:A:962:MET:HB3	1.98	0.45
1:A:978:LEU:HD12	1:A:983:THR:HG22	1.98	0.45
1:A:2234:CYS:O	1:A:2236:PHE:C	2.58	0.45
1:B:899:ASP:CB	1:B:902:LYS:HB2	2.33	0.45
1:B:978:LEU:HD12	1:B:983:THR:HG22	1.98	0.45
1:B:2795:TYR:CZ	1:B:2803:LYS:HG2	2.52	0.45
7:B:8005:PCW:H231	7:B:8005:PCW:H20	1.72	0.45
1:C:872:ARG:CG	1:C:927:GLY:HA2	2.46	0.45
1:C:880:HIS:CE1	1:C:914:LEU:HD22	2.52	0.45
1:C:892:TRP:HB3	1:C:908:LEU:CD1	2.46	0.45
1:C:2746:VAL:HG22	1:C:2747:ILE:H	1.81	0.45
1:C:3540:ARG:O	1:C:3541:TYR:C	2.57	0.45
1:D:723:TRP:CZ2	1:D:728:ALA:HB2	2.51	0.45
1:A:892:TRP:HB3	1:A:908:LEU:CD1	2.46	0.45
1:A:3108:VAL:HG23	1:A:3176:LEU:CD1	2.46	0.45
1:A:4703:VAL:O	1:A:4706:THR:OG1	2.34	0.45
1:B:723:TRP:CZ2	1:B:728:ALA:HB2	2.51	0.45
1:B:872:ARG:CG	1:B:927:GLY:HA2	2.46	0.45
1:B:883:TRP:HE1	1:B:887:ARG:HH11	1.64	0.45
1:B:1875:GLU:HA	1:B:1875:GLU:OE2	2.17	0.45
1:B:4729:ILE:N	1:B:4729:ILE:HD12	2.30	0.45
1:C:3384:ALA:O	1:C:3388:ALA:HB2	2.16	0.45
1:D:879:ILE:HA	1:D:882:LEU:CD1	2.45	0.45
1:D:931:LYS:HE2	1:D:931:LYS:HB3	1.69	0.45
1:D:2234:CYS:HB3	1:D:2238:CYS:HB2	1.63	0.45
1:D:2876:ALA:HB3	1:D:2921:ARG:HH12	1.79	0.45
1:D:4796:MET:HE1	7:D:8006:PCW:H212	1.98	0.45
1:A:971:LEU:H	1:A:971:LEU:HG	1.52	0.45
1:A:1001:ARG:NH2	1:A:1004:GLN:OE1	2.49	0.45
1:A:1252:GLU:N	1:A:1252:GLU:OE2	2.48	0.45
1:A:1273:LEU:HD22	1:A:1290:LEU:HD11	1.98	0.45
1:A:3282:LEU:HD12	1:A:3316:LEU:HD22	1.98	0.45
1:A:4796:MET:HE1	7:A:8006:PCW:H212	1.97	0.45
1:B:892:TRP:HB3	1:B:908:LEU:CD1	2.46	0.45
1:B:2876:ALA:HB3	1:B:2921:ARG:HH12	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:879:ILE:HA	1:C:882:LEU:CD1	2.44	0.45
1:C:893:THR:O	1:C:904:LEU:HA	2.15	0.45
1:C:2218:GLY:O	1:C:2225:ARG:NH1	2.38	0.45
1:C:2795:TYR:CZ	1:C:2803:LYS:HG2	2.51	0.45
1:D:4729:ILE:N	1:D:4729:ILE:HD12	2.30	0.45
1:A:2234:CYS:HB2	1:A:2271:SER:HB3	1.99	0.45
1:B:158:ARG:HG2	1:B:158:ARG:HH11	1.81	0.45
1:B:871:ILE:H	1:B:871:ILE:HG13	1.40	0.45
1:B:956:LEU:CD1	1:B:968:PRO:HD2	2.47	0.45
1:C:1116:LEU:HD13	1:C:1124:VAL:HG11	1.98	0.45
1:C:3282:LEU:HD12	1:C:3316:LEU:HD22	1.98	0.45
1:C:4893:GLY:N	1:C:4897:ASP:OD1	2.41	0.45
1:D:978:LEU:HB3	1:D:983:THR:HG23	1.98	0.45
1:D:3282:LEU:HD12	1:D:3316:LEU:HD22	1.98	0.45
1:D:3686:GLU:OE1	1:D:3686:GLU:N	2.46	0.45
1:A:892:TRP:CE3	1:A:905:HIS:HB2	2.52	0.45
1:A:3600:VAL:HG12	1:A:3604:LEU:CD1	2.46	0.45
1:B:880:HIS:CE1	1:B:914:LEU:HD22	2.52	0.45
1:B:2746:VAL:HG22	1:B:2747:ILE:H	1.81	0.45
1:C:894:TYR:HB3	1:C:964:ASN:H	1.80	0.45
1:C:978:LEU:HB3	1:C:983:THR:HG23	1.98	0.45
1:C:4796:MET:HE1	7:C:8006:PCW:H20	1.98	0.45
1:D:880:HIS:CE1	1:D:914:LEU:HD22	2.52	0.45
1:D:2795:TYR:CZ	1:D:2803:LYS:HG2	2.51	0.45
1:A:871:ILE:H	1:A:871:ILE:HG13	1.40	0.45
1:A:902:LYS:CB	1:A:904:LEU:HG	2.47	0.45
1:A:3384:ALA:O	1:A:3388:ALA:HB2	2.16	0.45
1:B:1740:THR:HG22	1:B:2147:VAL:HG22	1.98	0.45
1:B:2747:ILE:N	1:B:2747:ILE:HD12	2.31	0.45
1:B:2947:LEU:O	1:B:2950:SER:OG	2.26	0.45
1:C:872:ARG:NH2	1:C:873:GLU:HA	2.30	0.45
1:C:883:TRP:HE1	1:C:887:ARG:HH11	1.64	0.45
1:C:893:THR:HG22	1:C:904:LEU:HD13	1.98	0.45
7:C:8006:PCW:H411	1:D:4848:LEU:HD22	1.99	0.45
1:D:158:ARG:HG2	1:D:158:ARG:HH11	1.81	0.45
1:D:3108:VAL:HG23	1:D:3176:LEU:CD1	2.47	0.45
1:A:882:LEU:HD23	1:A:970:PRO:CB	2.47	0.45
1:A:882:LEU:HD23	1:A:970:PRO:HB3	1.99	0.45
1:B:3540:ARG:O	1:B:3541:TYR:C	2.57	0.45
7:B:8006:PCW:H411	1:C:4848:LEU:HD22	1.99	0.45
1:C:893:THR:HG23	1:C:963:SER:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:892:TRP:CE3	1:D:905:HIS:HB2	2.52	0.45
1:D:1273:LEU:HD22	1:D:1290:LEU:HD11	1.98	0.45
1:D:3384:ALA:O	1:D:3388:ALA:HB2	2.16	0.45
1:D:4796:MET:HE1	7:D:8006:PCW:H2O	1.98	0.45
1:A:158:ARG:HH11	1:A:158:ARG:HG2	1.81	0.45
1:A:2795:TYR:CZ	1:A:2803:LYS:HG2	2.51	0.45
1:A:3421:ARG:CG	1:A:3521:ILE:HD11	2.47	0.45
1:B:882:LEU:HD23	1:B:970:PRO:HB3	1.99	0.45
1:B:931:LYS:HE2	1:B:931:LYS:HB3	1.69	0.45
1:B:978:LEU:HB3	1:B:983:THR:HG23	1.98	0.45
1:B:1252:GLU:N	1:B:1252:GLU:OE2	2.48	0.45
1:C:892:TRP:CE3	1:C:905:HIS:HB2	2.52	0.45
1:C:2747:ILE:N	1:C:2747:ILE:HD12	2.31	0.45
1:C:3108:VAL:HG23	1:C:3176:LEU:CD1	2.47	0.45
1:D:894:TYR:HB3	1:D:962:MET:HB3	1.98	0.45
1:A:1740:THR:HG22	1:A:2147:VAL:HG22	1.98	0.45
1:B:892:TRP:CE3	1:B:905:HIS:HB2	2.52	0.45
1:C:843:PRO:O	1:C:1197:PRO:HA	2.17	0.45
1:D:1012:GLN:OE1	1:D:1014:ILE:HD11	2.17	0.45
1:A:879:ILE:HA	1:A:882:LEU:CD1	2.44	0.45
1:B:956:LEU:CB	1:B:967:LYS:HD2	2.47	0.45
1:B:1001:ARG:NH2	1:B:1004:GLN:OE1	2.49	0.45
1:B:1113:ASP:OD1	1:B:1113:ASP:N	2.41	0.45
1:B:2234:CYS:HB2	1:B:2271:SER:HB3	1.99	0.45
1:B:3421:ARG:CG	1:B:3521:ILE:HD11	2.47	0.45
1:B:3600:VAL:HG12	1:B:3604:LEU:CD1	2.46	0.45
1:C:882:LEU:HD23	1:C:970:PRO:HB3	1.99	0.45
1:C:1740:THR:HG22	1:C:2147:VAL:HG22	1.98	0.45
1:D:882:LEU:HD23	1:D:970:PRO:HB3	1.99	0.45
1:D:2234:CYS:HB2	1:D:2271:SER:HB3	1.99	0.45
1:A:978:LEU:HB3	1:A:983:THR:HG23	1.98	0.44
1:B:2755:PHE:CZ	1:B:2931:LEU:HG	2.52	0.44
1:C:957:PRO:HG2	1:C:960:TYR:CB	2.44	0.44
1:C:2755:PHE:CZ	1:C:2931:LEU:HG	2.52	0.44
1:D:865:PRO:HD2	1:D:868:LEU:CD1	2.47	0.44
1:D:882:LEU:HD23	1:D:970:PRO:CB	2.47	0.44
1:D:883:TRP:HE1	1:D:887:ARG:HH11	1.64	0.44
1:D:1875:GLU:OE2	1:D:1875:GLU:HA	2.17	0.44
1:A:843:PRO:O	1:A:1197:PRO:HA	2.17	0.44
1:A:872:ARG:CG	1:A:927:GLY:HA2	2.46	0.44
1:A:1042:GLN:O	1:A:1046:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2755:PHE:CZ	1:A:2931:LEU:HG	2.52	0.44
1:A:3283:PRO:HG3	1:A:3346:ILE:HG22	2.00	0.44
1:B:865:PRO:HD2	1:B:868:LEU:CD1	2.47	0.44
1:B:1012:GLN:OE1	1:B:1014:ILE:HD11	2.17	0.44
1:C:865:PRO:HD2	1:C:868:LEU:CD1	2.47	0.44
1:C:1273:LEU:HD22	1:C:1290:LEU:HD11	1.98	0.44
1:C:1940:MET:HA	1:C:1940:MET:HE3	2.00	0.44
1:C:3004:LEU:HB2	1:C:3005:PRO:HD3	1.99	0.44
1:D:1116:LEU:HD13	1:D:1124:VAL:HG11	1.98	0.44
1:D:2746:VAL:HG22	1:D:2747:ILE:H	1.81	0.44
1:D:2780:GLU:OE1	1:D:2780:GLU:N	2.44	0.44
1:D:3600:VAL:HG12	1:D:3604:LEU:CD1	2.46	0.44
1:D:4703:VAL:O	1:D:4706:THR:OG1	2.34	0.44
1:A:893:THR:HG23	1:A:963:SER:HB3	1.99	0.44
1:A:925:MET:O	1:A:929:THR:HG23	2.18	0.44
1:A:1217:ILE:HD13	1:D:3422:ALA:HB1	2.00	0.44
1:A:2234:CYS:SG	1:A:2271:SER:HB3	2.57	0.44
1:A:2746:VAL:HG22	1:A:2747:ILE:H	1.81	0.44
1:B:879:ILE:HD12	1:B:879:ILE:HA	1.78	0.44
1:B:893:THR:HG22	1:B:904:LEU:HD13	1.98	0.44
1:B:3423:HIS:ND1	1:B:3423:HIS:C	2.76	0.44
1:B:3605:TYR:C	1:B:3605:TYR:CD1	2.92	0.44
1:C:158:ARG:HG2	1:C:158:ARG:HH11	1.81	0.44
1:C:868:LEU:HD23	1:C:868:LEU:HA	1.77	0.44
1:C:2757:ASN:O	1:C:2761:GLU:OE1	2.35	0.44
1:C:3450:HIS:O	1:C:3450:HIS:ND1	2.35	0.44
1:D:872:ARG:NH2	1:D:873:GLU:HA	2.30	0.44
1:D:3548:GLU:CD	1:D:3548:GLU:H	2.25	0.44
1:A:880:HIS:CE1	1:A:914:LEU:HD22	2.52	0.44
1:A:956:LEU:CD1	1:A:968:PRO:HD2	2.47	0.44
1:A:1116:LEU:HD13	1:A:1124:VAL:HG11	1.98	0.44
1:B:843:PRO:O	1:B:1197:PRO:HA	2.17	0.44
1:B:902:LYS:CB	1:B:904:LEU:HG	2.47	0.44
1:B:925:MET:O	1:B:929:THR:HG23	2.18	0.44
1:B:1940:MET:HA	1:B:1940:MET:HE3	2.00	0.44
1:C:925:MET:O	1:C:929:THR:HG23	2.18	0.44
1:C:3105:GLU:OE2	1:C:3168:ARG:NE	2.51	0.44
1:D:925:MET:O	1:D:929:THR:HG23	2.18	0.44
1:D:2747:ILE:HG22	1:D:2748:ILE:N	2.33	0.44
1:D:2755:PHE:CZ	1:D:2931:LEU:HG	2.52	0.44
1:D:2757:ASN:O	1:D:2761:GLU:OE1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:957:PRO:HG2	1:A:960:TYR:CB	2.44	0.44
1:A:1113:ASP:OD1	1:A:1113:ASP:N	2.41	0.44
1:A:3592:LYS:O	1:A:3596:ARG:HG2	2.18	0.44
1:B:882:LEU:HD23	1:B:970:PRO:CB	2.47	0.44
1:B:1116:LEU:HD13	1:B:1124:VAL:HG11	1.98	0.44
1:B:3004:LEU:HB2	1:B:3005:PRO:HD3	1.99	0.44
1:B:3283:PRO:HG3	1:B:3346:ILE:HG22	2.00	0.44
1:C:882:LEU:HD23	1:C:970:PRO:CB	2.47	0.44
1:C:1875:GLU:HA	1:C:1875:GLU:OE2	2.17	0.44
1:C:2234:CYS:HB2	1:C:2271:SER:HB3	1.99	0.44
1:C:2761:GLU:OE2	1:C:2795:TYR:CD1	2.71	0.44
1:D:892:TRP:HB3	1:D:908:LEU:CD1	2.46	0.44
1:D:1940:MET:HA	1:D:1940:MET:HE3	2.00	0.44
1:D:3224:SER:OG	1:D:3227:GLU:OE2	2.31	0.44
1:A:1012:GLN:OE1	1:A:1014:ILE:HD11	2.17	0.44
1:B:1042:GLN:O	1:B:1046:THR:HG23	2.17	0.44
1:B:3548:GLU:H	1:B:3548:GLU:CD	2.25	0.44
1:C:902:LYS:CB	1:C:904:LEU:HG	2.47	0.44
1:C:2234:CYS:SG	1:C:2271:SER:HB3	2.57	0.44
1:D:843:PRO:O	1:D:1197:PRO:HA	2.17	0.44
1:D:902:LYS:HD2	1:D:902:LYS:HA	1.42	0.44
1:D:956:LEU:CB	1:D:967:LYS:HD2	2.47	0.44
1:D:1740:THR:HG22	1:D:2147:VAL:HG22	1.98	0.44
1:D:2234:CYS:SG	1:D:2271:SER:HB3	2.57	0.44
1:D:2782:ILE:HG23	1:D:2790:PRO:CD	2.48	0.44
1:D:3240:MET:HE2	1:D:3240:MET:HA	2.00	0.44
1:A:956:LEU:CB	1:A:967:LYS:HD2	2.47	0.44
1:C:1012:GLN:OE1	1:C:1014:ILE:HD11	2.17	0.44
1:C:2747:ILE:HG22	1:C:2748:ILE:N	2.33	0.44
1:C:2755:PHE:HB2	1:C:2936:TYR:CZ	2.53	0.44
1:C:2782:ILE:HG23	1:C:2790:PRO:CD	2.48	0.44
1:D:893:THR:HG23	1:D:963:SER:HB3	1.99	0.44
1:D:956:LEU:CD1	1:D:968:PRO:HD2	2.47	0.44
1:D:2755:PHE:HB2	1:D:2936:TYR:CZ	2.53	0.44
1:D:4830:HIS:NE2	1:D:4940:GLU:OE1	2.48	0.44
1:A:70:LEU:HD21	1:A:203:MET:HE1	2.00	0.44
1:A:3450:HIS:O	1:A:3450:HIS:ND1	2.35	0.44
2:F:30:MET:HE3	2:F:30:MET:HB2	1.95	0.44
2:H:30:MET:HE3	2:H:30:MET:HB2	1.95	0.44
1:B:956:LEU:HD22	1:B:956:LEU:HA	1.75	0.44
1:B:1273:LEU:HD22	1:B:1290:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4059:GLU:HG2	1:B:4169:LEU:HD13	2.00	0.44
1:C:956:LEU:CD1	1:C:968:PRO:HD2	2.47	0.44
1:C:4825:LEU:HD21	1:D:4841:LEU:HD21	2.00	0.44
1:D:3283:PRO:HG3	1:D:3346:ILE:HG22	2.00	0.44
1:A:1875:GLU:HA	1:A:1875:GLU:OE2	2.17	0.44
1:A:2747:ILE:HG22	1:A:2748:ILE:N	2.33	0.44
1:A:2761:GLU:OE2	1:A:2795:TYR:CD1	2.71	0.44
1:A:2782:ILE:HG23	1:A:2790:PRO:CD	2.48	0.44
1:A:3548:GLU:CD	1:A:3548:GLU:H	2.25	0.44
1:B:2600:GLN:O	1:B:2604:ILE:HG13	2.18	0.44
1:B:2761:GLU:OE2	1:B:2795:TYR:CD1	2.71	0.44
1:C:1054:ILE:C	1:C:1054:ILE:HD12	2.43	0.44
1:C:3584:GLU:OE1	1:C:3584:GLU:N	2.43	0.44
1:D:909:VAL:HB	1:D:910:ASN:H	1.72	0.44
1:D:1042:GLN:O	1:D:1046:THR:HG23	2.17	0.44
1:D:3547:ASP:N	1:D:3547:ASP:OD1	2.51	0.44
1:A:892:TRP:NE1	1:A:903:ARG:HD3	2.33	0.43
1:A:1940:MET:HA	1:A:1940:MET:HE3	2.00	0.43
1:B:70:LEU:HD21	1:B:203:MET:HE1	2.00	0.43
1:B:2782:ILE:HG23	1:B:2790:PRO:CD	2.48	0.43
1:B:3291:GLU:CG	1:B:3291:GLU:O	2.66	0.43
1:C:70:LEU:HD21	1:C:203:MET:HE1	2.00	0.43
1:C:1042:GLN:O	1:C:1046:THR:HG23	2.17	0.43
1:C:2600:GLN:O	1:C:2604:ILE:HG13	2.18	0.43
1:C:3283:PRO:HG3	1:C:3346:ILE:HG22	2.00	0.43
1:D:70:LEU:HD21	1:D:203:MET:HE1	2.00	0.43
1:D:3592:LYS:O	1:D:3596:ARG:HG2	2.18	0.43
1:A:1054:ILE:C	1:A:1054:ILE:HD12	2.43	0.43
1:A:4789:TYR:OH	1:A:4813:ASP:OD1	2.28	0.43
1:B:1055:GLU:O	1:B:1056:PRO:C	2.61	0.43
1:B:2605:GLU:O	1:B:2609:MET:HG2	2.18	0.43
1:B:2747:ILE:HG22	1:B:2748:ILE:N	2.33	0.43
1:B:2757:ASN:O	1:B:2761:GLU:OE1	2.35	0.43
1:B:3592:LYS:O	1:B:3596:ARG:HG2	2.18	0.43
1:C:956:LEU:CB	1:C:967:LYS:HD2	2.47	0.43
1:C:2581:ASP:OD1	1:C:2581:ASP:C	2.61	0.43
1:C:3006:LEU:O	1:C:3007:ILE:C	2.62	0.43
1:C:3548:GLU:CD	1:C:3548:GLU:H	2.25	0.43
1:D:1054:ILE:C	1:D:1054:ILE:HD12	2.43	0.43
1:D:2225:ARG:N	1:D:2225:ARG:HD3	2.33	0.43
1:D:2600:GLN:O	1:D:2604:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2761:GLU:OE2	1:D:2795:TYR:CD1	2.71	0.43
1:D:3176:LEU:HD22	1:D:3191:LEU:HD13	2.00	0.43
1:D:3291:GLU:CG	1:D:3291:GLU:O	2.66	0.43
1:D:3421:ARG:CG	1:D:3521:ILE:HD11	2.47	0.43
1:D:4869:GLU:HA	1:D:4869:GLU:OE2	2.18	0.43
1:A:931:LYS:HE2	1:A:931:LYS:HB3	1.69	0.43
1:A:2225:ARG:HD3	1:A:2225:ARG:N	2.33	0.43
1:A:3291:GLU:O	1:A:3291:GLU:CG	2.66	0.43
1:A:4932:GLY:HA2	1:D:4935:ILE:HG12	1.99	0.43
1:B:921:TYR:CE2	1:B:925:MET:HE2	2.54	0.43
1:C:3423:HIS:ND1	1:C:3423:HIS:C	2.76	0.43
1:C:4789:TYR:OH	1:C:4813:ASP:OD1	2.28	0.43
1:D:921:TYR:CE2	1:D:925:MET:HE2	2.53	0.43
1:D:975:HIS:CD2	1:D:975:HIS:H	2.36	0.43
1:D:3105:GLU:OE2	1:D:3168:ARG:NE	2.51	0.43
1:A:919:ARG:HG3	1:A:923:LEU:HD11	2.01	0.43
1:A:1055:GLU:O	1:A:1056:PRO:C	2.61	0.43
1:A:2804:GLU:O	1:A:2811:LYS:NZ	2.51	0.43
1:A:3006:LEU:O	1:A:3007:ILE:C	2.62	0.43
1:B:2234:CYS:SG	1:B:2271:SER:HB3	2.57	0.43
1:B:3176:LEU:HD22	1:B:3191:LEU:HD13	2.00	0.43
1:B:4825:LEU:HD21	1:C:4841:LEU:HD21	2.00	0.43
1:C:948:GLU:HA	1:C:1050:TYR:HA	2.01	0.43
1:D:2804:GLU:O	1:D:2811:LYS:NZ	2.51	0.43
1:D:3004:LEU:HB2	1:D:3005:PRO:HD3	1.99	0.43
1:A:882:LEU:CB	1:A:970:PRO:HB3	2.49	0.43
1:A:2761:GLU:OE2	1:A:2761:GLU:CA	2.67	0.43
1:A:3176:LEU:HD22	1:A:3191:LEU:HD13	2.00	0.43
1:A:3761:MET:HE2	1:A:3761:MET:HA	2.00	0.43
1:B:893:THR:HG23	1:B:963:SER:HB3	1.99	0.43
1:B:1054:ILE:C	1:B:1054:ILE:HD12	2.43	0.43
1:B:2225:ARG:HD3	1:B:2225:ARG:N	2.33	0.43
1:B:2755:PHE:HB2	1:B:2936:TYR:CZ	2.53	0.43
1:B:3761:MET:HE2	1:B:3761:MET:HA	2.01	0.43
1:B:4709:PHE:CD1	1:B:4709:PHE:C	2.93	0.43
7:B:8006:PCW:C41	1:C:4848:LEU:HD22	2.48	0.43
1:C:947:ALA:HA	1:C:950:ASN:ND2	2.34	0.43
1:C:3421:ARG:CG	1:C:3521:ILE:HD11	2.47	0.43
1:C:3592:LYS:O	1:C:3596:ARG:HG2	2.18	0.43
1:D:948:GLU:HA	1:D:1050:TYR:HA	2.01	0.43
1:D:3447:SER:O	1:D:3453:LYS:NZ	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LYS:NZ	1:D:2374:GLY:O	2.52	0.43
1:A:921:TYR:CE2	1:A:925:MET:HE2	2.53	0.43
1:A:2092:PRO:O	1:A:2097:GLU:OE1	2.37	0.43
1:A:2266:LEU:O	1:A:2269:GLN:NE2	2.52	0.43
1:A:3004:LEU:HB2	1:A:3005:PRO:HD3	1.99	0.43
1:A:3423:HIS:ND1	1:A:3423:HIS:C	2.76	0.43
1:B:892:TRP:NE1	1:B:903:ARG:HD3	2.33	0.43
1:B:4828:VAL:CG2	1:C:4929:ILE:HD11	2.49	0.43
1:C:2605:GLU:O	1:C:2609:MET:HG2	2.18	0.43
1:C:2804:GLU:O	1:C:2811:LYS:NZ	2.51	0.43
1:D:919:ARG:HG3	1:D:923:LEU:HD11	2.01	0.43
1:D:2047:LEU:HD22	1:D:2047:LEU:N	2.34	0.43
1:D:3541:TYR:OH	1:D:3598:GLN:NE2	2.48	0.43
1:A:2605:GLU:O	1:A:2609:MET:HG2	2.18	0.43
1:A:3847:LEU:HD13	1:B:77:ARG:HH11	1.82	0.43
1:A:4869:GLU:HA	1:A:4869:GLU:OE2	2.18	0.43
1:B:947:ALA:HA	1:B:950:ASN:ND2	2.34	0.43
1:C:892:TRP:NE1	1:C:903:ARG:HD3	2.33	0.43
1:C:919:ARG:HG3	1:C:923:LEU:HD11	2.01	0.43
1:C:3761:MET:HE2	1:C:3761:MET:HA	2.00	0.43
1:D:892:TRP:NE1	1:D:903:ARG:HD3	2.33	0.43
1:D:947:ALA:HA	1:D:950:ASN:ND2	2.34	0.43
1:D:2605:GLU:O	1:D:2609:MET:HG2	2.18	0.43
1:D:3041:THR:HA	1:D:3076:LEU:HD21	2.01	0.43
1:A:34:LEU:HD12	1:A:54:SER:HB2	2.01	0.43
1:A:947:ALA:HA	1:A:950:ASN:ND2	2.34	0.43
1:A:979:THR:HG23	1:A:982:GLN:CD	2.44	0.43
1:A:2600:GLN:O	1:A:2604:ILE:HG13	2.18	0.43
1:A:3041:THR:HA	1:A:3076:LEU:HD21	2.01	0.43
1:A:3227:GLU:O	1:A:3228:ARG:HB2	2.19	0.43
1:B:2581:ASP:C	1:B:2581:ASP:OD1	2.62	0.43
1:B:3450:HIS:HD1	1:B:3450:HIS:C	2.25	0.43
1:C:985:LEU:HD23	1:C:1054:ILE:HD13	2.01	0.43
1:C:2266:LEU:O	1:C:2269:GLN:NE2	2.52	0.43
1:C:2795:TYR:HA	1:C:2798:PHE:HB3	2.01	0.43
1:C:3176:LEU:HD22	1:C:3191:LEU:HD13	2.00	0.43
1:C:3291:GLU:CG	1:C:3291:GLU:O	2.66	0.43
1:C:4050:MET:HE3	1:C:4050:MET:HB3	1.96	0.43
1:C:4869:GLU:HA	1:C:4869:GLU:OE2	2.18	0.43
1:A:691:GLU:OE2	1:A:691:GLU:HA	2.19	0.43
1:A:865:PRO:HD2	1:A:868:LEU:CD1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2047:LEU:HD22	1:A:2047:LEU:N	2.34	0.43
1:A:2757:ASN:O	1:A:2761:GLU:OE1	2.35	0.43
1:B:691:GLU:HA	1:B:691:GLU:OE2	2.19	0.43
1:B:2761:GLU:OE2	1:B:2761:GLU:CA	2.67	0.43
1:B:4869:GLU:HA	1:B:4869:GLU:OE2	2.19	0.43
1:C:2225:ARG:HD3	1:C:2225:ARG:N	2.33	0.43
1:D:902:LYS:CB	1:D:904:LEU:HG	2.47	0.43
1:D:2761:GLU:OE2	1:D:2761:GLU:CA	2.67	0.43
1:D:3006:LEU:O	1:D:3007:ILE:C	2.62	0.43
1:A:422:PHE:O	1:A:423:SER:C	2.62	0.43
1:A:1171:MET:CE	1:D:3472:THR:HG23	2.49	0.43
1:A:2755:PHE:HB2	1:A:2936:TYR:CZ	2.53	0.43
1:B:2092:PRO:O	1:B:2097:GLU:OE1	2.37	0.43
1:B:3240:MET:HE2	1:B:3240:MET:HA	2.00	0.43
1:C:691:GLU:HA	1:C:691:GLU:OE2	2.19	0.43
1:C:1479:ASP:N	1:C:1482:GLY:O	2.47	0.43
1:C:2761:GLU:OE2	1:C:2761:GLU:CA	2.67	0.43
1:C:3240:MET:HA	1:C:3240:MET:HE2	2.00	0.43
1:C:3591:GLU:HA	1:C:3594:VAL:HG22	2.01	0.43
1:C:4059:GLU:HG2	1:C:4169:LEU:HD13	2.00	0.43
1:C:4649:THR:OG1	1:C:4801:HIS:NE2	2.39	0.43
1:D:882:LEU:H	1:D:882:LEU:HG	1.55	0.43
1:D:985:LEU:HD23	1:D:1054:ILE:HD13	2.01	0.43
1:D:2795:TYR:HA	1:D:2798:PHE:HB3	2.01	0.43
1:D:4671:ARG:NH1	1:D:4700:ASP:OD1	2.52	0.43
1:A:894:TYR:CZ	1:A:896:PRO:HA	2.54	0.42
1:A:2780:GLU:OE1	1:A:2780:GLU:N	2.44	0.42
1:A:2863:LEU:HA	1:A:2933:MET:HE1	2.01	0.42
1:A:4059:GLU:HG2	1:A:4169:LEU:HD13	2.00	0.42
2:E:30:MET:HE3	2:E:30:MET:HB2	1.95	0.42
1:B:887:ARG:O	1:B:892:TRP:HB2	2.19	0.42
1:B:979:THR:HG23	1:B:982:GLN:CD	2.44	0.42
1:B:3106:LYS:O	1:B:3109:GLU:HG3	2.19	0.42
1:B:4050:MET:HE3	1:B:4050:MET:HB3	1.96	0.42
1:B:4752:ASN:HB3	1:B:4754:ARG:CZ	2.49	0.42
1:C:921:TYR:CE2	1:C:925:MET:HE2	2.53	0.42
1:C:979:THR:HG23	1:C:982:GLN:CD	2.44	0.42
1:C:3761:MET:HE3	1:C:4717:PHE:HE1	1.84	0.42
1:D:953:LYS:HE2	1:D:953:LYS:HB2	1.47	0.42
1:D:2575:HIS:CD2	1:D:2575:HIS:H	2.37	0.42
1:D:2581:ASP:OD1	1:D:2581:ASP:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3423:HIS:C	1:D:3423:HIS:ND1	2.76	0.42
1:A:948:GLU:HA	1:A:1050:TYR:HA	2.01	0.42
1:A:3240:MET:HE2	1:A:3240:MET:HA	2.00	0.42
1:A:4050:MET:HE3	1:A:4050:MET:HB3	1.96	0.42
1:B:33:GLN:OE1	1:B:33:GLN:HA	2.19	0.42
1:B:882:LEU:CB	1:B:970:PRO:HB3	2.48	0.42
1:B:948:GLU:HA	1:B:1050:TYR:HA	2.01	0.42
1:C:33:GLN:OE1	1:C:33:GLN:HA	2.19	0.42
1:D:872:ARG:CG	1:D:927:GLY:HA2	2.46	0.42
1:D:882:LEU:CB	1:D:970:PRO:HB3	2.49	0.42
1:D:1479:ASP:N	1:D:1482:GLY:O	2.47	0.42
1:D:2922:GLU:O	1:D:2926:GLU:HG2	2.20	0.42
1:D:3761:MET:HE3	1:D:4717:PHE:HE1	1.84	0.42
1:A:2795:TYR:HA	1:A:2798:PHE:HB3	2.01	0.42
1:B:34:LEU:HD12	1:B:54:SER:HB2	2.01	0.42
1:B:919:ARG:HG3	1:B:923:LEU:HD11	2.01	0.42
1:B:2804:GLU:O	1:B:2811:LYS:NZ	2.51	0.42
1:B:3227:GLU:O	1:B:3228:ARG:HB2	2.19	0.42
1:B:3410:TYR:N	1:B:3411:PRO:HD2	2.34	0.42
1:C:422:PHE:O	1:C:423:SER:C	2.62	0.42
1:C:3227:GLU:O	1:C:3228:ARG:HB2	2.19	0.42
1:C:3410:TYR:N	1:C:3411:PRO:HD2	2.34	0.42
1:D:1830:ASP:OD1	1:D:1830:ASP:N	2.52	0.42
1:A:879:ILE:HD12	1:A:879:ILE:HA	1.79	0.42
1:A:942:MET:HE3	1:A:945:GLU:OE2	2.20	0.42
1:A:2575:HIS:H	1:A:2575:HIS:CD2	2.37	0.42
1:B:1642:ILE:HD11	1:B:1649:MET:HE3	2.02	0.42
1:B:2922:GLU:O	1:B:2926:GLU:HG2	2.20	0.42
1:B:2978:LEU:HD23	1:B:2978:LEU:O	2.19	0.42
1:B:3006:LEU:O	1:B:3007:ILE:C	2.62	0.42
1:B:3570:LEU:HD22	1:B:3570:LEU:N	2.35	0.42
1:C:2334:ASP:HA	1:C:2337:ARG:HD3	2.01	0.42
1:D:979:THR:HG23	1:D:982:GLN:CD	2.44	0.42
1:D:2266:LEU:O	1:D:2269:GLN:NE2	2.52	0.42
1:D:2334:ASP:HA	1:D:2337:ARG:HD3	2.01	0.42
1:D:3410:TYR:N	1:D:3411:PRO:HD2	2.34	0.42
1:A:3570:LEU:HD22	1:A:3570:LEU:N	2.35	0.42
1:A:3974:GLY:N	1:A:3975:PRO:HA	2.35	0.42
1:B:942:MET:HE3	1:B:945:GLU:OE2	2.20	0.42
1:B:2183:ILE:HG23	1:B:2236:PHE:HB2	2.02	0.42
1:B:2266:LEU:O	1:B:2269:GLN:NE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2795:TYR:HA	1:B:2798:PHE:HB3	2.01	0.42
1:C:2629:PHE:CD1	1:C:2629:PHE:C	2.98	0.42
1:C:2863:LEU:HA	1:C:2933:MET:HE1	2.01	0.42
1:C:2978:LEU:HD23	1:C:2978:LEU:O	2.19	0.42
1:D:422:PHE:O	1:D:423:SER:C	2.62	0.42
1:D:2183:ILE:HG23	1:D:2236:PHE:HB2	2.02	0.42
1:D:2863:LEU:HA	1:D:2933:MET:HE1	2.02	0.42
1:D:3974:GLY:N	1:D:3975:PRO:HA	2.35	0.42
1:A:1830:ASP:OD1	1:A:1830:ASP:N	2.52	0.42
1:A:3761:MET:HE3	1:A:4717:PHE:HE1	1.84	0.42
1:B:894:TYR:CZ	1:B:896:PRO:HA	2.54	0.42
1:B:2863:LEU:CD2	1:B:2933:MET:SD	3.08	0.42
1:B:3686:GLU:OE1	1:B:3686:GLU:N	2.46	0.42
1:C:887:ARG:O	1:C:892:TRP:HB2	2.19	0.42
1:C:1926:GLY:O	1:C:1930:MET:HG3	2.20	0.42
1:C:3106:LYS:O	1:C:3109:GLU:HG3	2.19	0.42
1:C:3847:LEU:HD13	1:D:77:ARG:HH11	1.84	0.42
7:C:8006:PCW:C41	1:D:4848:LEU:HD22	2.49	0.42
1:D:894:TYR:CZ	1:D:896:PRO:HA	2.54	0.42
1:D:2863:LEU:CD2	1:D:2933:MET:SD	3.08	0.42
1:D:3227:GLU:O	1:D:3228:ARG:HB2	2.19	0.42
1:A:956:LEU:HD12	1:A:967:LYS:HB2	2.01	0.42
1:A:2183:ILE:HG23	1:A:2236:PHE:HB2	2.02	0.42
1:A:2817:MET:SD	1:A:2822:TRP:HE3	2.42	0.42
1:A:3105:GLU:OE2	1:A:3168:ARG:NE	2.51	0.42
1:A:3639:MET:HE3	1:A:3639:MET:HB2	1.98	0.42
1:A:4671:ARG:NH1	1:A:4700:ASP:OD1	2.52	0.42
1:B:1926:GLY:O	1:B:1930:MET:HG3	2.19	0.42
1:B:2234:CYS:HB3	1:B:2238:CYS:HB2	1.62	0.42
1:B:4247:GLU:OE2	1:B:4247:GLU:HA	2.20	0.42
1:B:4671:ARG:NH1	1:B:4700:ASP:OD1	2.52	0.42
1:C:2047:LEU:HD22	1:C:2047:LEU:N	2.34	0.42
1:C:2817:MET:SD	1:C:2822:TRP:HE3	2.42	0.42
1:C:4828:VAL:CG2	1:D:4929:ILE:HD11	2.49	0.42
1:D:2092:PRO:O	1:D:2097:GLU:OE1	2.37	0.42
1:D:2224:ILE:HD11	1:D:2268:MET:HE1	2.02	0.42
1:D:3591:GLU:HA	1:D:3594:VAL:HG22	2.01	0.42
1:D:4753:GLU:OE1	1:D:4753:GLU:N	2.53	0.42
1:A:1044:VAL:HG12	1:A:1048:LEU:HD12	2.02	0.42
1:A:2229:MET:HE3	1:A:2229:MET:HB3	1.99	0.42
1:A:2922:GLU:O	1:A:2926:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:985:LEU:HD23	1:B:1054:ILE:HD13	2.01	0.42
1:C:490:ASN:O	1:C:494:ARG:HG2	2.20	0.42
1:C:879:ILE:HD12	1:C:879:ILE:HA	1.79	0.42
1:C:942:MET:HE3	1:C:945:GLU:OE2	2.20	0.42
1:C:2009:MET:HE3	1:C:2009:MET:HB3	1.94	0.42
1:C:2092:PRO:O	1:C:2097:GLU:OE1	2.37	0.42
1:C:2224:ILE:HD11	1:C:2268:MET:HE1	2.02	0.42
1:C:2756:ILE:HG23	1:C:2810:ILE:HB	2.02	0.42
1:C:3468:MET:SD	1:D:1174:SER:O	2.78	0.42
1:C:4649:THR:HG1	1:C:4801:HIS:CD2	2.33	0.42
1:C:4752:ASN:HB3	1:C:4754:ARG:CZ	2.49	0.42
7:C:8006:PCW:H272	7:C:8006:PCW:H483	2.02	0.42
1:D:169:ASP:OD1	1:D:169:ASP:N	2.53	0.42
1:D:942:MET:HE3	1:D:945:GLU:OE2	2.20	0.42
1:D:1044:VAL:HG12	1:D:1048:LEU:HD12	2.02	0.42
1:D:2817:MET:SD	1:D:2822:TRP:HE3	2.42	0.42
1:A:985:LEU:HD23	1:A:1054:ILE:HD13	2.01	0.42
1:A:2863:LEU:CD2	1:A:2933:MET:SD	3.08	0.42
1:A:3106:LYS:O	1:A:3109:GLU:HG3	2.19	0.42
1:A:3721:TYR:HA	1:A:3724:MET:HE3	2.02	0.42
1:A:4247:GLU:HA	1:A:4247:GLU:OE2	2.20	0.42
1:A:4752:ASN:HB3	1:A:4754:ARG:CZ	2.49	0.42
2:G:30:MET:HE3	2:G:30:MET:HB2	1.95	0.42
1:B:956:LEU:HD12	1:B:967:LYS:HB2	2.01	0.42
1:C:34:LEU:HD12	1:C:54:SER:HB2	2.01	0.42
1:C:894:TYR:CZ	1:C:896:PRO:HA	2.54	0.42
1:C:1642:ILE:HD11	1:C:1649:MET:HE3	2.02	0.42
1:C:2183:ILE:HG23	1:C:2236:PHE:HB2	2.02	0.42
1:C:2863:LEU:CD2	1:C:2933:MET:SD	3.08	0.42
1:D:3293:PRO:O	1:D:3295:PRO:CD	2.68	0.42
1:D:3761:MET:HE2	1:D:3761:MET:HA	2.00	0.42
1:A:957:PRO:HG2	1:A:960:TYR:CG	2.55	0.42
1:A:2629:PHE:CD1	1:A:2629:PHE:C	2.98	0.42
1:A:3547:ASP:N	1:A:3547:ASP:OD1	2.51	0.42
1:A:3591:GLU:HA	1:A:3594:VAL:HG22	2.01	0.42
1:B:2445:GLN:OE1	1:B:2445:GLN:HA	2.20	0.42
1:B:2863:LEU:HA	1:B:2933:MET:HE1	2.02	0.42
1:B:3105:GLU:OE2	1:B:3168:ARG:NE	2.51	0.42
1:B:3721:TYR:HA	1:B:3724:MET:HE3	2.02	0.42
1:C:882:LEU:CB	1:C:970:PRO:HB3	2.49	0.42
1:C:1044:VAL:HG12	1:C:1048:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1055:GLU:O	1:C:1056:PRO:C	2.61	0.42
1:C:3570:LEU:HD22	1:C:3570:LEU:N	2.35	0.42
1:D:490:ASN:O	1:D:494:ARG:HG2	2.20	0.42
1:D:956:LEU:HD22	1:D:956:LEU:HA	1.75	0.42
1:D:2445:GLN:OE1	1:D:2445:GLN:HA	2.20	0.42
1:D:3106:LYS:O	1:D:3109:GLU:HG3	2.19	0.42
1:D:4059:GLU:HG2	1:D:4169:LEU:HD13	2.00	0.42
1:D:4752:ASN:HB3	1:D:4754:ARG:CZ	2.49	0.42
1:A:4821:LEU:HD23	1:A:4821:LEU:HA	1.92	0.41
7:A:8006:PCW:H341	7:A:8006:PCW:O31	2.20	0.41
1:B:957:PRO:HG2	1:B:960:TYR:CG	2.55	0.41
1:B:2817:MET:SD	1:B:2822:TRP:HE3	2.42	0.41
1:B:3041:THR:HA	1:B:3076:LEU:HD21	2.01	0.41
1:B:3108:VAL:CG2	1:B:3176:LEU:HB2	2.50	0.41
1:B:3974:GLY:N	1:B:3975:PRO:HA	2.35	0.41
1:C:956:LEU:HD12	1:C:967:LYS:HB2	2.01	0.41
1:C:1830:ASP:N	1:C:1830:ASP:OD1	2.52	0.41
1:C:3041:THR:HA	1:C:3076:LEU:HD21	2.01	0.41
1:C:3865:ASP:HA	1:C:3868:VAL:HG22	2.02	0.41
1:C:4247:GLU:OE2	1:C:4247:GLU:HA	2.20	0.41
1:D:34:LEU:HD12	1:D:54:SER:HB2	2.01	0.41
1:D:887:ARG:O	1:D:892:TRP:HB2	2.19	0.41
1:D:956:LEU:HD12	1:D:967:LYS:HB2	2.01	0.41
1:D:1926:GLY:O	1:D:1930:MET:HG3	2.20	0.41
1:D:2215:VAL:HG11	1:D:2229:MET:CE	2.50	0.41
1:D:4050:MET:HE3	1:D:4050:MET:HB3	1.96	0.41
1:A:902:LYS:HA	1:A:902:LYS:HD2	1.41	0.41
1:A:953:LYS:CB	1:A:971:LEU:HA	2.45	0.41
1:A:1642:ILE:HD11	1:A:1649:MET:HE3	2.02	0.41
1:A:3410:TYR:N	1:A:3411:PRO:HD2	2.34	0.41
1:B:882:LEU:H	1:B:882:LEU:HG	1.55	0.41
1:B:4890:ARG:NH1	1:C:4897:ASP:OD2	2.53	0.41
7:B:8006:PCW:O31	7:B:8006:PCW:H341	2.20	0.41
1:D:696:TYR:CD2	1:D:1241:LYS:HD2	2.55	0.41
1:D:2978:LEU:O	1:D:2978:LEU:HD23	2.19	0.41
1:D:3721:TYR:HA	1:D:3724:MET:HE3	2.02	0.41
7:D:8006:PCW:H341	7:D:8006:PCW:O31	2.20	0.41
1:A:887:ARG:O	1:A:892:TRP:HB2	2.19	0.41
1:A:938:CYS:HB3	1:A:1057:PRO:HD3	2.02	0.41
1:A:3108:VAL:CG2	1:A:3176:LEU:HB2	2.50	0.41
1:A:3781:MET:HE2	1:A:3781:MET:HB3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2645:LEU:HD13	1:B:2679:LEU:HD21	2.03	0.41
1:B:3293:PRO:O	1:B:3295:PRO:CD	2.68	0.41
1:C:169:ASP:OD1	1:C:169:ASP:N	2.53	0.41
1:C:760:ILE:HG23	1:C:760:ILE:O	2.20	0.41
1:C:931:LYS:HE2	1:C:931:LYS:HB3	1.69	0.41
1:D:999:ARG:HH11	1:D:999:ARG:HG2	1.86	0.41
1:D:4227:GLU:O	1:D:4227:GLU:CG	2.69	0.41
1:A:1964:GLU:HA	1:A:3651:CYS:SG	2.61	0.41
1:A:2525:VAL:HG23	1:A:2526:GLY:N	2.36	0.41
1:A:2747:ILE:HD12	1:A:2747:ILE:H	1.86	0.41
1:A:4753:GLU:OE1	1:A:4753:GLU:N	2.53	0.41
1:B:953:LYS:HB2	1:B:953:LYS:HE2	1.46	0.41
1:B:1044:VAL:HG12	1:B:1048:LEU:HD12	2.02	0.41
1:B:2334:ASP:HA	1:B:2337:ARG:HD3	2.01	0.41
1:B:3108:VAL:HG23	1:B:3176:LEU:HD12	2.02	0.41
1:B:3458:ASN:O	1:B:3459:PHE:C	2.63	0.41
1:B:3468:MET:SD	1:C:1174:SER:O	2.78	0.41
1:B:3761:MET:HE3	1:B:4717:PHE:HE1	1.84	0.41
1:C:3108:VAL:CG2	1:C:3176:LEU:HB2	2.50	0.41
1:C:3721:TYR:HA	1:C:3724:MET:HE3	2.02	0.41
1:D:33:GLN:HA	1:D:33:GLN:OE1	2.19	0.41
1:D:691:GLU:HA	1:D:691:GLU:OE2	2.19	0.41
1:D:1116:LEU:HD23	1:D:1116:LEU:HA	1.95	0.41
1:D:2525:VAL:HG23	1:D:2526:GLY:N	2.36	0.41
1:A:1926:GLY:O	1:A:1930:MET:HG3	2.20	0.41
1:A:2224:ILE:HD11	1:A:2268:MET:HE1	2.02	0.41
1:A:2445:GLN:OE1	1:A:2445:GLN:HA	2.20	0.41
1:A:2581:ASP:OD1	1:A:2581:ASP:C	2.62	0.41
1:A:2645:LEU:HD13	1:A:2679:LEU:HD21	2.02	0.41
1:A:3108:VAL:HG23	1:A:3176:LEU:HD12	2.02	0.41
1:A:3293:PRO:O	1:A:3295:PRO:CD	2.68	0.41
1:B:804:LEU:HD22	1:B:804:LEU:HA	1.96	0.41
1:B:938:CYS:HB3	1:B:1057:PRO:HD3	2.02	0.41
1:B:1749:PHE:HB2	1:B:1757:ASP:HA	2.03	0.41
1:B:2047:LEU:HD22	1:B:2047:LEU:N	2.34	0.41
1:B:4753:GLU:OE1	1:B:4753:GLU:N	2.53	0.41
7:B:8006:PCW:H272	7:B:8006:PCW:H483	2.02	0.41
1:C:2922:GLU:O	1:C:2926:GLU:HG2	2.20	0.41
1:C:3108:VAL:HG23	1:C:3176:LEU:HD12	2.02	0.41
1:C:4227:GLU:O	1:C:4227:GLU:CG	2.69	0.41
1:C:4753:GLU:OE1	1:C:4753:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:885:LEU:HD12	1:D:960:TYR:CE2	2.55	0.41
1:D:2629:PHE:CD1	1:D:2629:PHE:C	2.98	0.41
1:D:3108:VAL:CG2	1:D:3176:LEU:HB2	2.50	0.41
1:D:3600:VAL:HG12	1:D:3604:LEU:HD12	2.02	0.41
1:A:33:GLN:OE1	1:A:33:GLN:HA	2.19	0.41
1:A:3521:ILE:N	1:A:3521:ILE:HD12	2.36	0.41
1:B:169:ASP:N	1:B:169:ASP:OD1	2.53	0.41
1:B:760:ILE:HG23	1:B:760:ILE:O	2.20	0.41
1:B:999:ARG:HG2	1:B:999:ARG:HH11	1.86	0.41
1:B:4691:GLU:CD	1:B:4691:GLU:N	2.79	0.41
1:C:871:ILE:H	1:C:871:ILE:HG13	1.40	0.41
1:C:938:CYS:HB3	1:C:1057:PRO:HD3	2.02	0.41
1:C:2575:HIS:CD2	1:C:2575:HIS:H	2.37	0.41
1:C:3541:TYR:OH	1:C:3598:GLN:NE2	2.48	0.41
1:C:3607:LEU:HD23	1:C:3607:LEU:HA	1.93	0.41
1:D:2640:MET:HE3	1:D:2640:MET:HB3	2.00	0.41
1:D:3291:GLU:O	1:D:3291:GLU:HG2	2.21	0.41
1:D:3570:LEU:HD22	1:D:3570:LEU:N	2.35	0.41
1:A:999:ARG:HG2	1:A:999:ARG:HH11	1.86	0.41
1:A:2215:VAL:HG11	1:A:2229:MET:CE	2.50	0.41
1:A:2942:LEU:H	1:A:2942:LEU:HD12	1.86	0.41
1:A:3231:LEU:HD12	1:A:3231:LEU:H	1.86	0.41
1:B:490:ASN:O	1:B:494:ARG:HG2	2.20	0.41
1:B:696:TYR:CD2	1:B:1241:LYS:HD2	2.55	0.41
1:B:753:VAL:HB	1:B:754:PRO:C	2.46	0.41
1:B:971:LEU:H	1:B:971:LEU:HG	1.52	0.41
1:B:1830:ASP:N	1:B:1830:ASP:OD1	2.52	0.41
1:B:3591:GLU:HA	1:B:3594:VAL:HG22	2.01	0.41
1:C:999:ARG:HH11	1:C:999:ARG:HG2	1.86	0.41
1:C:2799:SER:O	1:C:2802:ASP:OD1	2.39	0.41
1:C:3293:PRO:O	1:C:3295:PRO:CD	2.68	0.41
1:C:3600:VAL:HG12	1:C:3604:LEU:HD12	2.02	0.41
1:C:4691:GLU:CD	1:C:4691:GLU:N	2.79	0.41
1:D:760:ILE:O	1:D:760:ILE:HG23	2.20	0.41
1:D:914:LEU:HD21	1:D:919:ARG:CB	2.51	0.41
1:D:953:LYS:H	1:D:953:LYS:HG3	1.64	0.41
1:D:982:GLN:CG	1:D:1054:ILE:HD11	2.51	0.41
1:D:2645:LEU:HD13	1:D:2679:LEU:HD21	2.03	0.41
1:D:2756:ILE:HG23	1:D:2810:ILE:HB	2.02	0.41
1:D:3458:ASN:O	1:D:3459:PHE:C	2.63	0.41
1:D:3865:ASP:HA	1:D:3868:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:VAL:HB	1:A:754:PRO:C	2.46	0.41
1:A:760:ILE:HG23	1:A:760:ILE:O	2.20	0.41
1:A:2978:LEU:O	1:A:2978:LEU:HD23	2.19	0.41
7:A:8006:PCW:H272	7:A:8006:PCW:H483	2.02	0.41
1:B:218:GLY:N	1:B:263:LEU:O	2.48	0.41
1:B:422:PHE:O	1:B:423:SER:C	2.62	0.41
1:B:982:GLN:CG	1:B:1054:ILE:HD11	2.51	0.41
1:B:2756:ILE:HG23	1:B:2810:ILE:HB	2.02	0.41
1:B:2799:SER:O	1:B:2802:ASP:OD1	2.39	0.41
1:C:753:VAL:HB	1:C:754:PRO:C	2.46	0.41
1:C:3521:ILE:N	1:C:3521:ILE:HD12	2.36	0.41
1:C:3974:GLY:N	1:C:3975:PRO:HA	2.35	0.41
1:D:938:CYS:HB3	1:D:1057:PRO:HD3	2.02	0.41
1:D:1055:GLU:O	1:D:1056:PRO:C	2.61	0.41
1:D:4691:GLU:N	1:D:4691:GLU:CD	2.79	0.41
1:A:696:TYR:CD2	1:A:1241:LYS:HD2	2.55	0.41
1:A:885:LEU:HD12	1:A:960:TYR:CE2	2.56	0.41
1:A:2769:PHE:O	1:A:2773:GLN:HG2	2.21	0.41
1:A:2800:GLU:HA	1:A:2803:LYS:HD3	2.03	0.41
1:A:3388:ALA:O	1:A:3392:GLU:N	2.39	0.41
1:A:3458:ASN:O	1:A:3459:PHE:C	2.63	0.41
1:A:3865:ASP:HA	1:A:3868:VAL:HG22	2.02	0.41
1:B:885:LEU:HD12	1:B:960:TYR:CE2	2.56	0.41
1:B:1964:GLU:HA	1:B:3651:CYS:SG	2.61	0.41
1:B:2224:ILE:HD11	1:B:2268:MET:HE1	2.02	0.41
1:B:2413:GLU:HB2	1:B:2416:ARG:HE	1.86	0.41
1:B:2575:HIS:CD2	1:B:2575:HIS:H	2.37	0.41
1:B:2701:MET:HB3	1:B:2702:PRO:HD3	2.03	0.41
1:B:3639:MET:HE3	1:B:3639:MET:HB2	1.98	0.41
1:B:3639:MET:O	1:B:3641:PRO:HD3	2.21	0.41
1:B:3865:ASP:HA	1:B:3868:VAL:HG22	2.03	0.41
1:C:696:TYR:CD2	1:C:1241:LYS:HD2	2.55	0.41
1:C:885:LEU:HD12	1:C:960:TYR:CE2	2.56	0.41
1:C:1964:GLU:HA	1:C:3651:CYS:SG	2.60	0.41
1:C:2215:VAL:HG11	1:C:2229:MET:CE	2.50	0.41
1:C:2445:GLN:OE1	1:C:2445:GLN:HA	2.20	0.41
1:C:2863:LEU:CD1	1:C:2926:GLU:OE1	2.68	0.41
1:C:3291:GLU:O	1:C:3291:GLU:HG2	2.21	0.41
1:C:3547:ASP:N	1:C:3547:ASP:OD1	2.51	0.41
1:C:4890:ARG:NH1	1:D:4897:ASP:OD2	2.54	0.41
1:D:1642:ILE:HD11	1:D:1649:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2747:ILE:HD12	1:D:2747:ILE:H	1.86	0.41
1:D:2918:ALA:HA	1:D:2921:ARG:HB3	2.03	0.41
1:D:2942:LEU:HD12	1:D:2942:LEU:H	1.86	0.41
1:D:3639:MET:HE3	1:D:3639:MET:HB2	1.98	0.41
1:D:3639:MET:O	1:D:3641:PRO:HD3	2.21	0.41
7:D:8006:PCW:H272	7:D:8006:PCW:H483	2.02	0.41
1:A:490:ASN:O	1:A:494:ARG:HG2	2.20	0.41
1:A:822:LEU:HD23	1:A:823:HIS:N	2.36	0.41
1:A:2334:ASP:HA	1:A:2337:ARG:HD3	2.01	0.41
1:A:3639:MET:O	1:A:3641:PRO:HD3	2.21	0.41
1:B:3224:SER:OG	1:B:3227:GLU:OE2	2.31	0.41
1:C:957:PRO:HG2	1:C:960:TYR:CG	2.55	0.41
1:C:2480:LEU:HD11	1:C:2484:GLY:HA2	2.03	0.41
1:D:1788:LEU:HD12	1:D:1788:LEU:HA	1.95	0.41
1:A:1063:GLN:OE1	1:A:1063:GLN:N	2.55	0.40
1:A:3540:ARG:NH2	1:A:3549:GLU:C	2.80	0.40
1:A:3540:ARG:NH1	1:A:3545:ASP:OD2	2.54	0.40
1:B:2629:PHE:CD1	1:B:2629:PHE:C	2.98	0.40
1:B:3547:ASP:N	1:B:3547:ASP:OD1	2.51	0.40
1:B:3600:VAL:HG12	1:B:3604:LEU:HD12	2.02	0.40
1:C:1063:GLN:N	1:C:1063:GLN:OE1	2.54	0.40
1:C:2701:MET:HB3	1:C:2702:PRO:HD3	2.03	0.40
1:C:3330:ILE:O	1:C:3404:ARG:NH2	2.53	0.40
1:D:908:LEU:C	1:D:909:VAL:HG22	2.46	0.40
1:D:1063:GLN:OE1	1:D:1063:GLN:N	2.55	0.40
1:D:2635:ASN:OD1	1:D:2635:ASN:C	2.65	0.40
1:D:3108:VAL:HG23	1:D:3176:LEU:HD12	2.03	0.40
1:D:4796:MET:HE1	7:D:8006:PCW:C21	2.51	0.40
1:A:1788:LEU:HD12	1:A:1788:LEU:HA	1.95	0.40
1:A:2635:ASN:OD1	1:A:2635:ASN:C	2.65	0.40
1:A:3600:VAL:HG12	1:A:3604:LEU:HD12	2.02	0.40
1:A:4796:MET:HE1	7:A:8006:PCW:C21	2.51	0.40
1:B:2009:MET:HE3	1:B:2009:MET:HB3	1.94	0.40
1:B:2769:PHE:O	1:B:2773:GLN:HG2	2.21	0.40
1:B:2942:LEU:H	1:B:2942:LEU:HD12	1.86	0.40
1:B:3351:ARG:HH11	1:B:3351:ARG:HG2	1.87	0.40
1:B:3521:ILE:HD12	1:B:3521:ILE:N	2.36	0.40
1:C:908:LEU:C	1:C:909:VAL:HG22	2.46	0.40
1:C:975:HIS:CD2	1:C:975:HIS:H	2.36	0.40
1:C:2215:VAL:HG21	1:C:2229:MET:HE3	2.04	0.40
1:C:3589:ASP:OD1	1:C:3590:PRO:CD	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:957:PRO:HG2	1:D:960:TYR:CG	2.55	0.40
1:D:1964:GLU:HA	1:D:3651:CYS:SG	2.60	0.40
1:D:3540:ARG:NH2	1:D:3549:GLU:C	2.80	0.40
1:A:323:LYS:O	1:A:323:LYS:HG3	2.21	0.40
1:A:2723:LYS:O	1:A:2724:THR:C	2.65	0.40
1:A:2918:ALA:HA	1:A:2921:ARG:HB3	2.03	0.40
1:A:3589:ASP:OD1	1:A:3590:PRO:CD	2.70	0.40
1:A:4754:ARG:HD2	1:A:4754:ARG:N	2.37	0.40
1:B:71:GLU:OE1	1:B:111:ARG:NE	2.38	0.40
1:B:2215:VAL:HG21	1:B:2229:MET:HE3	2.04	0.40
1:B:2514:GLU:C	1:B:2514:GLU:OE2	2.65	0.40
1:B:2525:VAL:HG23	1:B:2526:GLY:N	2.36	0.40
1:B:2747:ILE:H	1:B:2747:ILE:HD12	1.86	0.40
1:B:2863:LEU:CD1	1:B:2926:GLU:OE1	2.68	0.40
1:B:2863:LEU:HD22	1:B:2933:MET:SD	2.61	0.40
1:B:3589:ASP:OD1	1:B:3590:PRO:CD	2.70	0.40
1:B:4140:ARG:HH11	1:B:4140:ARG:HG2	1.86	0.40
1:B:4754:ARG:HD2	1:B:4754:ARG:N	2.37	0.40
1:C:505:ALA:HB2	1:C:513:ALA:CB	2.51	0.40
1:C:864:LEU:HB3	1:C:869:GLU:HG2	2.04	0.40
1:C:953:LYS:HB2	1:C:953:LYS:HE2	1.47	0.40
1:C:2863:LEU:HD22	1:C:2933:MET:SD	2.61	0.40
1:C:2928:LEU:O	1:C:2932:GLN:HG2	2.21	0.40
1:C:3540:ARG:NH1	1:C:3545:ASP:OD2	2.54	0.40
1:C:4796:MET:HE1	7:C:8006:PCW:C21	2.51	0.40
1:D:505:ALA:HB2	1:D:513:ALA:CB	2.51	0.40
1:D:753:VAL:HB	1:D:754:PRO:C	2.46	0.40
1:A:975:HIS:CD2	1:A:975:HIS:H	2.36	0.40
1:A:978:LEU:HD22	1:A:978:LEU:HA	1.89	0.40
1:A:982:GLN:CG	1:A:1054:ILE:HD11	2.51	0.40
1:A:2413:GLU:HB2	1:A:2416:ARG:HE	1.86	0.40
1:A:2514:GLU:OE2	1:A:2514:GLU:C	2.65	0.40
1:A:4140:ARG:HH11	1:A:4140:ARG:HG2	1.87	0.40
1:A:4691:GLU:CD	1:A:4691:GLU:N	2.79	0.40
1:B:505:ALA:HB2	1:B:513:ALA:CB	2.51	0.40
1:B:882:LEU:HA	1:B:970:PRO:HG3	2.03	0.40
1:B:2800:GLU:HA	1:B:2803:LYS:HD3	2.03	0.40
1:B:2975:ILE:HD13	1:B:2975:ILE:HA	1.93	0.40
1:B:3540:ARG:NH1	1:B:3545:ASP:OD2	2.54	0.40
1:B:3847:LEU:HD13	1:C:77:ARG:HH11	1.84	0.40
1:C:2514:GLU:C	1:C:2514:GLU:OE2	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:868:LEU:HD23	1:D:868:LEU:HA	1.77	0.40
1:D:2799:SER:O	1:D:2802:ASP:OD1	2.39	0.40
1:D:2928:LEU:O	1:D:2932:GLN:HG2	2.21	0.40
1:D:3008:ASN:OD1	1:D:3008:ASN:C	2.65	0.40
1:A:914:LEU:HD21	1:A:919:ARG:CB	2.51	0.40
1:A:2640:MET:HE3	1:A:2640:MET:HB3	2.00	0.40
1:A:2947:LEU:O	1:A:2950:SER:OG	2.26	0.40
1:A:3541:TYR:OH	1:A:3598:GLN:NE2	2.48	0.40
1:B:874:LYS:H	1:B:874:LYS:HG3	1.63	0.40
1:B:1063:GLN:OE1	1:B:1063:GLN:N	2.54	0.40
1:B:1116:LEU:HD23	1:B:1116:LEU:HA	1.95	0.40
1:B:1479:ASP:N	1:B:1482:GLY:O	2.47	0.40
1:B:2215:VAL:HG11	1:B:2229:MET:CE	2.50	0.40
1:B:2928:LEU:O	1:B:2932:GLN:HG2	2.21	0.40
1:B:2971:SER:HA	1:B:2974:PHE:CD2	2.57	0.40
1:B:4227:GLU:CG	1:B:4227:GLU:O	2.69	0.40
1:B:4248:MET:HE1	1:B:4987:MET:HE1	2.04	0.40
1:C:1749:PHE:HB2	1:C:1757:ASP:HA	2.03	0.40
1:C:2747:ILE:H	1:C:2747:ILE:HD12	1.86	0.40
1:C:4754:ARG:HD2	1:C:4754:ARG:N	2.37	0.40
1:D:2723:LYS:O	1:D:2724:THR:C	2.65	0.40
1:D:2769:PHE:O	1:D:2773:GLN:HG2	2.21	0.40
1:D:3521:ILE:HD12	1:D:3521:ILE:N	2.36	0.40
1:D:4140:ARG:HG2	1:D:4140:ARG:HH11	1.86	0.40
7:D:8005:PCW:H231	7:D:8005:PCW:H20	1.72	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	4345/5035 (86%)	4217 (97%)	126 (3%)	2 (0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	4345/5035 (86%)	4218 (97%)	125 (3%)	2 (0%)	100	100
1	C	4345/5035 (86%)	4217 (97%)	126 (3%)	2 (0%)	100	100
1	D	4345/5035 (86%)	4216 (97%)	127 (3%)	2 (0%)	100	100
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
All	All	17800/20572 (86%)	17276 (97%)	516 (3%)	8 (0%)	100	100

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	909	VAL
1	B	909	VAL
1	C	909	VAL
1	D	909	VAL
1	A	2283	ASP
1	B	2283	ASP
1	C	2283	ASP
1	D	2283	ASP

### 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	3806/4296 (89%)	3670 (96%)	136 (4%)	30	56
1	B	3806/4296 (89%)	3668 (96%)	138 (4%)	30	56
1	C	3806/4296 (89%)	3665 (96%)	141 (4%)	29	55
1	D	3806/4296 (89%)	3669 (96%)	137 (4%)	30	56
2	E	89/90 (99%)	86 (97%)	3 (3%)	32	58
2	F	89/90 (99%)	86 (97%)	3 (3%)	32	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	89/90 (99%)	86 (97%)	3 (3%)	32	58
2	H	89/90 (99%)	86 (97%)	3 (3%)	32	58
All	All	15580/17544 (89%)	15016 (96%)	564 (4%)	32	56

All (564) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	147	CYS
1	A	210	CYS
1	A	269	SER
1	A	275	LEU
1	A	326	VAL
1	A	347	CYS
1	A	390	SER
1	A	393	ARG
1	A	397	GLU
1	A	417	LYS
1	A	429	SER
1	A	457	SER
1	A	485	LEU
1	A	589	SER
1	A	746	SER
1	A	748	CYS
1	A	755	SER
1	A	804	LEU
1	A	848	SER
1	A	864	LEU
1	A	869	GLU
1	A	870	ARG
1	A	871	ILE
1	A	872	ARG
1	A	874	LYS
1	A	875	LEU
1	A	878	ASN
1	A	879	ILE
1	A	880	HIS
1	A	882	LEU
1	A	885	LEU
1	A	893	THR
1	A	897	VAL

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Mol	Chain	Res	Type
1	A	898	ARG
1	A	900	ASP
1	A	902	LYS
1	A	903	ARG
1	A	908	LEU
1	A	909	VAL
1	A	910	ASN
1	A	912	HIS
1	A	914	LEU
1	A	919	ARG
1	A	925	MET
1	A	928	GLU
1	A	930	LEU
1	A	931	LYS
1	A	934	LEU
1	A	938	CYS
1	A	939	HIS
1	A	940	VAL
1	A	942	MET
1	A	949	ASP
1	A	952	LYS
1	A	953	LYS
1	A	954	THR
1	A	955	LYS
1	A	956	LEU
1	A	959	THR
1	A	960	TYR
1	A	961	MET
1	A	962	MET
1	A	963	SER
1	A	964	ASN
1	A	966	TYR
1	A	967	LYS
1	A	971	LEU
1	A	972	ASP
1	A	973	LEU
1	A	974	SER
1	A	976	VAL
1	A	977	ARG
1	A	978	LEU
1	A	979	THR
1	A	1007	SER

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Mol	Chain	Res	Type
1	A	1035	SER
1	A	1053	ASN
1	A	1054	ILE
1	A	1071	ASP
1	A	1174	SER
1	A	1210	SER
1	A	1267	THR
1	A	1487	SER
1	A	1503	SER
1	A	1513	THR
1	A	1604	VAL
1	A	1757	ASP
1	A	1788	LEU
1	A	1967	VAL
1	A	2007	ILE
1	A	2093	GLN
1	A	2146	SER
1	A	2155	SER
1	A	2229	MET
1	A	2282	ILE
1	A	2337	ARG
1	A	2508	ASP
1	A	2660	THR
1	A	2669	SER
1	A	2761	GLU
1	A	2824	VAL
1	A	2973	GLU
1	A	2975	ILE
1	A	2990	SER
1	A	3035	LYS
1	A	3040	ILE
1	A	3156	ASP
1	A	3233	LEU
1	A	3236	SER
1	A	3273	ILE
1	A	3297	LEU
1	A	3324	ILE
1	A	3374	VAL
1	A	3400	SER
1	A	3447	SER
1	A	3449	SER
1	A	3509	SER

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Mol	Chain	Res	Type
1	A	3529	THR
1	A	3557	ASN
1	A	3564	VAL
1	A	3612	HIS
1	A	3659	LYS
1	A	3708	ARG
1	A	3752	VAL
1	A	3806	SER
1	A	3869	ILE
1	A	4054	SER
1	A	4077	SER
1	A	4086	ASP
1	A	4092	SER
1	A	4128	CYS
1	A	4154	SER
1	A	4181	LEU
1	A	4711	SER
1	A	4762	LEU
2	E	3	VAL
2	E	26	HIS
2	E	68	SER
2	F	3	VAL
2	F	26	HIS
2	F	68	SER
2	G	3	VAL
2	G	26	HIS
2	G	68	SER
2	H	3	VAL
2	H	26	HIS
2	H	68	SER
1	B	145	GLU
1	B	147	CYS
1	B	210	CYS
1	B	269	SER
1	B	275	LEU
1	B	326	VAL
1	B	347	CYS
1	B	390	SER
1	B	393	ARG
1	B	397	GLU
1	B	417	LYS
1	B	429	SER

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Mol	Chain	Res	Type
1	B	457	SER
1	B	485	LEU
1	B	589	SER
1	B	746	SER
1	B	748	CYS
1	B	755	SER
1	B	804	LEU
1	B	848	SER
1	B	864	LEU
1	B	869	GLU
1	B	870	ARG
1	B	871	ILE
1	B	872	ARG
1	B	874	LYS
1	B	875	LEU
1	B	878	ASN
1	B	879	ILE
1	B	880	HIS
1	B	882	LEU
1	B	885	LEU
1	B	893	THR
1	B	897	VAL
1	B	898	ARG
1	B	900	ASP
1	B	902	LYS
1	B	903	ARG
1	B	908	LEU
1	B	909	VAL
1	B	910	ASN
1	B	912	HIS
1	B	914	LEU
1	B	919	ARG
1	B	925	MET
1	B	928	GLU
1	B	930	LEU
1	B	931	LYS
1	B	934	LEU
1	B	938	CYS
1	B	939	HIS
1	B	940	VAL
1	B	942	MET
1	B	949	ASP

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Mol	Chain	Res	Type
1	B	952	LYS
1	B	953	LYS
1	B	954	THR
1	B	955	LYS
1	B	956	LEU
1	B	959	THR
1	B	960	TYR
1	B	961	MET
1	B	962	MET
1	B	963	SER
1	B	964	ASN
1	B	966	TYR
1	B	967	LYS
1	B	971	LEU
1	B	972	ASP
1	B	973	LEU
1	B	974	SER
1	B	976	VAL
1	B	977	ARG
1	B	978	LEU
1	B	979	THR
1	B	1007	SER
1	B	1035	SER
1	B	1038	ASP
1	B	1053	ASN
1	B	1054	ILE
1	B	1071	ASP
1	B	1174	SER
1	B	1210	SER
1	B	1267	THR
1	B	1487	SER
1	B	1503	SER
1	B	1513	THR
1	B	1604	VAL
1	B	1757	ASP
1	B	1788	LEU
1	B	1967	VAL
1	B	2007	ILE
1	B	2093	GLN
1	B	2146	SER
1	B	2155	SER
1	B	2229	MET

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Mol	Chain	Res	Type
1	B	2282	ILE
1	B	2337	ARG
1	B	2508	ASP
1	B	2660	THR
1	B	2669	SER
1	B	2761	GLU
1	B	2824	VAL
1	B	2973	GLU
1	B	2975	ILE
1	B	2990	SER
1	B	2996	ILE
1	B	3035	LYS
1	B	3040	ILE
1	B	3156	ASP
1	B	3233	LEU
1	B	3236	SER
1	B	3273	ILE
1	B	3297	LEU
1	B	3324	ILE
1	B	3374	VAL
1	B	3400	SER
1	B	3447	SER
1	B	3449	SER
1	B	3509	SER
1	B	3529	THR
1	B	3557	ASN
1	B	3564	VAL
1	B	3612	HIS
1	B	3659	LYS
1	B	3708	ARG
1	B	3752	VAL
1	B	3806	SER
1	B	3869	ILE
1	B	4054	SER
1	B	4077	SER
1	B	4086	ASP
1	B	4092	SER
1	B	4128	CYS
1	B	4154	SER
1	B	4181	LEU
1	B	4711	SER
1	B	4762	LEU

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Mol	Chain	Res	Type
1	C	145	GLU
1	C	147	CYS
1	C	210	CYS
1	C	269	SER
1	C	275	LEU
1	C	326	VAL
1	C	347	CYS
1	C	390	SER
1	C	393	ARG
1	C	397	GLU
1	C	417	LYS
1	C	429	SER
1	C	457	SER
1	C	485	LEU
1	C	589	SER
1	C	746	SER
1	C	748	CYS
1	C	755	SER
1	C	804	LEU
1	C	846	CYS
1	C	848	SER
1	C	864	LEU
1	C	869	GLU
1	C	870	ARG
1	C	871	ILE
1	C	872	ARG
1	C	874	LYS
1	C	875	LEU
1	C	878	ASN
1	C	879	ILE
1	C	880	HIS
1	C	882	LEU
1	C	885	LEU
1	C	893	THR
1	C	897	VAL
1	C	898	ARG
1	C	900	ASP
1	C	902	LYS
1	C	903	ARG
1	C	908	LEU
1	C	909	VAL
1	C	910	ASN

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Mol	Chain	Res	Type
1	C	912	HIS
1	C	914	LEU
1	C	919	ARG
1	C	925	MET
1	C	928	GLU
1	C	930	LEU
1	C	931	LYS
1	C	934	LEU
1	C	938	CYS
1	C	939	HIS
1	C	940	VAL
1	C	942	MET
1	C	949	ASP
1	C	952	LYS
1	C	953	LYS
1	C	954	THR
1	C	955	LYS
1	C	956	LEU
1	C	959	THR
1	C	960	TYR
1	C	961	MET
1	C	962	MET
1	C	963	SER
1	C	964	ASN
1	C	966	TYR
1	C	967	LYS
1	C	971	LEU
1	C	972	ASP
1	C	973	LEU
1	C	974	SER
1	C	976	VAL
1	C	977	ARG
1	C	978	LEU
1	C	979	THR
1	C	1007	SER
1	C	1035	SER
1	C	1053	ASN
1	C	1054	ILE
1	C	1071	ASP
1	C	1174	SER
1	C	1210	SER
1	C	1267	THR

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Mol	Chain	Res	Type
1	C	1429	LEU
1	C	1487	SER
1	C	1503	SER
1	C	1513	THR
1	C	1604	VAL
1	C	1757	ASP
1	C	1967	VAL
1	C	2007	ILE
1	C	2093	GLN
1	C	2146	SER
1	C	2155	SER
1	C	2181	GLN
1	C	2229	MET
1	C	2282	ILE
1	C	2337	ARG
1	C	2508	ASP
1	C	2660	THR
1	C	2669	SER
1	C	2761	GLU
1	C	2824	VAL
1	C	2973	GLU
1	C	2975	ILE
1	C	2990	SER
1	C	2996	ILE
1	C	3035	LYS
1	C	3040	ILE
1	C	3156	ASP
1	C	3233	LEU
1	C	3236	SER
1	C	3273	ILE
1	C	3297	LEU
1	C	3324	ILE
1	C	3374	VAL
1	C	3400	SER
1	C	3447	SER
1	C	3449	SER
1	C	3509	SER
1	C	3529	THR
1	C	3557	ASN
1	C	3564	VAL
1	C	3612	HIS
1	C	3659	LYS

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Mol	Chain	Res	Type
1	C	3708	ARG
1	C	3752	VAL
1	C	3806	SER
1	C	3828	GLU
1	C	3869	ILE
1	C	4054	SER
1	C	4077	SER
1	C	4086	ASP
1	C	4092	SER
1	C	4128	CYS
1	C	4154	SER
1	C	4181	LEU
1	C	4711	SER
1	C	4762	LEU
1	C	4979	GLU
1	D	145	GLU
1	D	147	CYS
1	D	210	CYS
1	D	269	SER
1	D	275	LEU
1	D	326	VAL
1	D	347	CYS
1	D	390	SER
1	D	393	ARG
1	D	397	GLU
1	D	417	LYS
1	D	429	SER
1	D	457	SER
1	D	485	LEU
1	D	589	SER
1	D	746	SER
1	D	748	CYS
1	D	755	SER
1	D	804	LEU
1	D	848	SER
1	D	864	LEU
1	D	869	GLU
1	D	870	ARG
1	D	871	ILE
1	D	872	ARG
1	D	874	LYS
1	D	875	LEU

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Mol	Chain	Res	Type
1	D	878	ASN
1	D	879	ILE
1	D	880	HIS
1	D	882	LEU
1	D	885	LEU
1	D	893	THR
1	D	897	VAL
1	D	898	ARG
1	D	900	ASP
1	D	902	LYS
1	D	903	ARG
1	D	908	LEU
1	D	909	VAL
1	D	910	ASN
1	D	912	HIS
1	D	914	LEU
1	D	919	ARG
1	D	925	MET
1	D	928	GLU
1	D	930	LEU
1	D	931	LYS
1	D	934	LEU
1	D	938	CYS
1	D	939	HIS
1	D	940	VAL
1	D	942	MET
1	D	949	ASP
1	D	952	LYS
1	D	953	LYS
1	D	954	THR
1	D	955	LYS
1	D	956	LEU
1	D	959	THR
1	D	960	TYR
1	D	961	MET
1	D	962	MET
1	D	963	SER
1	D	964	ASN
1	D	966	TYR
1	D	967	LYS
1	D	971	LEU
1	D	972	ASP

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Mol	Chain	Res	Type
1	D	973	LEU
1	D	974	SER
1	D	976	VAL
1	D	977	ARG
1	D	978	LEU
1	D	979	THR
1	D	1007	SER
1	D	1035	SER
1	D	1038	ASP
1	D	1053	ASN
1	D	1054	ILE
1	D	1071	ASP
1	D	1174	SER
1	D	1210	SER
1	D	1267	THR
1	D	1487	SER
1	D	1503	SER
1	D	1513	THR
1	D	1604	VAL
1	D	1757	ASP
1	D	1967	VAL
1	D	2007	ILE
1	D	2093	GLN
1	D	2146	SER
1	D	2155	SER
1	D	2229	MET
1	D	2282	ILE
1	D	2337	ARG
1	D	2508	ASP
1	D	2660	THR
1	D	2669	SER
1	D	2761	GLU
1	D	2824	VAL
1	D	2973	GLU
1	D	2975	ILE
1	D	2990	SER
1	D	2996	ILE
1	D	3035	LYS
1	D	3040	ILE
1	D	3156	ASP
1	D	3233	LEU
1	D	3236	SER

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Mol	Chain	Res	Type
1	D	3273	ILE
1	D	3297	LEU
1	D	3324	ILE
1	D	3374	VAL
1	D	3400	SER
1	D	3447	SER
1	D	3449	SER
1	D	3509	SER
1	D	3529	THR
1	D	3557	ASN
1	D	3564	VAL
1	D	3612	HIS
1	D	3659	LYS
1	D	3708	ARG
1	D	3752	VAL
1	D	3806	SER
1	D	3869	ILE
1	D	4054	SER
1	D	4077	SER
1	D	4086	ASP
1	D	4092	SER
1	D	4128	CYS
1	D	4154	SER
1	D	4181	LEU
1	D	4711	SER
1	D	4762	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (157) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	HIS
1	A	350	GLN
1	A	395	GLN
1	A	400	GLN
1	A	462	HIS
1	A	766	GLN
1	A	878	ASN
1	A	880	HIS
1	A	922	ASN
1	A	950	ASN
1	A	1485	HIS
1	A	1564	GLN

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Mol	Chain	Res	Type
1	A	1570	GLN
1	A	1939	GLN
1	A	2030	GLN
1	A	2757	ASN
1	A	2932	GLN
1	A	2977	HIS
1	A	3031	HIS
1	A	3326	ASN
1	A	3419	ASN
1	A	3463	ASN
1	A	3609	GLN
1	A	3809	ASN
1	A	3917	ASN
1	A	3963	GLN
1	A	3981	GLN
1	A	4097	GLN
1	A	4112	GLN
1	A	4212	GLN
1	A	4219	GLN
1	A	4226	ASN
1	A	4660	ASN
2	E	44	ASN
2	E	66	GLN
2	E	88	HIS
2	F	44	ASN
2	F	66	GLN
2	F	95	HIS
2	G	44	ASN
2	G	66	GLN
2	G	88	HIS
2	G	95	HIS
2	H	44	ASN
2	H	66	GLN
2	H	95	HIS
1	B	182	HIS
1	B	204	ASN
1	B	350	GLN
1	B	395	GLN
1	B	400	GLN
1	B	462	HIS
1	B	766	GLN
1	B	878	ASN

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Mol	Chain	Res	Type
1	B	880	HIS
1	B	922	ASN
1	B	950	ASN
1	B	1485	HIS
1	B	1559	HIS
1	B	1564	GLN
1	B	1570	GLN
1	B	1826	GLN
1	B	1939	GLN
1	B	2030	GLN
1	B	2096	GLN
1	B	2254	HIS
1	B	2575	HIS
1	B	2757	ASN
1	B	2932	GLN
1	B	2977	HIS
1	B	3031	HIS
1	B	3326	ASN
1	B	3463	ASN
1	B	3598	GLN
1	B	3609	GLN
1	B	3809	ASN
1	B	3917	ASN
1	B	3963	GLN
1	B	3981	GLN
1	B	4097	GLN
1	B	4112	GLN
1	B	4212	GLN
1	B	4219	GLN
1	B	4226	ASN
1	B	4660	ASN
1	B	4855	ASN
1	C	182	HIS
1	C	204	ASN
1	C	350	GLN
1	C	395	GLN
1	C	400	GLN
1	C	462	HIS
1	C	766	GLN
1	C	878	ASN
1	C	880	HIS
1	C	922	ASN

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Mol	Chain	Res	Type
1	C	950	ASN
1	C	1485	HIS
1	C	1559	HIS
1	C	1564	GLN
1	C	1570	GLN
1	C	1939	GLN
1	C	2030	GLN
1	C	2096	GLN
1	C	2575	HIS
1	C	2757	ASN
1	C	2932	GLN
1	C	2977	HIS
1	C	3031	HIS
1	C	3326	ASN
1	C	3463	ASN
1	C	3609	GLN
1	C	3809	ASN
1	C	3917	ASN
1	C	3963	GLN
1	C	3981	GLN
1	C	4097	GLN
1	C	4112	GLN
1	C	4219	GLN
1	C	4226	ASN
1	C	4660	ASN
1	C	4855	ASN
1	D	182	HIS
1	D	350	GLN
1	D	395	GLN
1	D	400	GLN
1	D	462	HIS
1	D	766	GLN
1	D	878	ASN
1	D	880	HIS
1	D	922	ASN
1	D	950	ASN
1	D	1485	HIS
1	D	1559	HIS
1	D	1564	GLN
1	D	1570	GLN
1	D	1826	GLN
1	D	1939	GLN

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Mol	Chain	Res	Type
1	D	2030	GLN
1	D	2575	HIS
1	D	2757	ASN
1	D	2932	GLN
1	D	2977	HIS
1	D	3031	HIS
1	D	3326	ASN
1	D	3463	ASN
1	D	3598	GLN
1	D	3609	GLN
1	D	3917	ASN
1	D	3963	GLN
1	D	3981	GLN
1	D	4097	GLN
1	D	4112	GLN
1	D	4219	GLN
1	D	4226	ASN
1	D	4660	ASN
1	D	4855	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 36 ligands modelled in this entry, 8 are monoatomic - leaving 28 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$
7	PCW	D	8005	-	53,53,53	1.23	7 (13%)	59,61,61	1.20	5 (8%)
8	A1BYZ	B	8009	-	32,32,32	0.45	0	40,47,47	2.04	5 (12%)
5	ATP	D	8003	-	28,33,33	0.65	0	34,52,52	0.89	2 (5%)
5	ATP	C	8003	-	28,33,33	0.65	0	34,52,52	0.88	2 (5%)
7	PCW	A	8005	-	53,53,53	1.23	7 (13%)	59,61,61	1.20	5 (8%)
7	PCW	B	8006	-	53,53,53	1.25	7 (13%)	59,61,61	1.11	4 (6%)
7	PCW	C	8006	-	53,53,53	1.25	7 (13%)	59,61,61	1.11	4 (6%)
4	CFF	A	8002	-	8,15,15	2.20	4 (50%)	8,23,23	1.42	1 (12%)
7	PCW	A	8006	-	53,53,53	1.25	7 (13%)	59,61,61	1.11	4 (6%)
8	A1BYZ	D	8008	-	32,32,32	0.78	1 (3%)	40,47,47	0.94	2 (5%)
4	CFF	D	8002	-	8,15,15	2.20	4 (50%)	8,23,23	1.42	1 (12%)
4	CFF	C	8002	-	8,15,15	2.19	4 (50%)	8,23,23	1.41	1 (12%)
7	PCW	D	8006	-	53,53,53	1.25	7 (13%)	59,61,61	1.11	4 (6%)
8	A1BYZ	A	8009	-	32,32,32	0.45	0	40,47,47	2.04	5 (12%)
5	ATP	A	8003	-	28,33,33	0.65	0	34,52,52	0.88	2 (5%)
5	ATP	B	8007	-	28,33,33	0.67	0	34,52,52	0.92	1 (2%)
5	ATP	D	8007	-	28,33,33	0.66	0	34,52,52	0.92	1 (2%)
8	A1BYZ	D	8009	-	32,32,32	0.45	0	40,47,47	2.04	5 (12%)
7	PCW	C	8005	-	53,53,53	1.23	7 (13%)	59,61,61	1.20	5 (8%)
8	A1BYZ	C	8008	-	32,32,32	0.77	1 (3%)	40,47,47	0.94	2 (5%)
7	PCW	B	8005	-	53,53,53	1.23	7 (13%)	59,61,61	1.20	5 (8%)
4	CFF	B	8002	-	8,15,15	2.19	4 (50%)	8,23,23	1.42	1 (12%)
8	A1BYZ	C	8009	-	32,32,32	0.45	0	40,47,47	2.03	5 (12%)
5	ATP	B	8003	-	28,33,33	0.65	0	34,52,52	0.88	2 (5%)
8	A1BYZ	B	8008	-	32,32,32	0.78	1 (3%)	40,47,47	0.95	2 (5%)
8	A1BYZ	A	8008	-	32,32,32	0.78	1 (3%)	40,47,47	0.94	2 (5%)
5	ATP	C	8007	-	28,33,33	0.66	0	34,52,52	0.92	1 (2%)
5	ATP	A	8007	-	28,33,33	0.66	0	34,52,52	0.92	1 (2%)

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
7	PCW	D	8005	-	-	22/57/57/57	-
8	A1BYZ	B	8009	-	-	5/18/59/59	0/3/3/3
5	ATP	D	8003	-	-	6/18/38/38	0/3/3/3
5	ATP	C	8003	-	-	6/18/38/38	0/3/3/3
7	PCW	A	8005	-	-	22/57/57/57	-
7	PCW	B	8006	-	-	28/57/57/57	-
7	PCW	C	8006	-	-	28/57/57/57	-
4	CFF	A	8002	-	-	-	0/2/2/2
7	PCW	A	8006	-	-	28/57/57/57	-
8	A1BYZ	D	8008	-	-	5/18/59/59	0/3/3/3
4	CFF	D	8002	-	-	-	0/2/2/2
4	CFF	C	8002	-	-	-	0/2/2/2
7	PCW	D	8006	-	-	28/57/57/57	-
8	A1BYZ	A	8009	-	-	5/18/59/59	0/3/3/3
5	ATP	A	8003	-	-	6/18/38/38	0/3/3/3
5	ATP	B	8007	-	-	8/18/38/38	0/3/3/3
5	ATP	D	8007	-	-	8/18/38/38	0/3/3/3
8	A1BYZ	D	8009	-	-	5/18/59/59	0/3/3/3
7	PCW	C	8005	-	-	22/57/57/57	-
8	A1BYZ	C	8008	-	-	5/18/59/59	0/3/3/3
7	PCW	B	8005	-	-	23/57/57/57	-
8	A1BYZ	C	8009	-	-	5/18/59/59	0/3/3/3
4	CFF	B	8002	-	-	-	0/2/2/2
5	ATP	B	8003	-	-	6/18/38/38	0/3/3/3
8	A1BYZ	B	8008	-	-	5/18/59/59	0/3/3/3
8	A1BYZ	A	8008	-	-	5/18/59/59	0/3/3/3
5	ATP	C	8007	-	-	8/18/38/38	0/3/3/3
5	ATP	A	8007	-	-	8/18/38/38	0/3/3/3

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	8008	A1BYZ	C16-C15	-3.94	1.50	1.54
8	A	8008	A1BYZ	C16-C15	-3.93	1.50	1.54
8	B	8008	A1BYZ	C16-C15	-3.90	1.50	1.54
8	C	8008	A1BYZ	C16-C15	-3.86	1.50	1.54
4	B	8002	CFF	C5-C4	-3.59	1.33	1.39
4	D	8002	CFF	C5-C4	-3.59	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	8002	CFF	C5-C4	-3.58	1.33	1.39
4	A	8002	CFF	C6-N1	-3.58	1.32	1.38
4	D	8002	CFF	C6-N1	-3.58	1.32	1.38
4	C	8002	CFF	C5-C4	-3.56	1.33	1.39
4	C	8002	CFF	C6-N1	-3.56	1.32	1.38
4	B	8002	CFF	C6-N1	-3.53	1.32	1.38
7	C	8006	PCW	O3-C11	3.03	1.42	1.33
7	A	8006	PCW	O3-C11	3.03	1.42	1.33
7	B	8006	PCW	O3-C11	3.03	1.42	1.33
7	D	8006	PCW	O3-C11	3.03	1.42	1.33
7	D	8005	PCW	O3-C11	2.95	1.41	1.33
7	A	8005	PCW	O3-C11	2.94	1.41	1.33
7	C	8005	PCW	O3-C11	2.93	1.41	1.33
7	B	8005	PCW	O3-C11	2.93	1.41	1.33
7	B	8005	PCW	O2-C31	2.86	1.42	1.34
7	C	8005	PCW	O2-C31	2.85	1.42	1.34
7	A	8005	PCW	O2-C31	2.83	1.42	1.34
7	D	8005	PCW	O2-C31	2.82	1.42	1.34
7	A	8006	PCW	O2-C31	2.69	1.41	1.34
7	B	8006	PCW	O2-C31	2.67	1.41	1.34
7	C	8006	PCW	O2-C31	2.67	1.41	1.34
7	D	8006	PCW	O2-C31	2.67	1.41	1.34
7	D	8006	PCW	P-O4P	2.60	1.69	1.59
7	C	8006	PCW	P-O4P	2.59	1.69	1.59
7	A	8006	PCW	P-O4P	2.58	1.69	1.59
7	B	8006	PCW	P-O4P	2.58	1.69	1.59
7	C	8005	PCW	P-O4P	2.53	1.69	1.59
7	A	8005	PCW	P-O4P	2.52	1.69	1.59
7	B	8005	PCW	P-O4P	2.52	1.69	1.59
7	D	8005	PCW	P-O4P	2.51	1.69	1.59
7	D	8006	PCW	O2-C2	-2.49	1.40	1.46
4	C	8002	CFF	O13-C6	-2.48	1.18	1.24
4	D	8002	CFF	O13-C6	-2.48	1.18	1.24
4	A	8002	CFF	O13-C6	-2.48	1.18	1.24
4	B	8002	CFF	O13-C6	-2.47	1.18	1.24
7	A	8006	PCW	O2-C2	-2.47	1.40	1.46
7	C	8006	PCW	O2-C2	-2.45	1.40	1.46
7	B	8006	PCW	O2-C2	-2.44	1.40	1.46
7	C	8005	PCW	O2-C2	-2.42	1.40	1.46
7	A	8005	PCW	O2-C2	-2.38	1.41	1.46
7	D	8005	PCW	O2-C2	-2.38	1.41	1.46
7	B	8005	PCW	O2-C2	-2.37	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	8006	PCW	C5-C4	2.34	1.58	1.51
7	C	8005	PCW	C5-C4	2.34	1.58	1.51
7	D	8006	PCW	C5-C4	2.33	1.58	1.51
7	D	8005	PCW	C5-C4	2.32	1.58	1.51
7	A	8006	PCW	C5-C4	2.32	1.58	1.51
7	A	8005	PCW	C5-C4	2.32	1.58	1.51
7	B	8005	PCW	C5-C4	2.31	1.58	1.51
7	B	8006	PCW	C5-C4	2.31	1.58	1.51
7	D	8005	PCW	C32-C31	2.18	1.57	1.50
7	A	8005	PCW	C32-C31	2.16	1.57	1.50
7	B	8005	PCW	C32-C31	2.15	1.56	1.50
7	C	8005	PCW	C32-C31	2.15	1.56	1.50
7	D	8006	PCW	C32-C31	2.15	1.56	1.50
7	B	8005	PCW	P-O3P	2.14	1.67	1.59
7	A	8006	PCW	P-O3P	2.13	1.67	1.59
7	C	8006	PCW	C32-C31	2.12	1.56	1.50
7	B	8006	PCW	P-O3P	2.12	1.67	1.59
7	A	8005	PCW	P-O3P	2.12	1.67	1.59
7	C	8005	PCW	P-O3P	2.12	1.67	1.59
7	B	8006	PCW	C32-C31	2.12	1.56	1.50
7	A	8006	PCW	C32-C31	2.11	1.56	1.50
7	C	8006	PCW	P-O3P	2.11	1.67	1.59
7	D	8006	PCW	P-O3P	2.11	1.67	1.59
7	D	8005	PCW	P-O3P	2.10	1.67	1.59
4	C	8002	CFF	C5-C6	-2.07	1.37	1.41
4	A	8002	CFF	C5-C6	-2.05	1.37	1.41
4	B	8002	CFF	C5-C6	-2.05	1.37	1.41
4	D	8002	CFF	C5-C6	-2.02	1.37	1.41

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	8009	A1BYZ	C14-C15-C16	9.69	115.84	110.70
8	A	8009	A1BYZ	C14-C15-C16	9.67	115.83	110.70
8	B	8009	A1BYZ	C14-C15-C16	9.63	115.81	110.70
8	C	8009	A1BYZ	C14-C15-C16	9.59	115.79	110.70
8	C	8009	A1BYZ	C24-C25-C26	-4.37	109.12	116.30
8	B	8009	A1BYZ	C24-C25-C26	-4.36	109.14	116.30
8	A	8009	A1BYZ	C24-C25-C26	-4.35	109.15	116.30
8	D	8009	A1BYZ	C24-C25-C26	-4.35	109.16	116.30
7	A	8005	PCW	C21-C20-C19	4.22	156.42	124.83
7	B	8005	PCW	C21-C20-C19	4.22	156.42	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	8005	PCW	C21-C20-C19	4.21	156.41	124.83
7	C	8005	PCW	C21-C20-C19	4.21	156.38	124.83
8	C	8009	A1BYZ	C15-C16-C17	4.10	113.37	110.88
8	B	8009	A1BYZ	C15-C16-C17	4.09	113.37	110.88
8	A	8009	A1BYZ	C15-C16-C17	4.05	113.35	110.88
8	D	8009	A1BYZ	C15-C16-C17	4.03	113.34	110.88
7	C	8006	PCW	C21-C20-C19	3.96	154.53	124.83
7	A	8006	PCW	C21-C20-C19	3.96	154.53	124.83
7	B	8006	PCW	C21-C20-C19	3.96	154.52	124.83
7	D	8006	PCW	C21-C20-C19	3.96	154.50	124.83
7	A	8005	PCW	O2-C31-C32	3.80	119.69	111.48
7	D	8005	PCW	O2-C31-C32	3.80	119.69	111.48
7	C	8005	PCW	O2-C31-C32	3.79	119.68	111.48
7	B	8005	PCW	O2-C31-C32	3.78	119.66	111.48
8	C	8009	A1BYZ	C15-C14-C13	3.54	113.95	110.21
8	B	8009	A1BYZ	C15-C14-C13	3.50	113.92	110.21
8	A	8009	A1BYZ	C15-C14-C13	3.50	113.91	110.21
8	B	8008	A1BYZ	C15-C16-C17	-3.49	108.75	110.88
8	D	8009	A1BYZ	C15-C14-C13	3.48	113.89	110.21
8	A	8008	A1BYZ	C15-C16-C17	-3.37	108.82	110.88
8	C	8008	A1BYZ	C15-C16-C17	-3.36	108.83	110.88
8	D	8008	A1BYZ	C15-C16-C17	-3.36	108.83	110.88
7	C	8006	PCW	O2-C31-C32	3.28	118.58	111.48
7	D	8006	PCW	O2-C31-C32	3.28	118.57	111.48
7	A	8006	PCW	O2-C31-C32	3.27	118.55	111.48
7	B	8006	PCW	O2-C31-C32	3.27	118.55	111.48
4	C	8002	CFF	C14-N7-C8	-2.98	111.11	125.43
4	A	8002	CFF	C14-N7-C8	-2.96	111.16	125.43
4	B	8002	CFF	C14-N7-C8	-2.96	111.17	125.43
4	D	8002	CFF	C14-N7-C8	-2.95	111.22	125.43
7	D	8005	PCW	C18-C19-C20	2.93	146.76	124.83
7	B	8005	PCW	C18-C19-C20	2.93	146.75	124.83
7	C	8005	PCW	C18-C19-C20	2.93	146.75	124.83
7	A	8005	PCW	C18-C19-C20	2.92	146.73	124.83
8	D	8009	A1BYZ	C20-C15-C16	-2.63	111.18	112.87
8	B	8009	A1BYZ	C20-C15-C16	-2.63	111.18	112.87
7	B	8006	PCW	C18-C19-C20	2.62	144.48	124.83
7	C	8006	PCW	C18-C19-C20	2.62	144.48	124.83
7	A	8006	PCW	C18-C19-C20	2.62	144.45	124.83
7	D	8006	PCW	C18-C19-C20	2.62	144.44	124.83
8	A	8009	A1BYZ	C20-C15-C16	-2.60	111.20	112.87
8	C	8009	A1BYZ	C20-C15-C16	-2.56	111.22	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	8006	PCW	O3-C11-C12	2.53	119.54	111.83
7	D	8006	PCW	O3-C11-C12	2.53	119.54	111.83
7	A	8006	PCW	O3-C11-C12	2.52	119.51	111.83
7	C	8006	PCW	O3-C11-C12	2.51	119.49	111.83
7	B	8005	PCW	C2-O2-C31	-2.46	111.90	117.80
7	A	8005	PCW	C2-O2-C31	-2.46	111.91	117.80
7	D	8005	PCW	C2-O2-C31	-2.46	111.92	117.80
7	C	8005	PCW	C2-O2-C31	-2.45	111.93	117.80
7	D	8005	PCW	O3-C11-C12	2.42	119.22	111.83
7	A	8005	PCW	O3-C11-C12	2.42	119.22	111.83
7	C	8005	PCW	O3-C11-C12	2.42	119.21	111.83
7	B	8005	PCW	O3-C11-C12	2.41	119.20	111.83
8	B	8008	A1BYZ	C24-C25-C26	-2.40	112.35	116.30
8	C	8008	A1BYZ	C24-C25-C26	-2.40	112.35	116.30
8	A	8008	A1BYZ	C24-C25-C26	-2.40	112.36	116.30
8	D	8008	A1BYZ	C24-C25-C26	-2.40	112.37	116.30
5	B	8007	ATP	C5-C6-N6	2.34	123.87	120.31
5	D	8007	ATP	C5-C6-N6	2.34	123.87	120.31
5	A	8007	ATP	C5-C6-N6	2.32	123.85	120.31
5	C	8007	ATP	C5-C6-N6	2.32	123.85	120.31
5	B	8003	ATP	C5-C6-N6	2.31	123.83	120.31
5	D	8003	ATP	C5-C6-N6	2.31	123.83	120.31
5	A	8003	ATP	C5-C6-N6	2.30	123.81	120.31
5	C	8003	ATP	C5-C6-N6	2.29	123.80	120.31
5	B	8003	ATP	O3'-C3'-C2'	-2.02	105.33	111.82
5	C	8003	ATP	O3'-C3'-C2'	-2.02	105.36	111.82
5	A	8003	ATP	O3'-C3'-C2'	-2.01	105.37	111.82
5	D	8003	ATP	O3'-C3'-C2'	-2.01	105.38	111.82

There are no chirality outliers.

All (297) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	8003	ATP	C5'-O5'-PA-O1A
5	A	8003	ATP	C5'-O5'-PA-O3A
5	B	8003	ATP	C5'-O5'-PA-O1A
5	B	8003	ATP	C5'-O5'-PA-O3A
5	C	8003	ATP	C5'-O5'-PA-O1A
5	C	8003	ATP	C5'-O5'-PA-O3A
5	D	8003	ATP	C5'-O5'-PA-O1A
5	D	8003	ATP	C5'-O5'-PA-O3A
7	A	8005	PCW	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	A	8005	PCW	C32-C31-O2-C2
7	A	8006	PCW	O4P-C4-C5-N
7	A	8006	PCW	C4-O4P-P-O3P
7	B	8005	PCW	O3P-C1-C2-O2
7	B	8005	PCW	C32-C31-O2-C2
7	B	8006	PCW	O4P-C4-C5-N
7	B	8006	PCW	C4-O4P-P-O3P
7	C	8005	PCW	O3P-C1-C2-O2
7	C	8005	PCW	C32-C31-O2-C2
7	C	8006	PCW	O4P-C4-C5-N
7	C	8006	PCW	C4-O4P-P-O3P
7	D	8005	PCW	O3P-C1-C2-O2
7	D	8005	PCW	C32-C31-O2-C2
7	D	8006	PCW	O4P-C4-C5-N
7	D	8006	PCW	C4-O4P-P-O3P
8	A	8009	A1BYZ	C3-C6-O8-C9
8	A	8009	A1BYZ	O7-C6-O8-C9
8	B	8009	A1BYZ	C3-C6-O8-C9
8	B	8009	A1BYZ	O7-C6-O8-C9
8	C	8009	A1BYZ	C3-C6-O8-C9
8	C	8009	A1BYZ	O7-C6-O8-C9
8	D	8009	A1BYZ	C3-C6-O8-C9
8	D	8009	A1BYZ	O7-C6-O8-C9
8	A	8008	A1BYZ	C10-C9-O8-C6
8	B	8008	A1BYZ	C10-C9-O8-C6
8	C	8008	A1BYZ	C10-C9-O8-C6
8	D	8008	A1BYZ	C10-C9-O8-C6
7	A	8005	PCW	O31-C31-O2-C2
7	B	8005	PCW	O31-C31-O2-C2
7	C	8005	PCW	O31-C31-O2-C2
7	D	8005	PCW	O31-C31-O2-C2
7	A	8006	PCW	C32-C31-O2-C2
7	B	8006	PCW	C32-C31-O2-C2
7	C	8006	PCW	C32-C31-O2-C2
7	D	8006	PCW	C32-C31-O2-C2
7	A	8006	PCW	C22-C23-C24-C25
7	B	8006	PCW	C22-C23-C24-C25
7	C	8006	PCW	C22-C23-C24-C25
7	D	8006	PCW	C22-C23-C24-C25
7	A	8006	PCW	O31-C31-O2-C2
7	B	8006	PCW	O31-C31-O2-C2
7	C	8006	PCW	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
7	D	8006	PCW	O31-C31-O2-C2
8	A	8008	A1BYZ	C15-C20-C21-C22
8	B	8008	A1BYZ	C15-C20-C21-C22
8	C	8008	A1BYZ	C15-C20-C21-C22
8	D	8008	A1BYZ	C15-C20-C21-C22
7	A	8006	PCW	C11-C12-C13-C14
7	B	8006	PCW	C11-C12-C13-C14
7	C	8006	PCW	C11-C12-C13-C14
7	D	8006	PCW	C11-C12-C13-C14
7	A	8006	PCW	C36-C37-C38-C39
7	B	8006	PCW	C36-C37-C38-C39
7	C	8006	PCW	C36-C37-C38-C39
7	D	8006	PCW	C36-C37-C38-C39
7	A	8006	PCW	C33-C34-C35-C36
7	B	8006	PCW	C33-C34-C35-C36
7	C	8006	PCW	C33-C34-C35-C36
7	D	8006	PCW	C33-C34-C35-C36
7	B	8006	PCW	C12-C13-C14-C15
7	C	8006	PCW	C12-C13-C14-C15
7	A	8006	PCW	C12-C13-C14-C15
7	D	8006	PCW	C12-C13-C14-C15
7	A	8005	PCW	C12-C11-O3-C3
7	B	8005	PCW	C12-C11-O3-C3
7	C	8005	PCW	C12-C11-O3-C3
7	D	8005	PCW	C12-C11-O3-C3
7	B	8005	PCW	C35-C36-C37-C38
7	C	8005	PCW	C35-C36-C37-C38
7	A	8005	PCW	C35-C36-C37-C38
7	D	8005	PCW	C35-C36-C37-C38
7	A	8005	PCW	C41-C42-C43-C44
7	D	8005	PCW	C41-C42-C43-C44
7	B	8005	PCW	C41-C42-C43-C44
7	C	8005	PCW	C41-C42-C43-C44
7	A	8005	PCW	C24-C25-C26-C27
7	B	8005	PCW	C24-C25-C26-C27
7	C	8005	PCW	C24-C25-C26-C27
7	D	8005	PCW	C24-C25-C26-C27
7	A	8005	PCW	C43-C44-C45-C46
7	B	8005	PCW	C43-C44-C45-C46
7	D	8005	PCW	C43-C44-C45-C46
7	C	8005	PCW	C43-C44-C45-C46
7	A	8006	PCW	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
7	B	8006	PCW	C23-C24-C25-C26
7	C	8006	PCW	C23-C24-C25-C26
7	D	8006	PCW	C23-C24-C25-C26
7	A	8005	PCW	O11-C11-O3-C3
7	B	8005	PCW	O11-C11-O3-C3
7	C	8005	PCW	O11-C11-O3-C3
7	D	8005	PCW	O11-C11-O3-C3
7	A	8006	PCW	C21-C22-C23-C24
7	B	8006	PCW	C21-C22-C23-C24
7	C	8006	PCW	C21-C22-C23-C24
7	D	8006	PCW	C21-C22-C23-C24
7	A	8006	PCW	C16-C17-C18-C19
7	B	8006	PCW	C16-C17-C18-C19
7	C	8006	PCW	C16-C17-C18-C19
7	D	8006	PCW	C16-C17-C18-C19
7	A	8005	PCW	C42-C43-C44-C45
7	C	8005	PCW	C42-C43-C44-C45
7	D	8005	PCW	C42-C43-C44-C45
7	B	8005	PCW	C42-C43-C44-C45
7	A	8005	PCW	C32-C33-C34-C35
7	B	8005	PCW	C32-C33-C34-C35
7	C	8005	PCW	C32-C33-C34-C35
7	D	8005	PCW	C32-C33-C34-C35
7	D	8006	PCW	C35-C36-C37-C38
7	A	8006	PCW	C35-C36-C37-C38
7	B	8006	PCW	C35-C36-C37-C38
7	C	8006	PCW	C35-C36-C37-C38
7	A	8005	PCW	C20-C21-C22-C23
7	B	8005	PCW	C20-C21-C22-C23
7	C	8005	PCW	C20-C21-C22-C23
7	D	8005	PCW	C20-C21-C22-C23
7	D	8006	PCW	C17-C18-C19-C20
7	A	8005	PCW	O3P-C1-C2-C3
7	B	8005	PCW	O3P-C1-C2-C3
7	C	8005	PCW	O3P-C1-C2-C3
7	D	8005	PCW	O3P-C1-C2-C3
7	A	8006	PCW	C17-C18-C19-C20
7	B	8006	PCW	C17-C18-C19-C20
7	C	8006	PCW	C17-C18-C19-C20
7	C	8006	PCW	C42-C43-C44-C45
7	B	8006	PCW	C42-C43-C44-C45
7	A	8006	PCW	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
7	D	8006	PCW	C42-C43-C44-C45
7	A	8006	PCW	C19-C20-C21-C22
7	B	8006	PCW	C19-C20-C21-C22
7	C	8006	PCW	C19-C20-C21-C22
7	D	8006	PCW	C19-C20-C21-C22
7	B	8005	PCW	C45-C46-C47-C48
7	C	8005	PCW	C45-C46-C47-C48
7	D	8005	PCW	C45-C46-C47-C48
7	A	8005	PCW	C45-C46-C47-C48
7	A	8006	PCW	C45-C46-C47-C48
7	C	8006	PCW	C45-C46-C47-C48
7	D	8006	PCW	C45-C46-C47-C48
7	A	8006	PCW	C31-C32-C33-C34
7	B	8006	PCW	C31-C32-C33-C34
7	C	8006	PCW	C31-C32-C33-C34
7	B	8006	PCW	C45-C46-C47-C48
7	D	8006	PCW	C31-C32-C33-C34
7	A	8006	PCW	C25-C26-C27-C28
7	B	8006	PCW	C25-C26-C27-C28
7	C	8006	PCW	C25-C26-C27-C28
7	D	8006	PCW	C25-C26-C27-C28
7	C	8005	PCW	C13-C14-C15-C16
7	A	8005	PCW	C13-C14-C15-C16
7	B	8005	PCW	C13-C14-C15-C16
7	D	8005	PCW	C13-C14-C15-C16
7	B	8005	PCW	C21-C22-C23-C24
7	A	8005	PCW	C21-C22-C23-C24
7	B	8005	PCW	C15-C16-C17-C18
7	C	8005	PCW	C21-C22-C23-C24
7	D	8005	PCW	C21-C22-C23-C24
7	A	8005	PCW	C15-C16-C17-C18
7	C	8005	PCW	C15-C16-C17-C18
7	D	8005	PCW	C15-C16-C17-C18
7	A	8006	PCW	C5-C4-O4P-P
7	B	8006	PCW	C5-C4-O4P-P
7	C	8006	PCW	C5-C4-O4P-P
7	D	8006	PCW	C5-C4-O4P-P
7	D	8006	PCW	C34-C35-C36-C37
7	A	8006	PCW	C34-C35-C36-C37
7	B	8006	PCW	C34-C35-C36-C37
7	C	8006	PCW	C34-C35-C36-C37
7	A	8005	PCW	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
7	B	8005	PCW	C34-C35-C36-C37
7	C	8005	PCW	C34-C35-C36-C37
7	D	8005	PCW	C34-C35-C36-C37
5	A	8003	ATP	C5'-O5'-PA-O2A
5	A	8007	ATP	C5'-O5'-PA-O1A
5	A	8007	ATP	C5'-O5'-PA-O2A
5	A	8007	ATP	C5'-O5'-PA-O3A
5	B	8003	ATP	C5'-O5'-PA-O2A
5	B	8007	ATP	C5'-O5'-PA-O1A
5	B	8007	ATP	C5'-O5'-PA-O2A
5	B	8007	ATP	C5'-O5'-PA-O3A
5	C	8003	ATP	C5'-O5'-PA-O2A
5	C	8007	ATP	C5'-O5'-PA-O1A
5	C	8007	ATP	C5'-O5'-PA-O2A
5	C	8007	ATP	C5'-O5'-PA-O3A
5	D	8003	ATP	C5'-O5'-PA-O2A
5	D	8007	ATP	C5'-O5'-PA-O1A
5	D	8007	ATP	C5'-O5'-PA-O2A
5	D	8007	ATP	C5'-O5'-PA-O3A
7	A	8005	PCW	C4-O4P-P-O1P
7	A	8006	PCW	C4-O4P-P-O2P
7	B	8005	PCW	C4-O4P-P-O1P
7	B	8006	PCW	C4-O4P-P-O2P
7	C	8005	PCW	C4-O4P-P-O1P
7	C	8006	PCW	C4-O4P-P-O2P
7	D	8005	PCW	C4-O4P-P-O1P
7	D	8006	PCW	C4-O4P-P-O2P
7	A	8005	PCW	C25-C26-C27-C28
7	B	8005	PCW	C25-C26-C27-C28
7	D	8005	PCW	C25-C26-C27-C28
5	A	8007	ATP	PB-O3A-PA-O1A
5	A	8007	ATP	PB-O3A-PA-O2A
5	B	8007	ATP	PB-O3A-PA-O1A
5	B	8007	ATP	PB-O3A-PA-O2A
5	C	8007	ATP	PB-O3A-PA-O1A
5	C	8007	ATP	PB-O3A-PA-O2A
5	D	8007	ATP	PB-O3A-PA-O1A
5	D	8007	ATP	PB-O3A-PA-O2A
7	C	8005	PCW	C25-C26-C27-C28
5	A	8007	ATP	C3'-C4'-C5'-O5'
5	B	8007	ATP	C3'-C4'-C5'-O5'
5	C	8007	ATP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	D	8007	ATP	C3'-C4'-C5'-O5'
7	D	8006	PCW	C41-C42-C43-C44
7	B	8006	PCW	C41-C42-C43-C44
7	A	8006	PCW	C41-C42-C43-C44
7	C	8006	PCW	C41-C42-C43-C44
7	A	8006	PCW	C12-C11-O3-C3
7	B	8006	PCW	C12-C11-O3-C3
7	C	8006	PCW	C12-C11-O3-C3
7	D	8006	PCW	C12-C11-O3-C3
7	A	8006	PCW	O11-C11-O3-C3
7	B	8006	PCW	O11-C11-O3-C3
7	D	8006	PCW	O11-C11-O3-C3
5	A	8003	ATP	PA-O3A-PB-O3B
5	B	8003	ATP	PA-O3A-PB-O3B
5	C	8003	ATP	PA-O3A-PB-O3B
5	D	8003	ATP	PA-O3A-PB-O3B
8	A	8009	A1BYZ	C15-C20-C21-C22
8	B	8009	A1BYZ	C15-C20-C21-C22
8	C	8009	A1BYZ	C15-C20-C21-C22
8	D	8009	A1BYZ	C15-C20-C21-C22
7	C	8006	PCW	O11-C11-O3-C3
7	A	8006	PCW	C39-C40-C41-C42
7	B	8006	PCW	C39-C40-C41-C42
7	C	8006	PCW	C39-C40-C41-C42
7	D	8006	PCW	C39-C40-C41-C42
8	A	8009	A1BYZ	C16-C15-C20-C21
8	B	8009	A1BYZ	C16-C15-C20-C21
8	C	8009	A1BYZ	C16-C15-C20-C21
8	D	8009	A1BYZ	C16-C15-C20-C21
8	A	8008	A1BYZ	C2-C3-C6-O7
8	A	8009	A1BYZ	C2-C3-C6-O7
8	B	8008	A1BYZ	C2-C3-C6-O7
8	B	8009	A1BYZ	C2-C3-C6-O7
8	C	8008	A1BYZ	C2-C3-C6-O7
8	C	8009	A1BYZ	C2-C3-C6-O7
8	D	8008	A1BYZ	C2-C3-C6-O7
8	D	8009	A1BYZ	C2-C3-C6-O7
7	A	8006	PCW	C32-C33-C34-C35
7	B	8006	PCW	C32-C33-C34-C35
7	D	8006	PCW	C32-C33-C34-C35
7	C	8006	PCW	C32-C33-C34-C35
7	A	8005	PCW	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
7	B	8005	PCW	C17-C18-C19-C20
7	C	8005	PCW	C17-C18-C19-C20
7	D	8005	PCW	C17-C18-C19-C20
5	A	8007	ATP	PB-O3B-PG-O3G
5	B	8007	ATP	PB-O3B-PG-O3G
5	C	8007	ATP	PB-O3B-PG-O3G
5	D	8007	ATP	PB-O3B-PG-O3G
7	D	8006	PCW	C15-C16-C17-C18
7	A	8006	PCW	C15-C16-C17-C18
7	B	8006	PCW	C15-C16-C17-C18
7	C	8006	PCW	C15-C16-C17-C18
7	B	8005	PCW	C5-C4-O4P-P
7	A	8005	PCW	C39-C40-C41-C42
7	B	8005	PCW	C39-C40-C41-C42
7	C	8005	PCW	C39-C40-C41-C42
7	D	8005	PCW	C39-C40-C41-C42
8	A	8008	A1BYZ	C4-C3-C6-O8
8	B	8008	A1BYZ	C4-C3-C6-O8
8	C	8008	A1BYZ	C4-C3-C6-O8
8	D	8008	A1BYZ	C4-C3-C6-O8
5	A	8003	ATP	PA-O3A-PB-O1B
5	B	8003	ATP	PA-O3A-PB-O1B
5	C	8003	ATP	PA-O3A-PB-O1B
5	D	8003	ATP	PA-O3A-PB-O1B
5	A	8003	ATP	O4'-C4'-C5'-O5'
5	A	8007	ATP	O4'-C4'-C5'-O5'
5	B	8003	ATP	O4'-C4'-C5'-O5'
5	B	8007	ATP	O4'-C4'-C5'-O5'
5	C	8003	ATP	O4'-C4'-C5'-O5'
5	C	8007	ATP	O4'-C4'-C5'-O5'
5	D	8003	ATP	O4'-C4'-C5'-O5'
5	D	8007	ATP	O4'-C4'-C5'-O5'
8	A	8008	A1BYZ	C4-C3-C6-O7
8	B	8008	A1BYZ	C4-C3-C6-O7
8	C	8008	A1BYZ	C4-C3-C6-O7
8	D	8008	A1BYZ	C4-C3-C6-O7

There are no ring outliers.

10 monomers are involved in 32 short contacts:

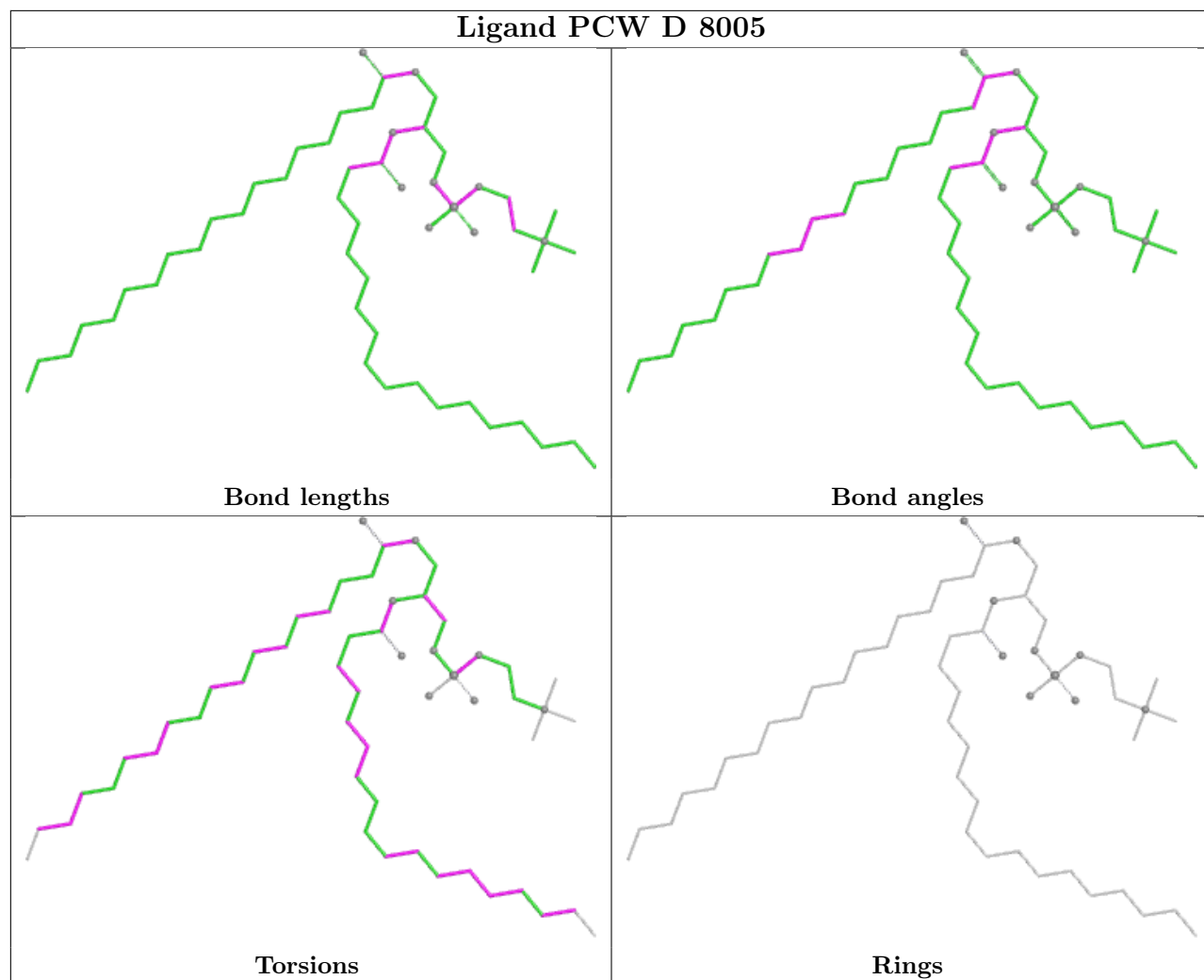
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	8005	PCW	1	0

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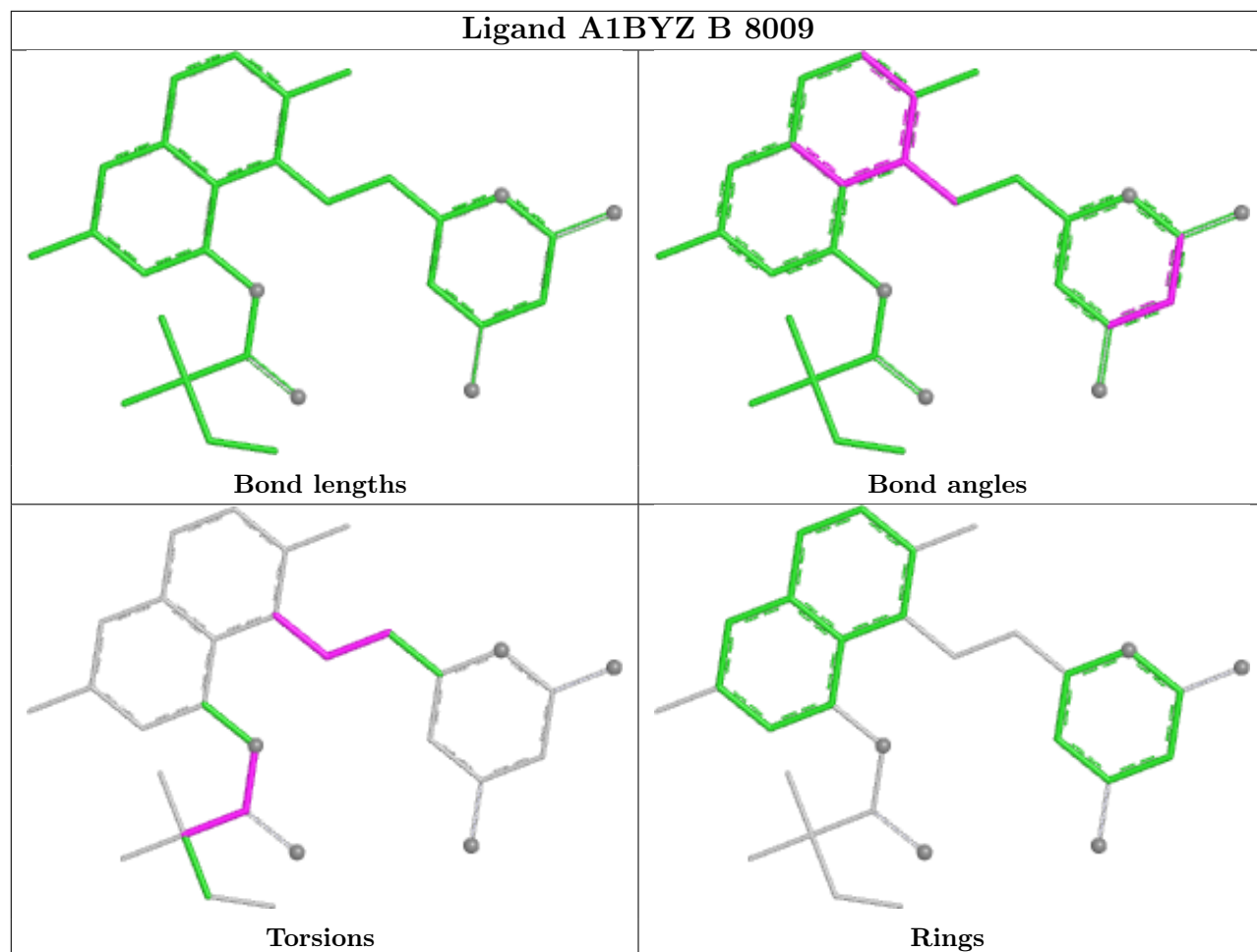
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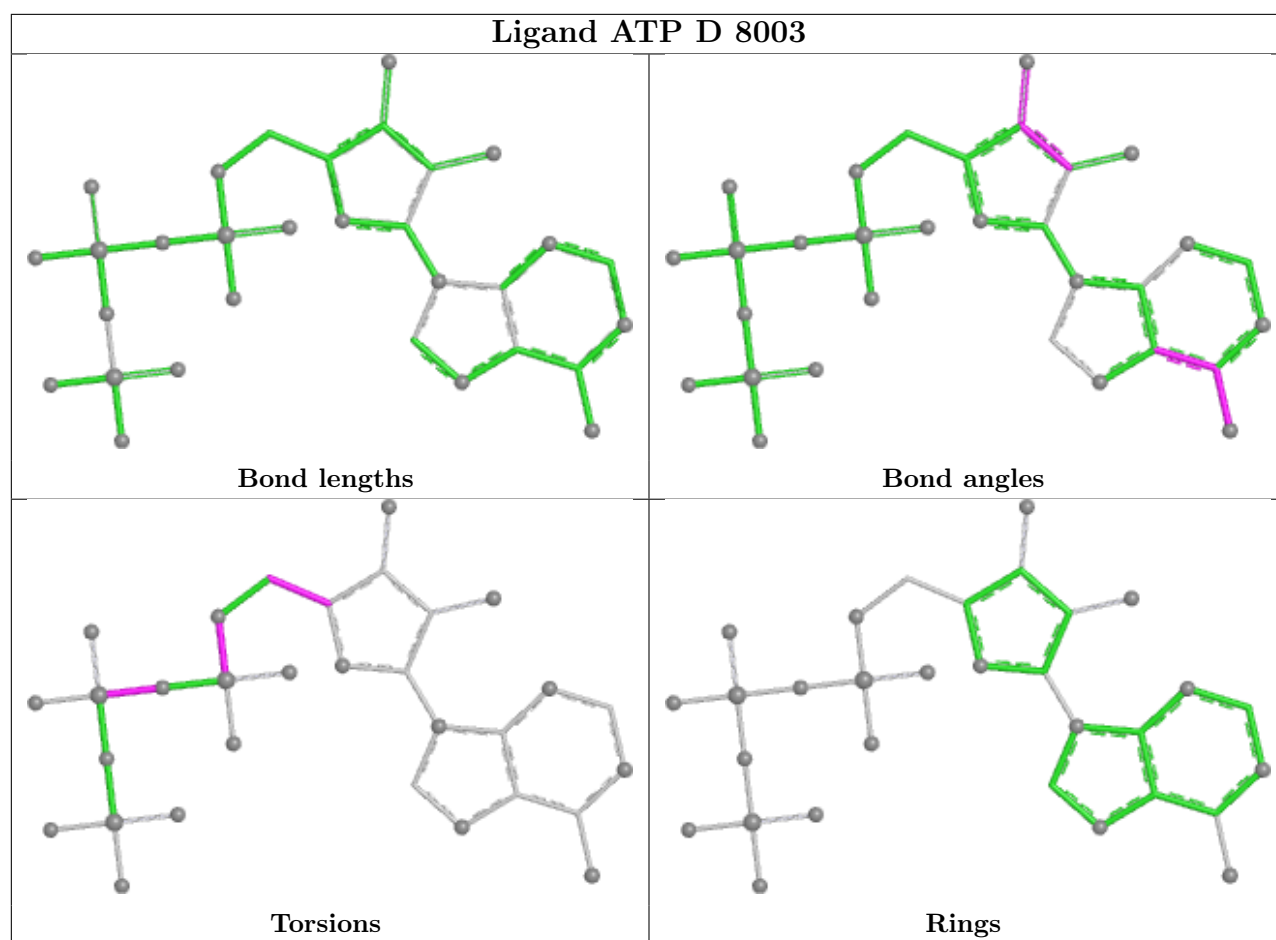
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	8009	A1BYZ	2	0
7	B	8006	PCW	6	0
7	C	8006	PCW	6	0
7	A	8006	PCW	5	0
7	D	8006	PCW	5	0
8	A	8009	A1BYZ	2	0
8	D	8009	A1BYZ	2	0
7	B	8005	PCW	1	0
8	C	8009	A1BYZ	2	0

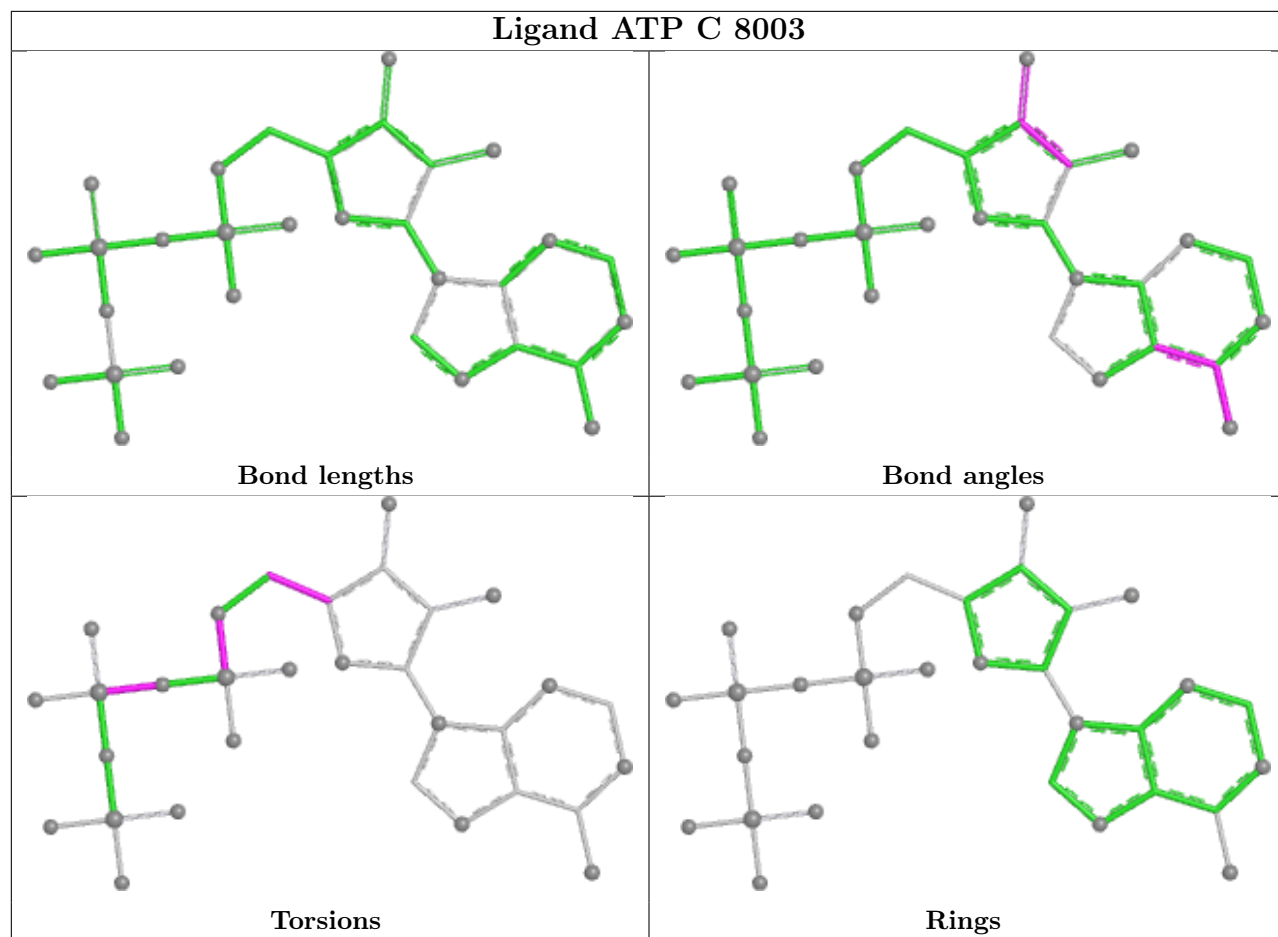
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



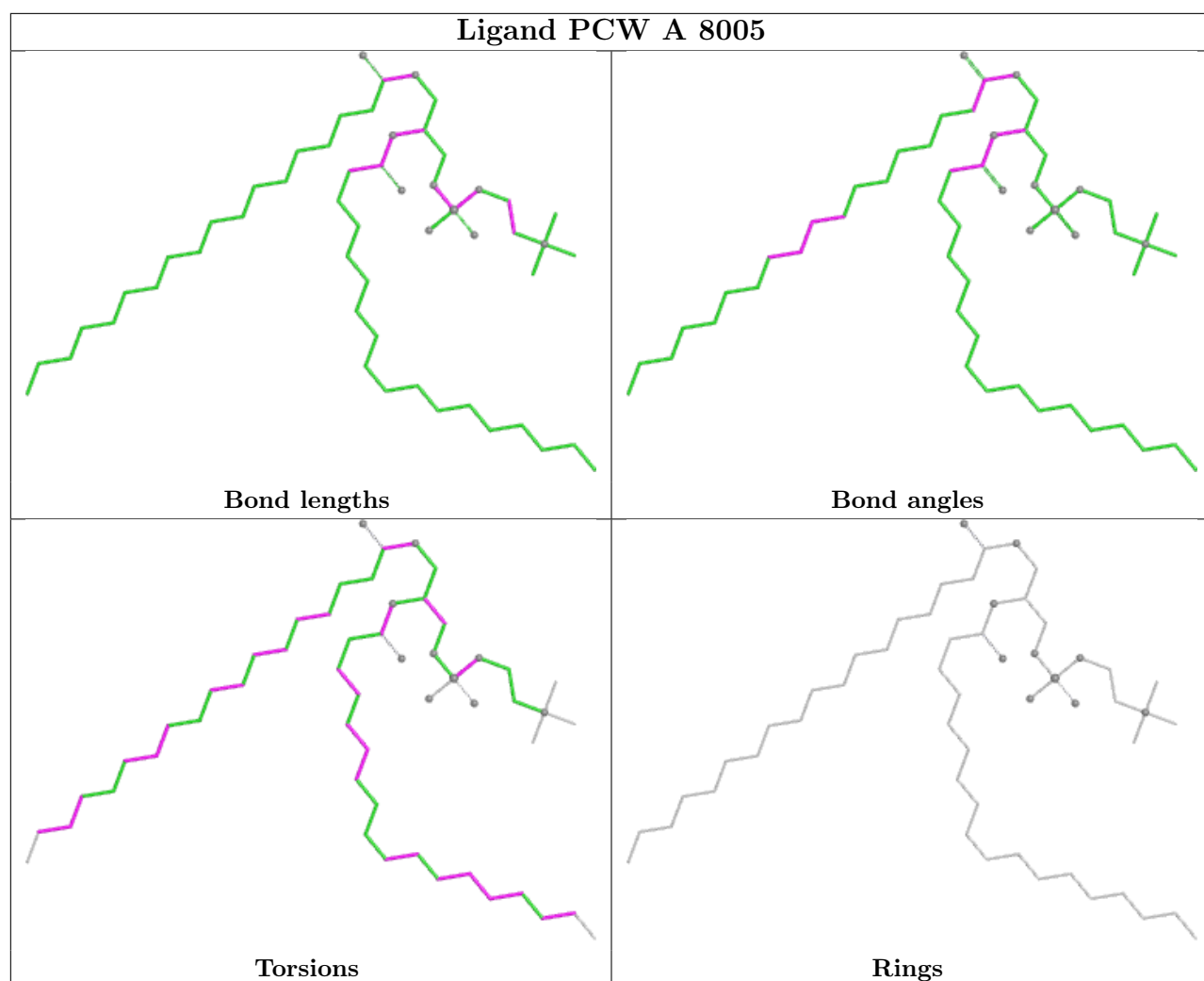
## Ligand A1BYZ B 8009

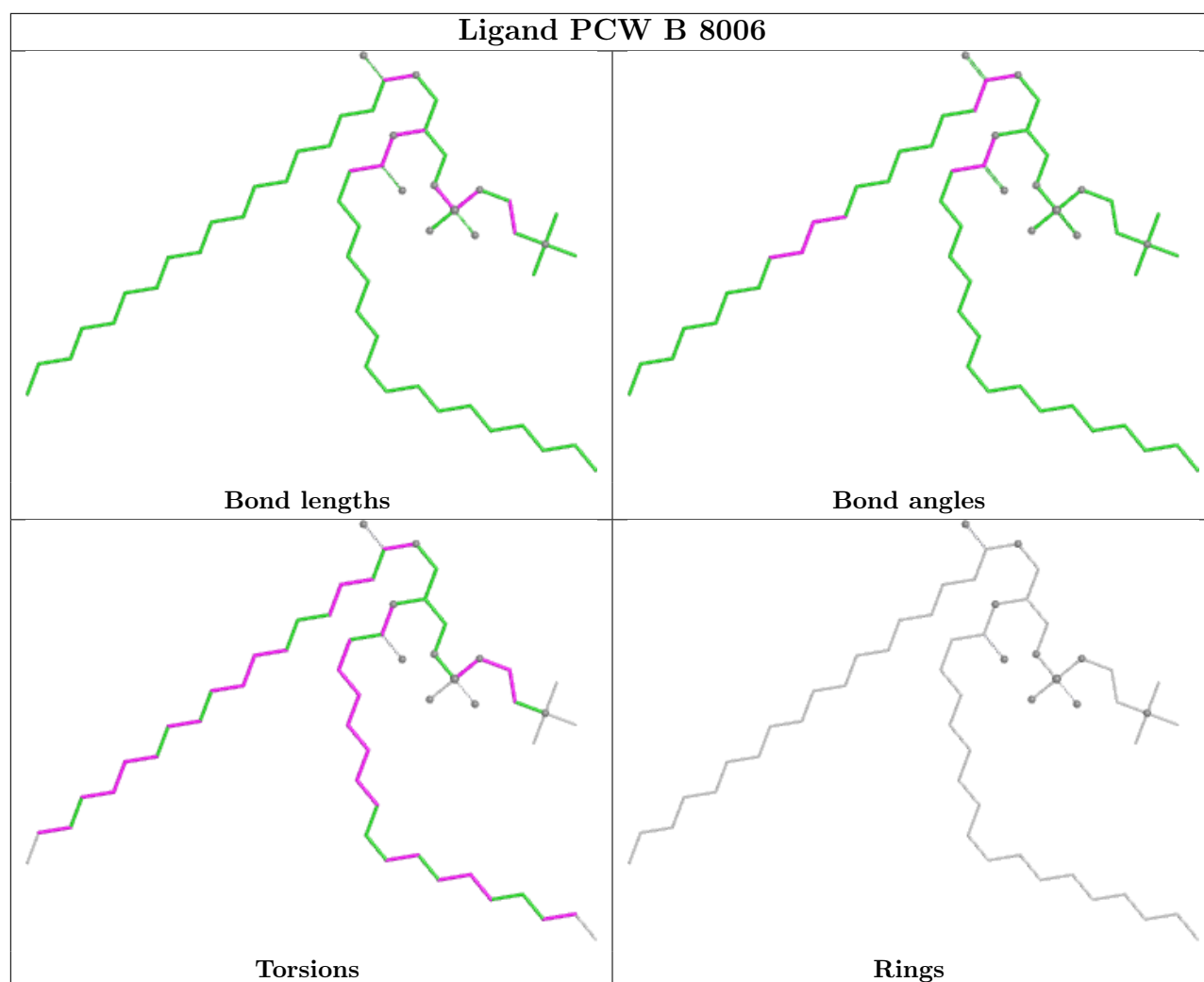


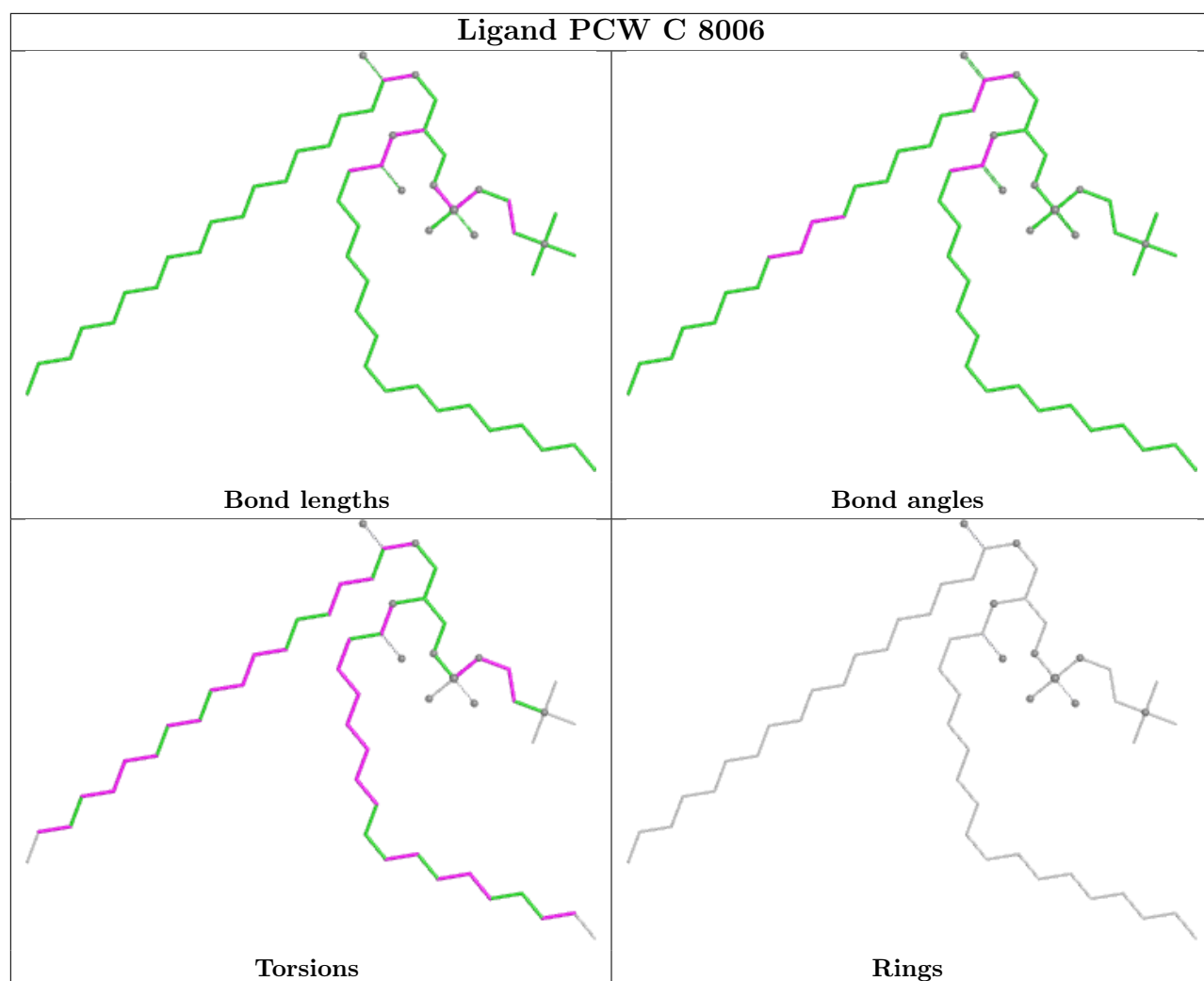


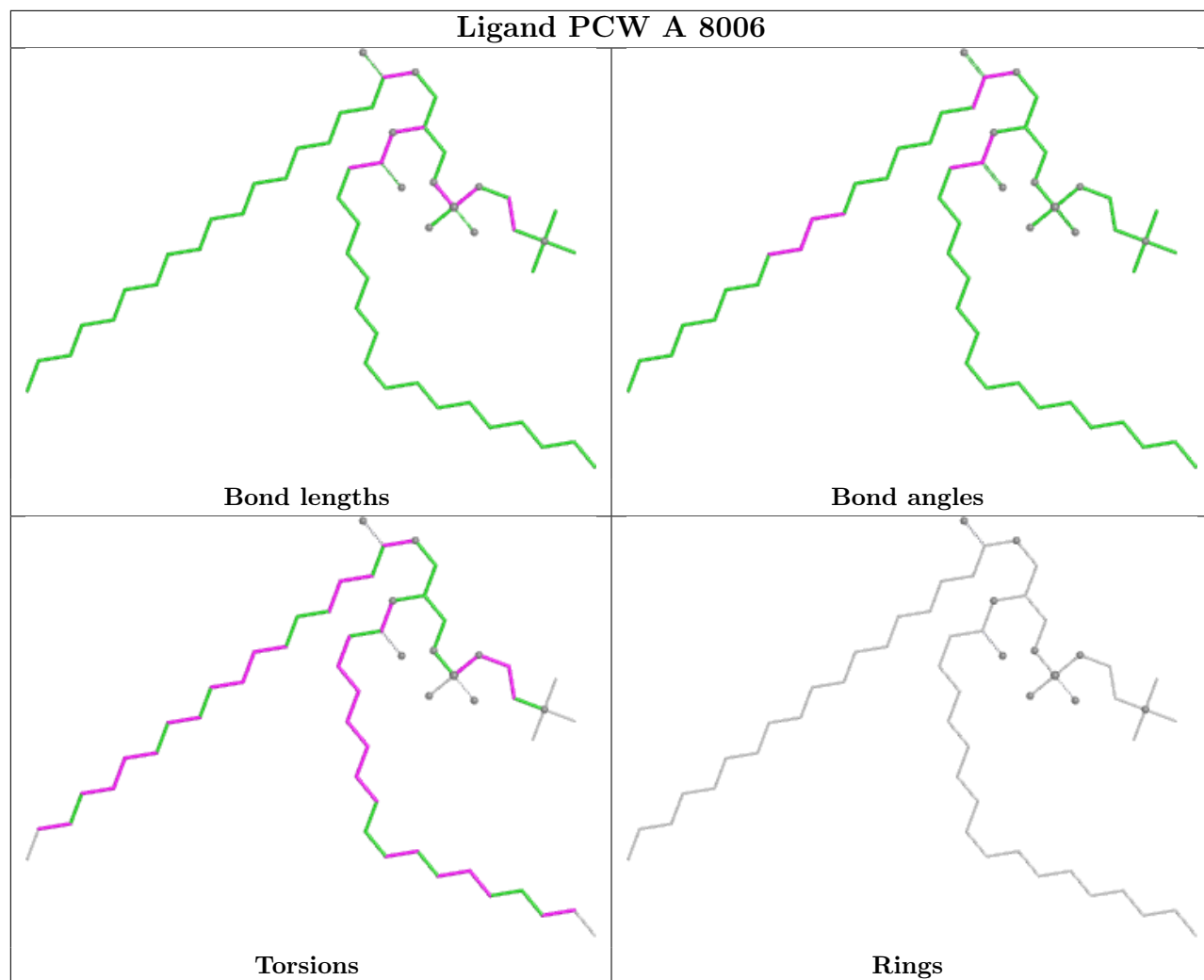




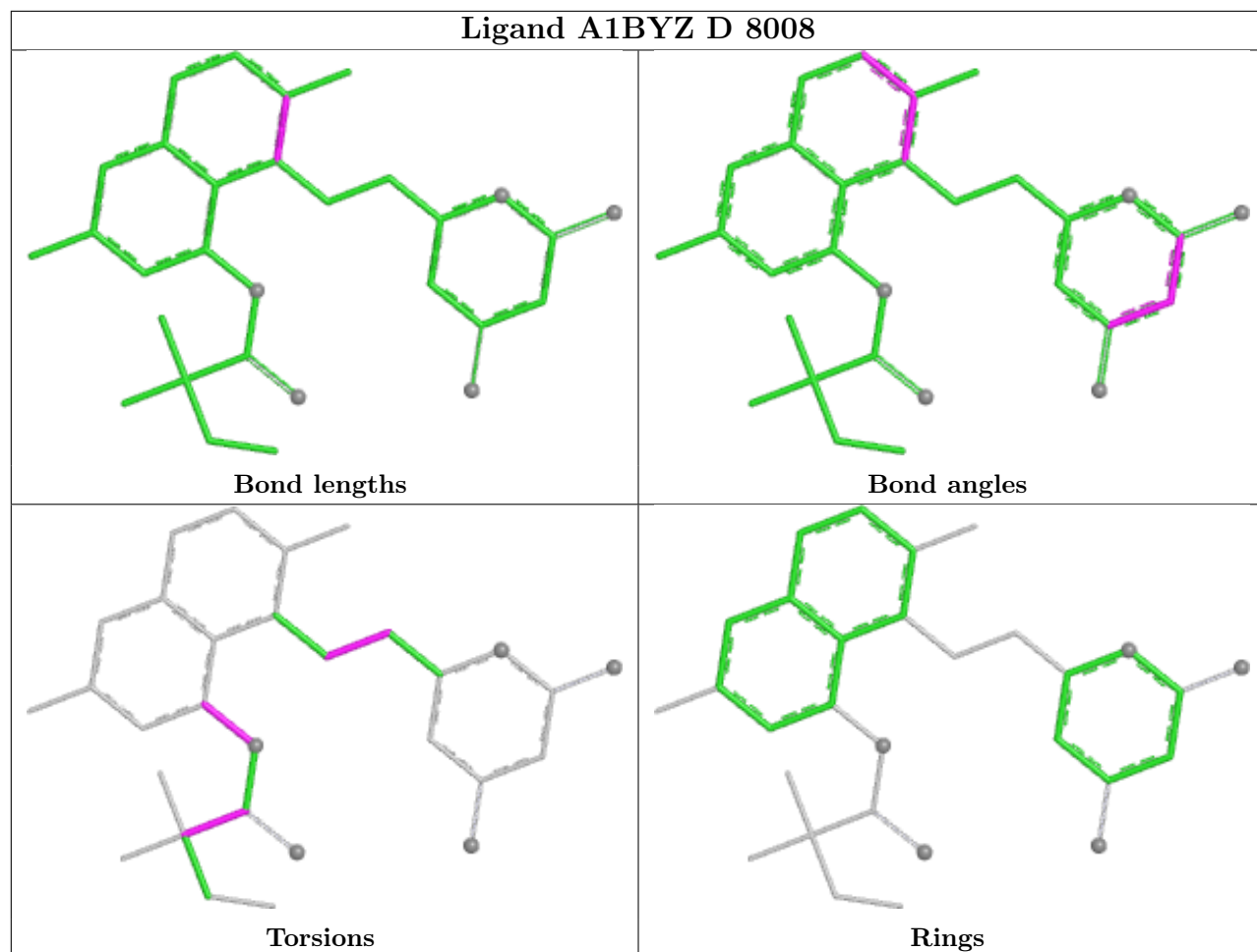


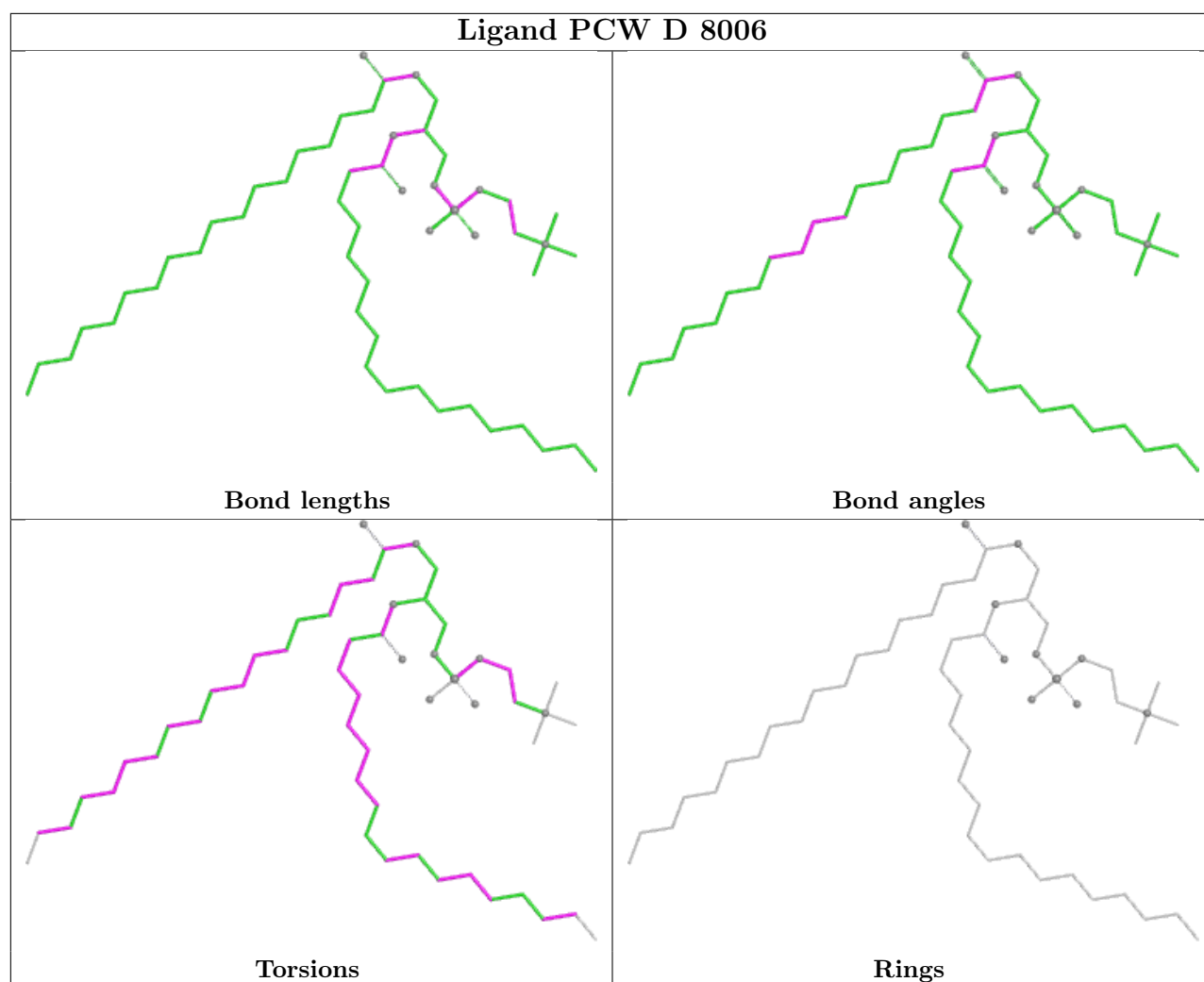




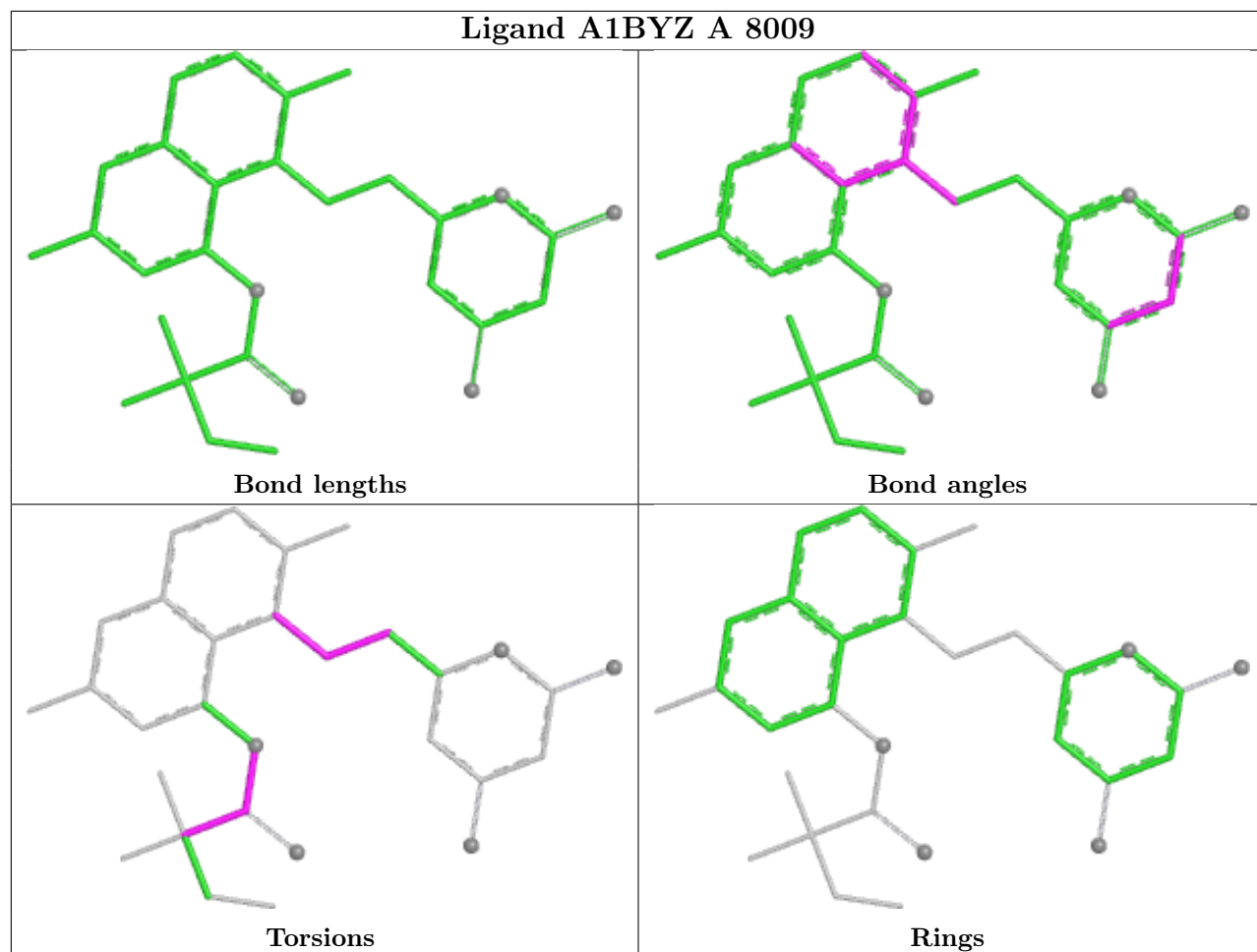


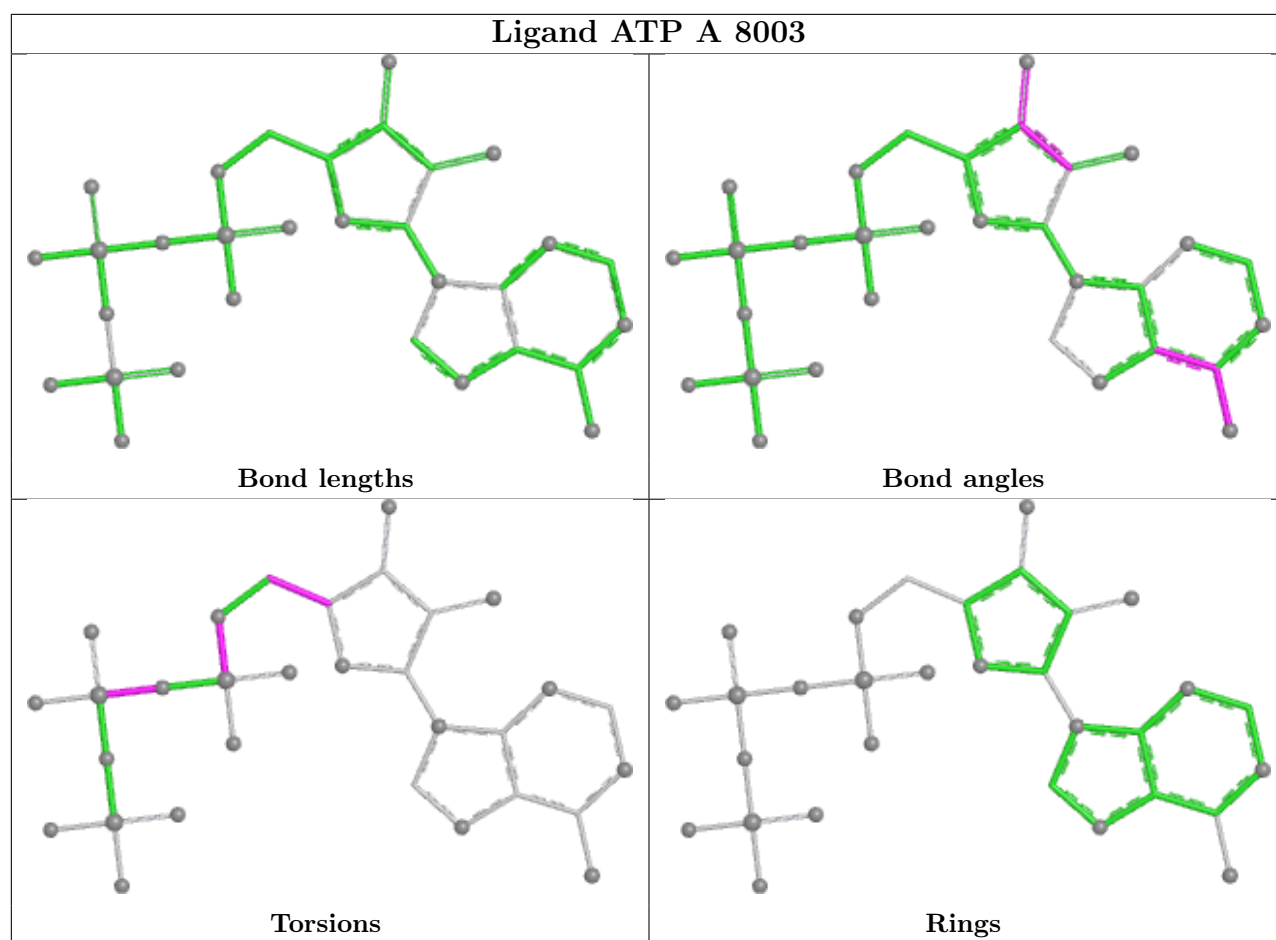
## Ligand A1BYZ D 8008



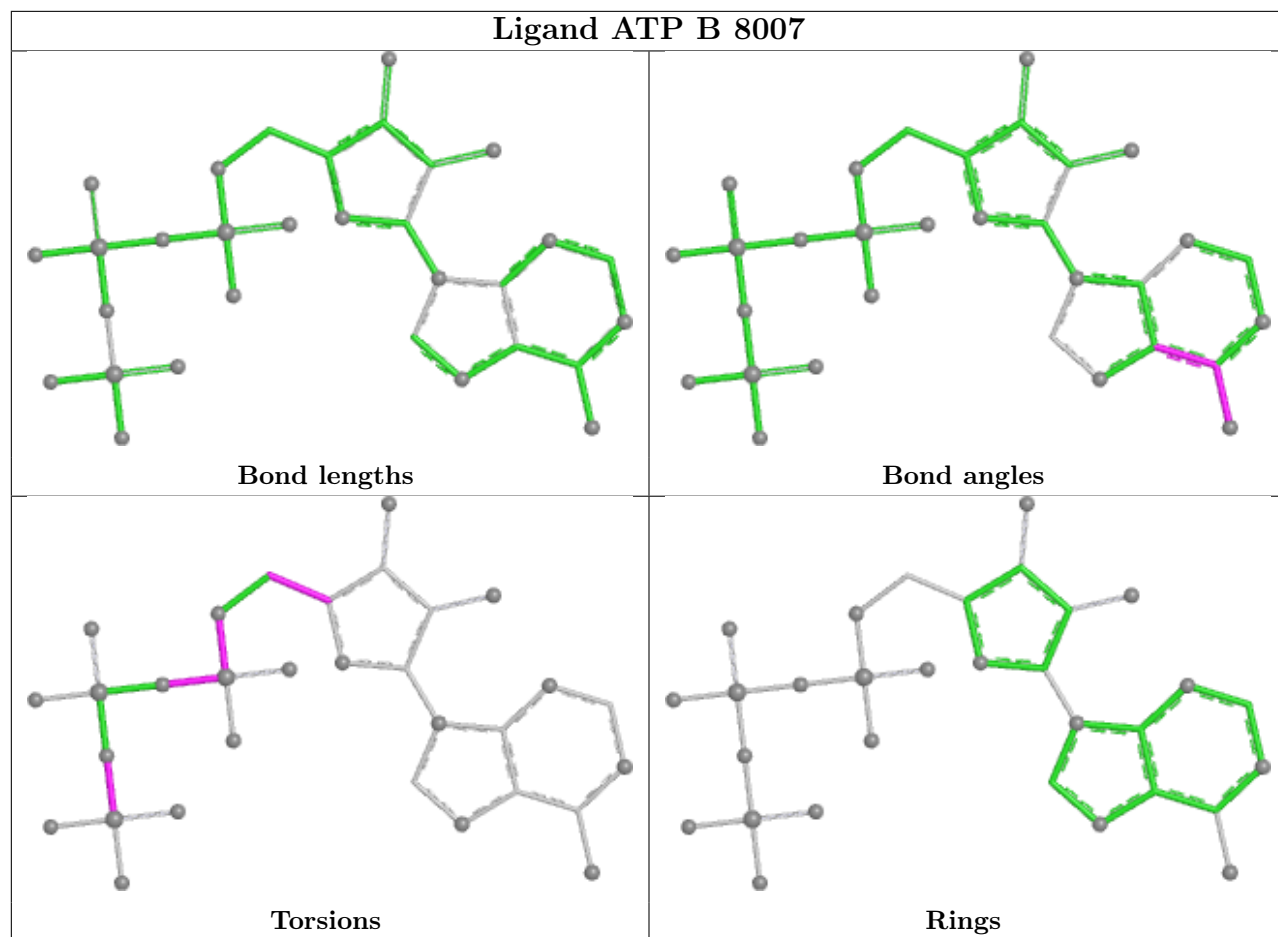


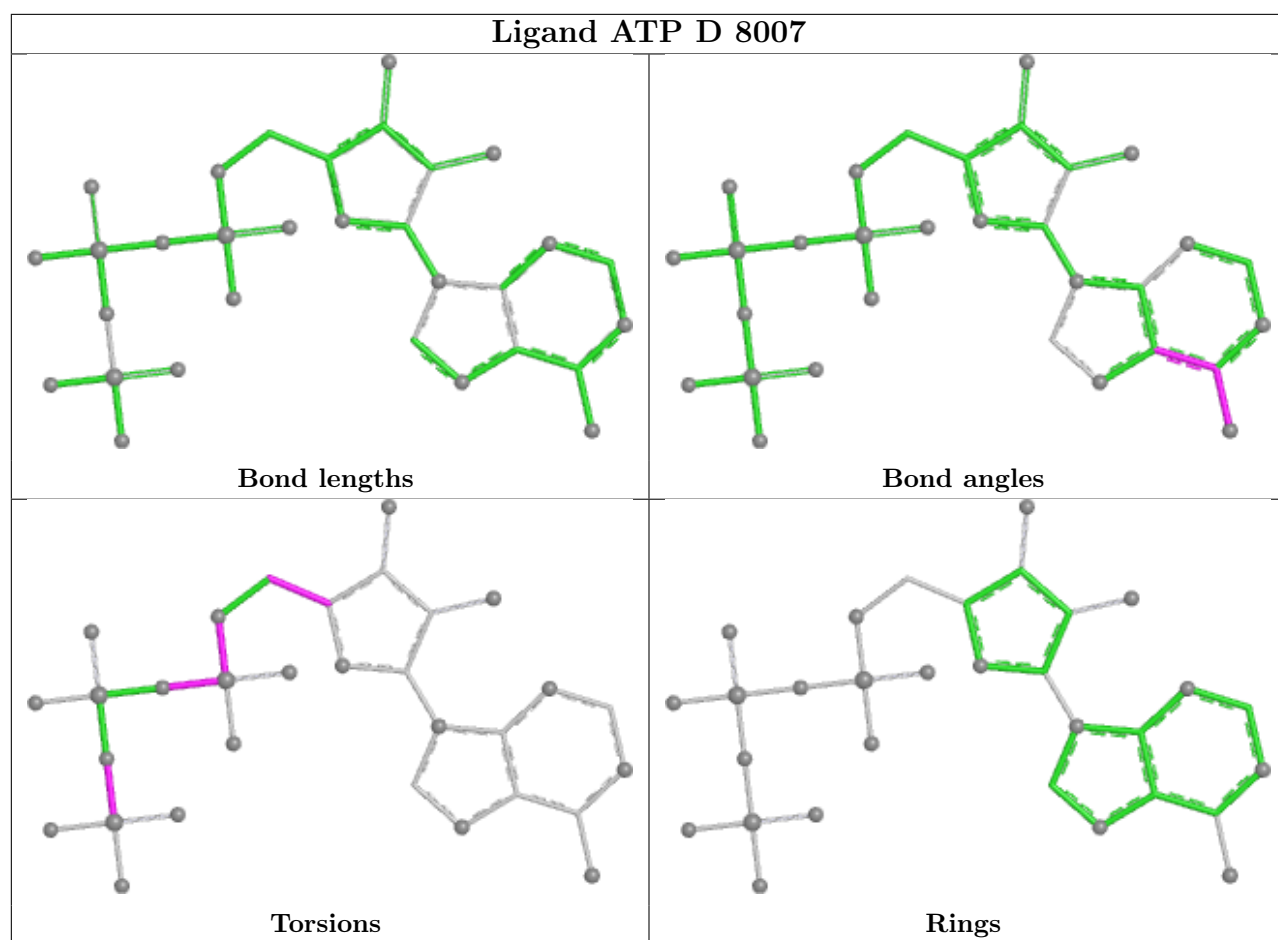
## Ligand A1BYZ A 8009



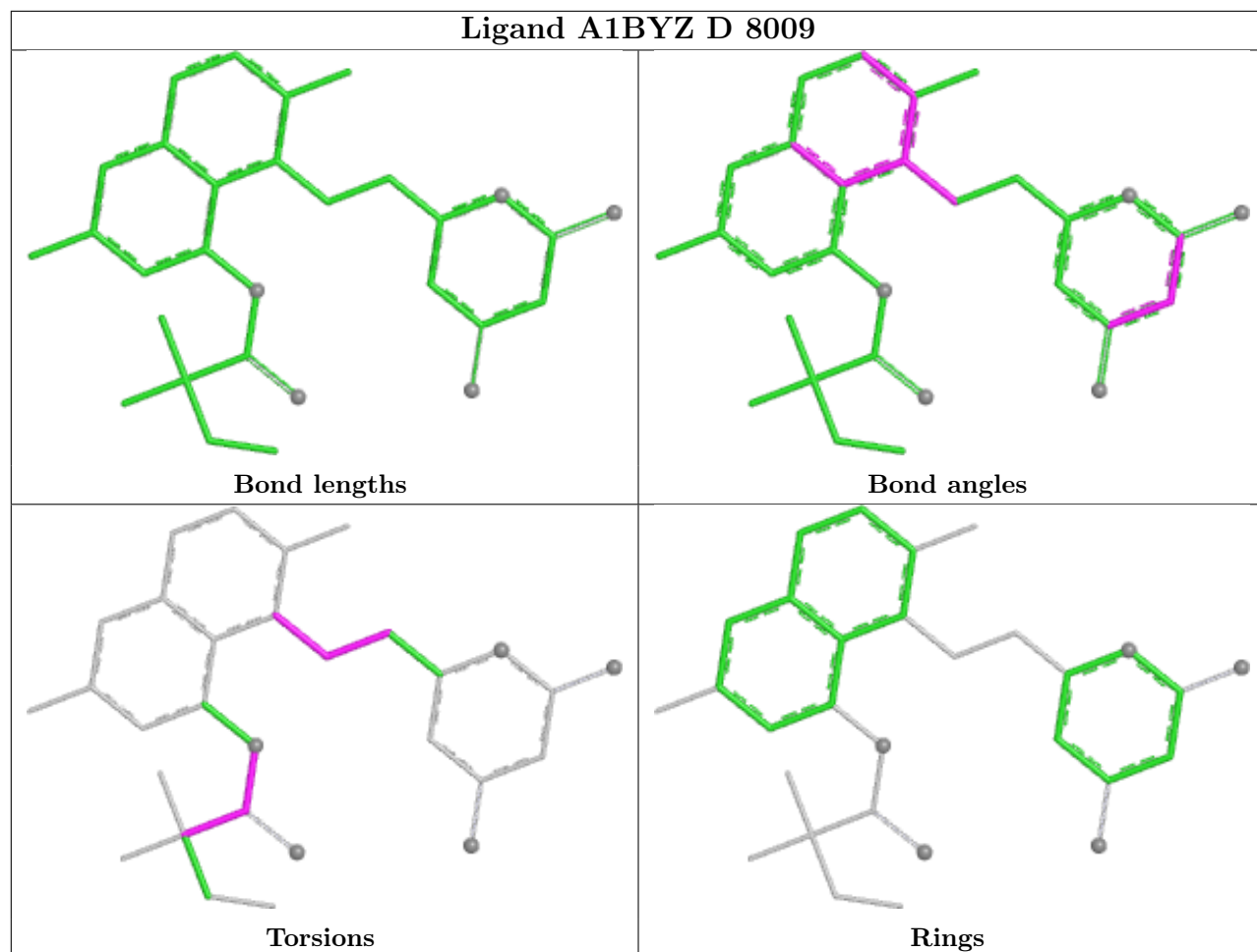


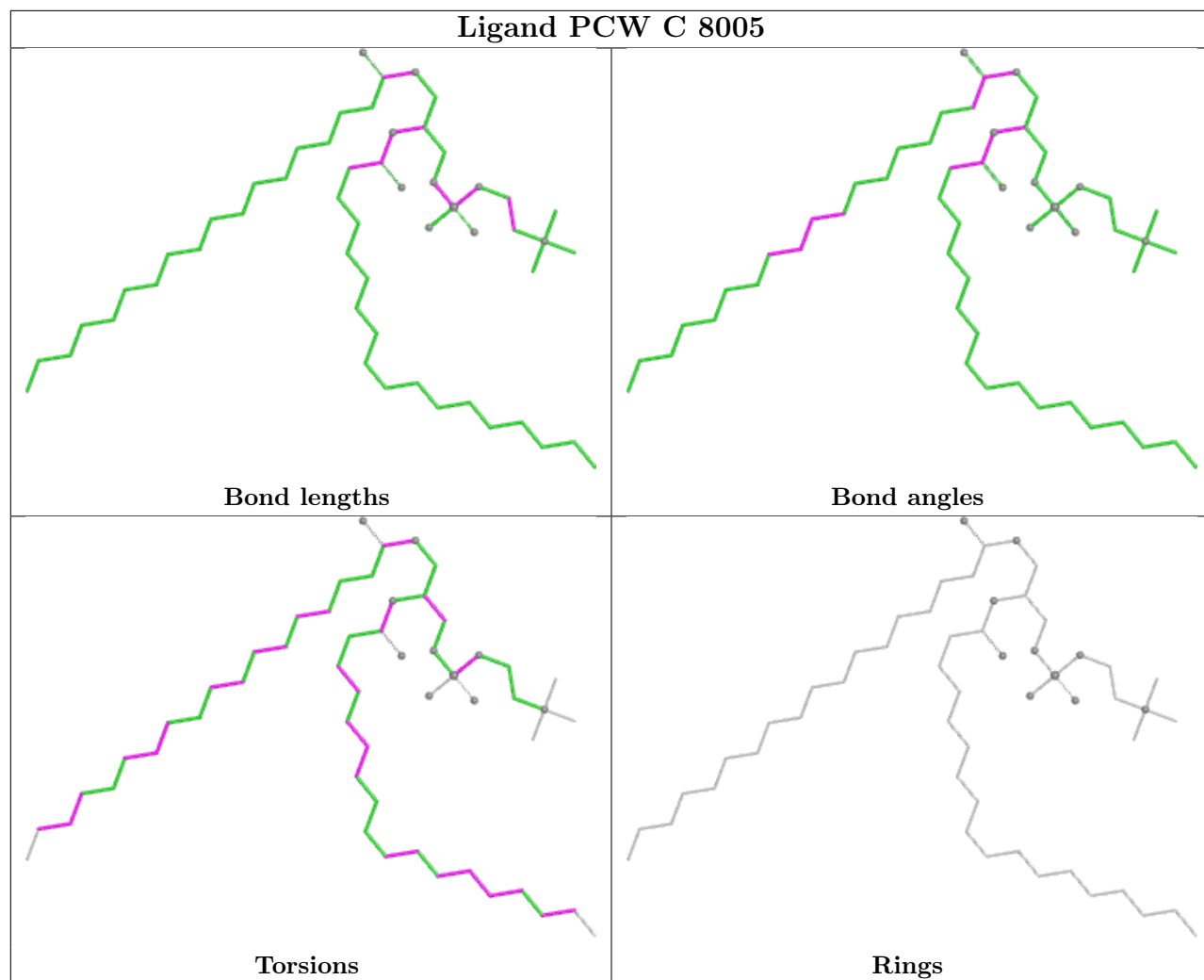




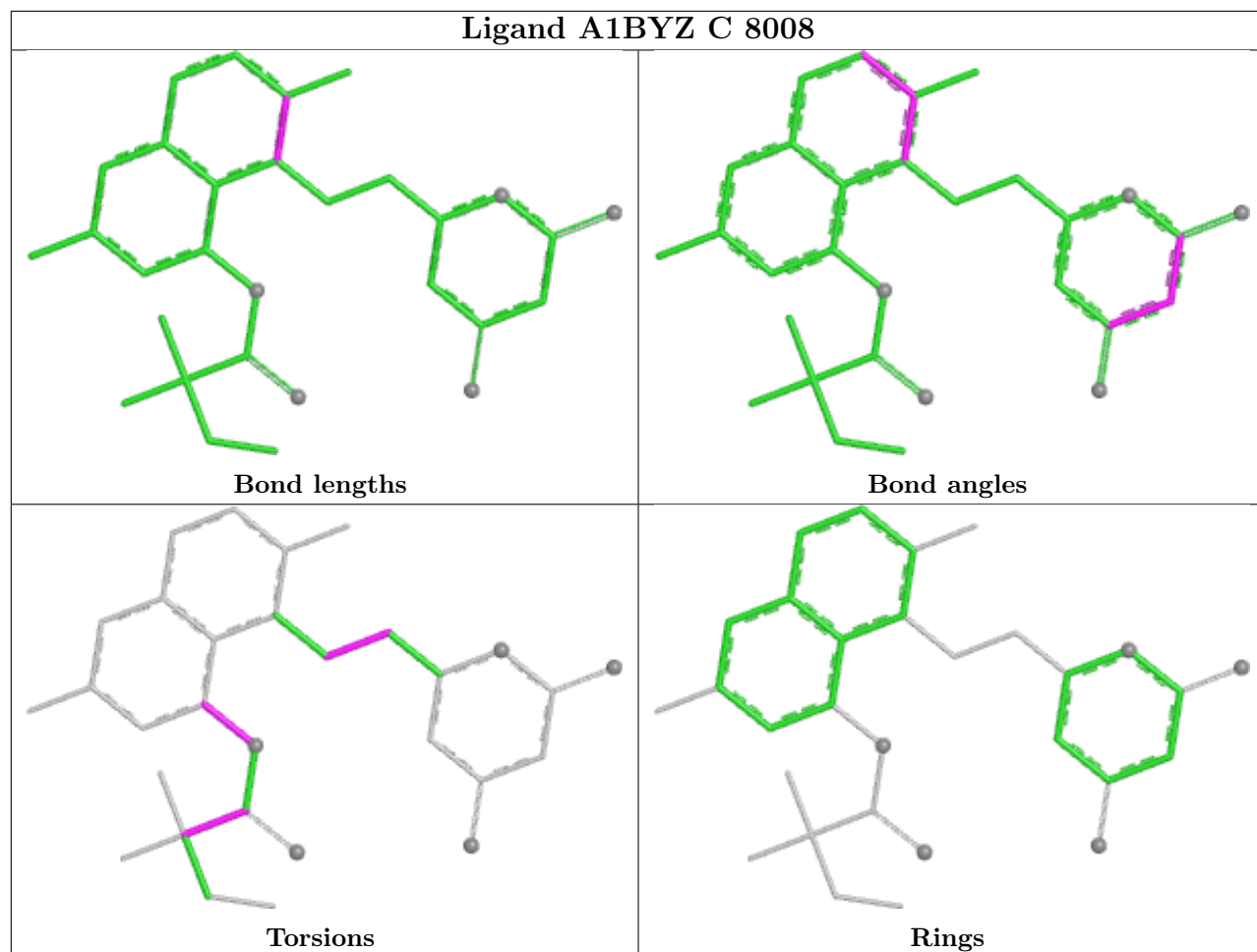


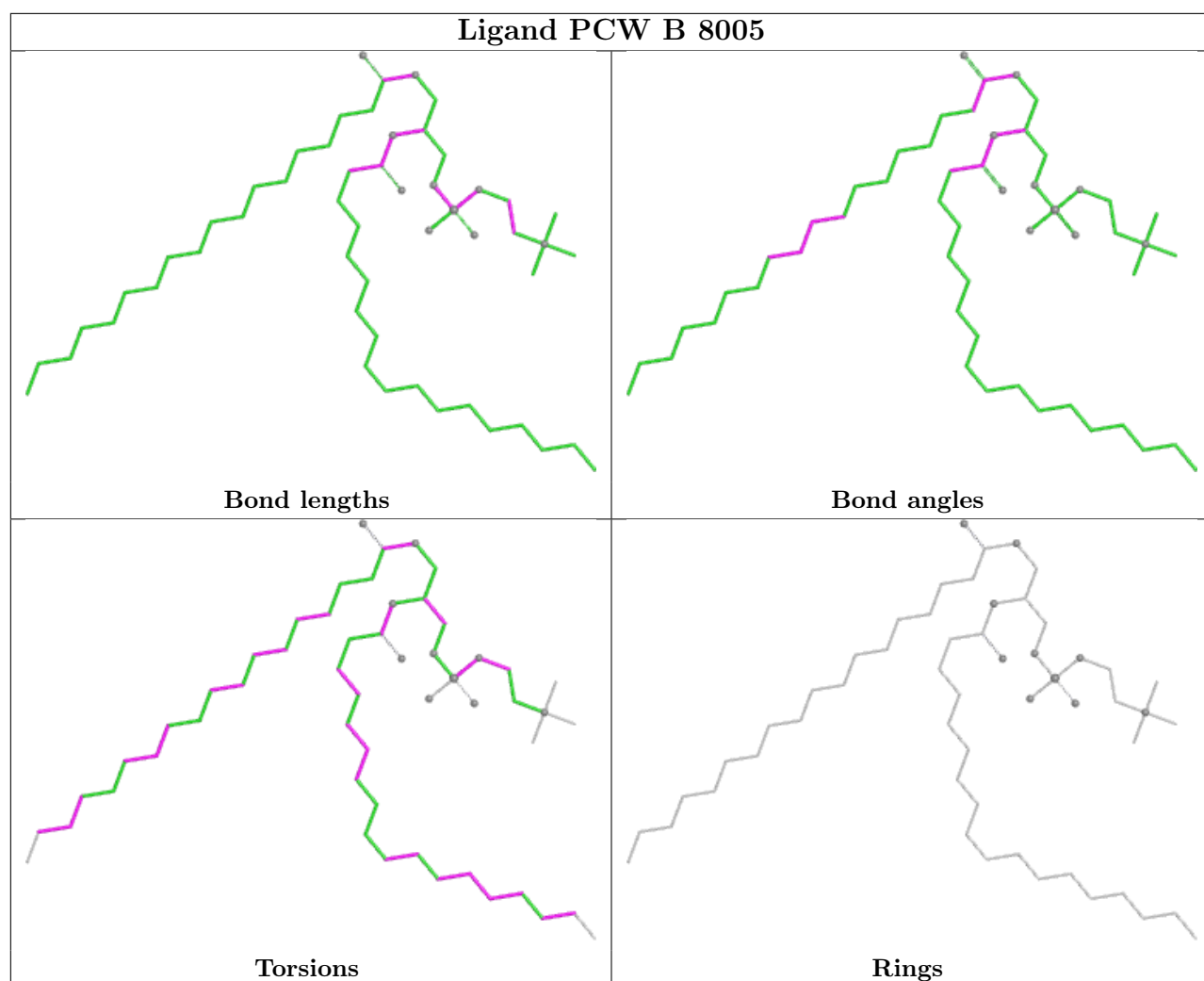
## Ligand A1BYZ D 8009



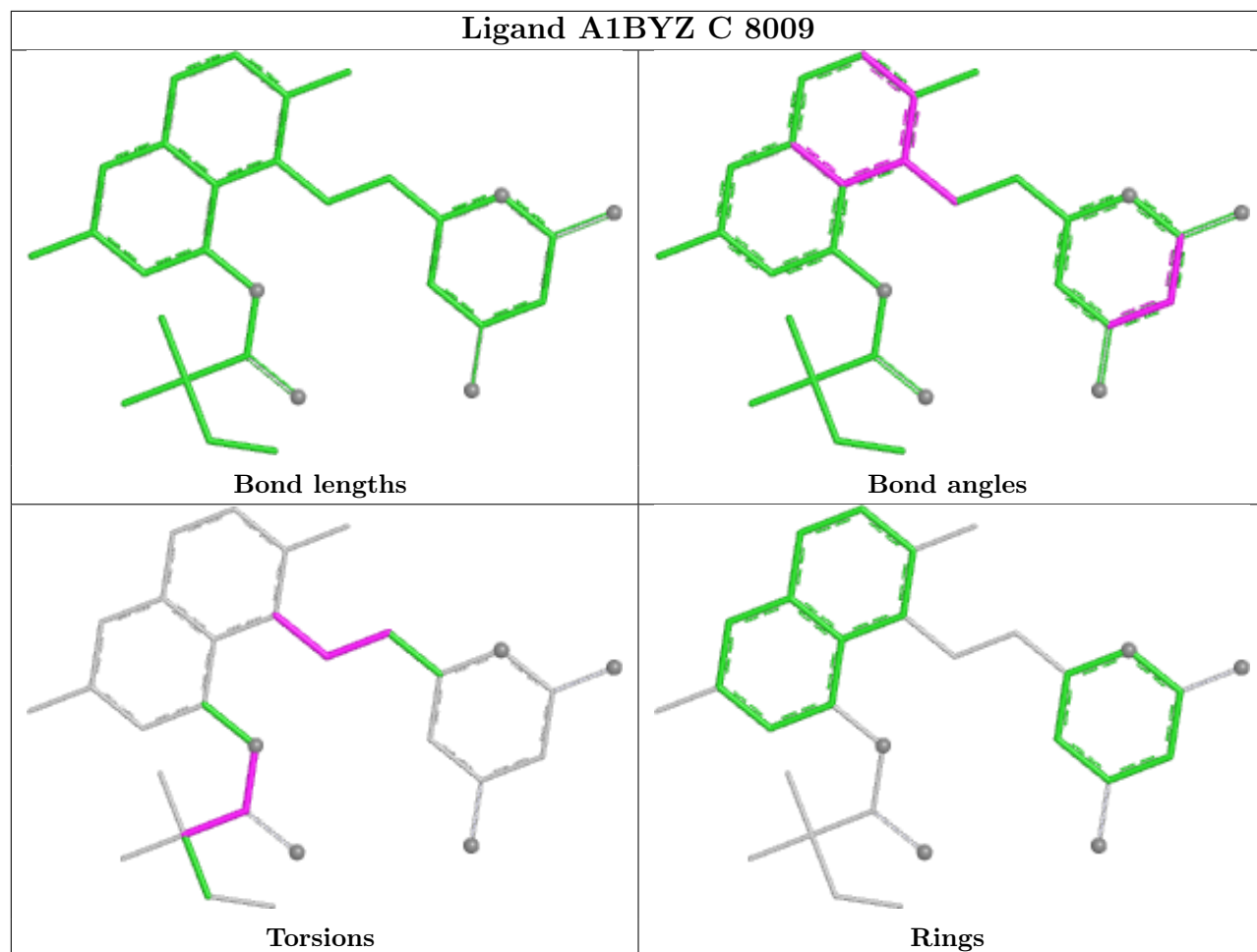


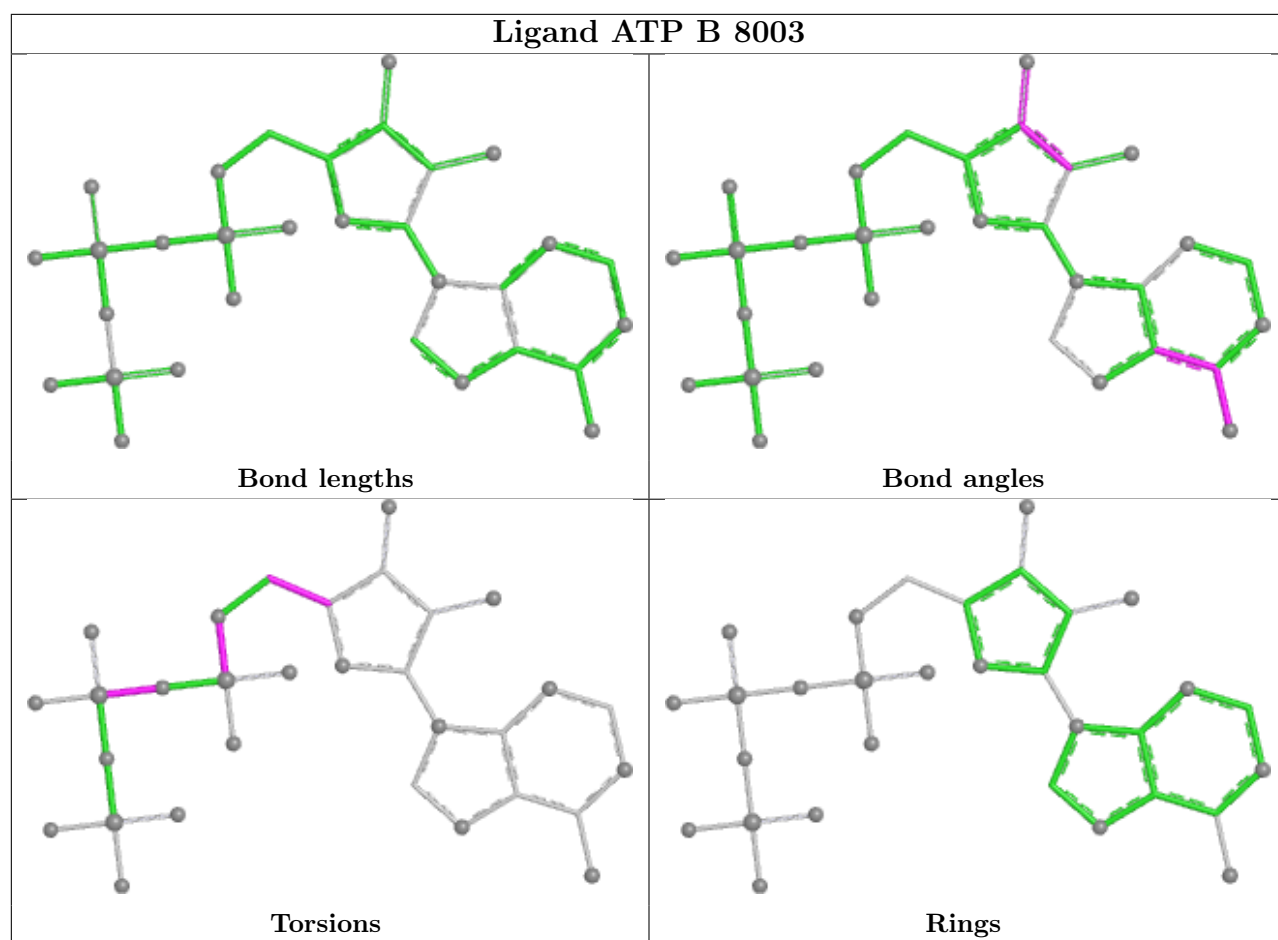
## Ligand A1BYZ C 8008





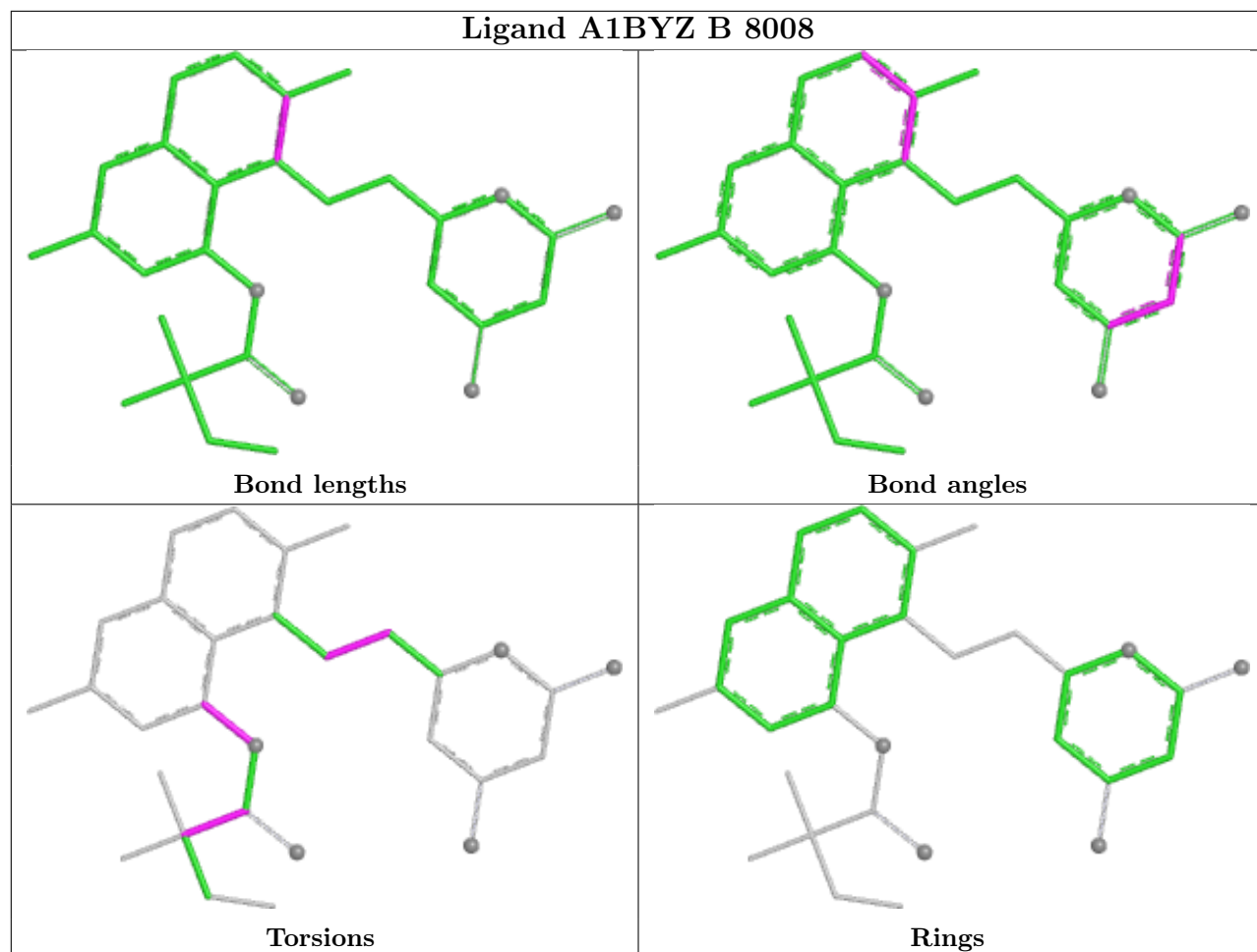
## Ligand A1BYZ C 8009



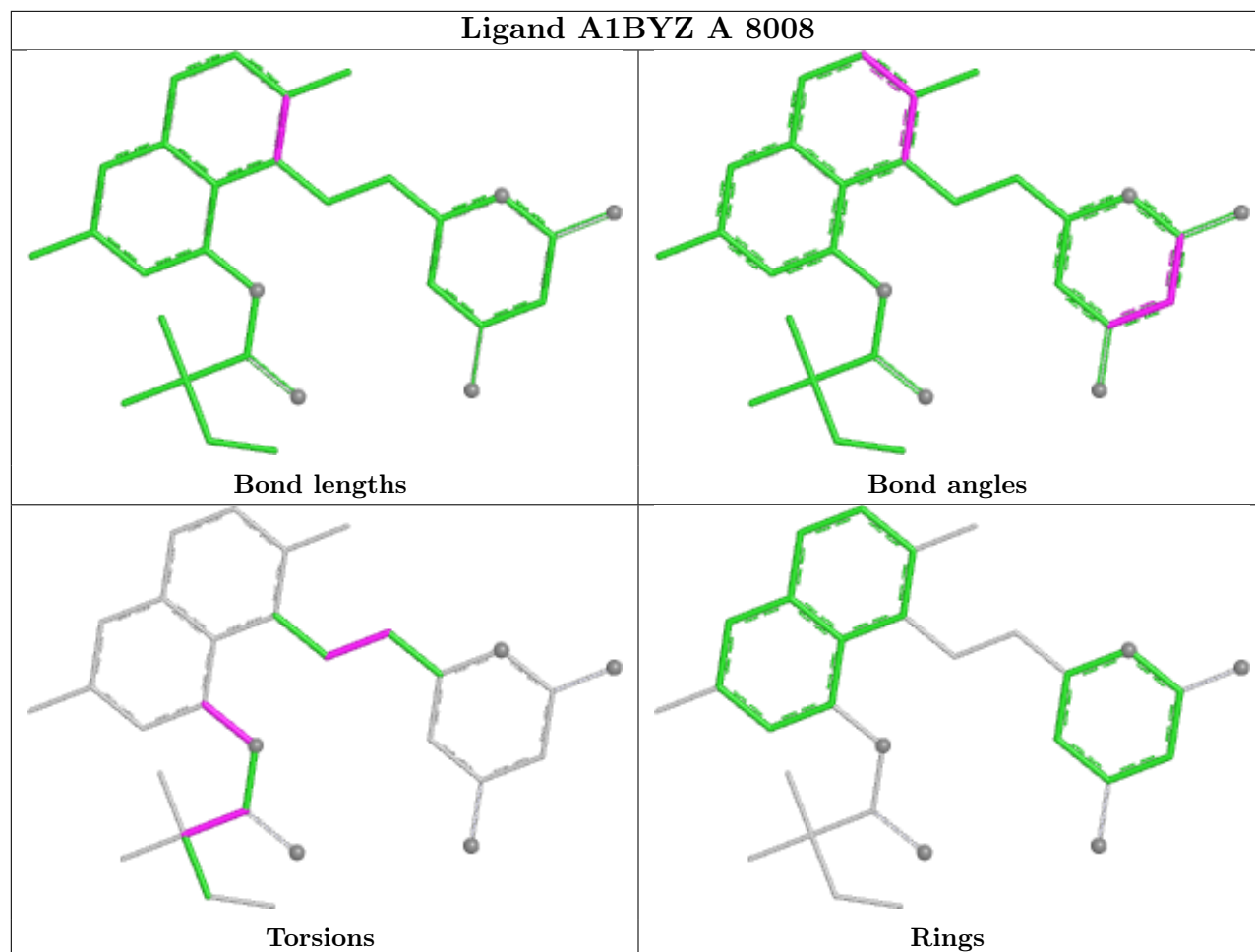


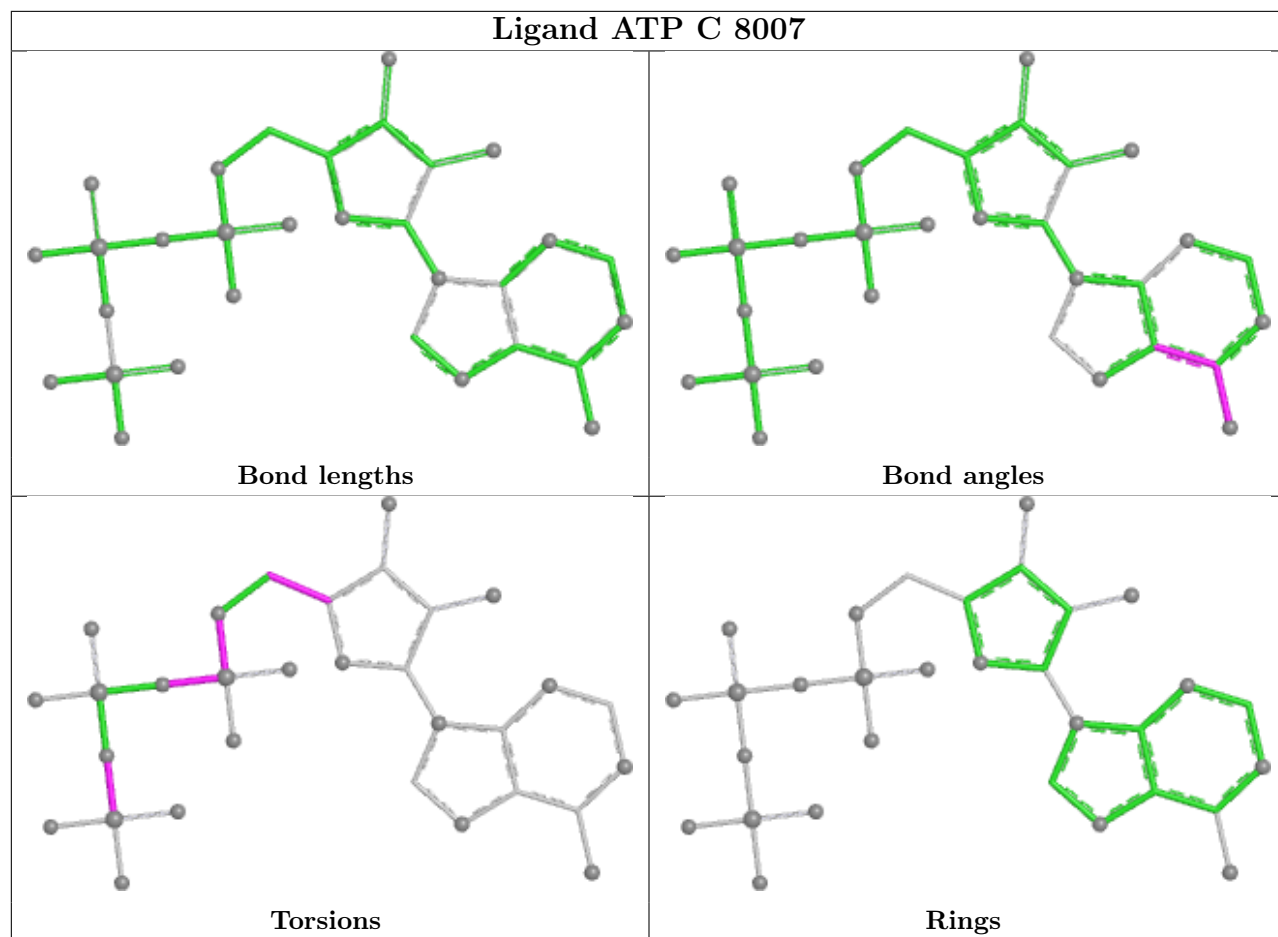


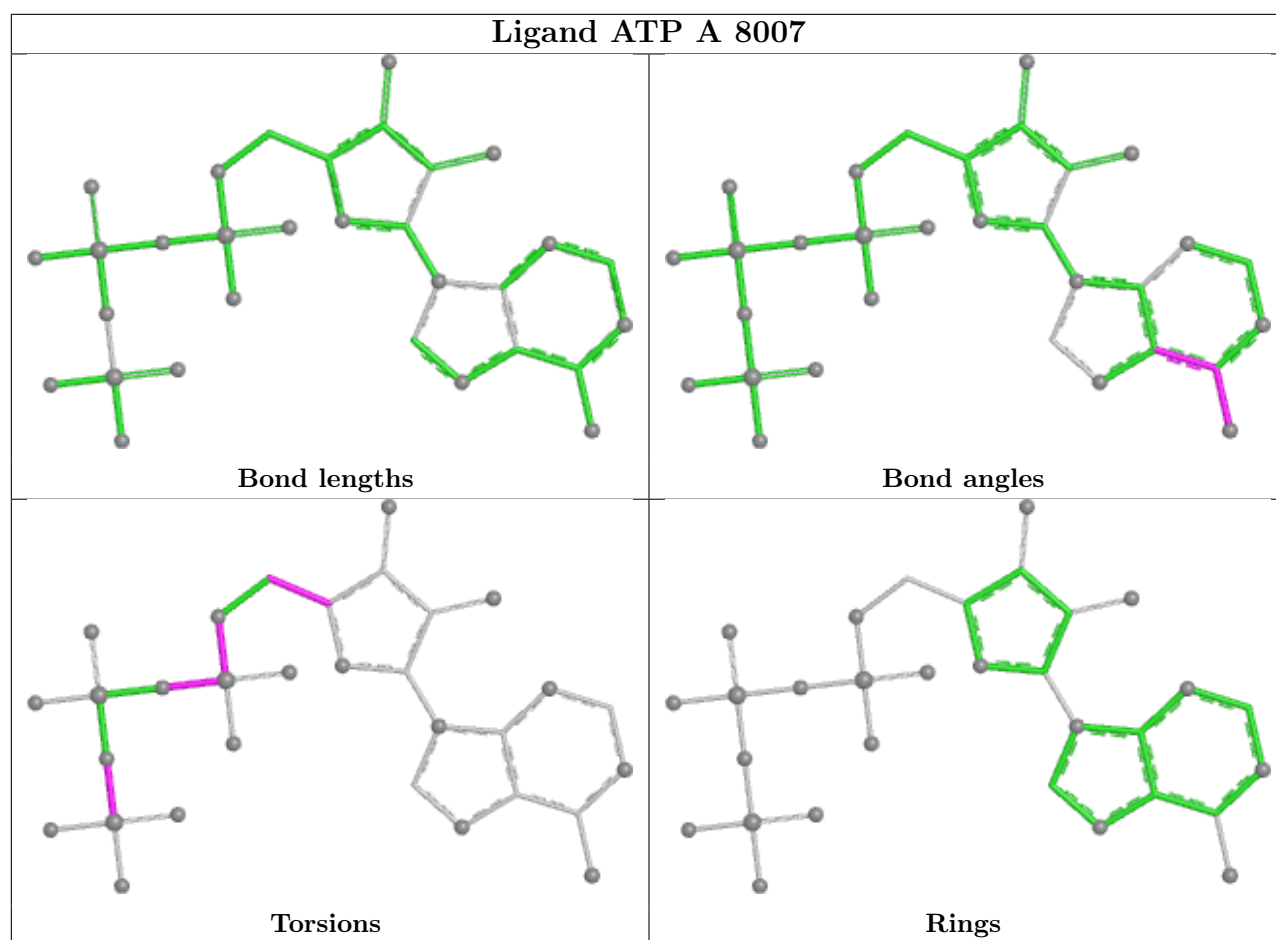
## Ligand A1BYZ B 8008



## Ligand A1BYZ A 8008







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

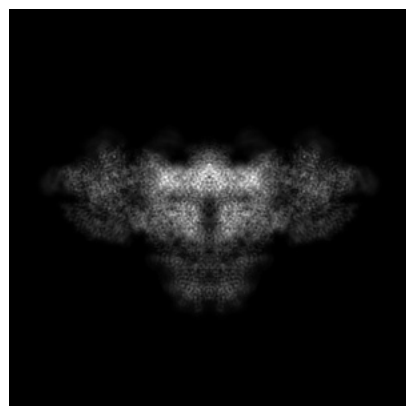
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49537. These allow visual inspection of the internal detail of the map and identification of artifacts.

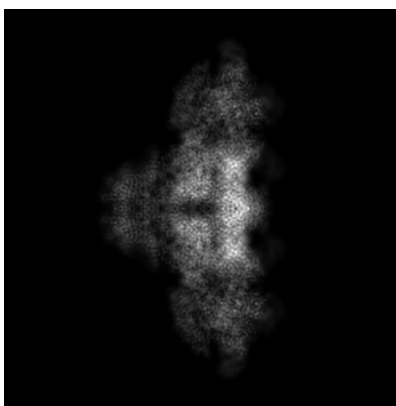
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

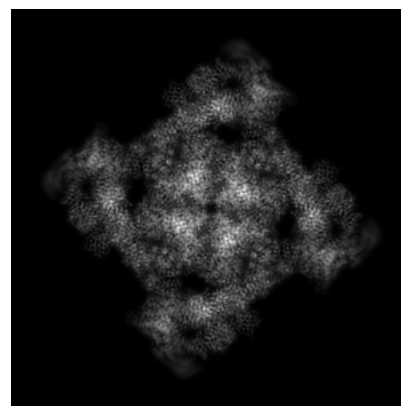
#### 6.1.1 Primary map



X

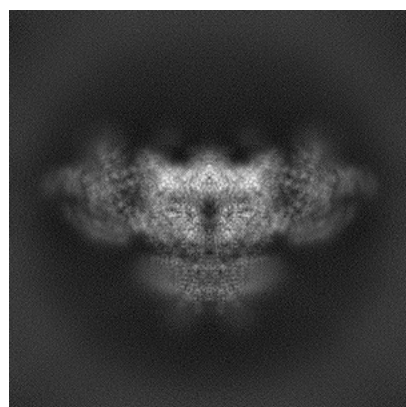


Y

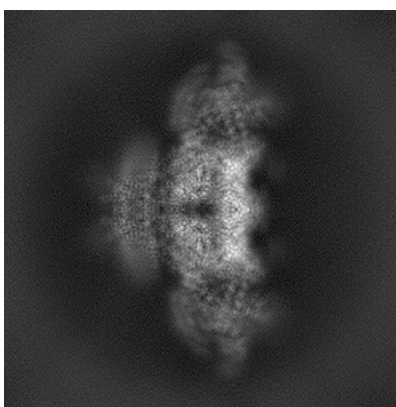


Z

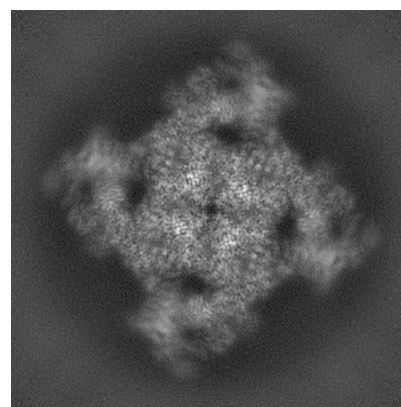
#### 6.1.2 Raw map



X



Y



Z

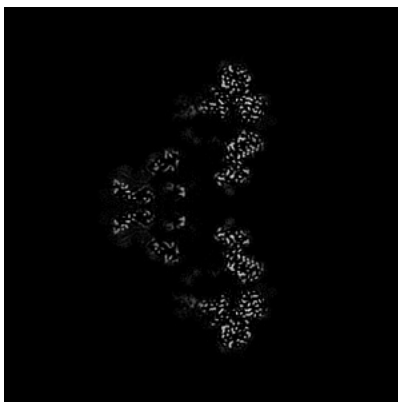
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

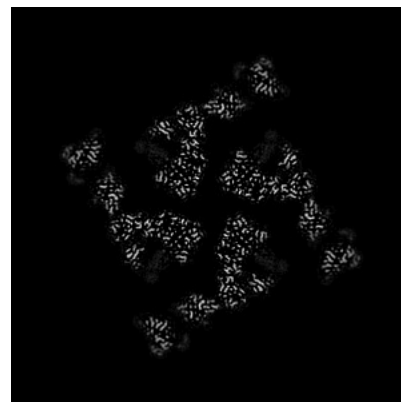
### 6.2.1 Primary map



X Index: 256

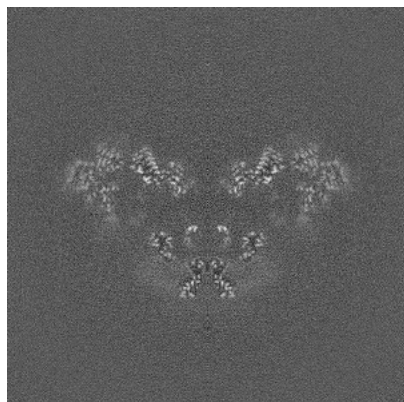


Y Index: 256

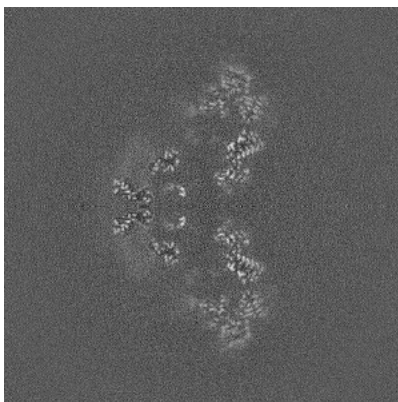


Z Index: 256

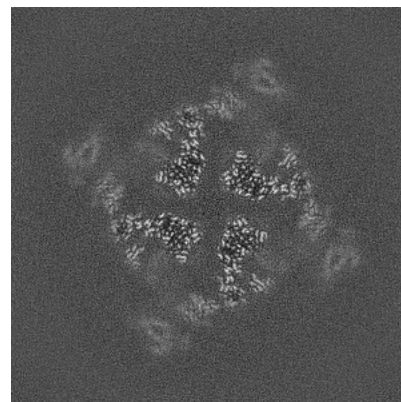
### 6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

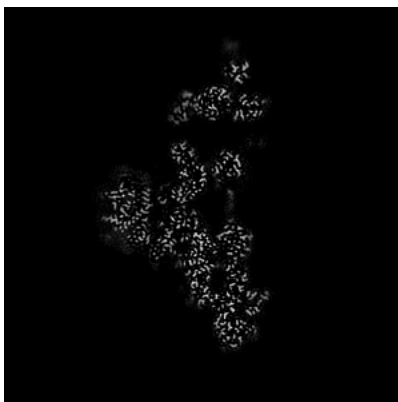
The images above show central slices of the map in three orthogonal directions.

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

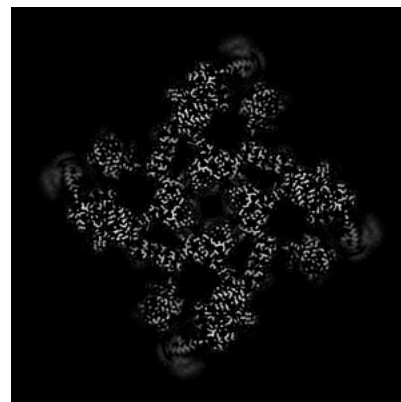
### 6.3.1 Primary map



X Index: 238

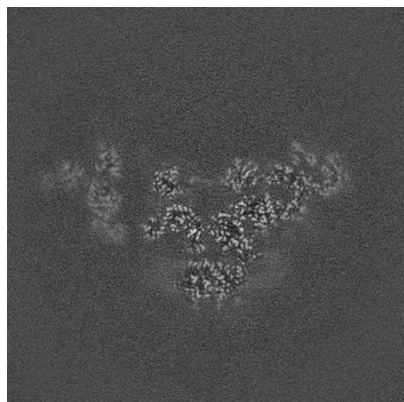


Y Index: 238

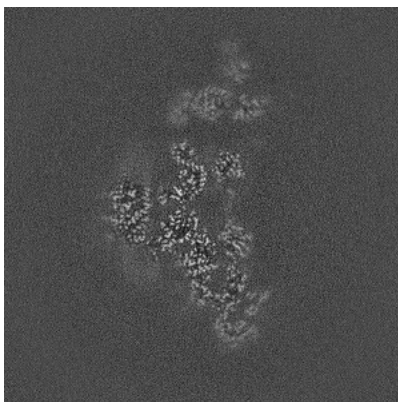


Z Index: 286

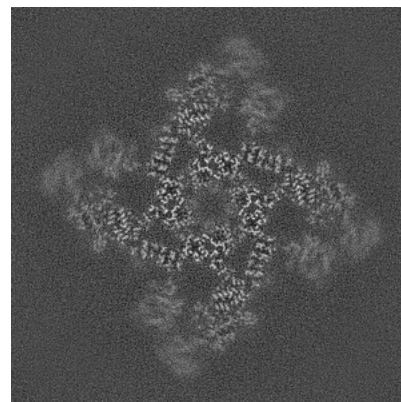
### 6.3.2 Raw map



X Index: 237



Y Index: 237



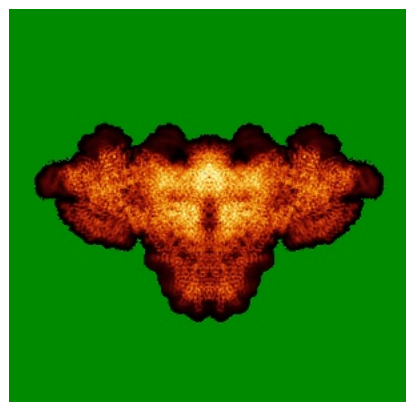
Z Index: 286

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

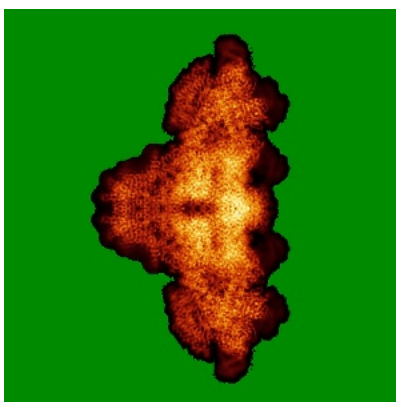


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

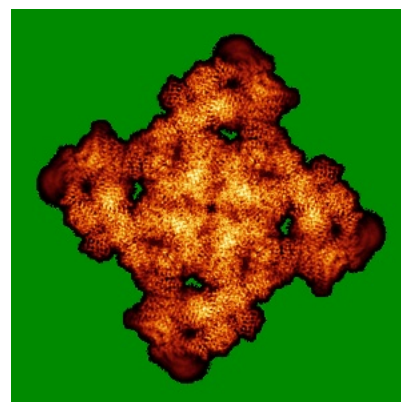
### 6.4.1 Primary map



X

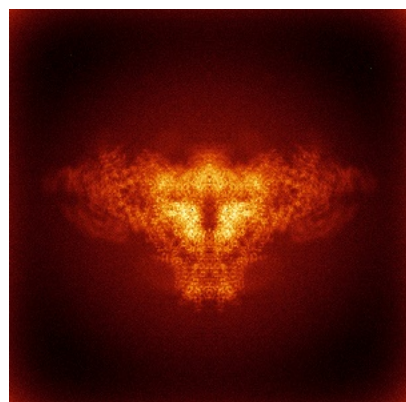


Y

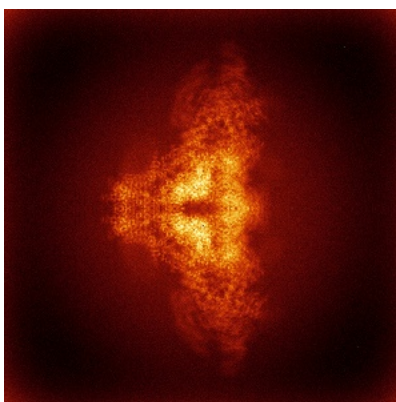


Z

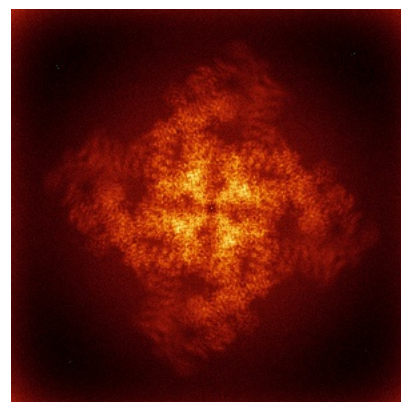
### 6.4.2 Raw map



X



Y



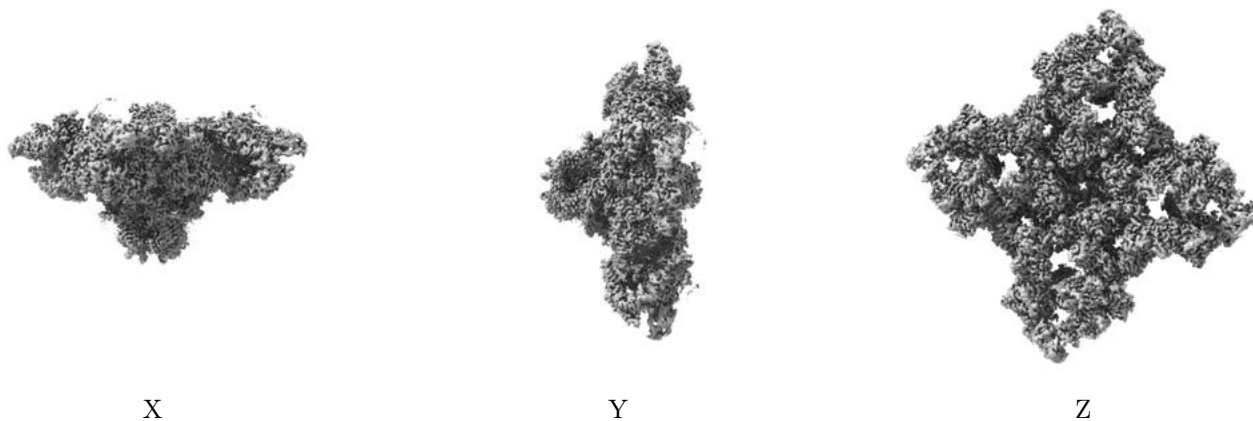
Z

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.



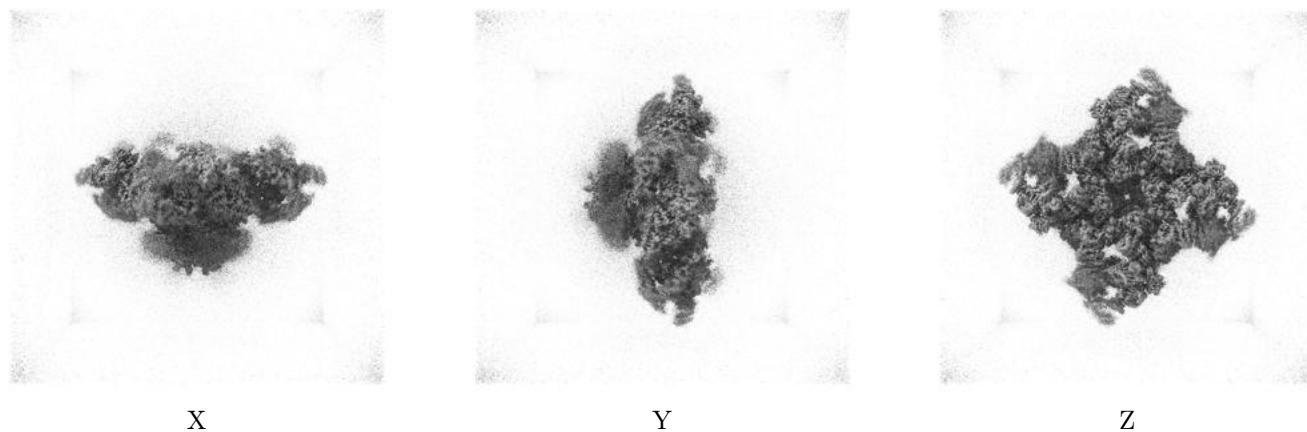
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

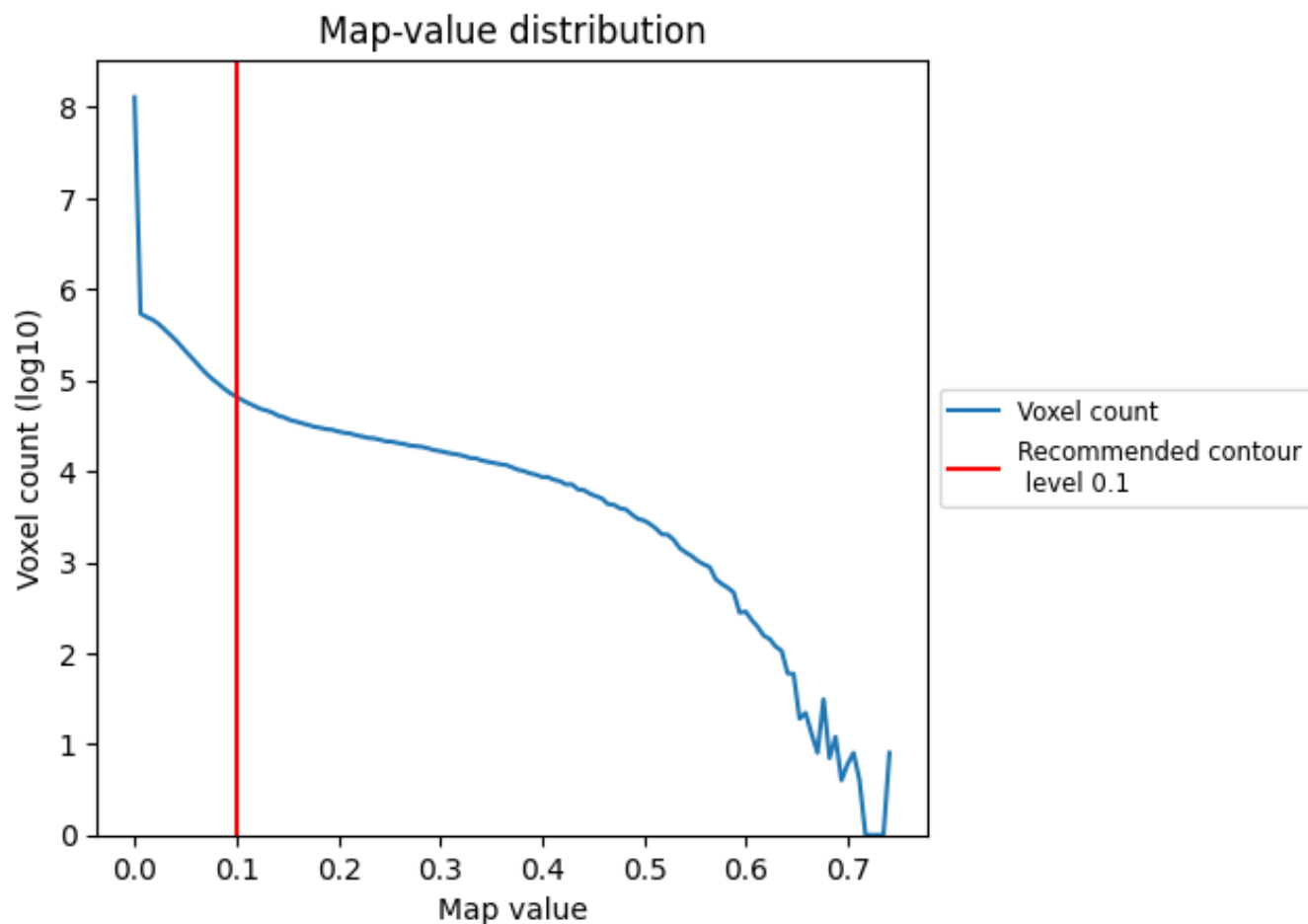
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

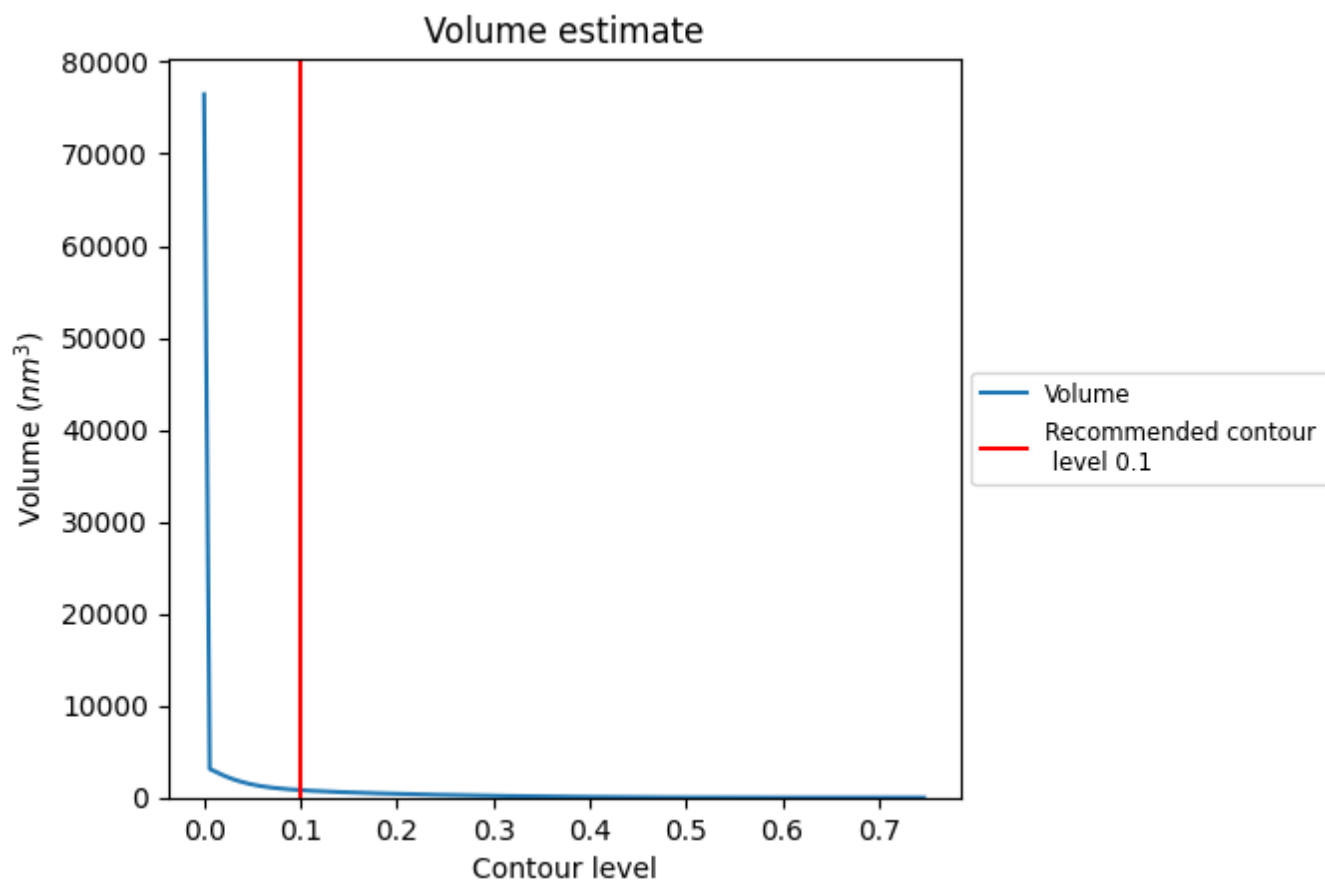
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

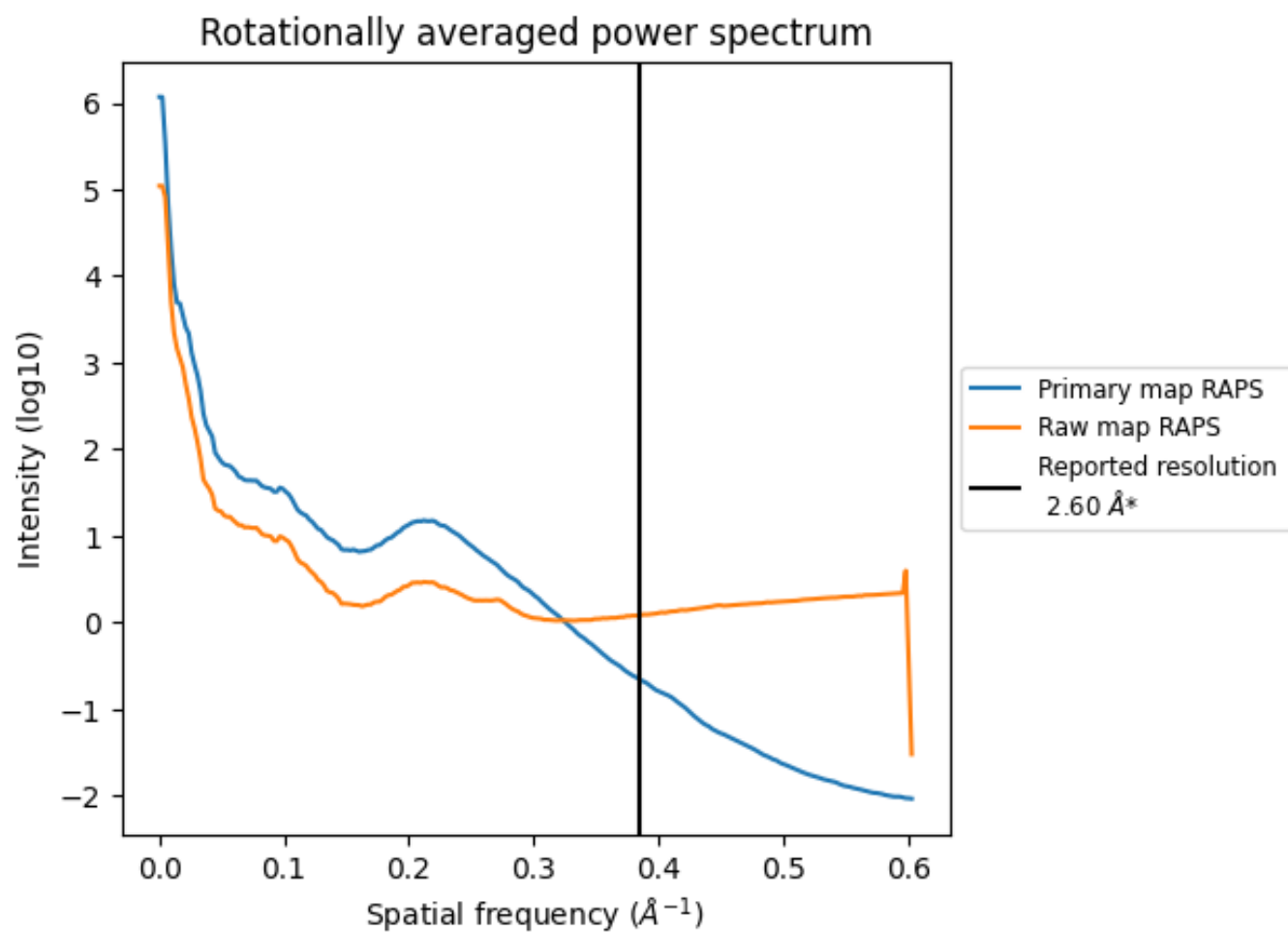
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 809 nm<sup>3</sup>; this corresponds to an approximate mass of 730 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 ⓘ

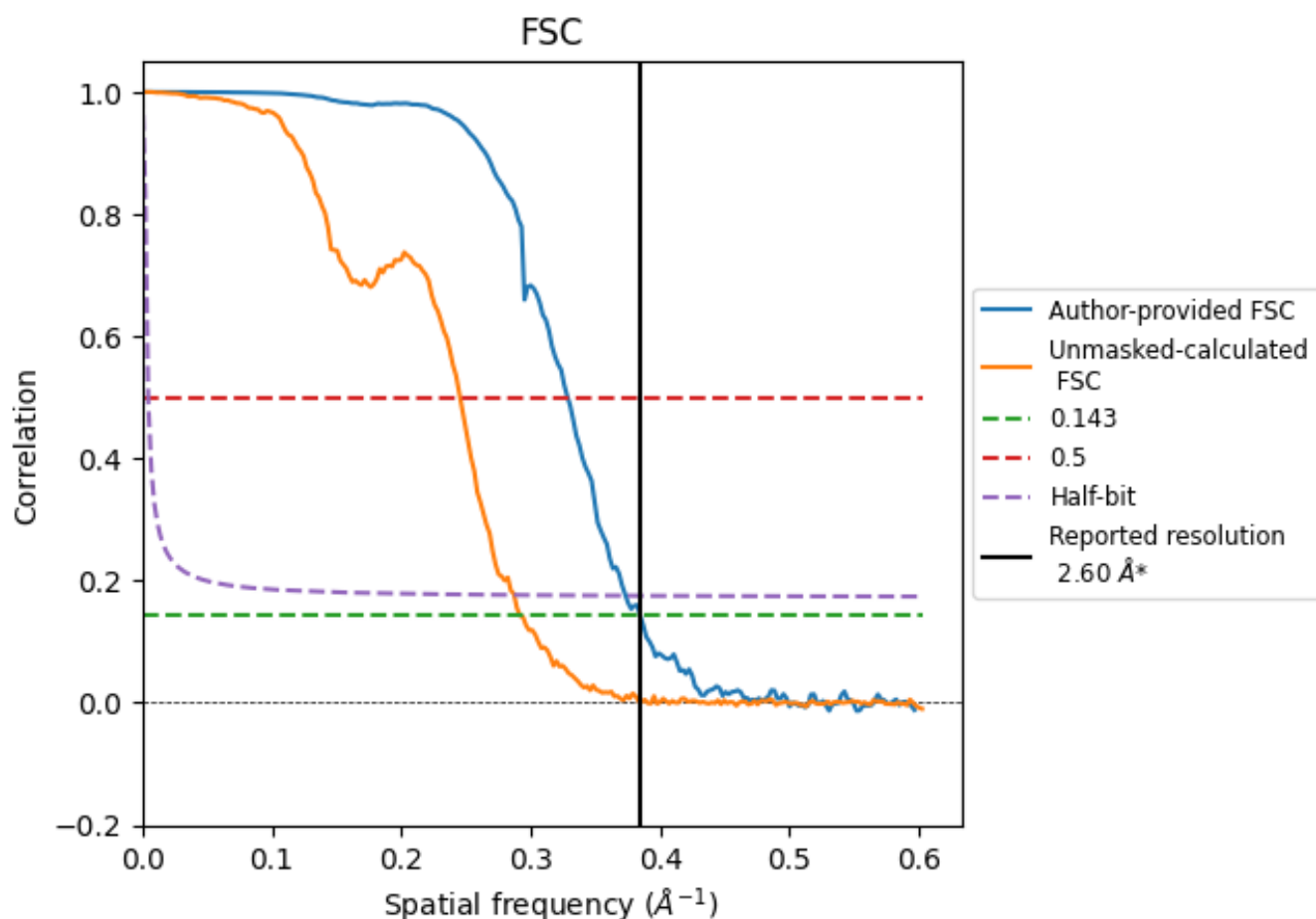


\*Reported resolution corresponds to spatial frequency of 0.385 Å<sup>-1</sup>

## 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 0.385  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

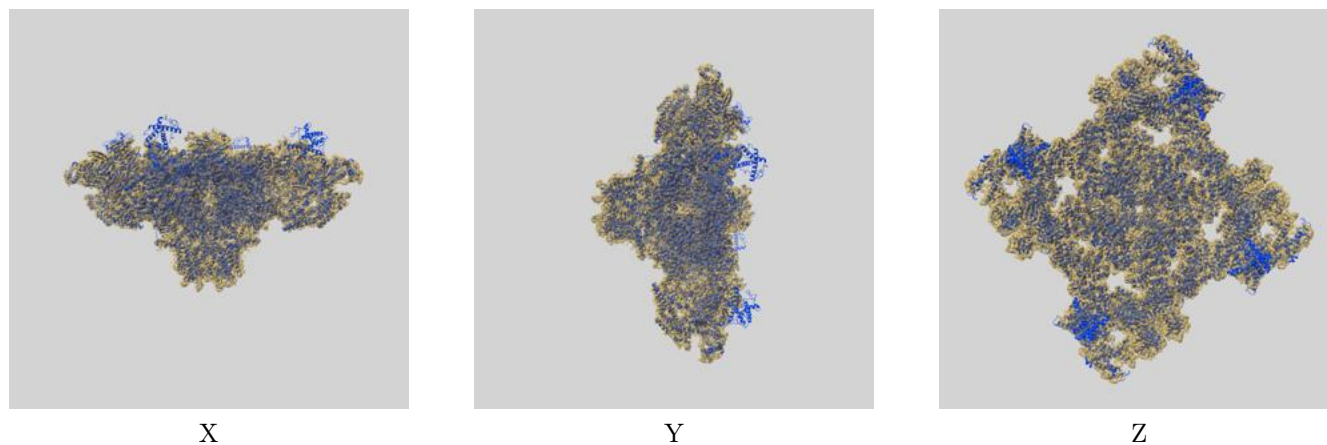
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.60	3.04	2.68
Unmasked-calculated*	3.43	4.07	3.48

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.43 differs from the reported value 2.6 by more than 10 %

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

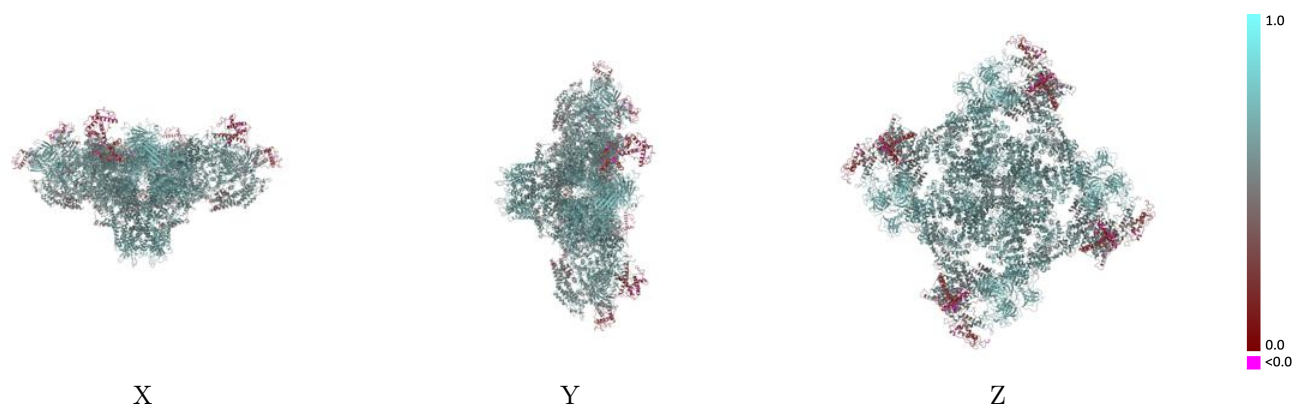
This section contains information regarding the fit between EMDB map EMD-49537 and PDB model 9NMQ. Per-residue inclusion information can be found in section [3](#) on page [9](#).

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



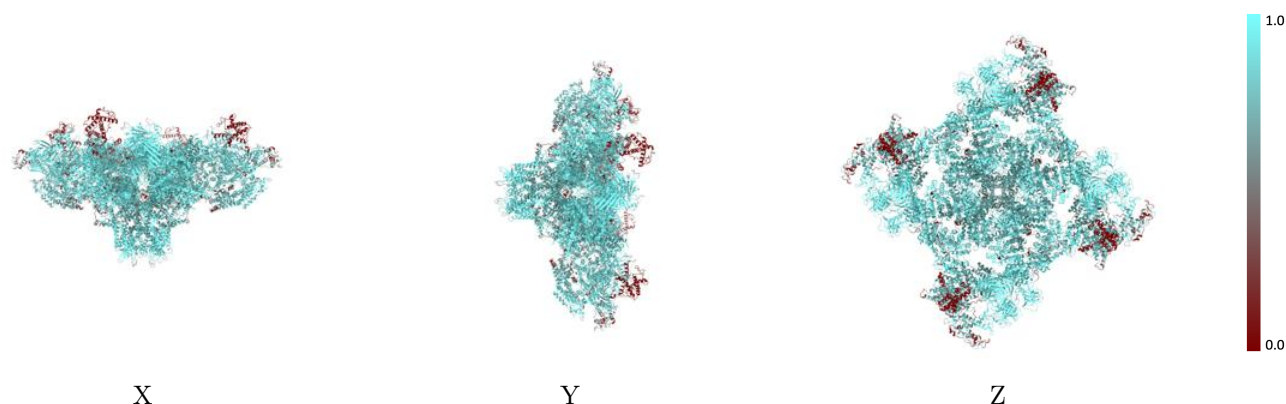
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

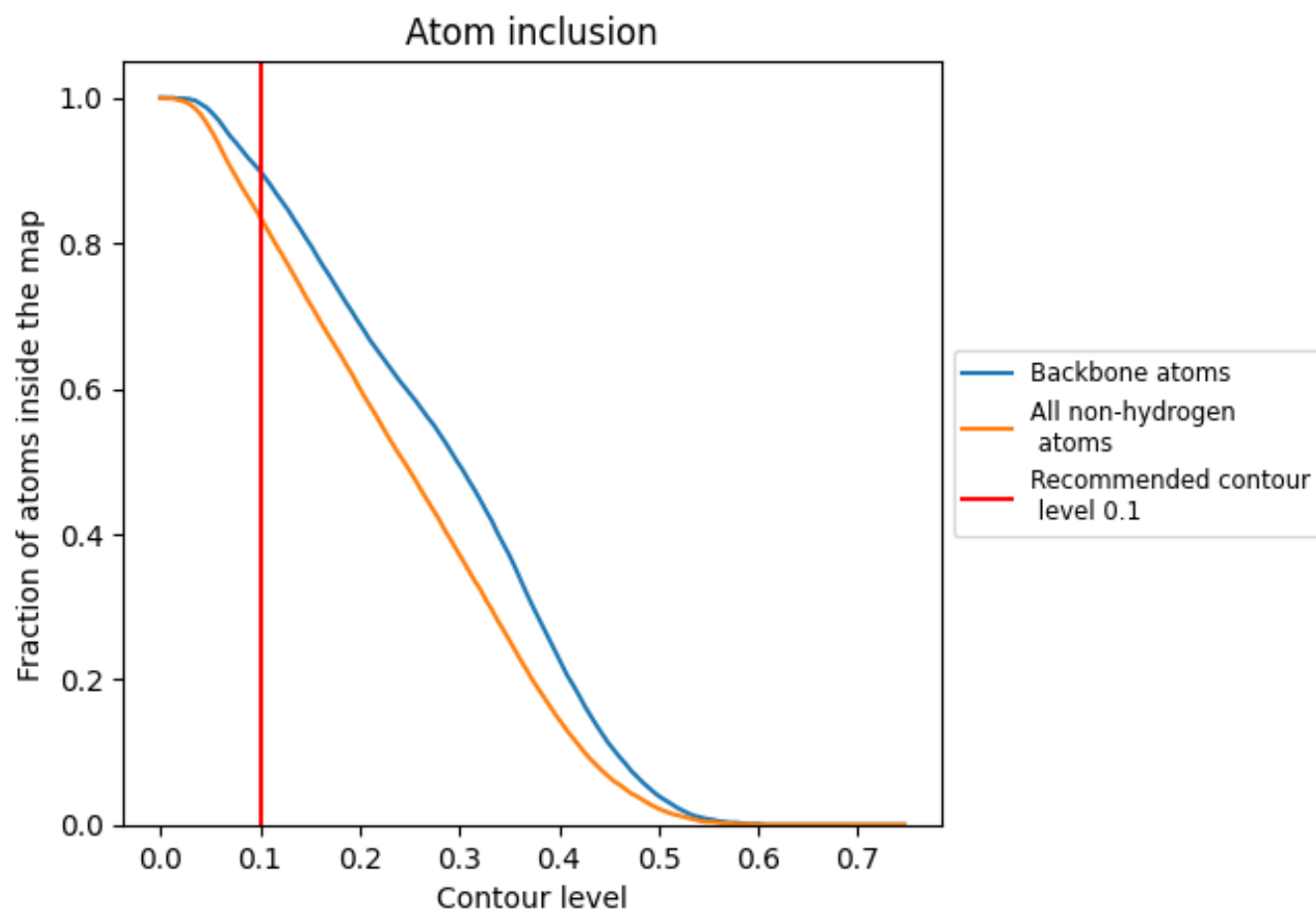
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 84% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8360	<div><div></div></div> 0.5810
A	<div><div></div></div> 0.8340	<div><div></div></div> 0.5800
B	<div><div></div></div> 0.8330	<div><div></div></div> 0.5780
C	<div><div></div></div> 0.8330	<div><div></div></div> 0.5790
D	<div><div></div></div> 0.8330	<div><div></div></div> 0.5780
E	<div><div></div></div> 0.9400	<div><div></div></div> 0.6410
F	<div><div></div></div> 0.9400	<div><div></div></div> 0.6440
G	<div><div></div></div> 0.9400	<div><div></div></div> 0.6430
H	<div><div></div></div> 0.9400	<div><div></div></div> 0.6430

1.0

0.0

<0.0