



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 01:57 AM UTC

PDB ID : 9NMO / pdb_00009nmo
EMDB ID : EMD-49535
Title : Structure of mouse RyR1 (Ca²⁺/CFF/ATP dataset; closed pore)
Authors : Weninger, G.; Marks, A.R.
Deposited on : 2025-03-04
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

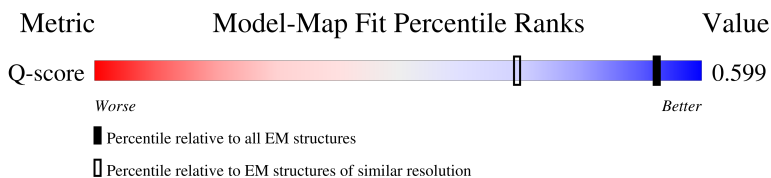
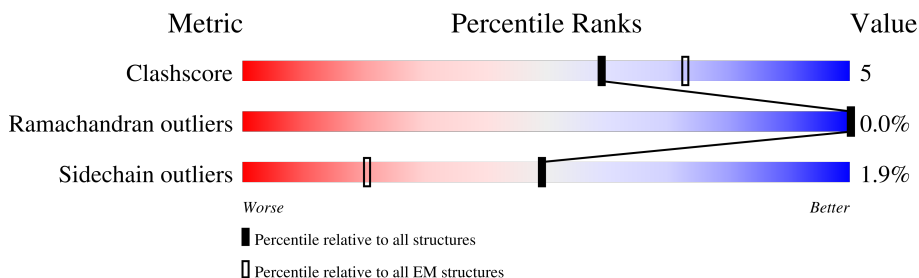
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 Å.

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







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5628 (1.90 - 2.90)

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

Mol	Chain	Length	Quality of chain
1	A	5035	
1	B	5035	
1	C	5035	
1	D	5035	

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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% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CFF	A	8002	-	X	-	-
4	CFF	B	8002	-	X	-	-
4	CFF	C	8002	-	X	-	-
4	CFF	D	8002	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 143248 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.

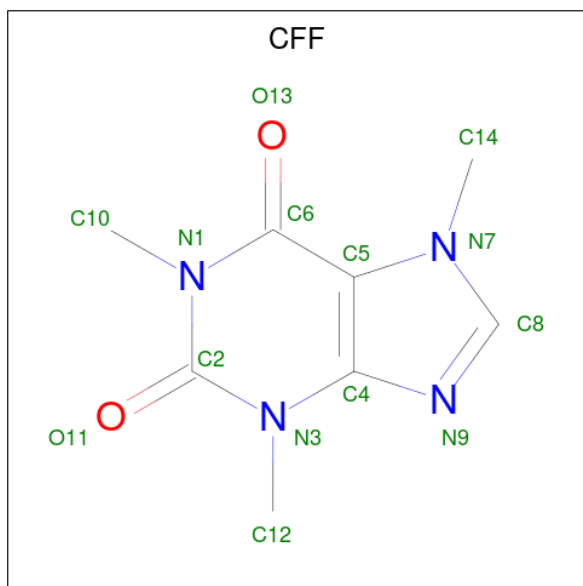
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
2	F	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
2	G	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
2	H	107	Total	C	N	O	S	0	0
			829	526	145	155	3		

- 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: C₈H₁₀N₄O₂) (labeled as "Ligand of

Interest" by depositor).



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: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

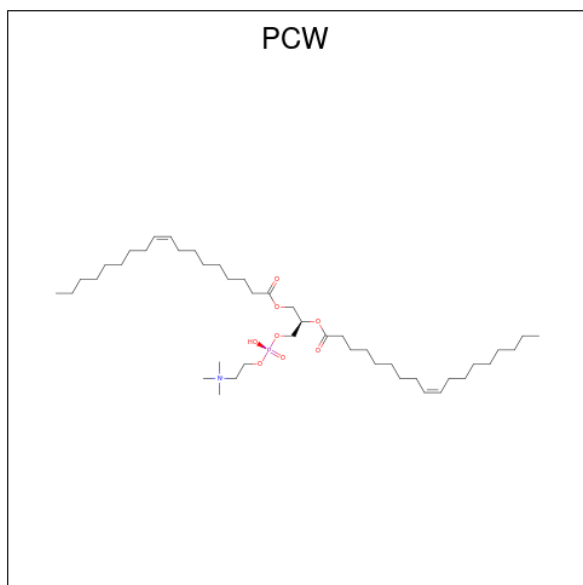
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total Ca 1 1	0
6	B	1	Total Ca 1 1	0
6	C	1	Total Ca 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total	Ca	0
			1	1	

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).

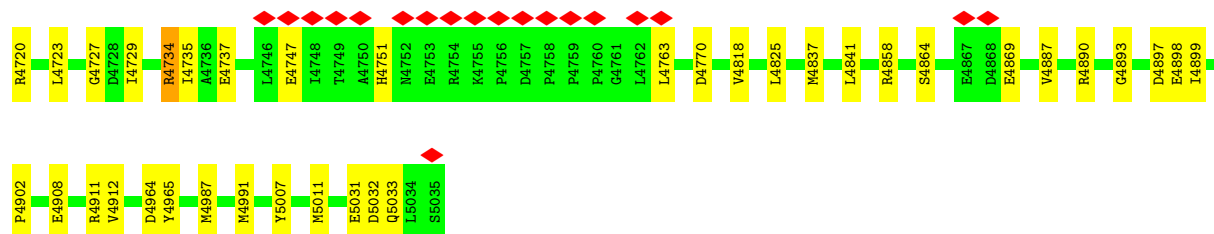


Mol	Chain	Residues	Atoms						AltConf
7	A	1	Total	C	N	O	P		0
			54	44	1	8	1		
7	A	1	Total	C	N	O	P		0
			54	44	1	8	1		
7	B	1	Total	C	N	O	P		0
			54	44	1	8	1		
7	B	1	Total	C	N	O	P		0
			54	44	1	8	1		
7	C	1	Total	C	N	O	P		0
			54	44	1	8	1		
7	C	1	Total	C	N	O	P		0
			54	44	1	8	1		
7	D	1	Total	C	N	O	P		0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

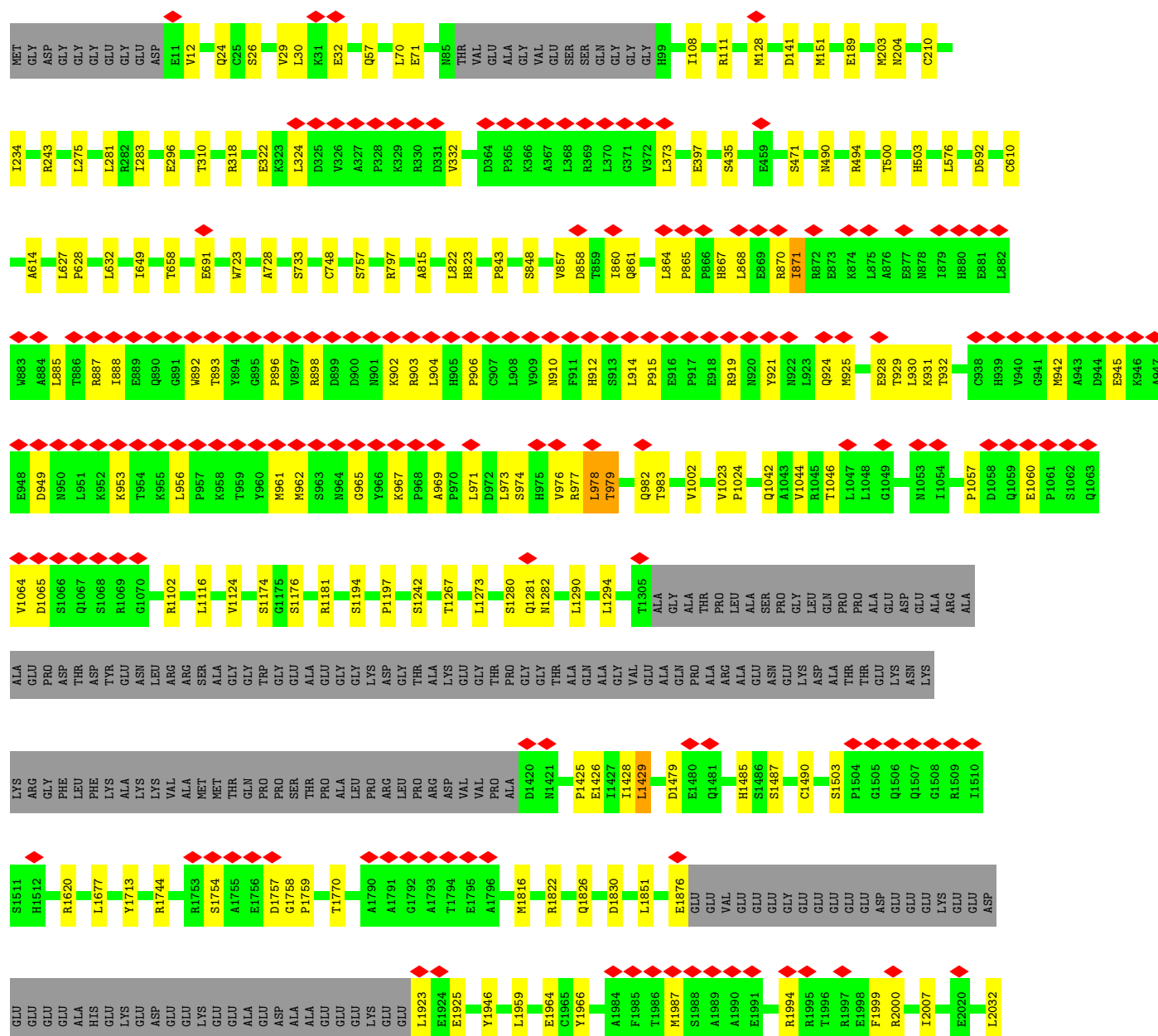
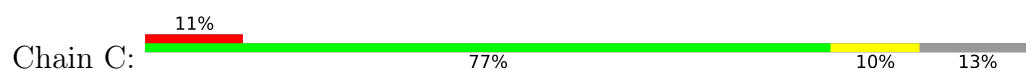




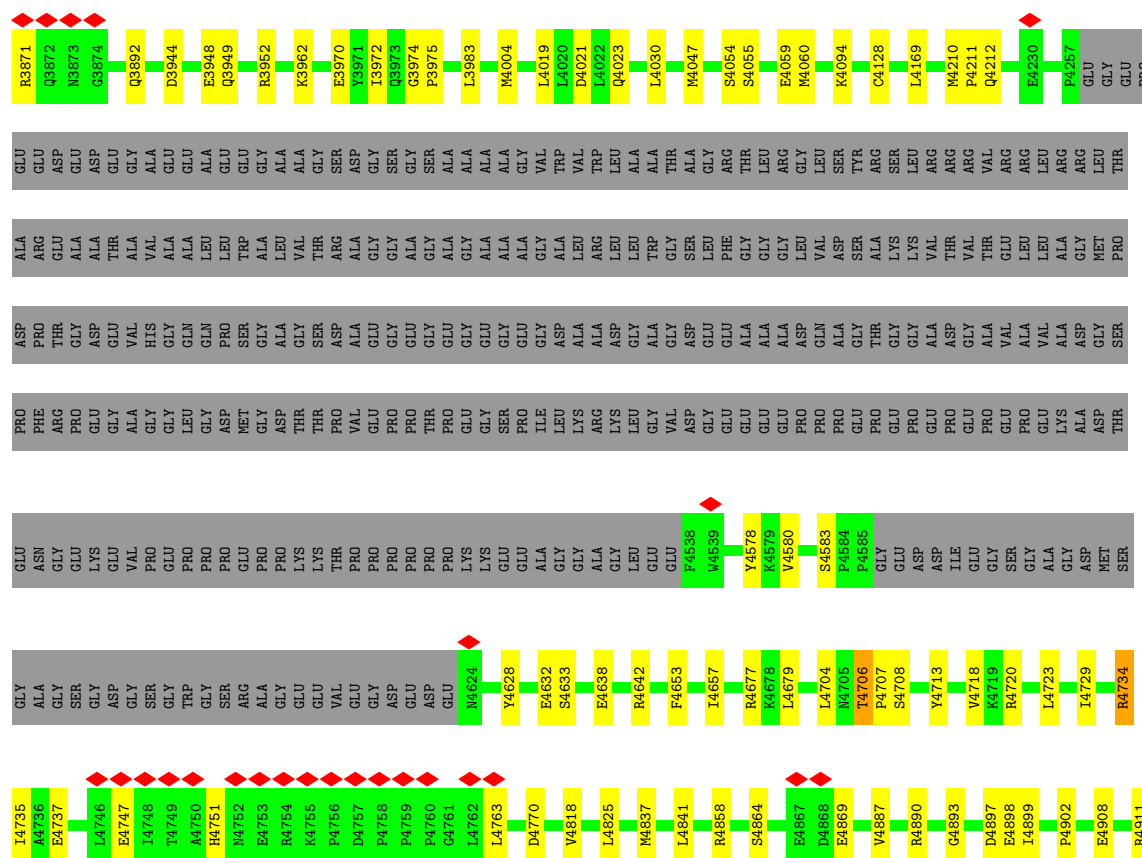




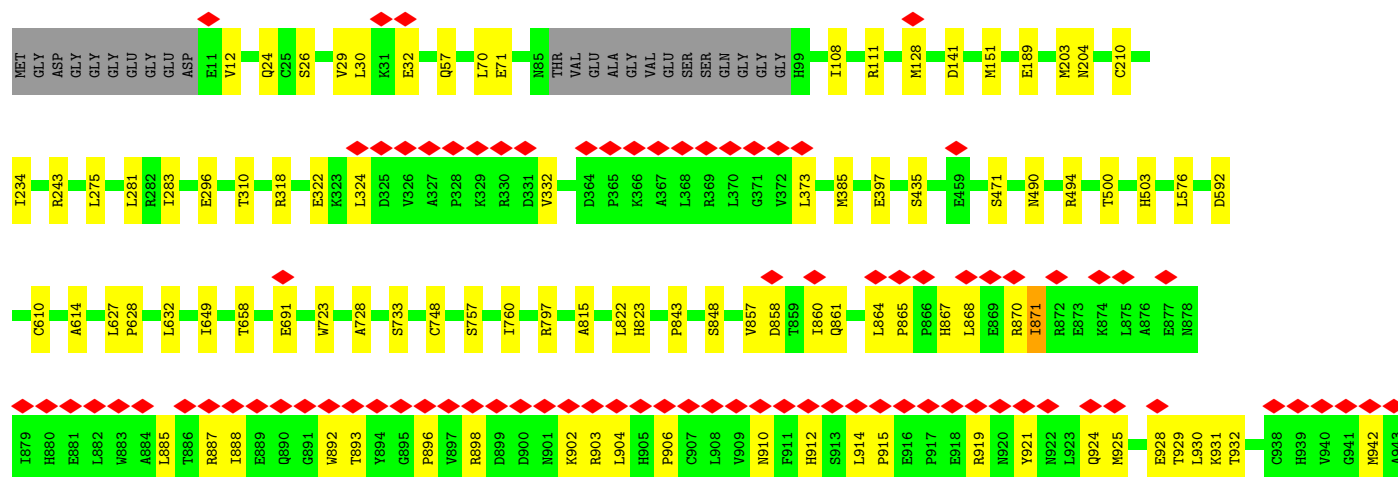
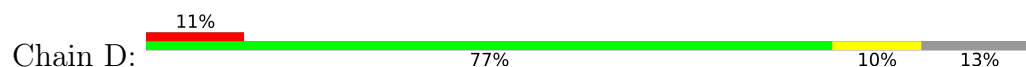
• Molecule 1: Ryanodine receptor 1

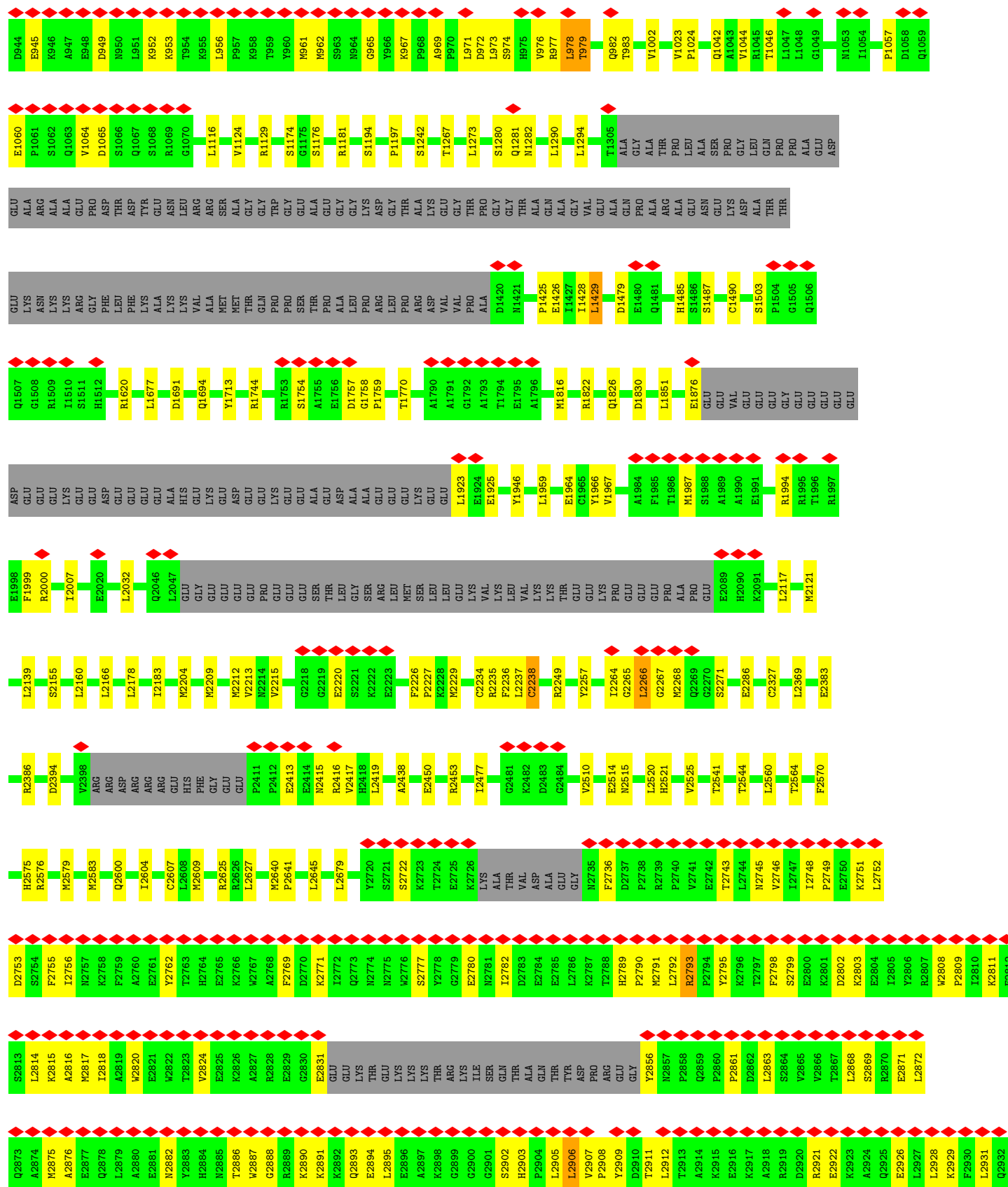




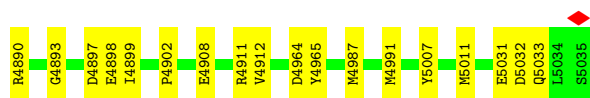


● Molecule 1: Ryanodine receptor 1









- 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	224439	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	0.565	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	427.776, 427.776, 427.776	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8355, 0.8355, 0.8355	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/35586	0.36	5/48203 (0.0%)
1	B	0.18	0/35586	0.36	6/48203 (0.0%)
1	C	0.18	0/35586	0.36	5/48203 (0.0%)
1	D	0.18	0/35586	0.36	5/48203 (0.0%)
2	E	0.14	0/847	0.33	0/1142
2	F	0.14	0/847	0.33	0/1142
2	G	0.14	0/847	0.33	0/1142
2	H	0.14	0/847	0.33	0/1142
All	All	0.18	0/145732	0.36	21/197380 (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	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2238	CYS	CA-CB-SG	7.13	130.80	114.40
1	C	2238	CYS	CA-CB-SG	7.13	130.80	114.40
1	D	2238	CYS	CA-CB-SG	7.12	130.78	114.40
1	B	2238	CYS	CA-CB-SG	7.11	130.75	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2908	PRO	CA-N-CD	-5.56	104.22	112.00
1	D	2908	PRO	CA-N-CD	-5.56	104.22	112.00
1	A	2908	PRO	CA-N-CD	-5.54	104.25	112.00
1	C	2908	PRO	CA-N-CD	-5.52	104.28	112.00
1	B	2238	CYS	N-CA-C	-5.24	106.94	113.38
1	A	2238	CYS	N-CA-C	-5.22	106.96	113.38
1	C	2238	CYS	N-CA-C	-5.22	106.96	113.38
1	D	2238	CYS	N-CA-C	-5.19	106.99	113.38
1	B	2238	CYS	CB-CA-C	5.14	118.59	109.65
1	A	2238	CYS	CB-CA-C	5.13	118.58	109.65
1	C	2238	CYS	CB-CA-C	5.12	118.56	109.65
1	D	2238	CYS	CB-CA-C	5.11	118.54	109.65
1	B	1057	PRO	CA-N-CD	-5.10	104.86	112.00
1	C	1057	PRO	CA-N-CD	-5.08	104.89	112.00
1	A	1057	PRO	CA-N-CD	-5.07	104.90	112.00
1	D	1057	PRO	CA-N-CD	-5.06	104.92	112.00
1	B	4727	GLY	N-CA-C	5.01	118.75	112.73

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2793	ARG	Sidechain
1	A	4720	ARG	Sidechain
1	A	4734	ARG	Sidechain
1	B	2793	ARG	Sidechain
1	B	4720	ARG	Sidechain
1	B	4734	ARG	Sidechain
1	C	2793	ARG	Sidechain
1	C	4720	ARG	Sidechain
1	C	4734	ARG	Sidechain
1	D	2793	ARG	Sidechain
1	D	4720	ARG	Sidechain
1	D	4734	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34797	0	34384	328	0
1	B	34797	0	34384	327	0
1	C	34797	0	34384	326	0
1	D	34797	0	34384	332	0
2	E	829	0	826	4	0
2	F	829	0	826	4	0
2	G	829	0	826	4	0
2	H	829	0	826	4	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	1	0
5	B	62	0	24	1	0
5	C	62	0	24	1	0
5	D	62	0	24	1	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	2	0
7	B	108	0	168	2	0
7	C	108	0	168	2	0
7	D	108	0	168	2	0
All	All	143248	0	141648	1317	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 5.

All (1317) 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:C:2215:VAL:HG11	1:C:2229:MET:HE1	1.43	0.99
1:D:2215:VAL:HG11	1:D:2229:MET:HE1	1.43	0.99
1:A:2215:VAL:HG11	1:A:2229:MET:HE1	1.43	0.97
1:B:2215:VAL:HG11	1:B:2229:MET:HE1	1.44	0.97
1:D:2875:MET:HE3	1:D:2875:MET:HA	1.55	0.88
1:A:2875:MET:HE3	1:A:2875:MET:HA	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2875:MET:HE3	1:C:2875:MET:HA	1.56	0.87
1:B:2875:MET:HE3	1:B:2875:MET:HA	1.55	0.85
1:D:2249:ARG:NH2	1:D:2286:GLU:OE2	2.14	0.81
1:C:2249:ARG:NH2	1:C:2286:GLU:OE2	2.14	0.81
1:B:2249:ARG:NH2	1:B:2286:GLU:OE2	2.14	0.81
1:A:2249:ARG:NH2	1:A:2286:GLU:OE2	2.14	0.81
1:C:860:ILE:HD12	1:C:861:GLN:N	1.97	0.80
1:A:860:ILE:HD12	1:A:861:GLN:N	1.97	0.80
1:D:860:ILE:HD12	1:D:861:GLN:N	1.97	0.79
1:C:318:ARG:NH2	1:C:322:GLU:O	2.16	0.78
1:B:860:ILE:HD12	1:B:861:GLN:N	1.97	0.78
1:B:318:ARG:NH2	1:B:322:GLU:O	2.16	0.77
1:A:318:ARG:NH2	1:A:322:GLU:O	2.17	0.77
1:D:318:ARG:NH2	1:D:322:GLU:O	2.17	0.77
1:C:962:MET:HE2	1:C:962:MET:HA	1.67	0.77
1:D:962:MET:HE2	1:D:962:MET:HA	1.66	0.76
1:B:962:MET:HE2	1:B:962:MET:HA	1.67	0.76
1:A:1042:GLN:O	1:A:1046:THR:HG23	1.86	0.76
1:B:2234:CYS:O	1:B:2235:ARG:C	2.29	0.76
1:A:962:MET:HE2	1:A:962:MET:HA	1.66	0.75
1:D:898:ARG:NH1	5:D:8005:ATP:O2G	2.20	0.75
1:D:1042:GLN:O	1:D:1046:THR:HG23	1.86	0.75
1:C:1042:GLN:O	1:C:1046:THR:HG23	1.86	0.75
1:C:898:ARG:NH1	5:C:8005:ATP:O2G	2.20	0.75
1:C:2234:CYS:O	1:C:2235:ARG:C	2.29	0.75
1:A:2234:CYS:O	1:A:2235:ARG:C	2.29	0.74
1:B:1042:GLN:O	1:B:1046:THR:HG23	1.86	0.74
1:C:2234:CYS:SG	1:C:2271:SER:OG	2.45	0.74
1:A:2234:CYS:SG	1:A:2271:SER:OG	2.44	0.74
1:D:2234:CYS:SG	1:D:2271:SER:OG	2.45	0.74
1:A:898:ARG:NH1	5:A:8005:ATP:O2G	2.20	0.74
1:B:2234:CYS:SG	1:B:2271:SER:OG	2.44	0.74
1:D:2234:CYS:O	1:D:2235:ARG:C	2.29	0.74
1:C:2981:VAL:O	1:C:2986:ARG:NH2	2.21	0.74
1:B:2981:VAL:O	1:B:2986:ARG:NH2	2.21	0.74
1:A:2981:VAL:O	1:A:2986:ARG:NH2	2.21	0.74
1:D:2981:VAL:O	1:D:2986:ARG:NH2	2.21	0.74
1:B:898:ARG:NH1	5:B:8005:ATP:O2G	2.20	0.73
1:B:2863:LEU:HD12	1:B:2926:GLU:OE1	1.89	0.73
1:D:2745:ASN:OD1	1:D:2746:VAL:N	2.22	0.73
1:B:2745:ASN:OD1	1:B:2746:VAL:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2160:LEU:HD13	1:D:2204:MET:HG2	1.72	0.72
1:A:2863:LEU:HD12	1:A:2926:GLU:OE1	1.89	0.72
1:B:2160:LEU:HD13	1:B:2204:MET:HG2	1.72	0.72
1:A:2160:LEU:HD13	1:A:2204:MET:HG2	1.72	0.72
1:D:4094:LYS:HE2	1:D:4094:LYS:H	1.55	0.72
1:A:4094:LYS:HE2	1:A:4094:LYS:H	1.55	0.72
1:A:2745:ASN:OD1	1:A:2746:VAL:N	2.22	0.72
1:B:1060:GLU:N	1:B:1060:GLU:OE1	2.23	0.72
1:C:2863:LEU:HD12	1:C:2926:GLU:OE1	1.89	0.72
1:C:2745:ASN:OD1	1:C:2746:VAL:N	2.22	0.72
1:D:2863:LEU:HD12	1:D:2926:GLU:OE1	1.89	0.72
1:C:4094:LYS:HE2	1:C:4094:LYS:H	1.55	0.71
1:C:2160:LEU:HD13	1:C:2204:MET:HG2	1.72	0.71
1:D:1060:GLU:N	1:D:1060:GLU:OE1	2.23	0.71
1:A:1060:GLU:N	1:A:1060:GLU:OE1	2.23	0.71
1:D:3530:ASP:OD2	1:D:3596:ARG:NH2	2.24	0.71
1:C:797:ARG:O	1:C:1620:ARG:NH2	2.24	0.71
1:C:2234:CYS:O	1:C:2236:PHE:N	2.24	0.71
1:C:3041:THR:HA	1:C:3076:LEU:HD11	1.73	0.71
1:D:797:ARG:O	1:D:1620:ARG:NH2	2.24	0.71
1:B:2234:CYS:O	1:B:2236:PHE:N	2.24	0.70
1:B:3530:ASP:OD2	1:B:3596:ARG:NH2	2.24	0.70
1:C:2564:THR:HG22	1:C:2607:CYS:HA	1.74	0.70
1:A:2564:THR:HG22	1:A:2607:CYS:HA	1.74	0.70
1:C:3531:GLN:O	1:C:3535:VAL:HG23	1.91	0.70
1:A:3041:THR:HA	1:A:3076:LEU:HD11	1.73	0.70
1:C:1060:GLU:N	1:C:1060:GLU:OE1	2.23	0.70
1:C:3530:ASP:OD2	1:C:3596:ARG:NH2	2.24	0.70
1:A:3531:GLN:O	1:A:3535:VAL:HG23	1.91	0.70
1:B:4094:LYS:H	1:B:4094:LYS:HE2	1.55	0.70
1:D:3531:GLN:O	1:D:3535:VAL:HG23	1.91	0.70
1:A:797:ARG:O	1:A:1620:ARG:NH2	2.24	0.70
1:A:3530:ASP:OD2	1:A:3596:ARG:NH2	2.24	0.70
1:B:2564:THR:HG22	1:B:2607:CYS:HA	1.74	0.70
1:D:2564:THR:HG22	1:D:2607:CYS:HA	1.74	0.70
1:D:3041:THR:HA	1:D:3076:LEU:HD11	1.73	0.69
1:A:2234:CYS:O	1:A:2236:PHE:N	2.24	0.69
1:B:1479:ASP:OD2	1:B:1485:HIS:NE2	2.26	0.69
1:B:3972:ILE:HG21	1:B:3983:LEU:HD12	1.74	0.69
1:C:2762:TYR:OH	1:C:2861:PRO:O	2.07	0.69
1:B:797:ARG:O	1:B:1620:ARG:NH2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3531:GLN:O	1:B:3535:VAL:HG23	1.91	0.69
1:D:2234:CYS:O	1:D:2236:PHE:N	2.24	0.69
1:D:3972:ILE:HG21	1:D:3983:LEU:HD12	1.74	0.69
1:A:1479:ASP:OD2	1:A:1485:HIS:NE2	2.26	0.69
1:B:3041:THR:HA	1:B:3076:LEU:HD11	1.73	0.69
1:C:4908:GLU:O	1:C:4912:VAL:HG13	1.93	0.69
1:C:2560:LEU:O	1:C:2564:THR:HG23	1.93	0.69
1:C:1479:ASP:OD2	1:C:1485:HIS:NE2	2.26	0.68
1:C:3972:ILE:HG21	1:C:3983:LEU:HD12	1.74	0.68
1:D:2215:VAL:CG1	1:D:2229:MET:HE1	2.22	0.68
1:B:2560:LEU:O	1:B:2564:THR:HG23	1.93	0.68
1:A:2560:LEU:O	1:A:2564:THR:HG23	1.93	0.68
1:D:2560:LEU:O	1:D:2564:THR:HG23	1.93	0.68
1:A:3972:ILE:HG21	1:A:3983:LEU:HD12	1.74	0.68
1:B:4908:GLU:O	1:B:4912:VAL:HG13	1.93	0.68
1:D:1479:ASP:OD2	1:D:1485:HIS:NE2	2.26	0.68
1:D:4908:GLU:O	1:D:4912:VAL:HG13	1.93	0.67
1:A:4908:GLU:O	1:A:4912:VAL:HG13	1.93	0.67
1:B:3367:ARG:NH1	1:B:3441:GLU:OE1	2.28	0.67
1:C:4965:TYR:OH	1:C:5031:GLU:OE1	2.10	0.67
1:B:1876:GLU:N	1:B:1876:GLU:OE1	2.27	0.66
1:C:1876:GLU:N	1:C:1876:GLU:OE1	2.27	0.66
1:A:2215:VAL:CG1	1:A:2229:MET:HE1	2.22	0.66
1:D:1876:GLU:N	1:D:1876:GLU:OE1	2.27	0.66
1:A:1876:GLU:OE1	1:A:1876:GLU:N	2.27	0.66
1:A:3367:ARG:NH1	1:A:3441:GLU:OE1	2.28	0.66
1:B:2890:LYS:O	1:B:2894:GLU:OE1	2.14	0.66
1:C:2215:VAL:CG1	1:C:2229:MET:HE1	2.22	0.66
1:C:3367:ARG:NH1	1:C:3441:GLU:OE1	2.28	0.66
1:D:2890:LYS:O	1:D:2894:GLU:OE1	2.14	0.66
1:D:3367:ARG:NH1	1:D:3441:GLU:OE1	2.28	0.65
1:A:2762:TYR:OH	1:A:2861:PRO:O	2.07	0.65
1:C:2890:LYS:O	1:C:2894:GLU:OE1	2.14	0.65
1:A:2890:LYS:O	1:A:2894:GLU:OE1	2.14	0.65
1:B:1023:VAL:HG22	1:B:1024:PRO:HD2	1.79	0.65
1:B:2752:LEU:HD12	1:B:2818:ILE:HD11	1.79	0.65
1:C:2752:LEU:HD12	1:C:2818:ILE:HD11	1.79	0.65
1:D:3962:LYS:NZ	1:D:4021:ASP:OD2	2.28	0.65
1:B:3347:VAL:HG11	1:B:3415:ARG:HB2	1.79	0.64
1:D:2752:LEU:HD12	1:D:2818:ILE:HD11	1.79	0.64
1:A:3347:VAL:HG11	1:A:3415:ARG:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:VAL:HG22	1:A:1024:PRO:HD2	1.79	0.64
1:B:2215:VAL:CG1	1:B:2229:MET:HE1	2.22	0.64
1:D:1281:GLN:O	1:D:1282:ASN:OD1	2.16	0.64
1:A:2752:LEU:HD12	1:A:2818:ILE:HD11	1.79	0.64
1:A:2753:ASP:HA	1:A:2756:ILE:HD12	1.80	0.64
1:B:3962:LYS:NZ	1:B:4021:ASP:OD2	2.28	0.64
1:B:2753:ASP:HA	1:B:2756:ILE:HD12	1.80	0.64
1:C:4890:ARG:NH1	1:D:4897:ASP:OD1	2.31	0.63
1:D:3538:LYS:NZ	1:D:3608:ASP:OD2	2.29	0.63
1:C:3347:VAL:HG11	1:C:3415:ARG:HB2	1.79	0.63
1:D:2753:ASP:HA	1:D:2756:ILE:HD12	1.80	0.63
1:A:2894:GLU:OE1	1:A:2894:GLU:N	2.31	0.63
1:C:1023:VAL:HG22	1:C:1024:PRO:HD2	1.79	0.63
1:C:1281:GLN:O	1:C:1282:ASN:OD1	2.16	0.63
1:C:2894:GLU:OE1	1:C:2894:GLU:N	2.31	0.63
1:D:71:GLU:OE1	1:D:111:ARG:NE	2.32	0.63
1:D:2762:TYR:OH	1:D:2861:PRO:O	2.07	0.63
1:D:1023:VAL:HG22	1:D:1024:PRO:HD2	1.79	0.63
1:B:1281:GLN:O	1:B:1282:ASN:OD1	2.16	0.63
1:B:4890:ARG:NH1	1:C:4897:ASP:OD1	2.32	0.63
1:B:2762:TYR:OH	1:B:2861:PRO:O	2.07	0.62
1:A:3538:LYS:NZ	1:A:3608:ASP:OD2	2.29	0.62
1:C:2753:ASP:HA	1:C:2756:ILE:HD12	1.80	0.62
1:D:3347:VAL:HG11	1:D:3415:ARG:HB2	1.79	0.62
1:C:71:GLU:OE1	1:C:111:ARG:NE	2.32	0.62
1:A:1281:GLN:O	1:A:1282:ASN:OD1	2.16	0.62
1:D:885:LEU:HD12	1:D:956:LEU:HD11	1.82	0.62
1:A:885:LEU:HD12	1:A:956:LEU:HD11	1.82	0.61
1:B:2477:ILE:HD12	1:B:2477:ILE:O	2.00	0.61
1:C:2872:LEU:HD22	1:C:2928:LEU:HD11	1.82	0.61
1:C:885:LEU:HD12	1:C:956:LEU:HD11	1.82	0.61
1:D:2894:GLU:OE1	1:D:2894:GLU:N	2.31	0.61
1:A:4887:VAL:HG12	1:A:4898:GLU:HG3	1.83	0.61
1:A:4890:ARG:NH1	1:B:4897:ASP:OD1	2.34	0.61
1:A:4897:ASP:OD1	1:D:4890:ARG:NH1	2.34	0.61
1:B:3538:LYS:NZ	1:B:3608:ASP:OD2	2.29	0.61
1:C:2477:ILE:O	1:C:2477:ILE:HD12	2.00	0.61
1:A:2477:ILE:HD12	1:A:2477:ILE:O	2.00	0.61
1:C:4887:VAL:HG12	1:C:4898:GLU:HG3	1.83	0.61
1:D:2872:LEU:HD22	1:D:2928:LEU:HD11	1.82	0.61
1:D:4887:VAL:HG12	1:D:4898:GLU:HG3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2872:LEU:HD22	1:A:2928:LEU:HD11	1.82	0.61
1:B:2872:LEU:HD22	1:B:2928:LEU:HD11	1.82	0.61
1:D:4965:TYR:OH	1:D:5031:GLU:OE1	2.10	0.61
1:B:885:LEU:HD12	1:B:956:LEU:HD11	1.82	0.61
1:B:2894:GLU:OE1	1:B:2894:GLU:N	2.31	0.61
1:D:2477:ILE:HD12	1:D:2477:ILE:O	2.00	0.61
1:C:3962:LYS:NZ	1:C:4021:ASP:OD2	2.28	0.60
1:B:2752:LEU:HD13	1:B:2814:LEU:HB3	1.83	0.60
1:A:2755:PHE:HD2	1:A:2814:LEU:HD11	1.66	0.60
1:B:4887:VAL:HG12	1:B:4898:GLU:HG3	1.83	0.60
1:D:2755:PHE:HD2	1:D:2814:LEU:HD11	1.66	0.60
1:C:3538:LYS:NZ	1:C:3608:ASP:OD2	2.29	0.60
1:A:2752:LEU:HD13	1:A:2814:LEU:HB3	1.83	0.60
1:A:4965:TYR:OH	1:A:5031:GLU:OE1	2.10	0.60
1:C:2755:PHE:HD2	1:C:2814:LEU:HD11	1.66	0.60
1:D:2752:LEU:HD13	1:D:2814:LEU:HB3	1.83	0.60
1:B:71:GLU:OE1	1:B:111:ARG:NE	2.32	0.60
1:A:71:GLU:OE1	1:A:111:ARG:NE	2.32	0.60
1:B:2755:PHE:HD2	1:B:2814:LEU:HD11	1.66	0.59
1:C:2645:LEU:HD13	1:C:2679:LEU:HD21	1.83	0.59
1:C:2752:LEU:HD13	1:C:2814:LEU:HB3	1.83	0.59
1:D:1116:LEU:HD12	1:D:1194:SER:HB2	1.85	0.59
1:A:925:MET:O	1:A:929:THR:HG23	2.03	0.59
1:B:2645:LEU:HD13	1:B:2679:LEU:HD21	1.83	0.59
1:A:1116:LEU:HD12	1:A:1194:SER:HB2	1.85	0.59
1:C:2875:MET:HE1	1:C:2940:ARG:HD2	1.85	0.59
1:D:2645:LEU:HD13	1:D:2679:LEU:HD21	1.83	0.59
1:A:2755:PHE:CD2	1:A:2814:LEU:HD11	2.38	0.59
1:C:925:MET:O	1:C:929:THR:HG23	2.03	0.59
1:D:2755:PHE:CD2	1:D:2814:LEU:HD11	2.38	0.59
1:A:2645:LEU:HD13	1:A:2679:LEU:HD21	1.83	0.58
1:B:1116:LEU:HD12	1:B:1194:SER:HB2	1.85	0.58
1:B:2755:PHE:CD2	1:B:2814:LEU:HD11	2.38	0.58
1:C:2265:GLY:O	1:C:2267:GLY:N	2.36	0.58
1:A:2265:GLY:O	1:A:2267:GLY:N	2.37	0.58
1:D:925:MET:O	1:D:929:THR:HG23	2.03	0.58
1:A:3541:TYR:HB3	1:A:3605:TYR:CD2	2.39	0.58
1:A:3962:LYS:NZ	1:A:4021:ASP:OD2	2.28	0.58
1:B:2265:GLY:O	1:B:2267:GLY:N	2.37	0.58
1:C:2755:PHE:CD2	1:C:2814:LEU:HD11	2.38	0.58
1:D:2875:MET:HE1	1:D:2940:ARG:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:928:GLU:O	1:B:932:THR:HG22	2.04	0.58
1:B:2875:MET:HE1	1:B:2940:ARG:HD2	1.85	0.58
1:B:925:MET:O	1:B:929:THR:HG23	2.03	0.57
1:D:928:GLU:O	1:D:932:THR:HG22	2.04	0.57
1:C:1116:LEU:HD12	1:C:1194:SER:HB2	1.85	0.57
1:C:3948:GLU:OE1	1:C:3952:ARG:NH2	2.37	0.57
1:D:2265:GLY:O	1:D:2267:GLY:N	2.36	0.57
1:A:658:THR:HG22	1:A:1002:VAL:HG21	1.86	0.57
1:A:979:THR:O	1:A:983:THR:HG23	2.04	0.57
1:B:2749:PRO:HD2	1:B:2752:LEU:HD12	1.87	0.57
1:D:3541:TYR:HB3	1:D:3605:TYR:CD2	2.39	0.57
1:A:1426:GLU:OE1	1:A:1426:GLU:N	2.35	0.57
1:A:3861:MET:N	1:A:3861:MET:HE3	2.20	0.57
1:A:2520:LEU:HD22	1:A:2579:MET:HE1	1.87	0.57
1:C:2749:PRO:HD2	1:C:2752:LEU:HD12	1.87	0.57
1:C:3236:SER:OG	1:C:3239:GLU:OE1	2.19	0.57
1:B:3861:MET:HE3	1:B:3861:MET:N	2.20	0.57
1:D:979:THR:O	1:D:983:THR:HG23	2.05	0.57
1:B:896:PRO:HD2	1:B:904:LEU:HD13	1.87	0.57
1:B:903:ARG:HE	1:B:903:ARG:HA	1.70	0.57
1:C:3541:TYR:HB3	1:C:3605:TYR:CD2	2.39	0.57
1:A:928:GLU:O	1:A:932:THR:HG22	2.04	0.57
1:A:2875:MET:HE1	1:A:2940:ARG:HD2	1.85	0.57
1:C:2520:LEU:HD22	1:C:2579:MET:HE1	1.87	0.57
1:A:57:GLN:O	1:A:310:THR:HG23	2.05	0.57
1:D:2520:LEU:HD22	1:D:2579:MET:HE1	1.87	0.57
1:D:3861:MET:N	1:D:3861:MET:HE3	2.20	0.57
1:B:3541:TYR:HB3	1:B:3605:TYR:CD2	2.39	0.56
1:C:57:GLN:O	1:C:310:THR:HG23	2.05	0.56
1:C:979:THR:O	1:C:983:THR:HG23	2.04	0.56
1:C:4628:TYR:OH	1:D:4858:ARG:NH1	2.38	0.56
1:D:3347:VAL:HG11	1:D:3415:ARG:CB	2.35	0.56
1:A:373:LEU:HD23	1:A:373:LEU:H	1.70	0.56
1:A:2815:LYS:HA	1:A:2818:ILE:HD12	1.86	0.56
1:A:2947:LEU:O	1:A:2950:SER:OG	2.23	0.56
1:B:57:GLN:O	1:B:310:THR:HG23	2.05	0.56
1:B:2815:LYS:HA	1:B:2818:ILE:HD12	1.86	0.56
1:B:3347:VAL:HG11	1:B:3415:ARG:CB	2.35	0.56
1:C:3861:MET:HE3	1:C:3861:MET:N	2.20	0.56
1:D:974:SER:O	1:D:977:ARG:NH2	2.39	0.56
1:A:903:ARG:HA	1:A:903:ARG:HE	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3860:GLY:C	1:A:3861:MET:HE3	2.31	0.56
1:A:3948:GLU:OE1	1:A:3952:ARG:NH2	2.37	0.56
1:B:979:THR:O	1:B:983:THR:HG23	2.05	0.56
1:C:658:THR:HG22	1:C:1002:VAL:HG21	1.87	0.56
1:C:928:GLU:O	1:C:932:THR:HG22	2.04	0.56
1:D:57:GLN:O	1:D:310:THR:HG23	2.05	0.56
1:D:2749:PRO:HD2	1:D:2752:LEU:HD12	1.87	0.56
1:A:974:SER:O	1:A:977:ARG:NH2	2.39	0.56
1:A:3347:VAL:HG11	1:A:3415:ARG:CB	2.35	0.56
1:B:4628:TYR:OH	1:C:4858:ARG:NH1	2.39	0.56
1:C:1426:GLU:N	1:C:1426:GLU:OE1	2.35	0.56
1:D:658:THR:HG22	1:D:1002:VAL:HG21	1.87	0.56
1:D:2815:LYS:HA	1:D:2818:ILE:HD12	1.86	0.56
1:D:3236:SER:OG	1:D:3239:GLU:OE1	2.19	0.56
1:B:2790:PRO:C	1:B:2791:MET:HE3	2.31	0.56
1:B:3236:SER:OG	1:B:3239:GLU:OE1	2.19	0.56
1:B:3860:GLY:C	1:B:3861:MET:HE3	2.31	0.56
1:C:2790:PRO:C	1:C:2791:MET:HE3	2.31	0.56
1:C:2815:LYS:HA	1:C:2818:ILE:HD12	1.86	0.56
1:C:3347:VAL:HG11	1:C:3415:ARG:CB	2.35	0.56
1:D:896:PRO:HD2	1:D:904:LEU:HD13	1.87	0.56
1:D:1426:GLU:OE1	1:D:1426:GLU:N	2.35	0.56
1:C:3771:SER:HA	1:C:3774:HIS:CD2	2.41	0.56
1:A:896:PRO:HD2	1:A:904:LEU:HD13	1.87	0.56
1:A:1758:GLY:N	1:A:1759:PRO:CD	2.69	0.56
1:B:373:LEU:H	1:B:373:LEU:HD23	1.70	0.56
1:C:896:PRO:HD2	1:C:904:LEU:HD13	1.87	0.56
1:C:903:ARG:HE	1:C:903:ARG:HA	1.70	0.56
1:C:3208:GLU:OE1	1:C:3306:THR:OG1	2.23	0.56
1:C:3860:GLY:C	1:C:3861:MET:HE3	2.31	0.56
1:D:373:LEU:HD23	1:D:373:LEU:H	1.70	0.56
1:A:3108:VAL:HG22	1:A:3176:LEU:HD12	1.88	0.56
1:A:4858:ARG:NH1	1:D:4628:TYR:OH	2.38	0.56
1:B:2520:LEU:HD22	1:B:2579:MET:HE1	1.87	0.56
1:B:2831:GLU:N	1:B:2831:GLU:OE1	2.39	0.56
1:B:2888:GLY:HA2	1:B:2891:LYS:HD2	1.88	0.56
1:D:903:ARG:HE	1:D:903:ARG:HA	1.70	0.56
1:D:3860:GLY:C	1:D:3861:MET:HE3	2.31	0.56
1:A:2749:PRO:HD2	1:A:2752:LEU:HD12	1.87	0.55
1:A:3771:SER:HA	1:A:3774:HIS:CD2	2.41	0.55
1:B:974:SER:O	1:B:977:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3208:GLU:OE1	1:B:3306:THR:OG1	2.23	0.55
1:B:3948:GLU:OE1	1:B:3952:ARG:NH2	2.37	0.55
1:D:3948:GLU:OE1	1:D:3952:ARG:NH2	2.37	0.55
1:D:3771:SER:HA	1:D:3774:HIS:CD2	2.41	0.55
1:A:3393:LEU:H	1:A:3393:LEU:HD22	1.72	0.55
1:B:658:THR:HG22	1:B:1002:VAL:HG21	1.87	0.55
1:B:3393:LEU:HD22	1:B:3393:LEU:H	1.72	0.55
1:B:3771:SER:HA	1:B:3774:HIS:CD2	2.41	0.55
1:C:967:LYS:NZ	1:C:969:ALA:HB2	2.22	0.55
1:D:967:LYS:NZ	1:D:969:ALA:HB2	2.21	0.55
1:B:2802:ASP:OD2	1:B:2803:LYS:N	2.40	0.55
1:C:1758:GLY:N	1:C:1759:PRO:CD	2.69	0.55
1:C:2986:ARG:HE	1:C:2986:ARG:N	2.05	0.55
1:D:3393:LEU:HD22	1:D:3393:LEU:H	1.72	0.55
1:A:2802:ASP:OD2	1:A:2803:LYS:N	2.40	0.55
1:A:2888:GLY:HA2	1:A:2891:LYS:HD2	1.88	0.55
1:C:373:LEU:HD23	1:C:373:LEU:H	1.70	0.55
1:C:974:SER:O	1:C:977:ARG:NH2	2.39	0.55
1:C:2802:ASP:OD2	1:C:2803:LYS:N	2.40	0.55
1:C:4723:LEU:HA	1:C:4735:ILE:HG21	1.89	0.55
1:D:1758:GLY:N	1:D:1759:PRO:CD	2.69	0.55
1:D:2790:PRO:C	1:D:2791:MET:HE3	2.31	0.55
1:D:2986:ARG:HE	1:D:2986:ARG:N	2.05	0.55
1:B:2000:ARG:O	1:B:3638:ARG:NH2	2.40	0.55
1:B:2450:GLU:OE1	1:B:2453:ARG:NH1	2.40	0.55
1:B:3108:VAL:HG22	1:B:3176:LEU:HD12	1.88	0.55
1:C:3108:VAL:HG22	1:C:3176:LEU:HD12	1.88	0.55
1:D:2947:LEU:O	1:D:2950:SER:OG	2.23	0.55
1:A:967:LYS:NZ	1:A:969:ALA:HB2	2.22	0.55
1:B:1758:GLY:N	1:B:1759:PRO:CD	2.69	0.55
1:B:2986:ARG:HE	1:B:2986:ARG:N	2.05	0.55
1:A:2790:PRO:C	1:A:2791:MET:HE3	2.31	0.55
1:A:2986:ARG:HE	1:A:2986:ARG:N	2.05	0.55
1:B:912:HIS:O	1:B:919:ARG:NH2	2.40	0.55
1:D:930:LEU:HD22	1:D:930:LEU:H	1.72	0.55
1:D:4723:LEU:HA	1:D:4735:ILE:HG21	1.89	0.55
1:B:1426:GLU:OE1	1:B:1426:GLU:N	2.35	0.54
1:B:2947:LEU:O	1:B:2950:SER:OG	2.23	0.54
1:C:2888:GLY:HA2	1:C:2891:LYS:HD2	1.89	0.54
1:C:3393:LEU:H	1:C:3393:LEU:HD22	1.72	0.54
1:A:912:HIS:O	1:A:919:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:967:LYS:NZ	1:B:969:ALA:HB2	2.22	0.54
1:C:32:GLU:OE2	1:C:32:GLU:HA	2.08	0.54
1:C:2450:GLU:OE1	1:C:2453:ARG:NH1	2.40	0.54
1:B:930:LEU:HD22	1:B:930:LEU:H	1.72	0.54
1:C:912:HIS:O	1:C:919:ARG:NH2	2.40	0.54
1:D:2831:GLU:N	1:D:2831:GLU:OE1	2.39	0.54
1:D:2906:LEU:O	1:D:2906:LEU:HD23	2.08	0.54
1:D:3108:VAL:HG22	1:D:3176:LEU:HD12	1.88	0.54
1:A:930:LEU:HD22	1:A:930:LEU:H	1.72	0.54
1:C:930:LEU:H	1:C:930:LEU:HD22	1.72	0.54
1:D:912:HIS:O	1:D:919:ARG:NH2	2.40	0.54
1:A:2450:GLU:OE1	1:A:2453:ARG:NH1	2.40	0.54
1:A:3837:ALA:O	1:A:3841:THR:HG23	2.08	0.54
1:C:2625:ARG:NH1	1:C:2911:THR:O	2.37	0.54
1:C:2906:LEU:HD23	1:C:2906:LEU:O	2.08	0.54
1:D:973:LEU:HD13	1:D:1046:THR:HA	1.90	0.54
1:D:2888:GLY:HA2	1:D:2891:LYS:HD2	1.88	0.54
1:A:2831:GLU:OE1	1:A:2831:GLU:N	2.39	0.54
1:A:2625:ARG:NH1	1:A:2911:THR:O	2.37	0.54
1:B:4723:LEU:HA	1:B:4735:ILE:HG21	1.89	0.54
1:D:2802:ASP:OD2	1:D:2803:LYS:N	2.40	0.54
1:B:973:LEU:HD13	1:B:1046:THR:HA	1.90	0.54
1:B:2215:VAL:HG21	1:B:2229:MET:CE	2.38	0.54
1:B:3576:LEU:O	1:B:3580:VAL:HG23	2.08	0.54
1:B:3837:ALA:O	1:B:3841:THR:HG23	2.08	0.54
1:A:2906:LEU:O	1:A:2906:LEU:HD23	2.08	0.53
1:A:4723:LEU:HA	1:A:4735:ILE:HG21	1.89	0.53
1:B:2906:LEU:HD23	1:B:2906:LEU:O	2.08	0.53
1:C:2215:VAL:HG21	1:C:2229:MET:CE	2.38	0.53
1:C:3837:ALA:O	1:C:3841:THR:HG23	2.08	0.53
1:C:4677:ARG:NH2	1:C:4713:TYR:OH	2.42	0.53
1:D:961:MET:HE2	1:D:965:GLY:O	2.09	0.53
1:D:2450:GLU:OE1	1:D:2453:ARG:NH1	2.40	0.53
1:A:4628:TYR:OH	1:B:4858:ARG:NH1	2.41	0.53
1:A:4677:ARG:NH2	1:A:4713:TYR:OH	2.42	0.53
1:B:32:GLU:HA	1:B:32:GLU:OE2	2.07	0.53
1:B:4653:PHE:CE2	1:B:4657:ILE:HD11	2.44	0.53
1:D:3837:ALA:O	1:D:3841:THR:HG23	2.08	0.53
1:C:860:ILE:HD12	1:C:861:GLN:H	1.72	0.53
1:C:2947:LEU:O	1:C:2950:SER:OG	2.23	0.53
1:D:29:VAL:HG12	1:D:30:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:GLU:OE2	1:D:32:GLU:HA	2.07	0.53
1:D:4653:PHE:CE2	1:D:4657:ILE:HD11	2.44	0.53
1:C:29:VAL:HG12	1:C:30:LEU:HD12	1.91	0.53
1:C:973:LEU:HD13	1:C:1046:THR:HA	1.90	0.53
1:A:2215:VAL:HG21	1:A:2229:MET:CE	2.38	0.53
1:D:2790:PRO:O	1:D:2791:MET:HE3	2.09	0.53
1:A:860:ILE:HD12	1:A:861:GLN:H	1.72	0.53
1:B:2756:ILE:HG13	1:B:2814:LEU:HD12	1.91	0.53
1:A:32:GLU:OE2	1:A:32:GLU:HA	2.07	0.53
1:B:961:MET:HE2	1:B:965:GLY:O	2.09	0.53
1:C:3576:LEU:O	1:C:3580:VAL:HG23	2.08	0.53
1:A:4653:PHE:CE2	1:A:4657:ILE:HD11	2.44	0.53
1:A:961:MET:HE2	1:A:965:GLY:O	2.09	0.52
1:A:2790:PRO:O	1:A:2791:MET:HE3	2.09	0.52
1:A:3576:LEU:O	1:A:3580:VAL:HG23	2.08	0.52
1:B:2791:MET:HA	1:B:2793:ARG:HH11	1.75	0.52
1:B:4677:ARG:NH2	1:B:4713:TYR:OH	2.42	0.52
1:C:397:GLU:OE1	1:C:471:SER:OG	2.24	0.52
1:C:961:MET:HE2	1:C:965:GLY:O	2.09	0.52
1:C:976:VAL:C	1:C:977:ARG:HE	2.17	0.52
1:C:2790:PRO:O	1:C:2791:MET:HE3	2.09	0.52
1:D:976:VAL:C	1:D:977:ARG:HE	2.17	0.52
1:B:860:ILE:HD12	1:B:861:GLN:H	1.72	0.52
1:B:2234:CYS:O	1:B:2237:LEU:N	2.42	0.52
1:C:864:LEU:HD11	1:C:931:LYS:HG3	1.92	0.52
1:C:4653:PHE:CE2	1:C:4657:ILE:HD11	2.44	0.52
1:D:2215:VAL:HG21	1:D:2229:MET:CE	2.38	0.52
1:D:3576:LEU:O	1:D:3580:VAL:HG23	2.08	0.52
1:B:2790:PRO:O	1:B:2791:MET:HE3	2.09	0.52
1:C:2234:CYS:O	1:C:2237:LEU:N	2.42	0.52
1:A:2000:ARG:O	1:A:3638:ARG:NH2	2.40	0.52
1:B:4059:GLU:HG2	1:B:4169:LEU:HD13	1.92	0.52
1:C:649:ILE:HG23	1:C:815:ALA:HB3	1.92	0.52
1:C:4747:GLU:O	1:C:4751:HIS:ND1	2.43	0.52
1:D:3580:VAL:HG21	1:D:3583:ARG:HH21	1.75	0.52
1:A:2791:MET:HA	1:A:2793:ARG:HH11	1.75	0.52
1:B:649:ILE:HG23	1:B:815:ALA:HB3	1.92	0.52
1:D:2234:CYS:O	1:D:2237:LEU:N	2.42	0.52
1:A:976:VAL:C	1:A:977:ARG:HE	2.17	0.52
1:D:864:LEU:HD11	1:D:931:LYS:HG3	1.92	0.52
1:A:4747:GLU:O	1:A:4751:HIS:ND1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3282:LEU:HD12	1:C:3316:LEU:HD22	1.92	0.52
1:D:860:ILE:HD12	1:D:861:GLN:H	1.72	0.52
1:D:2891:LYS:O	1:D:2895:LEU:HG	2.10	0.52
1:D:4902:PRO:HB3	1:D:4911:ARG:HG2	1.92	0.52
1:A:2234:CYS:O	1:A:2237:LEU:N	2.42	0.52
1:A:2756:ILE:HG13	1:A:2814:LEU:HD12	1.91	0.52
1:A:4902:PRO:HB3	1:A:4911:ARG:HG2	1.92	0.52
1:B:4902:PRO:HB3	1:B:4911:ARG:HG2	1.92	0.52
1:D:649:ILE:HG23	1:D:815:ALA:HB3	1.92	0.52
1:D:1176:SER:OG	1:D:1181:ARG:NH2	2.43	0.52
1:D:2777:SER:O	1:D:2789:HIS:N	2.43	0.52
1:A:649:ILE:HG23	1:A:815:ALA:HB3	1.92	0.52
1:A:2777:SER:O	1:A:2789:HIS:N	2.43	0.52
1:B:29:VAL:HG12	1:B:30:LEU:HD12	1.91	0.52
1:C:2756:ILE:HG13	1:C:2814:LEU:HD12	1.91	0.52
1:D:397:GLU:OE1	1:D:471:SER:OG	2.24	0.52
1:A:1987:MET:SD	1:A:1987:MET:N	2.82	0.51
1:C:2791:MET:HA	1:C:2793:ARG:HH11	1.75	0.51
1:C:4902:PRO:HB3	1:C:4911:ARG:HG2	1.92	0.51
1:A:29:VAL:HG12	1:A:30:LEU:HD12	1.91	0.51
1:A:973:LEU:HD13	1:A:1046:THR:HA	1.90	0.51
1:A:3282:LEU:HD12	1:A:3316:LEU:HD22	1.92	0.51
1:A:4059:GLU:HG2	1:A:4169:LEU:HD13	1.91	0.51
1:B:2777:SER:O	1:B:2789:HIS:N	2.43	0.51
1:B:864:LEU:HD11	1:B:931:LYS:HG3	1.92	0.51
1:B:976:VAL:C	1:B:977:ARG:HE	2.17	0.51
1:C:1176:SER:OG	1:C:1181:ARG:NH2	2.43	0.51
1:C:3580:VAL:HG21	1:C:3583:ARG:HH21	1.75	0.51
1:D:4677:ARG:NH2	1:D:4713:TYR:OH	2.42	0.51
1:A:864:LEU:HD11	1:A:931:LYS:HG3	1.92	0.51
1:B:2891:LYS:O	1:B:2895:LEU:HG	2.10	0.51
1:B:3331:ASP:N	1:B:3331:ASP:OD1	2.43	0.51
1:C:865:PRO:HD2	1:C:868:LEU:HD12	1.92	0.51
1:C:4059:GLU:HG2	1:C:4169:LEU:HD13	1.91	0.51
1:A:3236:SER:OG	1:A:3239:GLU:OE1	2.19	0.51
1:D:902:LYS:O	1:D:902:LYS:NZ	2.28	0.51
1:A:865:PRO:HD2	1:A:868:LEU:HD12	1.92	0.51
1:A:3331:ASP:OD1	1:A:3331:ASP:N	2.43	0.51
1:A:3580:VAL:HG21	1:A:3583:ARG:HH21	1.75	0.51
1:B:865:PRO:HD2	1:B:868:LEU:HD12	1.92	0.51
1:B:1176:SER:OG	1:B:1181:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4747:GLU:O	1:B:4751:HIS:ND1	2.43	0.51
1:C:2891:LYS:O	1:C:2895:LEU:HG	2.10	0.51
1:D:865:PRO:HD2	1:D:868:LEU:HD12	1.92	0.51
1:D:4747:GLU:O	1:D:4751:HIS:ND1	2.43	0.51
1:A:2942:LEU:HD12	1:A:2942:LEU:H	1.75	0.51
1:A:3344:GLN:O	1:A:3347:VAL:HG12	2.11	0.51
1:B:2625:ARG:NH1	1:B:2911:THR:O	2.37	0.51
1:B:3421:ARG:HG3	1:B:3521:ILE:HD11	1.92	0.51
1:D:2756:ILE:HG13	1:D:2814:LEU:HD12	1.91	0.51
1:A:2714:ASP:OD1	1:A:2714:ASP:N	2.41	0.51
1:B:3369:ARG:NH1	1:B:3405:ASP:OD2	2.41	0.51
1:C:1064:VAL:HG23	1:C:1065:ASP:N	2.26	0.51
1:C:2942:LEU:H	1:C:2942:LEU:HD12	1.75	0.51
1:D:3282:LEU:HD12	1:D:3316:LEU:HD22	1.92	0.51
1:D:3344:GLN:O	1:D:3347:VAL:HG12	2.11	0.51
1:B:3580:VAL:HG21	1:B:3583:ARG:HH21	1.75	0.51
1:D:2625:ARG:NH1	1:D:2911:THR:O	2.37	0.51
1:A:2891:LYS:O	1:A:2895:LEU:HG	2.10	0.51
1:B:902:LYS:O	1:B:902:LYS:NZ	2.28	0.51
1:B:1064:VAL:HG23	1:B:1065:ASP:N	2.26	0.51
1:B:2762:TYR:OH	1:B:2863:LEU:HG	2.11	0.51
1:D:1064:VAL:HG23	1:D:1065:ASP:N	2.26	0.51
1:D:2762:TYR:OH	1:D:2863:LEU:HG	2.11	0.51
1:B:2266:LEU:HD11	1:B:2327:CYS:HB3	1.93	0.50
1:B:2817:MET:HE1	1:B:2931:LEU:CD1	2.41	0.50
1:C:2777:SER:O	1:C:2789:HIS:N	2.43	0.50
1:C:2974:PHE:CD1	1:C:2974:PHE:C	2.89	0.50
1:C:3331:ASP:OD1	1:C:3331:ASP:N	2.43	0.50
1:C:3421:ARG:HG3	1:C:3521:ILE:HD11	1.92	0.50
1:A:1176:SER:OG	1:A:1181:ARG:NH2	2.43	0.50
1:B:2942:LEU:HD12	1:B:2942:LEU:H	1.75	0.50
1:C:2215:VAL:HG21	1:C:2229:MET:HE1	1.93	0.50
1:A:2215:VAL:HG21	1:A:2229:MET:HE1	1.93	0.50
1:B:3344:GLN:O	1:B:3347:VAL:HG12	2.11	0.50
1:C:2266:LEU:HD11	1:C:2327:CYS:HB3	1.94	0.50
1:C:4818:VAL:HG11	1:D:4837:MET:HE2	1.93	0.50
1:A:2974:PHE:CD1	1:A:2974:PHE:C	2.89	0.50
1:A:3421:ARG:HG3	1:A:3521:ILE:HD11	1.92	0.50
1:B:2215:VAL:HG21	1:B:2229:MET:HE1	1.93	0.50
1:B:3282:LEU:HD12	1:B:3316:LEU:HD22	1.92	0.50
1:C:1713:TYR:OH	1:C:1816:MET:HE3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2817:MET:HE1	1:C:2931:LEU:CD1	2.41	0.50
1:C:2831:GLU:OE1	1:C:2831:GLU:N	2.39	0.50
1:D:2215:VAL:HG21	1:D:2229:MET:HE1	1.93	0.50
1:A:1064:VAL:HG23	1:A:1065:ASP:N	2.26	0.50
1:A:2817:MET:HE1	1:A:2931:LEU:CD1	2.41	0.50
1:C:3344:GLN:O	1:C:3347:VAL:HG12	2.11	0.50
1:D:2791:MET:HA	1:D:2793:ARG:HH11	1.75	0.50
1:C:2762:TYR:OH	1:C:2863:LEU:HG	2.11	0.50
1:D:2817:MET:HE1	1:D:2931:LEU:CD1	2.41	0.50
1:D:2974:PHE:CD1	1:D:2974:PHE:C	2.89	0.50
1:D:2266:LEU:HD11	1:D:2327:CYS:HB3	1.94	0.50
1:D:2942:LEU:HD12	1:D:2942:LEU:H	1.75	0.50
1:D:3421:ARG:HG3	1:D:3521:ILE:HD11	1.92	0.50
1:D:4059:GLU:HG2	1:D:4169:LEU:HD13	1.92	0.50
1:A:2264:ILE:HD12	1:A:2264:ILE:C	2.37	0.50
1:B:397:GLU:OE1	1:B:471:SER:OG	2.24	0.50
1:B:1713:TYR:OH	1:B:1816:MET:HE3	2.12	0.50
1:C:2887:TRP:CG	1:C:2891:LYS:HE3	2.47	0.50
1:A:2762:TYR:OH	1:A:2863:LEU:HG	2.11	0.50
1:C:1987:MET:SD	1:C:1987:MET:N	2.82	0.50
1:A:1713:TYR:OH	1:A:1816:MET:HE3	2.12	0.49
1:A:2266:LEU:HD11	1:A:2327:CYS:HB3	1.94	0.49
2:H:62:GLU:O	2:H:66:GLN:HG3	2.12	0.49
1:B:2974:PHE:CD1	1:B:2974:PHE:C	2.89	0.49
1:C:2748:ILE:HD11	1:C:2752:LEU:HB3	1.94	0.49
1:D:2000:ARG:O	1:D:3638:ARG:NH2	2.40	0.49
2:G:80:ASP:OD1	2:G:80:ASP:N	2.46	0.49
1:D:2887:TRP:CG	1:D:2891:LYS:HE3	2.47	0.49
1:A:858:ASP:OD2	1:A:858:ASP:C	2.55	0.49
2:E:62:GLU:O	2:E:66:GLN:HG3	2.12	0.49
1:B:3861:MET:HE2	1:B:3871:ARG:HE	1.77	0.49
1:B:4210:MET:HE3	1:B:4211:PRO:HD2	1.94	0.49
1:D:2226:PHE:N	1:D:2227:PRO:HD3	2.28	0.49
1:D:2791:MET:CA	1:D:2793:ARG:HH11	2.26	0.49
1:A:2625:ARG:HD2	1:A:2907:VAL:HG21	1.95	0.49
1:B:4818:VAL:HG11	1:C:4837:MET:HE2	1.95	0.49
1:C:2000:ARG:O	1:C:3638:ARG:NH2	2.40	0.49
1:C:2226:PHE:N	1:C:2227:PRO:HD3	2.28	0.49
1:D:1713:TYR:OH	1:D:1816:MET:HE3	2.12	0.49
1:D:3208:GLU:OE1	1:D:3306:THR:OG1	2.23	0.49
1:D:4210:MET:HE3	1:D:4211:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2791:MET:CA	1:A:2793:ARG:HH11	2.26	0.49
1:A:2887:TRP:CG	1:A:2891:LYS:HE3	2.47	0.49
2:F:62:GLU:O	2:F:66:GLN:HG3	2.12	0.49
1:B:858:ASP:OD2	1:B:858:ASP:C	2.55	0.49
1:C:3861:MET:HE2	1:C:3871:ARG:HE	1.78	0.49
1:D:2906:LEU:HD23	1:D:2906:LEU:C	2.37	0.49
1:D:3861:MET:HE2	1:D:3871:ARG:HE	1.78	0.49
2:G:62:GLU:O	2:G:66:GLN:HG3	2.12	0.49
1:B:2264:ILE:C	1:B:2264:ILE:HD12	2.37	0.49
1:D:2264:ILE:C	1:D:2264:ILE:HD12	2.37	0.49
1:D:4893:GLY:N	1:D:4897:ASP:OD2	2.45	0.49
1:A:2906:LEU:HD23	1:A:2906:LEU:C	2.37	0.49
1:A:3208:GLU:OE1	1:A:3306:THR:OG1	2.23	0.49
1:C:2264:ILE:HD12	1:C:2264:ILE:C	2.37	0.49
1:D:1987:MET:SD	1:D:1987:MET:N	2.82	0.49
1:D:2748:ILE:HD11	1:D:2752:LEU:HB3	1.94	0.49
1:D:3526:CYS:SG	1:D:3600:VAL:HG21	2.53	0.49
1:B:3556:ASN:OD1	1:B:3557:ASN:OD1	2.31	0.49
1:C:4210:MET:HE3	1:C:4211:PRO:HD2	1.94	0.49
1:D:4638:GLU:OE1	1:D:4642:ARG:NH2	2.46	0.49
1:A:3369:ARG:NH1	1:A:3405:ASP:OD2	2.41	0.49
1:B:2226:PHE:N	1:B:2227:PRO:HD3	2.28	0.49
1:C:3556:ASN:OD1	1:C:3557:ASN:OD1	2.31	0.49
1:D:858:ASP:OD2	1:D:858:ASP:C	2.55	0.49
1:A:902:LYS:O	1:A:902:LYS:NZ	2.28	0.48
1:A:3861:MET:HE2	1:A:3871:ARG:HE	1.78	0.48
1:A:4638:GLU:OE1	1:A:4642:ARG:NH2	2.46	0.48
1:B:2748:ILE:HD11	1:B:2752:LEU:HB3	1.94	0.48
1:B:2791:MET:CA	1:B:2793:ARG:HH11	2.25	0.48
1:B:2906:LEU:HD23	1:B:2906:LEU:C	2.37	0.48
1:D:108:ILE:HG23	1:D:151:MET:HE2	1.95	0.48
1:A:978:LEU:HD13	1:A:982:GLN:HB3	1.96	0.48
1:C:858:ASP:C	1:C:858:ASP:OD2	2.55	0.48
2:F:80:ASP:OD1	2:F:80:ASP:N	2.46	0.48
1:B:871:ILE:HG22	1:B:871:ILE:O	2.13	0.48
1:B:2890:LYS:O	1:B:2893:GLN:N	2.46	0.48
1:B:3526:CYS:SG	1:B:3600:VAL:HG21	2.53	0.48
1:C:2906:LEU:HD23	1:C:2906:LEU:C	2.37	0.48
1:C:3369:ARG:NH1	1:C:3405:ASP:OD2	2.41	0.48
1:D:978:LEU:HD13	1:D:982:GLN:HB3	1.96	0.48
1:B:2887:TRP:CG	1:B:2891:LYS:HE3	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2945:MET:SD	1:B:2945:MET:C	2.97	0.48
1:C:108:ILE:HG23	1:C:151:MET:HE2	1.96	0.48
1:C:2791:MET:CA	1:C:2793:ARG:HH11	2.26	0.48
1:C:2945:MET:SD	1:C:2945:MET:C	2.97	0.48
1:C:5007:TYR:CZ	1:C:5011:MET:HE3	2.49	0.48
1:A:3176:LEU:O	1:A:3176:LEU:HD23	2.14	0.48
1:A:3526:CYS:SG	1:A:3600:VAL:HG21	2.53	0.48
1:A:3556:ASN:OD1	1:A:3557:ASN:OD1	2.31	0.48
1:A:4837:MET:HE2	1:D:4818:VAL:HG11	1.94	0.48
1:C:2929:LYS:O	1:C:2933:MET:SD	2.72	0.48
1:D:953:LYS:HE3	1:D:967:LYS:HZ3	1.79	0.48
1:A:3170:LEU:HD12	1:A:3195:LEU:HD11	1.96	0.48
1:A:3591:GLU:OE2	1:A:3591:GLU:N	2.43	0.48
1:A:4210:MET:HE3	1:A:4211:PRO:HD2	1.94	0.48
1:B:2929:LYS:O	1:B:2933:MET:SD	2.72	0.48
1:D:2890:LYS:O	1:D:2893:GLN:N	2.46	0.48
1:A:108:ILE:HG23	1:A:151:MET:HE2	1.96	0.48
1:A:2748:ILE:HD11	1:A:2752:LEU:HB3	1.94	0.48
1:A:3455:GLU:OE1	1:A:3455:GLU:HA	2.14	0.48
1:B:888:ILE:HD13	1:B:962:MET:CE	2.44	0.48
1:C:871:ILE:HG22	1:C:871:ILE:O	2.13	0.48
1:C:978:LEU:HD13	1:C:982:GLN:HB3	1.96	0.48
1:C:2625:ARG:HD2	1:C:2907:VAL:HG21	1.95	0.48
1:C:2780:GLU:OE1	1:C:2780:GLU:N	2.40	0.48
1:C:3526:CYS:SG	1:C:3600:VAL:HG21	2.53	0.48
1:D:2625:ARG:HD2	1:D:2907:VAL:HG21	1.95	0.48
1:D:2929:LYS:O	1:D:2933:MET:SD	2.72	0.48
1:A:2780:GLU:OE1	1:A:2780:GLU:N	2.40	0.48
1:A:4818:VAL:HG11	1:B:4837:MET:HE2	1.95	0.48
1:B:108:ILE:HG23	1:B:151:MET:HE2	1.95	0.48
1:B:2514:GLU:N	1:B:2514:GLU:OE2	2.47	0.48
1:B:3008:ASN:O	1:B:3012:THR:OG1	2.32	0.48
1:C:953:LYS:HE3	1:C:967:LYS:HZ3	1.79	0.48
1:D:5007:TYR:CZ	1:D:5011:MET:HE3	2.49	0.48
1:A:2226:PHE:N	1:A:2227:PRO:HD3	2.28	0.48
1:A:2945:MET:SD	1:A:2945:MET:C	2.97	0.48
1:B:2625:ARG:HD2	1:B:2907:VAL:HG21	1.95	0.48
1:D:2945:MET:SD	1:D:2945:MET:C	2.97	0.48
1:A:397:GLU:OE1	1:A:471:SER:OG	2.24	0.48
1:A:1116:LEU:HD13	1:A:1124:VAL:HG11	1.96	0.48
1:B:978:LEU:HD13	1:B:982:GLN:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3170:LEU:HD12	1:B:3195:LEU:HD11	1.96	0.48
1:D:3556:ASN:OD1	1:D:3557:ASN:OD1	2.31	0.48
1:A:888:ILE:HD13	1:A:962:MET:CE	2.44	0.47
1:A:2929:LYS:O	1:A:2933:MET:SD	2.72	0.47
1:C:3591:GLU:OE2	1:C:3591:GLU:N	2.43	0.47
1:C:4893:GLY:N	1:C:4897:ASP:OD2	2.45	0.47
1:D:3176:LEU:O	1:D:3176:LEU:HD23	2.14	0.47
1:A:871:ILE:HG22	1:A:871:ILE:O	2.13	0.47
1:A:5007:TYR:CZ	1:A:5011:MET:HE3	2.49	0.47
1:B:1116:LEU:HD13	1:B:1124:VAL:HG11	1.96	0.47
1:C:888:ILE:HD13	1:C:962:MET:CE	2.44	0.47
1:C:1116:LEU:HD13	1:C:1124:VAL:HG11	1.96	0.47
1:D:4706:THR:HG23	1:D:4708:SER:H	1.80	0.47
1:B:189:GLU:OE1	1:B:189:GLU:N	2.48	0.47
1:B:953:LYS:HE3	1:B:967:LYS:HZ3	1.79	0.47
1:B:1923:LEU:HD12	1:B:1925:GLU:H	1.80	0.47
1:B:3176:LEU:HD23	1:B:3176:LEU:O	2.14	0.47
1:B:3455:GLU:HA	1:B:3455:GLU:OE1	2.14	0.47
1:C:189:GLU:OE1	1:C:189:GLU:N	2.47	0.47
1:C:592:ASP:HA	1:C:632:LEU:HD21	1.97	0.47
1:C:2890:LYS:O	1:C:2893:GLN:N	2.46	0.47
1:C:4638:GLU:OE1	1:C:4642:ARG:NH2	2.46	0.47
1:B:4638:GLU:OE1	1:B:4642:ARG:NH2	2.46	0.47
1:C:3789:CYS:SG	1:C:3834:SER:OG	2.73	0.47
1:D:1923:LEU:HD12	1:D:1925:GLU:H	1.80	0.47
1:D:3789:CYS:SG	1:D:3834:SER:OG	2.73	0.47
1:B:1987:MET:SD	1:B:1987:MET:N	2.82	0.47
1:B:4706:THR:HG23	1:B:4708:SER:H	1.80	0.47
1:B:5007:TYR:CZ	1:B:5011:MET:HE3	2.49	0.47
1:C:2627:LEU:HD22	1:C:2641:PRO:HB3	1.96	0.47
1:C:3176:LEU:HD23	1:C:3176:LEU:O	2.14	0.47
1:D:888:ILE:HD13	1:D:962:MET:CE	2.44	0.47
1:D:3331:ASP:N	1:D:3331:ASP:OD1	2.43	0.47
1:A:1923:LEU:HD12	1:A:1925:GLU:H	1.80	0.47
1:A:2514:GLU:OE2	1:A:2514:GLU:N	2.47	0.47
1:A:4706:THR:HG23	1:A:4708:SER:H	1.80	0.47
1:A:4893:GLY:N	1:A:4897:ASP:OD2	2.45	0.47
1:B:2415:ASN:OD1	1:B:2416:ARG:NH2	2.48	0.47
1:B:2627:LEU:HD22	1:B:2641:PRO:HB3	1.96	0.47
1:C:2875:MET:HA	1:C:2875:MET:CE	2.38	0.47
1:C:2926:GLU:OE1	1:C:2926:GLU:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3455:GLU:OE1	1:C:3455:GLU:HA	2.14	0.47
1:D:2780:GLU:OE1	1:D:2780:GLU:N	2.40	0.47
1:D:3455:GLU:HA	1:D:3455:GLU:OE1	2.14	0.47
1:A:2627:LEU:HD22	1:A:2641:PRO:HB3	1.96	0.47
1:A:2890:LYS:O	1:A:2893:GLN:N	2.46	0.47
1:B:2755:PHE:HB2	1:B:2936:TYR:CZ	2.50	0.47
1:B:2926:GLU:OE1	1:B:2926:GLU:HA	2.15	0.47
1:C:2415:ASN:OD1	1:C:2416:ARG:NH2	2.48	0.47
1:B:592:ASP:HA	1:B:632:LEU:HD21	1.97	0.47
1:C:1923:LEU:HD12	1:C:1925:GLU:H	1.80	0.47
1:D:871:ILE:HG22	1:D:871:ILE:O	2.13	0.47
1:D:2627:LEU:HD22	1:D:2641:PRO:HB3	1.96	0.47
1:D:3170:LEU:HD12	1:D:3195:LEU:HD11	1.96	0.47
1:A:953:LYS:HE3	1:A:967:LYS:HZ3	1.79	0.47
1:A:3789:CYS:SG	1:A:3834:SER:OG	2.73	0.47
1:B:1744:ARG:NE	1:B:1964:GLU:OE2	2.48	0.47
1:C:902:LYS:O	1:C:902:LYS:NZ	2.28	0.47
1:C:2514:GLU:OE2	1:C:2514:GLU:N	2.47	0.47
1:C:3170:LEU:HD12	1:C:3195:LEU:HD11	1.96	0.47
1:D:1116:LEU:HD13	1:D:1124:VAL:HG11	1.96	0.47
1:D:2415:ASN:OD1	1:D:2416:ARG:NH2	2.48	0.47
1:D:2875:MET:HA	1:D:2875:MET:CE	2.38	0.47
1:D:3176:LEU:HD21	1:D:3184:VAL:HG22	1.97	0.47
1:B:822:LEU:HD23	1:B:823:HIS:N	2.31	0.46
1:B:867:HIS:HB3	1:B:942:MET:HE2	1.97	0.46
1:C:867:HIS:HB3	1:C:942:MET:HE2	1.97	0.46
1:C:4706:THR:HG23	1:C:4708:SER:H	1.80	0.46
1:D:275:LEU:HD21	1:D:281:LEU:HD22	1.97	0.46
1:D:592:ASP:HA	1:D:632:LEU:HD21	1.97	0.46
1:D:867:HIS:HB3	1:D:942:MET:HE2	1.97	0.46
1:D:2514:GLU:OE2	1:D:2514:GLU:N	2.47	0.46
1:A:592:ASP:HA	1:A:632:LEU:HD21	1.97	0.46
1:A:3176:LEU:HD21	1:A:3184:VAL:HG22	1.97	0.46
1:B:3176:LEU:HD21	1:B:3184:VAL:HG22	1.97	0.46
1:B:3591:GLU:OE2	1:B:3591:GLU:N	2.43	0.46
1:C:275:LEU:HD21	1:C:281:LEU:HD22	1.97	0.46
1:D:3591:GLU:OE2	1:D:3591:GLU:N	2.43	0.46
1:A:822:LEU:HD23	1:A:823:HIS:N	2.31	0.46
1:A:867:HIS:HB3	1:A:942:MET:HE2	1.97	0.46
1:A:1744:ARG:NE	1:A:1964:GLU:OE2	2.48	0.46
1:A:2755:PHE:HB2	1:A:2936:TYR:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:12:ASP:OD1	2:E:13:GLY:N	2.49	0.46
2:G:12:ASP:OD1	2:G:13:GLY:N	2.49	0.46
1:B:658:THR:HG22	1:B:1002:VAL:CG2	2.45	0.46
1:B:3789:CYS:SG	1:B:3834:SER:OG	2.73	0.46
1:C:1744:ARG:NE	1:C:1964:GLU:OE2	2.48	0.46
1:C:2736:PHE:CB	1:C:2906:LEU:HD21	2.46	0.46
1:C:4825:LEU:HD21	1:D:4841:LEU:HD21	1.97	0.46
1:A:2575:HIS:H	1:A:2575:HIS:CD2	2.33	0.46
1:B:3736:LEU:HD13	1:B:3809:ASN:HB3	1.98	0.46
1:C:141:ASP:OD1	1:C:141:ASP:N	2.49	0.46
1:D:2755:PHE:HB2	1:D:2936:TYR:CZ	2.50	0.46
1:A:2415:ASN:OD1	1:A:2416:ARG:NH2	2.48	0.46
1:A:3736:LEU:HD13	1:A:3809:ASN:HB3	1.98	0.46
1:B:3369:ARG:O	1:B:3373:VAL:HG23	2.16	0.46
1:C:822:LEU:HD23	1:C:823:HIS:N	2.31	0.46
1:C:4869:GLU:HA	1:C:4869:GLU:OE2	2.16	0.46
1:D:658:THR:HG22	1:D:1002:VAL:CG2	2.45	0.46
1:D:2736:PHE:CB	1:D:2906:LEU:HD21	2.46	0.46
1:D:2968:MET:HE1	1:D:2999:PHE:HE1	1.81	0.46
1:A:3369:ARG:O	1:A:3373:VAL:HG23	2.16	0.46
1:A:4825:LEU:HD21	1:B:4841:LEU:HD21	1.97	0.46
2:H:12:ASP:OD1	2:H:13:GLY:N	2.49	0.46
1:B:2968:MET:HE1	1:B:2999:PHE:HE1	1.81	0.46
1:B:4869:GLU:OE2	1:B:4869:GLU:HA	2.16	0.46
1:C:2968:MET:HE1	1:C:2999:PHE:HE1	1.81	0.46
1:D:3369:ARG:NH1	1:D:3405:ASP:OD2	2.41	0.46
1:A:2926:GLU:OE1	1:A:2926:GLU:HA	2.15	0.46
2:H:80:ASP:OD1	2:H:80:ASP:N	2.46	0.46
1:C:3589:ASP:OD1	1:C:3591:GLU:N	2.49	0.46
1:D:3369:ARG:O	1:D:3373:VAL:HG23	2.16	0.46
1:A:658:THR:HG22	1:A:1002:VAL:CG2	2.45	0.46
1:A:2736:PHE:CB	1:A:2906:LEU:HD21	2.46	0.46
2:E:80:ASP:OD1	2:E:80:ASP:N	2.46	0.46
1:B:1966:TYR:CZ	1:B:2032:LEU:HB2	2.51	0.46
1:B:3672:ASP:OD2	1:B:3735:HIS:NE2	2.48	0.46
1:C:2751:LYS:HE2	1:C:2936:TYR:CE2	2.51	0.46
1:D:189:GLU:N	1:D:189:GLU:OE1	2.48	0.46
1:A:189:GLU:N	1:A:189:GLU:OE1	2.47	0.46
1:A:1966:TYR:CZ	1:A:2032:LEU:HB2	2.51	0.46
1:A:2570:PHE:CE1	1:A:2583:MET:HE1	2.51	0.46
1:B:914:LEU:HD12	1:B:915:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2780:GLU:OE1	1:B:2780:GLU:N	2.40	0.46
1:B:3974:GLY:N	1:B:3975:PRO:HA	2.31	0.46
1:C:658:THR:HG22	1:C:1002:VAL:CG2	2.45	0.46
1:C:2755:PHE:HB2	1:C:2936:TYR:CZ	2.50	0.46
1:D:2751:LYS:HE2	1:D:2936:TYR:CE2	2.51	0.46
1:D:3672:ASP:OD2	1:D:3735:HIS:NE2	2.48	0.46
1:A:914:LEU:HD12	1:A:915:PRO:HD2	1.98	0.46
2:F:12:ASP:OD1	2:F:13:GLY:N	2.49	0.46
1:B:2971:SER:HA	1:B:2974:PHE:CE2	2.51	0.46
1:C:2575:HIS:H	1:C:2575:HIS:CD2	2.33	0.46
1:C:2971:SER:HA	1:C:2974:PHE:CE2	2.51	0.46
1:C:3974:GLY:N	1:C:3975:PRO:HA	2.31	0.46
1:D:1744:ARG:NE	1:D:1964:GLU:OE2	2.48	0.46
1:D:3540:ARG:HG3	1:D:3553:PHE:HD2	1.81	0.46
1:D:4869:GLU:OE2	1:D:4869:GLU:HA	2.16	0.46
1:A:275:LEU:HD21	1:A:281:LEU:HD22	1.97	0.45
1:A:2868:LEU:HD11	1:A:2929:LYS:HD3	1.98	0.45
1:A:3589:ASP:OD1	1:A:3591:GLU:N	2.49	0.45
1:B:141:ASP:OD1	1:B:141:ASP:N	2.49	0.45
1:B:2575:HIS:CD2	1:B:2575:HIS:H	2.33	0.45
1:B:2751:LYS:HE2	1:B:2936:TYR:CE2	2.51	0.45
1:B:4893:GLY:N	1:B:4897:ASP:OD2	2.45	0.45
1:C:914:LEU:HD12	1:C:915:PRO:HD2	1.98	0.45
1:C:3176:LEU:HD21	1:C:3184:VAL:HG22	1.97	0.45
1:A:2751:LYS:HE2	1:A:2936:TYR:CE2	2.51	0.45
1:A:3774:HIS:C	1:A:3774:HIS:ND1	2.75	0.45
1:A:4869:GLU:HA	1:A:4869:GLU:OE2	2.16	0.45
1:B:2736:PHE:CB	1:B:2906:LEU:HD21	2.46	0.45
1:C:2394:ASP:OD2	1:C:2419:LEU:N	2.50	0.45
1:D:914:LEU:HD12	1:D:915:PRO:HD2	1.98	0.45
1:D:3173:ILE:HB	1:D:3195:LEU:HD13	1.99	0.45
1:A:2971:SER:HA	1:A:2974:PHE:CE2	2.51	0.45
1:B:275:LEU:HD21	1:B:281:LEU:HD22	1.97	0.45
1:C:2814:LEU:HD23	1:C:2817:MET:HE3	1.98	0.45
1:C:3774:HIS:ND1	1:C:3774:HIS:C	2.75	0.45
1:D:141:ASP:OD1	1:D:141:ASP:N	2.49	0.45
1:D:870:ARG:NH1	1:D:942:MET:HE1	2.32	0.45
1:D:2971:SER:HA	1:D:2974:PHE:CE2	2.51	0.45
1:A:3974:GLY:N	1:A:3975:PRO:HA	2.31	0.45
7:A:8006:PCW:H412	7:D:8007:PCW:H412	1.97	0.45
1:B:1479:ASP:CG	1:B:1485:HIS:HE2	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2394:ASP:OD2	1:B:2419:LEU:N	2.50	0.45
1:B:2570:PHE:CE1	1:B:2583:MET:HE1	2.51	0.45
1:B:2814:LEU:HD23	1:B:2817:MET:HE3	1.98	0.45
1:C:870:ARG:NH1	1:C:942:MET:HE1	2.32	0.45
1:C:2570:PHE:CE1	1:C:2583:MET:HE1	2.51	0.45
1:C:3736:LEU:HD13	1:C:3809:ASN:HB3	1.98	0.45
1:D:2394:ASP:OD2	1:D:2419:LEU:N	2.50	0.45
1:D:2570:PHE:CE1	1:D:2583:MET:HE1	2.51	0.45
1:D:2575:HIS:CD2	1:D:2575:HIS:H	2.33	0.45
1:D:2868:LEU:HD11	1:D:2929:LYS:HD3	1.98	0.45
1:C:324:LEU:HD12	1:C:324:LEU:O	2.17	0.45
1:C:3369:ARG:O	1:C:3373:VAL:HG23	2.16	0.45
1:D:2814:LEU:HD23	1:D:2817:MET:HE3	1.98	0.45
1:D:3774:HIS:ND1	1:D:3774:HIS:C	2.75	0.45
1:A:1959:LEU:HD23	1:A:2139:LEU:HD21	1.99	0.45
1:A:2394:ASP:OD2	1:A:2419:LEU:N	2.50	0.45
1:A:2814:LEU:HD23	1:A:2817:MET:HE3	1.98	0.45
1:A:2968:MET:HE1	1:A:2999:PHE:HE1	1.81	0.45
1:B:2212:MET:O	1:B:2215:VAL:HG22	2.17	0.45
1:C:1966:TYR:CZ	1:C:2032:LEU:HB2	2.51	0.45
1:C:2869:SER:H	1:C:2872:LEU:HD12	1.81	0.45
1:C:3008:ASN:O	1:C:3012:THR:OG1	2.32	0.45
1:A:614:ALA:HB2	1:A:1677:LEU:HD12	1.99	0.45
1:A:870:ARG:NH1	1:A:942:MET:HE1	2.32	0.45
1:D:3736:LEU:HD13	1:D:3809:ASN:HB3	1.98	0.45
1:A:1758:GLY:N	1:A:1759:PRO:HD2	2.32	0.45
1:A:3173:ILE:HB	1:A:3195:LEU:HD13	1.99	0.45
1:A:3410:TYR:N	1:A:3411:PRO:HD2	2.32	0.45
1:B:324:LEU:HD12	1:B:324:LEU:O	2.17	0.45
1:B:1758:GLY:N	1:B:1759:PRO:HD2	2.32	0.45
1:C:924:GLN:NE2	1:C:925:MET:SD	2.90	0.45
1:D:864:LEU:H	1:D:864:LEU:HD22	1.82	0.45
1:D:3589:ASP:OD1	1:D:3591:GLU:N	2.49	0.45
1:B:2868:LEU:HD11	1:B:2929:LYS:HD3	1.98	0.45
1:B:3257:LEU:HD13	1:B:3267:MET:HE2	1.99	0.45
1:B:4825:LEU:HD21	1:C:4841:LEU:HD21	1.98	0.45
1:C:1479:ASP:CG	1:C:1485:HIS:HE2	2.25	0.45
1:D:1959:LEU:HD23	1:D:2139:LEU:HD21	1.99	0.45
1:D:2234:CYS:CA	1:D:2238:CYS:HB2	2.47	0.45
1:D:3974:GLY:N	1:D:3975:PRO:HA	2.31	0.45
1:A:2945:MET:SD	1:A:2946:GLU:N	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3257:LEU:HD13	1:A:3267:MET:HE2	1.99	0.45
1:A:3540:ARG:HG3	1:A:3553:PHE:HD2	1.81	0.45
1:B:3173:ILE:HB	1:B:3195:LEU:HD13	1.99	0.45
1:B:3774:HIS:ND1	1:B:3774:HIS:C	2.75	0.45
1:B:4987:MET:HE1	1:B:4991:MET:SD	2.57	0.45
1:C:864:LEU:HD22	1:C:864:LEU:H	1.82	0.45
1:C:2209:MET:O	1:C:2213:VAL:HG13	2.17	0.45
1:C:2868:LEU:HD11	1:C:2929:LYS:HD3	1.98	0.45
1:C:3173:ILE:HB	1:C:3195:LEU:HD13	1.99	0.45
1:D:3410:TYR:N	1:D:3411:PRO:HD2	2.32	0.45
1:A:2212:MET:O	1:A:2215:VAL:HG22	2.17	0.44
1:B:2945:MET:SD	1:B:2946:GLU:N	2.90	0.44
1:B:3540:ARG:HG3	1:B:3553:PHE:HD2	1.81	0.44
1:B:3589:ASP:OD1	1:B:3591:GLU:N	2.49	0.44
1:B:4707:PRO:HD2	1:B:4770:ASP:OD2	2.18	0.44
1:D:324:LEU:HD12	1:D:324:LEU:O	2.17	0.44
1:D:822:LEU:HD23	1:D:823:HIS:N	2.31	0.44
1:D:1758:GLY:N	1:D:1759:PRO:HD2	2.32	0.44
1:D:2212:MET:O	1:D:2215:VAL:HG22	2.17	0.44
1:D:3257:LEU:HD13	1:D:3267:MET:HE2	1.99	0.44
1:A:945:GLU:O	1:A:949:ASP:OD1	2.35	0.44
1:B:864:LEU:H	1:B:864:LEU:HD22	1.82	0.44
1:C:893:THR:HG22	1:C:903:ARG:O	2.17	0.44
1:D:885:LEU:HD23	1:D:885:LEU:C	2.43	0.44
1:D:2820:TRP:CH2	1:D:2882:ASN:HB2	2.52	0.44
1:D:2926:GLU:OE1	1:D:2926:GLU:HA	2.15	0.44
1:A:2234:CYS:CA	1:A:2238:CYS:HB2	2.47	0.44
1:A:2869:SER:H	1:A:2872:LEU:HD12	1.81	0.44
1:B:952:LYS:O	1:B:972:ASP:N	2.46	0.44
1:C:3257:LEU:HD13	1:C:3267:MET:HE2	1.99	0.44
1:D:1966:TYR:CZ	1:D:2032:LEU:HB2	2.51	0.44
1:D:2817:MET:HA	1:D:2820:TRP:HE3	1.82	0.44
1:D:2903:HIS:CE1	1:D:2905:LEU:HB2	2.53	0.44
1:A:885:LEU:C	1:A:885:LEU:HD23	2.43	0.44
1:A:893:THR:HG22	1:A:903:ARG:O	2.17	0.44
1:A:2817:MET:HA	1:A:2820:TRP:HE3	1.82	0.44
1:A:2820:TRP:CH2	1:A:2882:ASN:HB2	2.52	0.44
1:B:2209:MET:O	1:B:2213:VAL:HG13	2.17	0.44
1:C:3540:ARG:HG3	1:C:3553:PHE:HD2	1.81	0.44
1:D:924:GLN:NE2	1:D:925:MET:SD	2.90	0.44
1:D:4707:PRO:HD2	1:D:4770:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4987:MET:HE1	1:D:4991:MET:SD	2.57	0.44
1:A:128:MET:HE3	1:A:128:MET:HA	2.00	0.44
1:A:864:LEU:HD22	1:A:864:LEU:H	1.82	0.44
1:A:4707:PRO:HD2	1:A:4770:ASP:OD2	2.17	0.44
1:D:893:THR:HG22	1:D:903:ARG:O	2.17	0.44
1:D:973:LEU:HD23	1:D:973:LEU:N	2.33	0.44
1:A:324:LEU:HD12	1:A:324:LEU:O	2.17	0.44
1:A:691:GLU:OE2	1:A:691:GLU:HA	2.18	0.44
1:A:924:GLN:NE2	1:A:925:MET:SD	2.90	0.44
1:A:3949:GLN:OE1	1:A:3952:ARG:NH1	2.51	0.44
1:B:870:ARG:NH1	1:B:942:MET:HE1	2.32	0.44
1:B:893:THR:HG22	1:B:903:ARG:O	2.17	0.44
1:B:2817:MET:HA	1:B:2820:TRP:HE3	1.82	0.44
1:C:945:GLU:O	1:C:949:ASP:OD1	2.35	0.44
1:C:1758:GLY:N	1:C:1759:PRO:HD2	2.32	0.44
1:C:2212:MET:O	1:C:2215:VAL:HG22	2.17	0.44
1:C:2817:MET:HA	1:C:2820:TRP:HE3	1.82	0.44
1:C:2903:HIS:CE1	1:C:2905:LEU:HB2	2.53	0.44
1:C:3410:TYR:N	1:C:3411:PRO:HD2	2.32	0.44
1:C:4987:MET:HE1	1:C:4991:MET:SD	2.57	0.44
1:D:614:ALA:HB2	1:D:1677:LEU:HD12	1.99	0.44
1:D:952:LYS:O	1:D:972:ASP:N	2.46	0.44
1:D:2869:SER:H	1:D:2872:LEU:HD12	1.82	0.44
1:A:893:THR:HA	1:A:962:MET:HE1	2.00	0.44
1:A:962:MET:HA	1:A:962:MET:CE	2.44	0.44
1:A:4019:LEU:O	1:A:4023:GLN:HG3	2.18	0.44
1:B:924:GLN:NE2	1:B:925:MET:SD	2.90	0.44
1:B:2234:CYS:CA	1:B:2238:CYS:HB2	2.47	0.44
1:B:2903:HIS:CE1	1:B:2905:LEU:HB2	2.53	0.44
1:B:4965:TYR:OH	1:B:5031:GLU:OE1	2.10	0.44
1:C:885:LEU:C	1:C:885:LEU:HD23	2.43	0.44
1:C:973:LEU:N	1:C:973:LEU:HD23	2.33	0.44
1:C:3360:ILE:HB	1:C:3361:PRO:HD3	2.00	0.44
1:C:3949:GLN:OE1	1:C:3952:ARG:NH1	2.51	0.44
1:D:962:MET:HA	1:D:962:MET:CE	2.44	0.44
1:D:2209:MET:O	1:D:2213:VAL:HG13	2.17	0.44
1:D:3541:TYR:OH	1:D:3598:GLN:NE2	2.51	0.44
1:A:2903:HIS:CE1	1:A:2905:LEU:HB2	2.53	0.44
1:B:691:GLU:OE2	1:B:691:GLU:HA	2.18	0.44
1:B:1959:LEU:HD23	1:B:2139:LEU:HD21	1.99	0.44
1:B:2820:TRP:CH2	1:B:2882:ASN:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3360:ILE:HB	1:B:3361:PRO:HD3	2.00	0.44
1:C:2234:CYS:CA	1:C:2238:CYS:HB2	2.47	0.44
1:C:2791:MET:HA	1:C:2793:ARG:NH1	2.33	0.44
1:C:2945:MET:SD	1:C:2946:GLU:N	2.90	0.44
1:D:128:MET:HE3	1:D:128:MET:HA	2.00	0.44
1:A:903:ARG:HA	1:A:903:ARG:NE	2.33	0.44
2:F:19:ARG:NH1	2:F:19:ARG:HB3	2.33	0.44
1:B:614:ALA:HB2	1:B:1677:LEU:HD12	1.99	0.44
1:B:945:GLU:O	1:B:949:ASP:OD1	2.35	0.44
1:B:973:LEU:N	1:B:973:LEU:HD23	2.33	0.44
1:C:1851:LEU:HD22	1:C:1946:TYR:CE2	2.53	0.44
1:C:2820:TRP:CH2	1:C:2882:ASN:HB2	2.52	0.44
1:D:1479:ASP:CG	1:D:1485:HIS:HE2	2.25	0.44
1:D:2791:MET:HA	1:D:2793:ARG:NH1	2.33	0.44
1:D:4019:LEU:O	1:D:4023:GLN:HG3	2.18	0.44
2:E:19:ARG:HB3	2:E:19:ARG:NH1	2.33	0.43
1:B:500:THR:HG23	1:B:503:HIS:H	1.83	0.43
1:B:893:THR:HA	1:B:962:MET:HE1	2.00	0.43
1:B:2869:SER:H	1:B:2872:LEU:HD12	1.82	0.43
1:B:3949:GLN:OE1	1:B:3952:ARG:NH1	2.51	0.43
1:C:1959:LEU:HD23	1:C:2139:LEU:HD21	1.99	0.43
1:C:4707:PRO:HD2	1:C:4770:ASP:OD2	2.17	0.43
1:D:691:GLU:OE2	1:D:691:GLU:HA	2.18	0.43
1:D:945:GLU:O	1:D:949:ASP:OD1	2.35	0.43
1:D:1273:LEU:HD22	1:D:1290:LEU:HD11	2.00	0.43
1:D:1851:LEU:HD22	1:D:1946:TYR:CE2	2.53	0.43
1:D:3004:LEU:HB2	1:D:3005:PRO:HD3	2.00	0.43
1:D:3008:ASN:O	1:D:3012:THR:OG1	2.32	0.43
1:A:3008:ASN:O	1:A:3012:THR:OG1	2.32	0.43
1:A:3865:ASP:HA	1:A:3868:VAL:HG22	2.00	0.43
1:A:4029:MET:HE2	1:A:4029:MET:HB3	1.97	0.43
1:B:2871:GLU:OE2	1:B:2872:LEU:HD23	2.18	0.43
1:B:4030:LEU:O	1:B:4047:MET:HE1	2.18	0.43
1:C:2871:GLU:OE2	1:C:2872:LEU:HD23	2.18	0.43
1:C:3227:GLU:O	1:C:3228:ARG:HB2	2.19	0.43
1:C:3541:TYR:OH	1:C:3598:GLN:NE2	2.51	0.43
1:D:70:LEU:HD21	1:D:203:MET:HE1	2.00	0.43
1:D:903:ARG:HA	1:D:903:ARG:NE	2.33	0.43
1:D:2117:LEU:O	1:D:2121:MET:HG2	2.18	0.43
1:D:2413:GLU:O	1:D:2413:GLU:CD	2.62	0.43
1:A:2791:MET:HA	1:A:2793:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:19:ARG:HB3	2:G:19:ARG:NH1	2.33	0.43
1:B:885:LEU:HD23	1:B:885:LEU:C	2.42	0.43
1:B:3410:TYR:N	1:B:3411:PRO:HD2	2.32	0.43
1:B:3865:ASP:HA	1:B:3868:VAL:HG22	2.00	0.43
1:C:128:MET:HA	1:C:128:MET:HE3	2.00	0.43
1:C:614:ALA:HB2	1:C:1677:LEU:HD12	1.99	0.43
1:C:2117:LEU:O	1:C:2121:MET:HG2	2.19	0.43
1:C:2521:HIS:O	1:C:2525:VAL:HG22	2.18	0.43
1:C:3004:LEU:HB2	1:C:3005:PRO:HD3	2.00	0.43
1:D:2945:MET:SD	1:D:2946:GLU:N	2.90	0.43
1:D:3949:GLN:OE1	1:D:3952:ARG:NH1	2.51	0.43
1:A:324:LEU:HD12	1:A:324:LEU:C	2.43	0.43
1:A:888:ILE:HD13	1:A:962:MET:HE1	2.00	0.43
1:A:3360:ILE:HB	1:A:3361:PRO:HD3	2.00	0.43
1:A:3532:ASP:O	1:A:3536:LEU:HG	2.18	0.43
1:A:4987:MET:HE1	1:A:4991:MET:SD	2.57	0.43
7:A:8007:PCW:H412	7:B:8006:PCW:H412	2.00	0.43
1:B:921:TYR:O	1:B:924:GLN:HG3	2.19	0.43
1:B:1851:LEU:HD22	1:B:1946:TYR:CE2	2.53	0.43
1:B:2722:SER:OG	1:B:2944:ASP:OD2	2.32	0.43
1:C:324:LEU:HD12	1:C:324:LEU:C	2.43	0.43
1:C:4030:LEU:O	1:C:4047:MET:HE1	2.19	0.43
1:D:888:ILE:HD13	1:D:962:MET:HE1	2.00	0.43
1:D:2521:HIS:O	1:D:2525:VAL:HG22	2.18	0.43
1:D:3227:GLU:O	1:D:3228:ARG:HB2	2.19	0.43
1:D:4763:LEU:HD13	1:D:4763:LEU:C	2.43	0.43
1:B:2909:TYR:HA	1:B:2912:LEU:HD12	2.01	0.43
1:C:2722:SER:OG	1:C:2944:ASP:OD2	2.32	0.43
1:D:921:TYR:O	1:D:924:GLN:HG3	2.19	0.43
1:D:2520:LEU:HD13	1:D:2576:ARG:HG3	2.01	0.43
1:D:4030:LEU:O	1:D:4047:MET:HE1	2.18	0.43
1:A:500:THR:HG23	1:A:503:HIS:H	1.83	0.43
1:B:1994:ARG:HB3	1:B:1994:ARG:CZ	2.49	0.43
1:B:2756:ILE:CG1	1:B:2814:LEU:HD12	2.49	0.43
1:B:2791:MET:HA	1:B:2793:ARG:NH1	2.33	0.43
1:B:2795:TYR:HA	1:B:2798:PHE:HB2	2.00	0.43
1:C:1273:LEU:HD22	1:C:1290:LEU:HD11	2.00	0.43
1:D:2745:ASN:OD1	1:D:2745:ASN:C	2.62	0.43
1:A:70:LEU:HD21	1:A:203:MET:HE1	2.01	0.43
1:A:490:ASN:O	1:A:494:ARG:HG2	2.19	0.43
1:A:3227:GLU:O	1:A:3228:ARG:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4679:LEU:HD11	1:A:4704:LEU:HD22	2.01	0.43
1:A:5032:ASP:OD2	1:A:5033:GLN:NE2	2.52	0.43
1:B:324:LEU:HD12	1:B:324:LEU:C	2.43	0.43
1:C:2949:THR:O	1:C:2950:SER:C	2.62	0.43
1:D:3360:ILE:HB	1:D:3361:PRO:HD3	2.00	0.43
1:D:3865:ASP:HA	1:D:3868:VAL:HG22	2.00	0.43
1:A:24:GLN:OE1	1:A:204:ASN:ND2	2.52	0.43
1:A:2183:ILE:HG23	1:A:2236:PHE:HB2	2.01	0.43
1:A:2909:TYR:HA	1:A:2912:LEU:HD12	2.01	0.43
1:A:3004:LEU:HB2	1:A:3005:PRO:HD3	2.01	0.43
1:A:3385:LYS:O	1:A:3388:ALA:N	2.52	0.43
1:B:2413:GLU:CD	1:B:2413:GLU:O	2.62	0.43
1:C:1102:ARG:NH1	1:C:1116:LEU:O	2.48	0.43
1:C:1994:ARG:HB3	1:C:1994:ARG:CZ	2.49	0.43
1:C:2520:LEU:HD13	1:C:2576:ARG:HG3	2.01	0.43
1:D:324:LEU:HD12	1:D:324:LEU:C	2.43	0.43
1:D:1994:ARG:HB3	1:D:1994:ARG:CZ	2.49	0.43
1:D:2949:THR:O	1:D:2950:SER:C	2.62	0.43
1:D:3385:LYS:O	1:D:3388:ALA:N	2.52	0.43
1:D:3532:ASP:O	1:D:3536:LEU:HG	2.18	0.43
1:A:2209:MET:O	1:A:2213:VAL:HG13	2.17	0.43
1:A:2875:MET:CE	1:A:2940:ARG:HD2	2.49	0.43
1:B:2521:HIS:O	1:B:2525:VAL:HG22	2.18	0.43
1:B:3532:ASP:O	1:B:3536:LEU:HG	2.18	0.43
1:C:691:GLU:OE2	1:C:691:GLU:HA	2.18	0.43
1:C:5032:ASP:OD2	1:C:5033:GLN:NE2	2.52	0.43
1:D:2183:ILE:HG23	1:D:2236:PHE:HB2	2.01	0.43
1:D:2871:GLU:OE2	1:D:2872:LEU:HD23	2.18	0.43
1:D:5032:ASP:OD2	1:D:5033:GLN:NE2	2.52	0.43
1:A:2871:GLU:OE2	1:A:2872:LEU:HD23	2.18	0.43
1:A:4763:LEU:HD13	1:A:4763:LEU:C	2.43	0.43
2:H:19:ARG:HB3	2:H:19:ARG:NH1	2.33	0.43
1:B:128:MET:HE3	1:B:128:MET:HA	2.00	0.43
1:B:576:LEU:HD22	1:B:610:CYS:HB2	2.01	0.43
1:B:903:ARG:HA	1:B:903:ARG:NE	2.33	0.43
1:B:962:MET:HA	1:B:962:MET:CE	2.44	0.43
1:C:70:LEU:HD21	1:C:203:MET:HE1	2.01	0.43
1:C:903:ARG:HA	1:C:903:ARG:NE	2.33	0.43
1:C:2413:GLU:CD	1:C:2413:GLU:O	2.62	0.43
1:C:2756:ILE:CG1	1:C:2814:LEU:HD12	2.49	0.43
1:D:2886:THR:O	1:D:2890:LYS:HE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:LEU:HD22	1:A:610:CYS:HB2	2.01	0.42
1:A:1851:LEU:HD22	1:A:1946:TYR:CE2	2.53	0.42
1:A:2234:CYS:HA	1:A:2238:CYS:HB2	2.01	0.42
1:A:2876:ALA:C	1:A:2921:ARG:HH12	2.27	0.42
1:A:3672:ASP:OD2	1:A:3735:HIS:NE2	2.48	0.42
1:B:2886:THR:O	1:B:2890:LYS:HE2	2.19	0.42
1:B:3385:LYS:O	1:B:3388:ALA:N	2.52	0.42
1:B:3944:ASP:OD1	1:B:3944:ASP:N	2.52	0.42
1:B:5032:ASP:OD2	1:B:5033:GLN:NE2	2.52	0.42
1:C:576:LEU:HD22	1:C:610:CYS:HB2	2.01	0.42
1:C:893:THR:HA	1:C:962:MET:HE1	2.00	0.42
1:C:3532:ASP:O	1:C:3536:LEU:HG	2.18	0.42
1:C:3865:ASP:HA	1:C:3868:VAL:HG22	2.00	0.42
1:C:4763:LEU:HD13	1:C:4763:LEU:C	2.43	0.42
1:D:490:ASN:O	1:D:494:ARG:HG2	2.19	0.42
1:D:893:THR:HA	1:D:962:MET:HE1	2.00	0.42
1:D:2234:CYS:C	1:D:2236:PHE:N	2.77	0.42
1:A:1273:LEU:HD22	1:A:1290:LEU:HD11	2.00	0.42
1:B:490:ASN:O	1:B:494:ARG:HG2	2.19	0.42
1:B:888:ILE:HD13	1:B:962:MET:HE1	2.00	0.42
1:B:898:ARG:HE	1:B:906:PRO:HD2	1.84	0.42
1:B:1273:LEU:HD22	1:B:1290:LEU:HD11	2.00	0.42
1:B:2746:VAL:HG11	1:B:2815:LYS:O	2.20	0.42
1:B:2820:TRP:HH2	1:B:2882:ASN:HB2	1.85	0.42
1:B:3004:LEU:HB2	1:B:3005:PRO:HD3	2.00	0.42
1:B:4019:LEU:O	1:B:4023:GLN:HG3	2.18	0.42
1:C:921:TYR:O	1:C:924:GLN:HG3	2.19	0.42
1:C:2745:ASN:OD1	1:C:2745:ASN:C	2.62	0.42
1:D:3293:PRO:O	1:D:3295:PRO:CD	2.67	0.42
1:A:1830:ASP:N	1:A:1830:ASP:OD1	2.53	0.42
1:A:1994:ARG:HB3	1:A:1994:ARG:CZ	2.49	0.42
1:A:2795:TYR:HA	1:A:2798:PHE:HB2	2.00	0.42
1:A:4030:LEU:O	1:A:4047:MET:HE1	2.19	0.42
1:B:2117:LEU:O	1:B:2121:MET:HG2	2.19	0.42
1:B:2745:ASN:OD1	1:B:2745:ASN:C	2.62	0.42
1:B:2875:MET:CE	1:B:2940:ARG:HD2	2.49	0.42
1:B:3293:PRO:O	1:B:3295:PRO:CD	2.67	0.42
1:B:4004:MET:HG3	1:B:4060:MET:HE3	2.01	0.42
1:C:490:ASN:O	1:C:494:ARG:HG2	2.19	0.42
1:D:576:LEU:HD22	1:D:610:CYS:HB2	2.01	0.42
1:A:2413:GLU:O	1:A:2413:GLU:CD	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2520:LEU:HD13	1:A:2576:ARG:HG3	2.01	0.42
1:A:2521:HIS:O	1:A:2525:VAL:HG22	2.18	0.42
1:A:2820:TRP:HH2	1:A:2882:ASN:HB2	1.85	0.42
1:A:3293:PRO:O	1:A:3295:PRO:CD	2.67	0.42
1:B:24:GLN:OE1	1:B:204:ASN:ND2	2.52	0.42
1:B:723:TRP:CZ2	1:B:728:ALA:HB2	2.55	0.42
1:B:2234:CYS:HA	1:B:2238:CYS:HB2	2.01	0.42
1:B:2876:ALA:C	1:B:2921:ARG:HH12	2.27	0.42
1:C:888:ILE:HD13	1:C:962:MET:HE1	2.00	0.42
1:C:1830:ASP:OD1	1:C:1830:ASP:N	2.53	0.42
1:C:2183:ILE:HG23	1:C:2236:PHE:HB2	2.01	0.42
1:C:2383:GLU:OE1	1:C:2386:ARG:NH1	2.53	0.42
1:C:2746:VAL:HG11	1:C:2815:LYS:O	2.20	0.42
1:C:2795:TYR:HA	1:C:2798:PHE:HB2	2.00	0.42
1:A:973:LEU:N	1:A:973:LEU:HD23	2.33	0.42
1:A:2117:LEU:O	1:A:2121:MET:HG2	2.19	0.42
1:A:2383:GLU:OE1	1:A:2386:ARG:NH1	2.53	0.42
1:A:2609:MET:HE3	1:A:2609:MET:HB3	1.95	0.42
1:A:3944:ASP:OD1	1:A:3944:ASP:N	2.52	0.42
1:B:2183:ILE:HG23	1:B:2236:PHE:HB2	2.01	0.42
1:B:3227:GLU:O	1:B:3228:ARG:HB2	2.19	0.42
1:B:3376:GLU:OE2	1:B:3376:GLU:HA	2.20	0.42
1:C:24:GLN:OE1	1:C:204:ASN:ND2	2.52	0.42
1:C:898:ARG:HE	1:C:906:PRO:HD2	1.84	0.42
1:C:2771:LYS:HD3	1:C:2789:HIS:CG	2.55	0.42
1:D:723:TRP:CZ2	1:D:728:ALA:HB2	2.55	0.42
1:D:1691:ASP:OD2	1:D:1694:GLN:NE2	2.45	0.42
1:D:2722:SER:OG	1:D:2944:ASP:OD2	2.32	0.42
1:D:2771:LYS:HD3	1:D:2789:HIS:CG	2.55	0.42
1:D:2795:TYR:HA	1:D:2798:PHE:HB2	2.00	0.42
1:D:2922:GLU:O	1:D:2926:GLU:HG2	2.20	0.42
1:A:1425:PRO:HA	1:A:1428:ILE:HG22	2.01	0.42
1:A:1479:ASP:CG	1:A:1485:HIS:HE2	2.25	0.42
1:A:2872:LEU:O	1:A:2875:MET:HB2	2.20	0.42
1:A:2922:GLU:O	1:A:2926:GLU:HG2	2.20	0.42
1:B:4679:LEU:HD11	1:B:4704:LEU:HD22	2.01	0.42
1:C:500:THR:HG23	1:C:503:HIS:H	1.83	0.42
1:C:2820:TRP:HH2	1:C:2882:ASN:HB2	1.85	0.42
1:C:2876:ALA:C	1:C:2921:ARG:HH12	2.27	0.42
1:C:3385:LYS:O	1:C:3388:ALA:N	2.52	0.42
1:C:4019:LEU:O	1:C:4023:GLN:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2872:LEU:O	1:D:2875:MET:HB2	2.20	0.42
1:D:2876:ALA:C	1:D:2921:ARG:HH12	2.27	0.42
1:A:234:ILE:HD12	1:A:243:ARG:HB3	2.01	0.42
1:A:2756:ILE:CG1	1:A:2814:LEU:HD12	2.49	0.42
1:A:2886:THR:O	1:A:2890:LYS:HE2	2.19	0.42
1:B:1425:PRO:HA	1:B:1428:ILE:HG22	2.01	0.42
1:B:2520:LEU:HD13	1:B:2576:ARG:HG3	2.01	0.42
1:B:2872:LEU:O	1:B:2875:MET:HB2	2.20	0.42
1:B:4763:LEU:C	1:B:4763:LEU:HD13	2.43	0.42
1:C:2793:ARG:NH2	1:C:2798:PHE:HA	2.35	0.42
1:C:3376:GLU:HA	1:C:3376:GLU:OE2	2.20	0.42
1:D:2820:TRP:HH2	1:D:2882:ASN:HB2	1.84	0.42
1:A:2745:ASN:OD1	1:A:2745:ASN:C	2.62	0.42
1:A:2756:ILE:HD13	1:A:2811:LYS:HG2	2.02	0.42
1:A:2771:LYS:HD3	1:A:2789:HIS:CG	2.55	0.42
1:A:2949:THR:O	1:A:2950:SER:C	2.62	0.42
1:C:296:GLU:H	1:C:296:GLU:CD	2.27	0.42
1:C:2886:THR:O	1:C:2890:LYS:HE2	2.19	0.42
1:C:2909:TYR:HA	1:C:2912:LEU:HD12	2.01	0.42
1:C:4004:MET:HG3	1:C:4060:MET:HE3	2.01	0.42
1:D:898:ARG:HE	1:D:906:PRO:HD2	1.84	0.42
1:D:2746:VAL:HG11	1:D:2815:LYS:O	2.20	0.42
1:D:4632:GLU:HA	1:D:4632:GLU:OE1	2.20	0.42
1:A:921:TYR:O	1:A:924:GLN:HG3	2.19	0.42
1:A:1788:LEU:HD12	1:A:1788:LEU:HA	1.96	0.42
1:A:4841:LEU:HD21	1:D:4825:LEU:HD21	2.01	0.42
1:B:70:LEU:HD21	1:B:203:MET:HE1	2.00	0.42
1:B:2313:MET:HE2	1:B:2313:MET:HB3	1.98	0.42
1:B:2743:THR:HG22	1:B:2816:ALA:CA	2.50	0.42
1:B:3661:SER:O	1:B:3665:THR:OG1	2.34	0.42
7:B:8007:PCW:H412	7:C:8006:PCW:H412	2.01	0.42
1:C:1425:PRO:HA	1:C:1428:ILE:HG22	2.01	0.42
1:C:3293:PRO:O	1:C:3295:PRO:CD	2.67	0.42
1:D:296:GLU:H	1:D:296:GLU:CD	2.27	0.42
1:D:500:THR:HG23	1:D:503:HIS:H	1.83	0.42
1:D:2743:THR:HG22	1:D:2816:ALA:CA	2.50	0.42
1:D:2909:TYR:HA	1:D:2912:LEU:HD12	2.01	0.42
1:D:4004:MET:HG3	1:D:4060:MET:HE3	2.01	0.42
1:A:627:LEU:N	1:A:628:PRO:HD2	2.35	0.42
1:A:898:ARG:HE	1:A:906:PRO:HD2	1.84	0.42
1:A:967:LYS:HZ2	1:A:969:ALA:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2975:ILE:HD13	1:A:2975:ILE:HA	1.93	0.42
1:A:3376:GLU:OE2	1:A:3376:GLU:HA	2.20	0.42
1:B:627:LEU:N	1:B:628:PRO:HD2	2.35	0.42
1:B:2383:GLU:OE1	1:B:2386:ARG:NH1	2.53	0.42
1:B:2771:LYS:HD3	1:B:2789:HIS:CG	2.55	0.42
1:B:2793:ARG:NH2	1:B:2798:PHE:HA	2.35	0.42
1:B:4964:ASP:OD1	1:B:4965:TYR:N	2.53	0.42
1:C:1428:ILE:HG23	1:C:1429:LEU:HD22	2.02	0.42
1:C:3672:ASP:OD2	1:C:3735:HIS:NE2	2.48	0.42
1:D:2793:ARG:NH2	1:D:2798:PHE:HA	2.35	0.42
1:D:4964:ASP:OD1	1:D:4965:TYR:N	2.53	0.42
1:A:723:TRP:CZ2	1:A:728:ALA:HB2	2.55	0.41
1:A:2743:THR:HG22	1:A:2816:ALA:CA	2.50	0.41
1:B:2756:ILE:HD13	1:B:2811:LYS:HG2	2.02	0.41
1:D:2234:CYS:HA	1:D:2238:CYS:HB2	2.01	0.41
1:D:2756:ILE:CG1	1:D:2814:LEU:HD12	2.49	0.41
1:D:2808:TRP:HB3	1:D:2809:PRO:HD3	2.02	0.41
1:D:3376:GLU:OE2	1:D:3376:GLU:HA	2.20	0.41
1:A:2746:VAL:HG11	1:A:2815:LYS:O	2.20	0.41
1:A:4632:GLU:OE1	1:A:4632:GLU:HA	2.20	0.41
1:B:861:GLN:H	1:B:861:GLN:CD	2.28	0.41
1:C:2875:MET:HG3	1:C:2938:VAL:CG1	2.51	0.41
1:C:2922:GLU:O	1:C:2926:GLU:HG2	2.20	0.41
1:C:4679:LEU:HD11	1:C:4704:LEU:HD22	2.01	0.41
1:D:2609:MET:HE3	1:D:2609:MET:HB3	1.95	0.41
1:D:3892:GLN:HG3	1:D:3970:GLU:HG3	2.02	0.41
1:D:4679:LEU:HD11	1:D:4704:LEU:HD22	2.01	0.41
1:A:141:ASP:OD1	1:A:141:ASP:N	2.49	0.41
1:A:2793:ARG:NH2	1:A:2798:PHE:HA	2.35	0.41
1:A:2875:MET:HG3	1:A:2938:VAL:CG1	2.51	0.41
1:B:1999:PHE:CD2	1:B:1999:PHE:N	2.89	0.41
1:C:3944:ASP:OD1	1:C:3944:ASP:N	2.52	0.41
7:C:8007:PCW:H412	7:D:8006:PCW:H412	2.01	0.41
1:D:24:GLN:OE1	1:D:204:ASN:ND2	2.52	0.41
1:D:234:ILE:HD12	1:D:243:ARG:HB3	2.01	0.41
1:D:1425:PRO:HA	1:D:1428:ILE:HG22	2.01	0.41
1:A:1428:ILE:HG23	1:A:1429:LEU:HD22	2.02	0.41
1:A:2234:CYS:C	1:A:2236:PHE:N	2.77	0.41
1:A:2808:TRP:HB3	1:A:2809:PRO:HD3	2.03	0.41
1:A:4964:ASP:OD1	1:A:4965:TYR:N	2.53	0.41
1:B:234:ILE:HD12	1:B:243:ARG:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:967:LYS:HZ2	1:B:969:ALA:HB2	1.86	0.41
1:C:723:TRP:CZ2	1:C:728:ALA:HB2	2.55	0.41
1:C:843:PRO:O	1:C:1197:PRO:HA	2.21	0.41
1:C:2743:THR:HG22	1:C:2816:ALA:CA	2.50	0.41
1:C:4632:GLU:OE1	1:C:4632:GLU:HA	2.20	0.41
1:D:2752:LEU:CD1	1:D:2818:ILE:HD11	2.48	0.41
1:A:861:GLN:H	1:A:861:GLN:CD	2.29	0.41
1:A:3037:LYS:O	1:A:3040:ILE:HG22	2.20	0.41
1:A:4004:MET:HG3	1:A:4060:MET:HE3	2.01	0.41
1:B:2975:ILE:HD13	1:B:2975:ILE:HA	1.93	0.41
1:B:4632:GLU:HA	1:B:4632:GLU:OE1	2.20	0.41
1:C:861:GLN:H	1:C:861:GLN:CD	2.28	0.41
1:C:2215:VAL:HG11	1:C:2229:MET:CE	2.33	0.41
1:C:4964:ASP:OD1	1:C:4965:TYR:N	2.53	0.41
1:D:1822:ARG:O	1:D:1826:GLN:HG2	2.21	0.41
1:D:2383:GLU:OE1	1:D:2386:ARG:NH1	2.53	0.41
1:D:2640:MET:HB3	1:D:2641:PRO:HD3	2.02	0.41
1:B:690:SER:N	1:B:777:LEU:O	2.52	0.41
1:B:1822:ARG:O	1:B:1826:GLN:HG2	2.21	0.41
1:B:1830:ASP:OD1	1:B:1830:ASP:N	2.53	0.41
1:C:2234:CYS:HA	1:C:2238:CYS:HB2	2.01	0.41
1:C:2714:ASP:OD1	1:C:2714:ASP:N	2.41	0.41
1:C:3180:ARG:HG2	1:C:3180:ARG:HH11	1.85	0.41
1:C:3393:LEU:HD22	1:C:3393:LEU:N	2.35	0.41
1:D:1428:ILE:HG23	1:D:1429:LEU:HD22	2.02	0.41
1:D:3037:LYS:O	1:D:3040:ILE:HG22	2.20	0.41
1:A:1691:ASP:OD2	1:A:1694:GLN:NE2	2.45	0.41
1:B:2808:TRP:HB3	1:B:2809:PRO:HD3	2.03	0.41
1:C:2166:LEU:HD21	1:C:2178:LEU:HD23	2.03	0.41
1:C:3037:LYS:O	1:C:3040:ILE:HG22	2.20	0.41
1:D:1830:ASP:N	1:D:1830:ASP:OD1	2.53	0.41
1:D:2875:MET:CE	1:D:2940:ARG:HD2	2.49	0.41
1:B:1281:GLN:O	1:B:1282:ASN:CG	2.64	0.41
1:B:2922:GLU:O	1:B:2926:GLU:HG2	2.20	0.41
1:C:234:ILE:HD12	1:C:243:ARG:HB3	2.01	0.41
1:D:843:PRO:O	1:D:1197:PRO:HA	2.21	0.41
1:D:2875:MET:HG3	1:D:2938:VAL:CG1	2.51	0.41
1:A:385:MET:HE3	1:A:385:MET:HB3	1.98	0.41
1:A:2166:LEU:HD21	1:A:2178:LEU:HD23	2.03	0.41
1:A:2167:LEU:HD11	1:A:2207:THR:HG23	2.03	0.41
1:A:3892:GLN:HG3	1:A:3970:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2875:MET:HG3	1:B:2938:VAL:CG1	2.51	0.41
1:B:3202:MET:SD	1:B:3204:VAL:HG22	2.61	0.41
1:B:4899:ILE:HG13	1:B:4911:ARG:NH2	2.36	0.41
1:C:967:LYS:HZ1	1:C:969:ALA:HB2	1.84	0.41
1:C:2640:MET:HB3	1:C:2641:PRO:HD3	2.02	0.41
1:C:2792:LEU:HD12	1:C:2856:TYR:CE1	2.56	0.41
1:C:2808:TRP:HB3	1:C:2809:PRO:HD3	2.03	0.41
1:C:2872:LEU:O	1:C:2875:MET:HB2	2.20	0.41
1:C:2875:MET:CE	1:C:2940:ARG:HD2	2.49	0.41
1:D:385:MET:HE3	1:D:385:MET:HB3	1.98	0.41
1:D:861:GLN:H	1:D:861:GLN:CD	2.28	0.41
1:D:2166:LEU:HD21	1:D:2178:LEU:HD23	2.03	0.41
1:D:2756:ILE:HD13	1:D:2811:LYS:HG2	2.02	0.41
1:D:3202:MET:SD	1:D:3204:VAL:HG22	2.61	0.41
1:A:843:PRO:O	1:A:1197:PRO:HA	2.21	0.41
1:A:1281:GLN:O	1:A:1282:ASN:CG	2.64	0.41
1:A:2792:LEU:HD12	1:A:2856:TYR:CE1	2.56	0.41
1:B:885:LEU:HD13	1:B:970:PRO:HG3	2.03	0.41
1:B:2600:GLN:O	1:B:2604:ILE:HG13	2.21	0.41
1:B:2640:MET:HB3	1:B:2641:PRO:HD3	2.02	0.41
1:C:1281:GLN:O	1:C:1282:ASN:CG	2.64	0.41
1:C:2974:PHE:CE1	1:C:2996:ILE:HG12	2.56	0.41
1:D:2215:VAL:HG11	1:D:2229:MET:CE	2.33	0.41
1:D:2268:MET:HE2	1:D:2268:MET:HB2	2.01	0.41
1:A:1822:ARG:O	1:A:1826:GLN:HG2	2.21	0.40
1:B:2167:LEU:HD11	1:B:2207:THR:HG23	2.03	0.40
1:B:2974:PHE:CE1	1:B:2996:ILE:HG12	2.56	0.40
1:B:3317:LEU:HD21	1:B:3347:VAL:HG23	2.03	0.40
1:B:3892:GLN:HG3	1:B:3970:GLU:HG3	2.02	0.40
1:C:627:LEU:N	1:C:628:PRO:HD2	2.35	0.40
1:C:1822:ARG:O	1:C:1826:GLN:HG2	2.21	0.40
1:D:760:ILE:O	1:D:760:ILE:HG23	2.21	0.40
1:D:2438:ALA:HB2	1:D:2510:VAL:HG22	2.03	0.40
1:D:2600:GLN:O	1:D:2604:ILE:HG13	2.21	0.40
1:D:2792:LEU:HD12	1:D:2856:TYR:CE1	2.56	0.40
1:D:2931:LEU:HD22	1:D:2936:TYR:CB	2.51	0.40
1:A:2438:ALA:HB2	1:A:2510:VAL:HG22	2.03	0.40
1:A:2600:GLN:O	1:A:2604:ILE:HG13	2.21	0.40
1:A:2640:MET:HB3	1:A:2641:PRO:HD3	2.02	0.40
1:A:2931:LEU:HD22	1:A:2936:TYR:CB	2.51	0.40
1:A:2974:PHE:CE1	1:A:2996:ILE:HG12	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1428:ILE:HG23	1:B:1429:LEU:HD22	2.02	0.40
1:B:2792:LEU:HD12	1:B:2856:TYR:CE1	2.56	0.40
1:B:2931:LEU:HD22	1:B:2936:TYR:CB	2.51	0.40
1:B:3037:LYS:O	1:B:3040:ILE:HG22	2.20	0.40
1:B:3106:LYS:O	1:B:3109:GLU:HG3	2.22	0.40
1:C:887:ARG:HB3	1:C:892:TRP:HB2	2.04	0.40
1:C:2756:ILE:HD13	1:C:2811:LYS:HG2	2.02	0.40
1:C:4899:ILE:HG13	1:C:4911:ARG:NH2	2.36	0.40
1:D:1129:ARG:HB2	1:D:1129:ARG:NH1	2.36	0.40
1:D:1999:PHE:N	1:D:1999:PHE:CD2	2.89	0.40
1:D:3944:ASP:OD1	1:D:3944:ASP:N	2.52	0.40
1:A:760:ILE:O	1:A:760:ILE:HG23	2.21	0.40
1:A:3202:MET:SD	1:A:3204:VAL:HG22	2.61	0.40
1:B:1102:ARG:NH1	1:B:1116:LEU:O	2.48	0.40
1:B:1129:ARG:HB2	1:B:1129:ARG:NH1	2.36	0.40
1:B:1691:ASP:OD2	1:B:1694:GLN:NE2	2.45	0.40
1:B:2949:THR:O	1:B:2950:SER:C	2.62	0.40
1:B:3969:THR:HG23	1:B:4032:SER:OG	2.21	0.40
1:C:2600:GLN:O	1:C:2604:ILE:HG13	2.21	0.40
1:D:3111:LEU:O	1:D:3181:ASN:ND2	2.55	0.40
1:D:3180:ARG:HG2	1:D:3180:ARG:HH11	1.85	0.40
1:D:4899:ILE:HG13	1:D:4911:ARG:NH2	2.36	0.40
1:A:1102:ARG:NH1	1:A:1116:LEU:O	2.48	0.40
1:A:2752:LEU:CD1	1:A:2818:ILE:HD11	2.48	0.40
1:A:3106:LYS:O	1:A:3109:GLU:HG3	2.22	0.40
1:B:3180:ARG:HH11	1:B:3180:ARG:HG2	1.86	0.40
1:C:2887:TRP:O	1:C:2891:LYS:HD2	2.22	0.40
1:C:3111:LEU:O	1:C:3181:ASN:ND2	2.55	0.40
1:D:627:LEU:N	1:D:628:PRO:HD2	2.35	0.40
1:D:887:ARG:HB3	1:D:892:TRP:HB2	2.04	0.40
1:D:2213:VAL:HG11	1:D:2257:TYR:CE2	2.57	0.40
1:D:3393:LEU:HD22	1:D:3393:LEU:N	2.35	0.40
1:A:887:ARG:HB3	1:A:892:TRP:HB2	2.04	0.40
1:A:3385:LYS:O	1:A:3389:GLU:N	2.40	0.40
1:C:1999:PHE:CD2	1:C:1999:PHE:N	2.89	0.40
1:C:2213:VAL:HG11	1:C:2257:TYR:CE2	2.57	0.40
1:C:2907:VAL:HG23	1:C:2912:LEU:HG	2.04	0.40
1:C:2931:LEU:HD22	1:C:2936:TYR:CB	2.51	0.40
1:C:3892:GLN:HG3	1:C:3970:GLU:HG3	2.02	0.40
1:D:2997:LYS:HA	1:D:2997:LYS:HD2	1.95	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%)	4236 (98%)	108 (2%)	1 (0%)	100	100
1	B	4345/5035 (86%)	4234 (97%)	110 (2%)	1 (0%)	100	100
1	C	4345/5035 (86%)	4236 (98%)	108 (2%)	1 (0%)	100	100
1	D	4345/5035 (86%)	4236 (98%)	108 (2%)	1 (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%)	17350 (98%)	446 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2266	LEU
1	B	2266	LEU
1	C	2266	LEU
1	D	2266	LEU

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%)	3734 (98%)	72 (2%)	50	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	3806/4296 (89%)	3737 (98%)	69 (2%)	51	73
1	C	3806/4296 (89%)	3734 (98%)	72 (2%)	50	71
1	D	3806/4296 (89%)	3734 (98%)	72 (2%)	50	71
2	E	89/90 (99%)	87 (98%)	2 (2%)	45	67
2	F	89/90 (99%)	87 (98%)	2 (2%)	45	67
2	G	89/90 (99%)	87 (98%)	2 (2%)	45	67
2	H	89/90 (99%)	87 (98%)	2 (2%)	45	67
All	All	15580/17544 (89%)	15287 (98%)	293 (2%)	49	71

All (293) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	26	SER
1	A	210	CYS
1	A	283	ILE
1	A	332	VAL
1	A	435	SER
1	A	733	SER
1	A	748	CYS
1	A	757	SER
1	A	848	SER
1	A	857	VAL
1	A	871	ILE
1	A	910	ASN
1	A	971	LEU
1	A	978	LEU
1	A	979	THR
1	A	1044	VAL
1	A	1174	SER
1	A	1242	SER
1	A	1267	THR
1	A	1280	SER
1	A	1294	LEU
1	A	1429	LEU
1	A	1487	SER
1	A	1490	CYS
1	A	1503	SER
1	A	1754	SER
1	A	1757	ASP

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Mol	Chain	Res	Type
1	A	1770	THR
1	A	2007	ILE
1	A	2155	SER
1	A	2220	GLU
1	A	2369	LEU
1	A	2417	VAL
1	A	2515	ASN
1	A	2541	THR
1	A	2544	THR
1	A	2769	PHE
1	A	2782	ILE
1	A	2799	SER
1	A	2824	VAL
1	A	2902	SER
1	A	2906	LEU
1	A	2926	GLU
1	A	2933	MET
1	A	2975	ILE
1	A	3055	VAL
1	A	3060	THR
1	A	3170	LEU
1	A	3374	VAL
1	A	3509	SER
1	A	3607	LEU
1	A	3612	HIS
1	A	3640	THR
1	A	3659	LYS
1	A	3691	VAL
1	A	3752	VAL
1	A	3774	HIS
1	A	4054	SER
1	A	4055	SER
1	A	4128	CYS
1	A	4212	GLN
1	A	4578	TYR
1	A	4580	VAL
1	A	4583	SER
1	A	4633	SER
1	A	4706	THR
1	A	4718	VAL
1	A	4729	ILE
1	A	4734	ARG

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Mol	Chain	Res	Type
1	A	4737	GLU
1	A	4864	SER
2	E	15	THR
2	E	26	HIS
2	F	15	THR
2	F	26	HIS
2	G	15	THR
2	G	26	HIS
2	H	15	THR
2	H	26	HIS
1	B	12	VAL
1	B	26	SER
1	B	210	CYS
1	B	283	ILE
1	B	332	VAL
1	B	435	SER
1	B	733	SER
1	B	748	CYS
1	B	757	SER
1	B	848	SER
1	B	857	VAL
1	B	871	ILE
1	B	910	ASN
1	B	971	LEU
1	B	978	LEU
1	B	979	THR
1	B	1044	VAL
1	B	1174	SER
1	B	1242	SER
1	B	1267	THR
1	B	1280	SER
1	B	1294	LEU
1	B	1429	LEU
1	B	1487	SER
1	B	1490	CYS
1	B	1503	SER
1	B	1754	SER
1	B	1757	ASP
1	B	1770	THR
1	B	2007	ILE
1	B	2155	SER
1	B	2220	GLU

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Mol	Chain	Res	Type
1	B	2369	LEU
1	B	2417	VAL
1	B	2515	ASN
1	B	2541	THR
1	B	2544	THR
1	B	2769	PHE
1	B	2782	ILE
1	B	2799	SER
1	B	2824	VAL
1	B	2902	SER
1	B	2906	LEU
1	B	2933	MET
1	B	2975	ILE
1	B	3060	THR
1	B	3170	LEU
1	B	3374	VAL
1	B	3509	SER
1	B	3607	LEU
1	B	3612	HIS
1	B	3640	THR
1	B	3659	LYS
1	B	3691	VAL
1	B	3752	VAL
1	B	3774	HIS
1	B	4054	SER
1	B	4055	SER
1	B	4128	CYS
1	B	4212	GLN
1	B	4580	VAL
1	B	4583	SER
1	B	4633	SER
1	B	4706	THR
1	B	4718	VAL
1	B	4729	ILE
1	B	4734	ARG
1	B	4737	GLU
1	B	4864	SER
1	C	12	VAL
1	C	26	SER
1	C	210	CYS
1	C	283	ILE
1	C	332	VAL

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Mol	Chain	Res	Type
1	C	435	SER
1	C	733	SER
1	C	748	CYS
1	C	757	SER
1	C	848	SER
1	C	857	VAL
1	C	871	ILE
1	C	910	ASN
1	C	971	LEU
1	C	978	LEU
1	C	979	THR
1	C	1044	VAL
1	C	1174	SER
1	C	1242	SER
1	C	1267	THR
1	C	1280	SER
1	C	1294	LEU
1	C	1429	LEU
1	C	1487	SER
1	C	1490	CYS
1	C	1503	SER
1	C	1754	SER
1	C	1757	ASP
1	C	1770	THR
1	C	2007	ILE
1	C	2155	SER
1	C	2220	GLU
1	C	2369	LEU
1	C	2417	VAL
1	C	2515	ASN
1	C	2541	THR
1	C	2544	THR
1	C	2769	PHE
1	C	2782	ILE
1	C	2799	SER
1	C	2824	VAL
1	C	2902	SER
1	C	2906	LEU
1	C	2926	GLU
1	C	2933	MET
1	C	2975	ILE
1	C	3055	VAL

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Mol	Chain	Res	Type
1	C	3060	THR
1	C	3170	LEU
1	C	3374	VAL
1	C	3509	SER
1	C	3607	LEU
1	C	3612	HIS
1	C	3640	THR
1	C	3659	LYS
1	C	3691	VAL
1	C	3752	VAL
1	C	3774	HIS
1	C	4054	SER
1	C	4055	SER
1	C	4128	CYS
1	C	4212	GLN
1	C	4578	TYR
1	C	4580	VAL
1	C	4583	SER
1	C	4633	SER
1	C	4706	THR
1	C	4718	VAL
1	C	4729	ILE
1	C	4734	ARG
1	C	4737	GLU
1	C	4864	SER
1	D	12	VAL
1	D	26	SER
1	D	210	CYS
1	D	283	ILE
1	D	332	VAL
1	D	435	SER
1	D	733	SER
1	D	748	CYS
1	D	757	SER
1	D	848	SER
1	D	857	VAL
1	D	871	ILE
1	D	910	ASN
1	D	971	LEU
1	D	978	LEU
1	D	979	THR
1	D	1044	VAL

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Mol	Chain	Res	Type
1	D	1174	SER
1	D	1242	SER
1	D	1267	THR
1	D	1280	SER
1	D	1294	LEU
1	D	1429	LEU
1	D	1487	SER
1	D	1490	CYS
1	D	1503	SER
1	D	1754	SER
1	D	1757	ASP
1	D	1770	THR
1	D	1967	VAL
1	D	2007	ILE
1	D	2155	SER
1	D	2220	GLU
1	D	2369	LEU
1	D	2417	VAL
1	D	2515	ASN
1	D	2541	THR
1	D	2544	THR
1	D	2769	PHE
1	D	2782	ILE
1	D	2799	SER
1	D	2824	VAL
1	D	2902	SER
1	D	2906	LEU
1	D	2933	MET
1	D	2975	ILE
1	D	3055	VAL
1	D	3060	THR
1	D	3170	LEU
1	D	3374	VAL
1	D	3509	SER
1	D	3607	LEU
1	D	3612	HIS
1	D	3640	THR
1	D	3659	LYS
1	D	3691	VAL
1	D	3752	VAL
1	D	3774	HIS
1	D	4054	SER

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Mol	Chain	Res	Type
1	D	4055	SER
1	D	4128	CYS
1	D	4212	GLN
1	D	4578	TYR
1	D	4580	VAL
1	D	4583	SER
1	D	4633	SER
1	D	4706	THR
1	D	4718	VAL
1	D	4729	ILE
1	D	4734	ARG
1	D	4737	GLU
1	D	4864	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (144) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	HIS
1	A	395	GLN
1	A	400	GLN
1	A	462	HIS
1	A	659	GLN
1	A	766	GLN
1	A	912	HIS
1	A	1063	GLN
1	A	1245	GLN
1	A	1301	HIS
1	A	1506	GLN
1	A	1632	GLN
1	A	1950	GLN
1	A	2030	GLN
1	A	2246	GLN
1	A	2254	HIS
1	A	2488	GLN
1	A	2575	HIS
1	A	2600	GLN
1	A	2757	ASN
1	A	2773	GLN
1	A	2789	HIS
1	A	2857	ASN
1	A	2884	HIS
1	A	2903	HIS

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Mol	Chain	Res	Type
1	A	2977	HIS
1	A	3963	GLN
1	A	4057	ASN
1	A	4123	ASN
1	A	4165	ASN
1	A	4219	GLN
1	A	4545	GLN
1	A	4931	GLN
1	A	5033	GLN
2	E	88	HIS
2	E	95	HIS
2	F	88	HIS
2	F	95	HIS
2	G	88	HIS
2	G	95	HIS
2	H	88	HIS
2	H	95	HIS
1	B	139	GLN
1	B	219	HIS
1	B	395	GLN
1	B	400	GLN
1	B	462	HIS
1	B	496	ASN
1	B	659	GLN
1	B	766	GLN
1	B	912	HIS
1	B	1063	GLN
1	B	1245	GLN
1	B	1301	HIS
1	B	1506	GLN
1	B	1632	GLN
1	B	1950	GLN
1	B	2030	GLN
1	B	2181	GLN
1	B	2246	GLN
1	B	2254	HIS
1	B	2575	HIS
1	B	2600	GLN
1	B	2757	ASN
1	B	2773	GLN
1	B	2789	HIS
1	B	2857	ASN

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Mol	Chain	Res	Type
1	B	2884	HIS
1	B	2903	HIS
1	B	2977	HIS
1	B	3963	GLN
1	B	4057	ASN
1	B	4103	GLN
1	B	4123	ASN
1	B	4219	GLN
1	B	4545	GLN
1	B	4931	GLN
1	B	5033	GLN
1	C	219	HIS
1	C	395	GLN
1	C	400	GLN
1	C	462	HIS
1	C	659	GLN
1	C	766	GLN
1	C	912	HIS
1	C	1063	GLN
1	C	1301	HIS
1	C	1506	GLN
1	C	1632	GLN
1	C	1950	GLN
1	C	2030	GLN
1	C	2246	GLN
1	C	2254	HIS
1	C	2575	HIS
1	C	2600	GLN
1	C	2757	ASN
1	C	2773	GLN
1	C	2857	ASN
1	C	2884	HIS
1	C	2903	HIS
1	C	2977	HIS
1	C	3963	GLN
1	C	3997	HIS
1	C	4057	ASN
1	C	4103	GLN
1	C	4123	ASN
1	C	4219	GLN
1	C	4545	GLN
1	C	4931	GLN

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Mol	Chain	Res	Type
1	C	5033	GLN
1	D	139	GLN
1	D	219	HIS
1	D	395	GLN
1	D	400	GLN
1	D	462	HIS
1	D	659	GLN
1	D	766	GLN
1	D	890	GLN
1	D	912	HIS
1	D	1063	GLN
1	D	1245	GLN
1	D	1301	HIS
1	D	1506	GLN
1	D	1632	GLN
1	D	1950	GLN
1	D	2030	GLN
1	D	2246	GLN
1	D	2254	HIS
1	D	2575	HIS
1	D	2600	GLN
1	D	2773	GLN
1	D	2857	ASN
1	D	2884	HIS
1	D	2903	HIS
1	D	2977	HIS
1	D	3963	GLN
1	D	4057	ASN
1	D	4103	GLN
1	D	4123	ASN
1	D	4165	ASN
1	D	4219	GLN
1	D	4545	GLN
1	D	4931	GLN
1	D	5033	GLN

5.3.3 RNA ⓘ

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 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 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$
5	ATP	A	8005	-	32,33,33	0.27	0	48,52,52	0.68	0
5	ATP	B	8003	-	32,33,33	0.27	0	48,52,52	0.68	0
7	PCW	D	8006	-	53,53,53	1.25	7 (13%)	59,61,61	1.04	3 (5%)
5	ATP	D	8005	-	32,33,33	0.27	0	48,52,52	0.68	0
5	ATP	D	8003	-	32,33,33	0.27	0	48,52,52	0.68	0
4	CFF	C	8002	-	15,15,15	1.79	5 (33%)	23,23,23	2.92	12 (52%)
7	PCW	A	8007	-	53,53,53	1.26	7 (13%)	59,61,61	1.13	4 (6%)
7	PCW	B	8006	-	53,53,53	1.25	7 (13%)	59,61,61	1.04	3 (5%)
5	ATP	C	8003	-	32,33,33	0.27	0	48,52,52	0.68	0
5	ATP	C	8005	-	32,33,33	0.27	0	48,52,52	0.68	0
7	PCW	C	8006	-	53,53,53	1.25	7 (13%)	59,61,61	1.04	3 (5%)
4	CFF	D	8002	-	15,15,15	1.79	5 (33%)	23,23,23	2.93	13 (56%)
4	CFF	A	8002	-	15,15,15	1.79	5 (33%)	23,23,23	2.93	12 (52%)
7	PCW	D	8007	-	53,53,53	1.26	7 (13%)	59,61,61	1.13	4 (6%)
7	PCW	A	8006	-	53,53,53	1.25	7 (13%)	59,61,61	1.04	3 (5%)
7	PCW	B	8007	-	53,53,53	1.26	7 (13%)	59,61,61	1.13	4 (6%)
4	CFF	B	8002	-	15,15,15	1.79	5 (33%)	23,23,23	2.92	12 (52%)
5	ATP	A	8003	-	32,33,33	0.27	0	48,52,52	0.68	0
7	PCW	C	8007	-	53,53,53	1.26	7 (13%)	59,61,61	1.13	4 (6%)
5	ATP	B	8005	-	32,33,33	0.26	0	48,52,52	0.68	0

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
5	ATP	A	8005	-	-	8/22/38/38	0/3/3/3
5	ATP	B	8003	-	-	3/22/38/38	0/3/3/3
7	PCW	D	8006	-	-	25/57/57/57	-
5	ATP	D	8005	-	-	8/22/38/38	0/3/3/3
5	ATP	D	8003	-	-	3/22/38/38	0/3/3/3
4	CFF	C	8002	-	-	-	0/2/2/2
7	PCW	A	8007	-	-	27/57/57/57	-
7	PCW	B	8006	-	-	25/57/57/57	-
5	ATP	C	8003	-	-	3/22/38/38	0/3/3/3
5	ATP	C	8005	-	-	8/22/38/38	0/3/3/3
7	PCW	C	8006	-	-	25/57/57/57	-
4	CFF	D	8002	-	-	-	0/2/2/2
7	PCW	D	8007	-	-	27/57/57/57	-
4	CFF	A	8002	-	-	-	0/2/2/2
7	PCW	A	8006	-	-	25/57/57/57	-
7	PCW	B	8007	-	-	28/57/57/57	-
4	CFF	B	8002	-	-	-	0/2/2/2
5	ATP	A	8003	-	-	3/22/38/38	0/3/3/3
7	PCW	C	8007	-	-	27/57/57/57	-
5	ATP	B	8005	-	-	8/22/38/38	0/3/3/3

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	8002	CFF	C6-N1	-3.81	1.32	1.40
4	B	8002	CFF	C6-N1	-3.81	1.32	1.40
4	C	8002	CFF	C6-N1	-3.81	1.32	1.40
4	D	8002	CFF	C6-N1	-3.81	1.32	1.40
7	D	8006	PCW	O3-C11	3.04	1.42	1.33
7	B	8007	PCW	O3-C11	3.04	1.42	1.33
7	A	8006	PCW	O3-C11	3.02	1.42	1.33
7	B	8006	PCW	O3-C11	3.02	1.42	1.33
7	C	8006	PCW	O3-C11	3.02	1.42	1.33
7	A	8007	PCW	O3-C11	3.01	1.42	1.33
7	C	8007	PCW	O3-C11	3.01	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	8007	PCW	O3-C11	3.01	1.42	1.33
7	D	8007	PCW	O2-C31	2.90	1.42	1.34
7	A	8007	PCW	O2-C31	2.88	1.42	1.34
7	B	8007	PCW	O2-C31	2.88	1.42	1.34
7	C	8007	PCW	O2-C31	2.88	1.42	1.34
7	A	8006	PCW	O2-C31	2.86	1.42	1.34
7	B	8006	PCW	O2-C31	2.86	1.42	1.34
7	D	8006	PCW	O2-C31	2.86	1.42	1.34
7	C	8006	PCW	O2-C31	2.86	1.42	1.34
7	C	8007	PCW	P-O4P	2.57	1.69	1.59
7	D	8007	PCW	P-O4P	2.57	1.69	1.59
7	A	8007	PCW	P-O4P	2.55	1.69	1.59
7	A	8006	PCW	P-O4P	2.54	1.69	1.59
7	B	8006	PCW	P-O4P	2.54	1.69	1.59
7	C	8006	PCW	P-O4P	2.54	1.69	1.59
7	D	8006	PCW	P-O4P	2.54	1.69	1.59
4	B	8002	CFF	C5-N7	-2.54	1.34	1.38
7	B	8007	PCW	P-O4P	2.54	1.69	1.59
4	A	8002	CFF	C5-N7	-2.51	1.34	1.38
4	C	8002	CFF	C5-N7	-2.51	1.34	1.38
4	D	8002	CFF	C5-N7	-2.51	1.34	1.38
7	C	8006	PCW	O2-C2	-2.38	1.41	1.46
7	A	8006	PCW	O2-C2	-2.38	1.41	1.46
7	B	8006	PCW	O2-C2	-2.38	1.41	1.46
7	D	8006	PCW	O2-C2	-2.38	1.41	1.46
7	B	8006	PCW	C5-C4	2.38	1.58	1.51
7	C	8006	PCW	C5-C4	2.38	1.58	1.51
7	D	8006	PCW	C5-C4	2.38	1.58	1.51
7	A	8006	PCW	C5-C4	2.37	1.58	1.51
7	B	8007	PCW	O2-C2	-2.33	1.41	1.46
7	D	8007	PCW	C5-C4	2.33	1.58	1.51
7	A	8007	PCW	O2-C2	-2.32	1.41	1.46
7	A	8007	PCW	C5-C4	2.31	1.58	1.51
7	B	8007	PCW	C5-C4	2.31	1.58	1.51
7	D	8007	PCW	O2-C2	-2.30	1.41	1.46
7	C	8007	PCW	O2-C2	-2.28	1.41	1.46
7	C	8007	PCW	C5-C4	2.28	1.58	1.51
7	A	8006	PCW	C32-C31	2.23	1.57	1.50
7	B	8006	PCW	C32-C31	2.22	1.57	1.50
7	C	8006	PCW	C32-C31	2.22	1.57	1.50
7	D	8006	PCW	C32-C31	2.22	1.57	1.50
7	B	8006	PCW	P-O3P	2.21	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	8006	PCW	P-O3P	2.20	1.68	1.59
7	C	8006	PCW	P-O3P	2.19	1.68	1.59
7	D	8006	PCW	P-O3P	2.19	1.68	1.59
7	B	8007	PCW	C32-C31	2.17	1.57	1.50
7	A	8007	PCW	C32-C31	2.17	1.57	1.50
7	D	8007	PCW	C32-C31	2.17	1.57	1.50
4	A	8002	CFF	C4-N3	-2.16	1.34	1.38
4	C	8002	CFF	C4-N3	-2.16	1.34	1.38
4	D	8002	CFF	C4-N3	-2.16	1.34	1.38
7	C	8007	PCW	P-O3P	2.15	1.67	1.59
7	D	8007	PCW	P-O3P	2.15	1.67	1.59
7	C	8007	PCW	C32-C31	2.14	1.56	1.50
7	A	8007	PCW	P-O3P	2.14	1.67	1.59
7	B	8007	PCW	P-O3P	2.14	1.67	1.59
4	B	8002	CFF	O13-C6	-2.11	1.18	1.23
4	B	8002	CFF	C4-N3	-2.11	1.34	1.38
4	B	8002	CFF	C5-C6	-2.08	1.37	1.43
4	C	8002	CFF	C5-C6	-2.08	1.37	1.43
4	A	8002	CFF	O13-C6	-2.08	1.18	1.23
4	C	8002	CFF	O13-C6	-2.08	1.18	1.23
4	D	8002	CFF	O13-C6	-2.08	1.18	1.23
4	A	8002	CFF	C5-C6	-2.08	1.37	1.43
4	D	8002	CFF	C5-C6	-2.08	1.37	1.43

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	8002	CFF	C14-N7-C8	-8.09	111.14	126.28
4	B	8002	CFF	C14-N7-C8	-8.08	111.15	126.28
4	A	8002	CFF	C14-N7-C8	-8.07	111.17	126.28
4	D	8002	CFF	C14-N7-C8	-8.07	111.17	126.28
4	B	8002	CFF	C14-N7-C5	5.51	140.87	127.77
4	A	8002	CFF	C14-N7-C5	5.49	140.83	127.77
4	C	8002	CFF	C14-N7-C5	5.49	140.83	127.77
4	D	8002	CFF	C14-N7-C5	5.47	140.79	127.77
4	D	8002	CFF	C5-C6-N1	4.39	120.10	112.06
4	A	8002	CFF	C5-C6-N1	4.38	120.09	112.06
4	B	8002	CFF	C5-C6-N1	4.37	120.07	112.06
4	C	8002	CFF	C5-C6-N1	4.37	120.07	112.06
7	B	8007	PCW	C21-C20-C19	4.17	156.06	124.83
7	A	8007	PCW	C21-C20-C19	4.17	156.04	124.83
7	D	8007	PCW	C21-C20-C19	4.17	156.04	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	8007	PCW	C21-C20-C19	4.16	156.02	124.83
7	B	8006	PCW	C21-C20-C19	3.79	153.23	124.83
7	C	8006	PCW	C21-C20-C19	3.79	153.22	124.83
7	A	8006	PCW	C21-C20-C19	3.79	153.20	124.83
7	D	8006	PCW	C21-C20-C19	3.78	153.16	124.83
7	A	8007	PCW	O2-C31-C32	3.76	119.62	111.48
7	D	8007	PCW	O2-C31-C32	3.76	119.62	111.48
7	B	8007	PCW	O2-C31-C32	3.76	119.61	111.48
7	C	8007	PCW	O2-C31-C32	3.76	119.61	111.48
7	B	8006	PCW	O2-C31-C32	3.76	119.61	111.48
7	D	8006	PCW	O2-C31-C32	3.76	119.61	111.48
7	A	8006	PCW	O2-C31-C32	3.74	119.58	111.48
7	C	8006	PCW	O2-C31-C32	3.74	119.57	111.48
4	D	8002	CFF	N3-C4-N9	3.56	131.87	126.27
4	A	8002	CFF	N3-C4-N9	3.55	131.85	126.27
4	D	8002	CFF	C6-N1-C2	-3.55	119.89	125.66
4	A	8002	CFF	C6-N1-C2	-3.55	119.90	125.66
4	C	8002	CFF	N3-C4-N9	3.54	131.84	126.27
4	B	8002	CFF	N3-C4-N9	3.54	131.83	126.27
4	B	8002	CFF	C6-N1-C2	-3.54	119.91	125.66
4	C	8002	CFF	C6-N1-C2	-3.54	119.91	125.66
4	D	8002	CFF	O13-C6-C5	-3.25	119.72	126.38
4	A	8002	CFF	O13-C6-C5	-3.24	119.74	126.38
4	C	8002	CFF	O13-C6-C5	-3.23	119.76	126.38
4	B	8002	CFF	O13-C6-C5	-3.22	119.79	126.38
4	C	8002	CFF	N7-C8-N9	-3.05	107.95	113.48
4	D	8002	CFF	N7-C8-N9	-3.05	107.95	113.48
4	B	8002	CFF	N7-C8-N9	-3.04	107.97	113.48
4	A	8002	CFF	N7-C8-N9	-3.03	107.99	113.48
7	D	8007	PCW	C18-C19-C20	2.88	146.38	124.83
7	A	8007	PCW	C18-C19-C20	2.87	146.35	124.83
7	C	8007	PCW	C18-C19-C20	2.87	146.34	124.83
7	B	8007	PCW	C18-C19-C20	2.87	146.32	124.83
7	D	8007	PCW	O3-C11-C12	2.66	119.94	111.83
7	A	8007	PCW	O3-C11-C12	2.64	119.90	111.83
7	C	8007	PCW	O3-C11-C12	2.64	119.90	111.83
7	B	8007	PCW	O3-C11-C12	2.64	119.88	111.83
7	B	8006	PCW	O3-C11-C12	2.37	119.06	111.83
7	C	8006	PCW	O3-C11-C12	2.37	119.06	111.83
7	A	8006	PCW	O3-C11-C12	2.37	119.05	111.83
7	D	8006	PCW	O3-C11-C12	2.36	119.04	111.83
4	D	8002	CFF	C6-C5-C4	-2.35	119.96	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	8002	CFF	C6-C5-C4	-2.34	119.97	122.92
4	D	8002	CFF	N3-C2-N1	2.30	120.01	117.14
4	B	8002	CFF	C6-C5-C4	-2.30	120.02	122.92
4	C	8002	CFF	C6-C5-C4	-2.30	120.02	122.92
4	A	8002	CFF	N3-C2-N1	2.29	120.00	117.14
4	B	8002	CFF	N3-C2-N1	2.28	119.99	117.14
4	D	8002	CFF	C12-N3-C2	2.26	121.27	117.33
4	C	8002	CFF	N3-C2-N1	2.25	119.95	117.14
4	B	8002	CFF	C12-N3-C2	2.24	121.24	117.33
4	A	8002	CFF	C12-N3-C2	2.24	121.23	117.33
4	C	8002	CFF	C12-N3-C2	2.21	121.18	117.33
4	D	8002	CFF	C8-N9-C4	2.08	107.96	102.98
4	A	8002	CFF	C8-N9-C4	2.07	107.94	102.98
4	C	8002	CFF	C8-N9-C4	2.06	107.93	102.98
4	B	8002	CFF	C8-N9-C4	2.06	107.92	102.98
4	D	8002	CFF	C5-C4-N9	-2.05	108.03	112.10
4	A	8002	CFF	C5-C4-N9	-2.05	108.04	112.10
4	B	8002	CFF	C5-C4-N9	-2.02	108.09	112.10
4	C	8002	CFF	C5-C4-N9	-2.02	108.09	112.10
4	D	8002	CFF	C10-N1-C2	2.00	120.83	117.33

There are no chirality outliers.

All (253) 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	A	8005	ATP	PB-O3B-PG-O2G
5	A	8005	ATP	PB-O3A-PA-O5'
5	A	8005	ATP	C5'-O5'-PA-O2A
5	B	8003	ATP	C5'-O5'-PA-O1A
5	B	8003	ATP	C5'-O5'-PA-O3A
5	B	8005	ATP	PB-O3B-PG-O2G
5	B	8005	ATP	PB-O3A-PA-O5'
5	B	8005	ATP	C5'-O5'-PA-O2A
5	C	8003	ATP	C5'-O5'-PA-O1A
5	C	8003	ATP	C5'-O5'-PA-O3A
5	C	8005	ATP	PB-O3B-PG-O2G
5	C	8005	ATP	PB-O3A-PA-O5'
5	C	8005	ATP	C5'-O5'-PA-O2A
5	D	8003	ATP	C5'-O5'-PA-O1A
5	D	8003	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
5	D	8005	ATP	PB-O3B-PG-O2G
5	D	8005	ATP	PB-O3A-PA-O5'
5	D	8005	ATP	C5'-O5'-PA-O2A
7	A	8006	PCW	C1-O3P-P-O1P
7	A	8007	PCW	O4P-C4-C5-N
7	A	8007	PCW	C1-O3P-P-O2P
7	A	8007	PCW	C4-O4P-P-O2P
7	B	8006	PCW	C1-O3P-P-O1P
7	B	8007	PCW	O4P-C4-C5-N
7	B	8007	PCW	C1-O3P-P-O2P
7	B	8007	PCW	C4-O4P-P-O2P
7	C	8006	PCW	C1-O3P-P-O1P
7	C	8007	PCW	O4P-C4-C5-N
7	C	8007	PCW	C1-O3P-P-O2P
7	C	8007	PCW	C4-O4P-P-O2P
7	D	8006	PCW	C1-O3P-P-O1P
7	D	8007	PCW	O4P-C4-C5-N
7	D	8007	PCW	C1-O3P-P-O2P
7	D	8007	PCW	C4-O4P-P-O2P
7	A	8007	PCW	C36-C37-C38-C39
7	B	8007	PCW	C36-C37-C38-C39
7	C	8007	PCW	C36-C37-C38-C39
7	D	8007	PCW	C36-C37-C38-C39
5	A	8005	ATP	O4'-C4'-C5'-O5'
5	B	8005	ATP	O4'-C4'-C5'-O5'
5	C	8005	ATP	O4'-C4'-C5'-O5'
5	D	8005	ATP	O4'-C4'-C5'-O5'
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	O31-C31-O2-C2
7	B	8006	PCW	O31-C31-O2-C2
7	C	8006	PCW	O31-C31-O2-C2
7	D	8006	PCW	O31-C31-O2-C2
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	C32-C33-C34-C35
7	D	8006	PCW	C32-C33-C34-C35
7	B	8006	PCW	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
7	C	8006	PCW	C32-C33-C34-C35
7	A	8006	PCW	C44-C45-C46-C47
7	C	8006	PCW	C44-C45-C46-C47
7	D	8006	PCW	C44-C45-C46-C47
7	B	8006	PCW	C44-C45-C46-C47
7	A	8006	PCW	C43-C44-C45-C46
7	A	8007	PCW	C24-C25-C26-C27
7	B	8006	PCW	C43-C44-C45-C46
7	C	8006	PCW	C43-C44-C45-C46
7	C	8007	PCW	C24-C25-C26-C27
7	D	8006	PCW	C43-C44-C45-C46
7	B	8007	PCW	C24-C25-C26-C27
7	D	8007	PCW	C24-C25-C26-C27
7	A	8007	PCW	C22-C23-C24-C25
7	A	8007	PCW	C44-C45-C46-C47
7	B	8007	PCW	C22-C23-C24-C25
7	B	8007	PCW	C44-C45-C46-C47
7	C	8007	PCW	C44-C45-C46-C47
7	D	8007	PCW	C22-C23-C24-C25
7	D	8007	PCW	C44-C45-C46-C47
7	C	8007	PCW	C22-C23-C24-C25
5	A	8005	ATP	C4'-C5'-O5'-PA
5	B	8005	ATP	C4'-C5'-O5'-PA
5	C	8005	ATP	C4'-C5'-O5'-PA
5	D	8005	ATP	C4'-C5'-O5'-PA
7	A	8007	PCW	C43-C44-C45-C46
7	C	8007	PCW	C43-C44-C45-C46
7	D	8007	PCW	C43-C44-C45-C46
7	B	8007	PCW	C43-C44-C45-C46
7	A	8007	PCW	C40-C41-C42-C43
7	B	8007	PCW	C40-C41-C42-C43
7	C	8007	PCW	C40-C41-C42-C43
7	D	8007	PCW	C40-C41-C42-C43
7	A	8007	PCW	O3P-C1-C2-C3
7	B	8007	PCW	O3P-C1-C2-C3
7	C	8007	PCW	O3P-C1-C2-C3
7	D	8007	PCW	O3P-C1-C2-C3
7	A	8007	PCW	C32-C31-O2-C2
7	B	8007	PCW	C32-C31-O2-C2
7	C	8007	PCW	C32-C31-O2-C2
7	D	8007	PCW	C32-C31-O2-C2
7	A	8006	PCW	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
7	B	8006	PCW	C35-C36-C37-C38
7	C	8006	PCW	C35-C36-C37-C38
7	D	8006	PCW	C35-C36-C37-C38
5	A	8005	ATP	PB-O3B-PG-O1G
5	B	8005	ATP	PB-O3B-PG-O1G
5	C	8005	ATP	PB-O3B-PG-O1G
5	D	8005	ATP	PB-O3B-PG-O1G
7	A	8006	PCW	C20-C21-C22-C23
7	B	8006	PCW	C20-C21-C22-C23
7	C	8006	PCW	C20-C21-C22-C23
7	D	8006	PCW	C20-C21-C22-C23
7	D	8006	PCW	C23-C24-C25-C26
7	A	8006	PCW	C23-C24-C25-C26
7	B	8006	PCW	C23-C24-C25-C26
7	C	8006	PCW	C23-C24-C25-C26
7	A	8007	PCW	C12-C11-O3-C3
7	B	8007	PCW	C12-C11-O3-C3
7	C	8007	PCW	C12-C11-O3-C3
7	D	8007	PCW	C12-C11-O3-C3
7	A	8007	PCW	C34-C35-C36-C37
7	B	8007	PCW	C34-C35-C36-C37
7	C	8007	PCW	C34-C35-C36-C37
7	D	8007	PCW	C34-C35-C36-C37
7	A	8007	PCW	O2-C2-C3-O3
7	B	8007	PCW	O2-C2-C3-O3
7	C	8007	PCW	O2-C2-C3-O3
7	D	8007	PCW	O2-C2-C3-O3
7	A	8007	PCW	C12-C13-C14-C15
7	B	8007	PCW	C12-C13-C14-C15
7	C	8007	PCW	C12-C13-C14-C15
7	D	8007	PCW	C12-C13-C14-C15
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
7	B	8007	PCW	C31-C32-C33-C34
7	A	8007	PCW	C31-C32-C33-C34
7	C	8007	PCW	C31-C32-C33-C34
7	D	8007	PCW	C31-C32-C33-C34
7	A	8007	PCW	O11-C11-O3-C3
7	B	8007	PCW	O11-C11-O3-C3
7	C	8007	PCW	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
7	D	8007	PCW	O11-C11-O3-C3
7	A	8007	PCW	O31-C31-O2-C2
7	B	8007	PCW	O31-C31-O2-C2
7	C	8007	PCW	O31-C31-O2-C2
7	D	8007	PCW	O31-C31-O2-C2
5	A	8005	ATP	PG-O3B-PB-O2B
5	B	8005	ATP	PG-O3B-PB-O2B
5	C	8005	ATP	PG-O3B-PB-O2B
5	D	8005	ATP	PG-O3B-PB-O2B
7	A	8006	PCW	C19-C20-C21-C22
7	D	8006	PCW	C19-C20-C21-C22
7	B	8006	PCW	C19-C20-C21-C22
7	C	8006	PCW	C19-C20-C21-C22
7	A	8007	PCW	C33-C34-C35-C36
7	B	8007	PCW	C33-C34-C35-C36
7	C	8007	PCW	C33-C34-C35-C36
7	D	8007	PCW	C33-C34-C35-C36
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	O2-C2-C3-O3
7	B	8006	PCW	O2-C2-C3-O3
7	C	8006	PCW	O2-C2-C3-O3
7	D	8006	PCW	O2-C2-C3-O3
7	B	8007	PCW	C41-C42-C43-C44
7	D	8007	PCW	C41-C42-C43-C44
7	A	8007	PCW	C41-C42-C43-C44
7	C	8007	PCW	C41-C42-C43-C44
5	A	8003	ATP	C5'-O5'-PA-O2A
5	B	8003	ATP	C5'-O5'-PA-O2A
5	C	8003	ATP	C5'-O5'-PA-O2A
5	D	8003	ATP	C5'-O5'-PA-O2A
7	A	8006	PCW	C1-O3P-P-O2P
7	A	8006	PCW	C1-O3P-P-O4P
7	B	8006	PCW	C1-O3P-P-O2P
7	B	8006	PCW	C1-O3P-P-O4P
7	C	8006	PCW	C1-O3P-P-O2P
7	C	8006	PCW	C1-O3P-P-O4P
7	D	8006	PCW	C1-O3P-P-O2P
7	D	8006	PCW	C1-O3P-P-O4P
7	A	8006	PCW	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
7	B	8006	PCW	C31-C32-C33-C34
7	C	8006	PCW	C31-C32-C33-C34
7	D	8006	PCW	C31-C32-C33-C34
7	B	8006	PCW	C14-C15-C16-C17
7	D	8006	PCW	C14-C15-C16-C17
7	A	8006	PCW	C14-C15-C16-C17
7	C	8006	PCW	C14-C15-C16-C17
7	A	8007	PCW	O3P-C1-C2-O2
7	B	8007	PCW	O3P-C1-C2-O2
7	C	8007	PCW	O3P-C1-C2-O2
7	D	8007	PCW	O3P-C1-C2-O2
7	A	8006	PCW	C40-C41-C42-C43
7	B	8006	PCW	C40-C41-C42-C43
7	C	8006	PCW	C40-C41-C42-C43
7	D	8006	PCW	C40-C41-C42-C43
7	A	8007	PCW	C17-C18-C19-C20
7	B	8007	PCW	C17-C18-C19-C20
7	C	8007	PCW	C17-C18-C19-C20
7	D	8007	PCW	C17-C18-C19-C20
7	B	8007	PCW	C25-C26-C27-C28
7	A	8007	PCW	C25-C26-C27-C28
7	C	8007	PCW	C25-C26-C27-C28
7	D	8007	PCW	C25-C26-C27-C28
7	A	8006	PCW	C1-C2-C3-O3
7	B	8006	PCW	C1-C2-C3-O3
7	C	8006	PCW	C1-C2-C3-O3
7	D	8006	PCW	C1-C2-C3-O3
7	A	8007	PCW	C42-C43-C44-C45
7	B	8007	PCW	C42-C43-C44-C45
7	D	8007	PCW	C42-C43-C44-C45
7	C	8007	PCW	C42-C43-C44-C45
7	A	8006	PCW	C37-C38-C39-C40
7	A	8006	PCW	C13-C14-C15-C16
7	B	8006	PCW	C13-C14-C15-C16
7	C	8006	PCW	C13-C14-C15-C16
7	D	8006	PCW	C13-C14-C15-C16
7	D	8006	PCW	C37-C38-C39-C40
7	B	8006	PCW	C41-C42-C43-C44
7	C	8006	PCW	C41-C42-C43-C44
7	A	8006	PCW	C41-C42-C43-C44
7	D	8006	PCW	C41-C42-C43-C44
7	B	8006	PCW	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
7	C	8006	PCW	C37-C38-C39-C40
7	D	8007	PCW	C15-C16-C17-C18
7	A	8007	PCW	C15-C16-C17-C18
7	C	8007	PCW	C15-C16-C17-C18
7	B	8007	PCW	C15-C16-C17-C18
7	A	8007	PCW	C1-C2-C3-O3
7	B	8007	PCW	C1-C2-C3-O3
7	C	8007	PCW	C1-C2-C3-O3
7	D	8007	PCW	C1-C2-C3-O3
7	A	8006	PCW	O2-C31-C32-C33
7	B	8006	PCW	O2-C31-C32-C33
7	C	8006	PCW	O2-C31-C32-C33
7	D	8006	PCW	O2-C31-C32-C33
7	A	8007	PCW	C37-C38-C39-C40
7	B	8007	PCW	C37-C38-C39-C40
7	C	8007	PCW	C37-C38-C39-C40
7	D	8007	PCW	C37-C38-C39-C40
7	A	8006	PCW	O31-C31-C32-C33
7	B	8006	PCW	O31-C31-C32-C33
7	C	8006	PCW	O31-C31-C32-C33
7	D	8006	PCW	O31-C31-C32-C33
5	A	8005	ATP	PG-O3B-PB-O1B
5	B	8005	ATP	PG-O3B-PB-O1B
5	C	8005	ATP	PG-O3B-PB-O1B
5	D	8005	ATP	PG-O3B-PB-O1B
7	B	8007	PCW	C32-C33-C34-C35

There are no ring outliers.

12 monomers are involved in 8 short contacts:

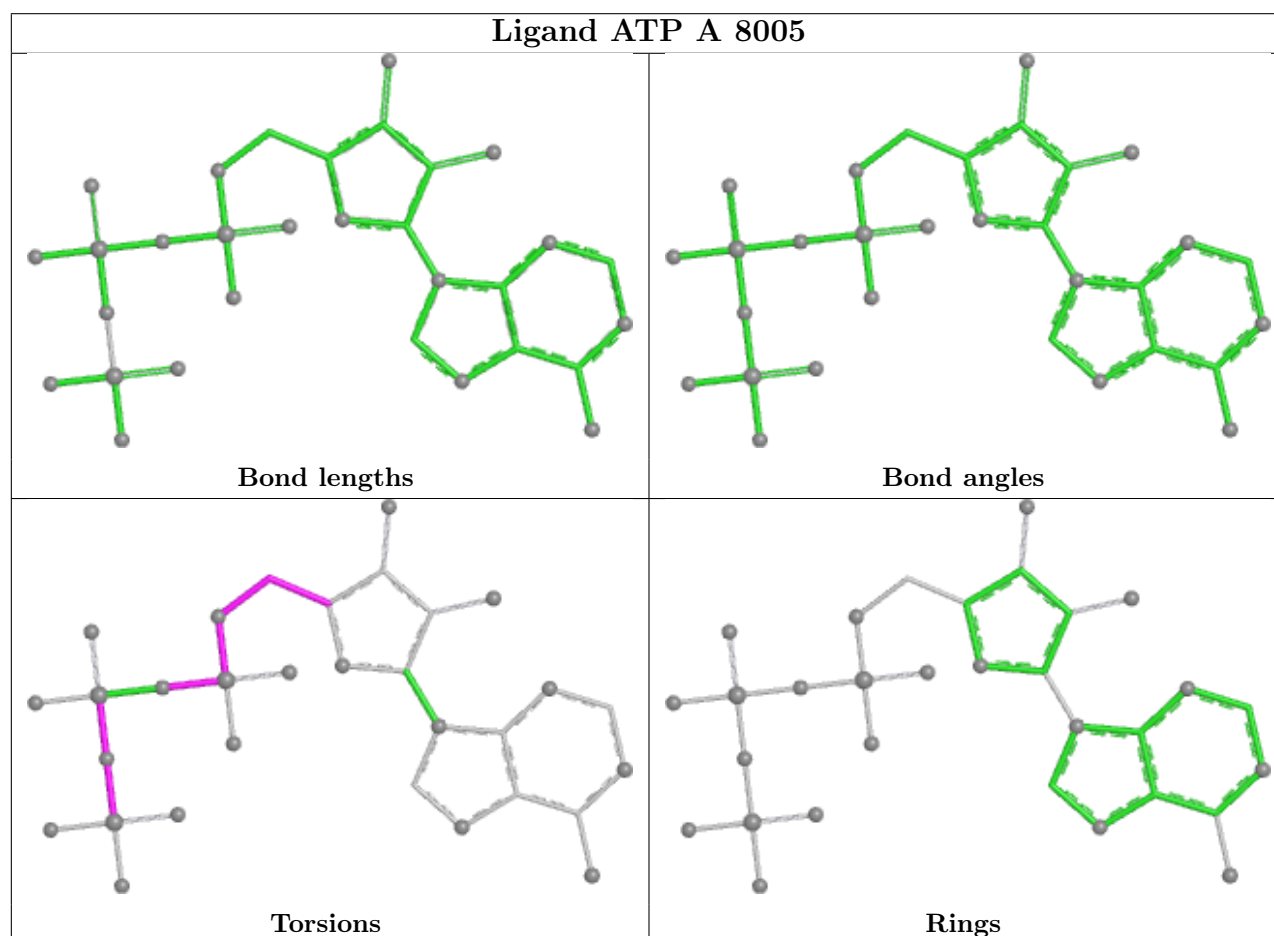
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8005	ATP	1	0
7	D	8006	PCW	1	0
5	D	8005	ATP	1	0
7	A	8007	PCW	1	0
7	B	8006	PCW	1	0
5	C	8005	ATP	1	0
7	C	8006	PCW	1	0
7	D	8007	PCW	1	0
7	A	8006	PCW	1	0
7	B	8007	PCW	1	0
7	C	8007	PCW	1	0

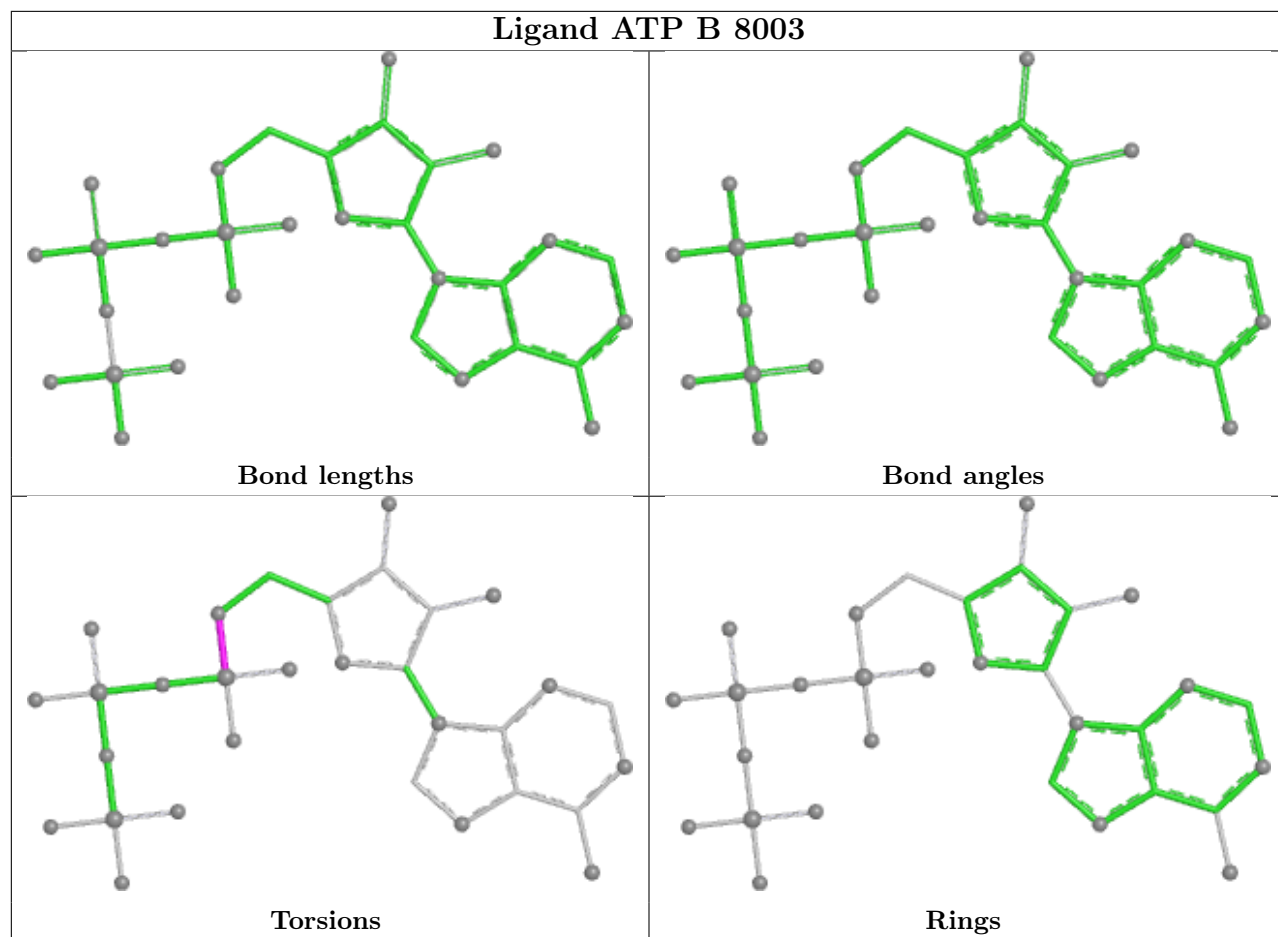
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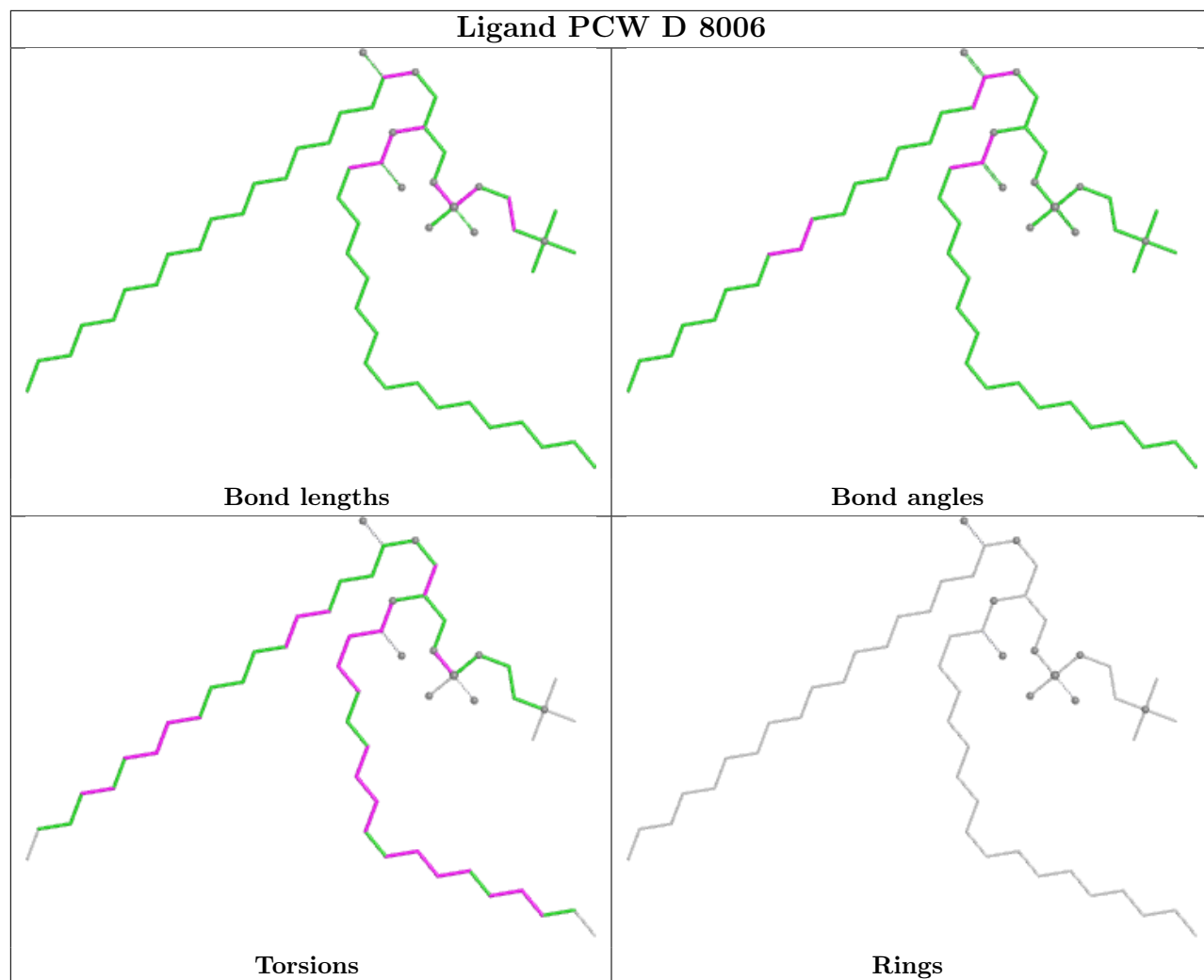
Continued from previous page...

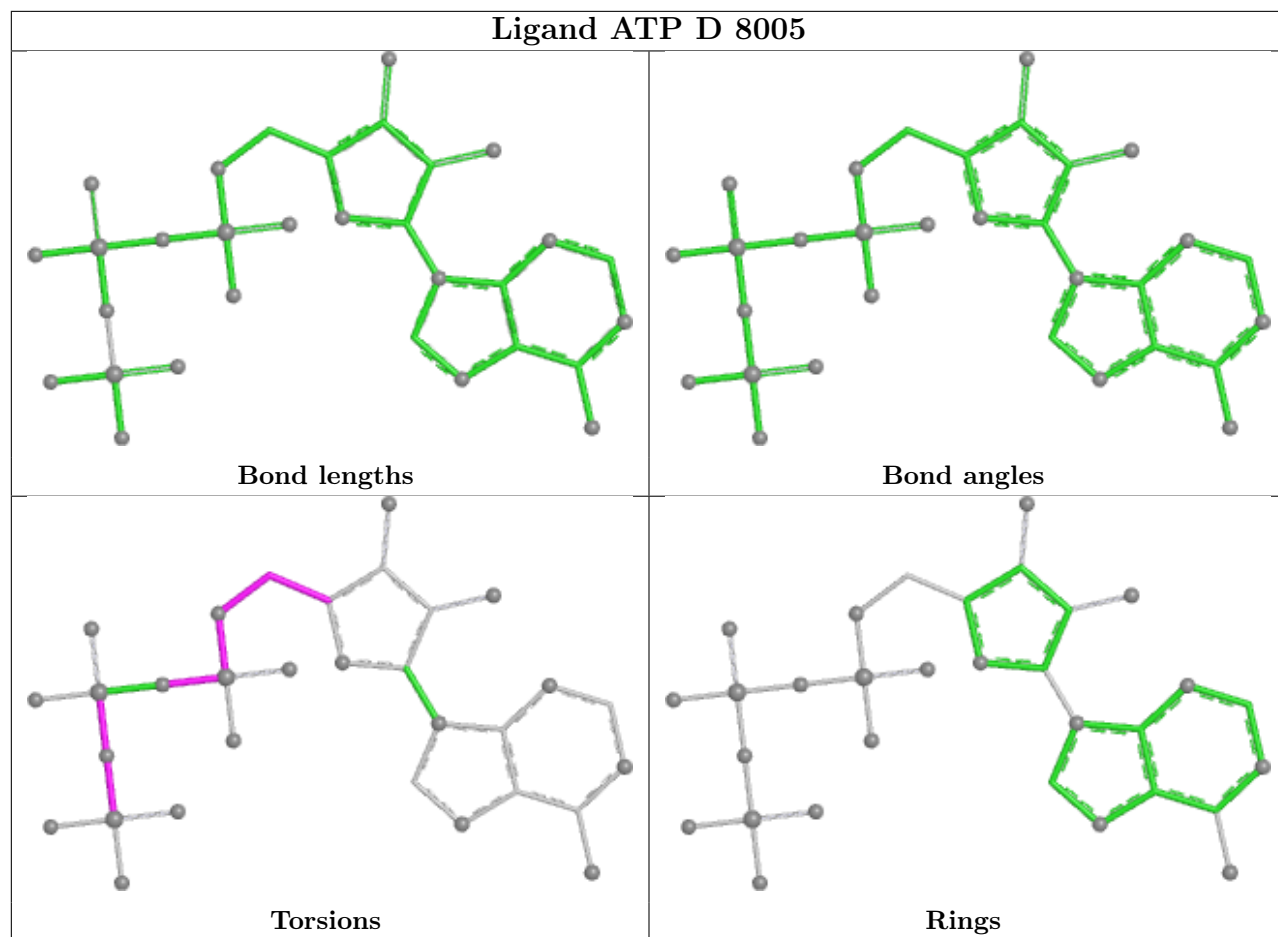
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	8005	ATP	1	0

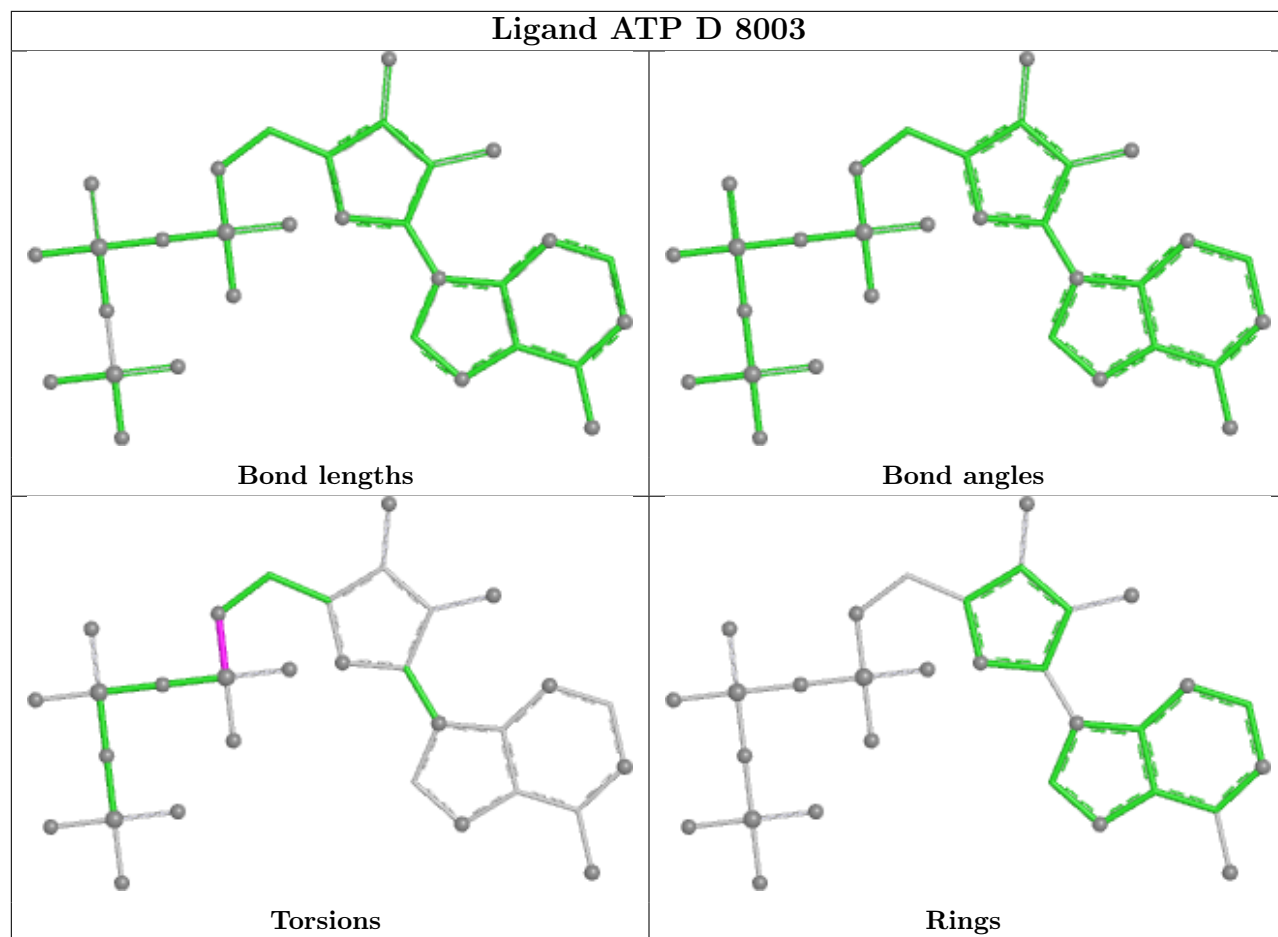
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

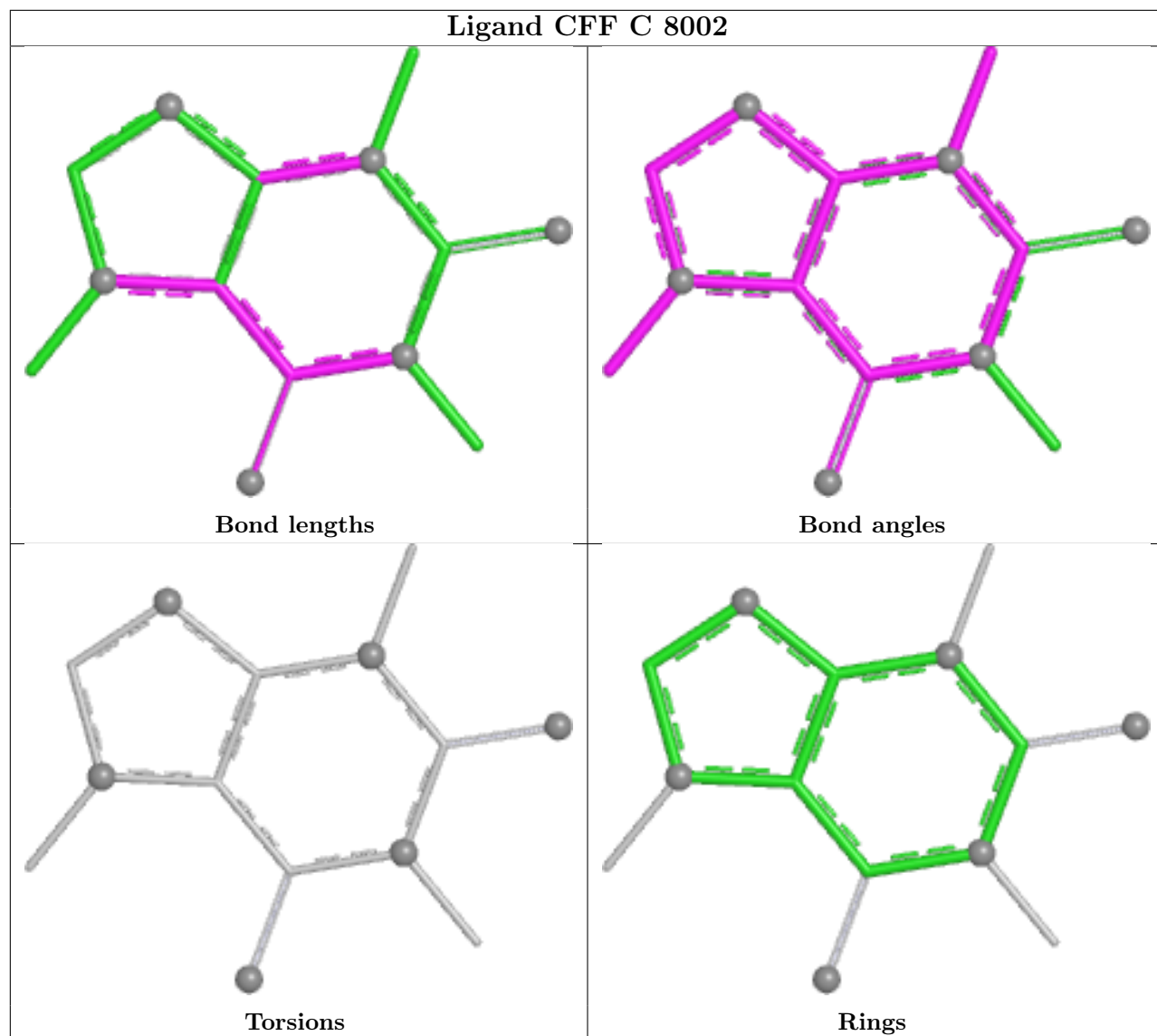


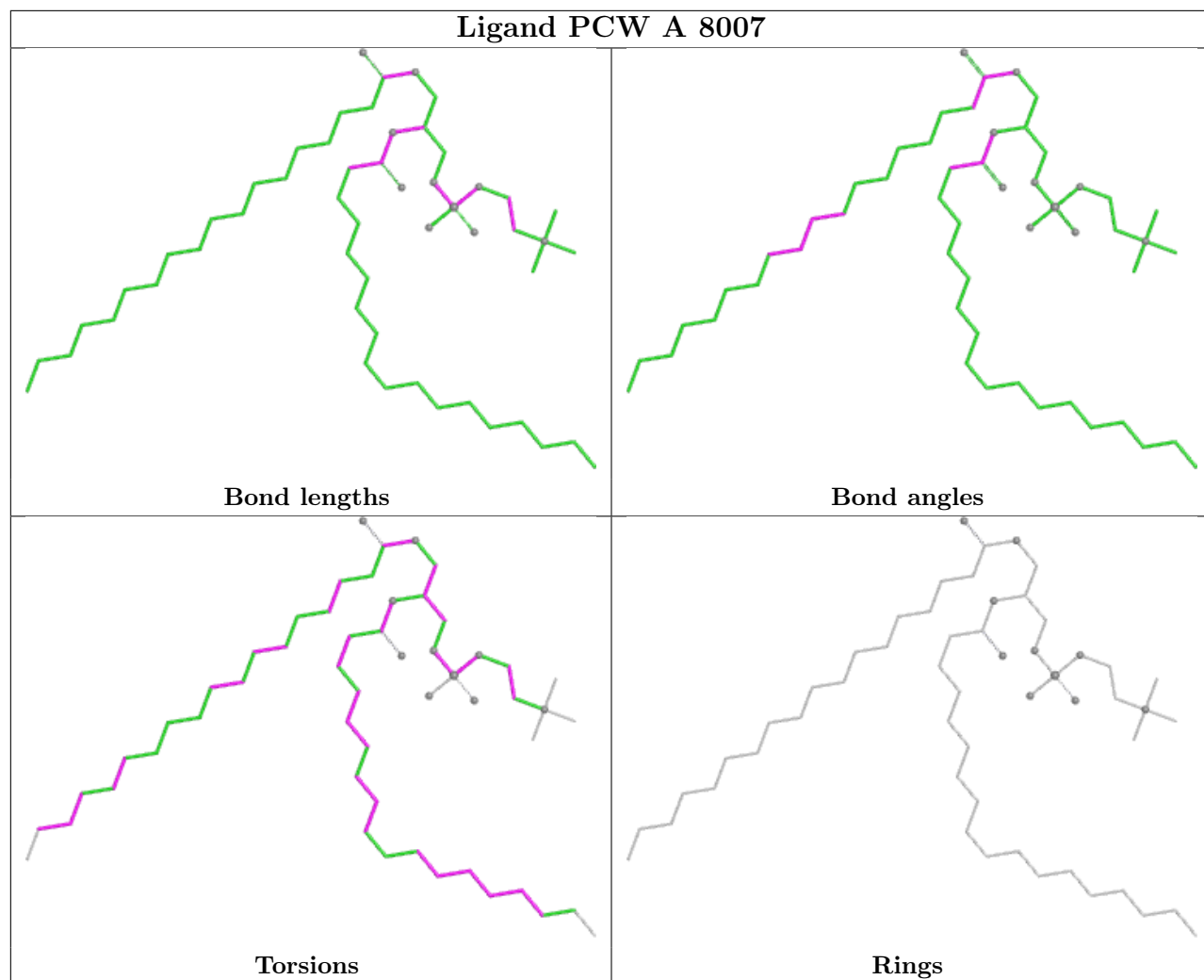


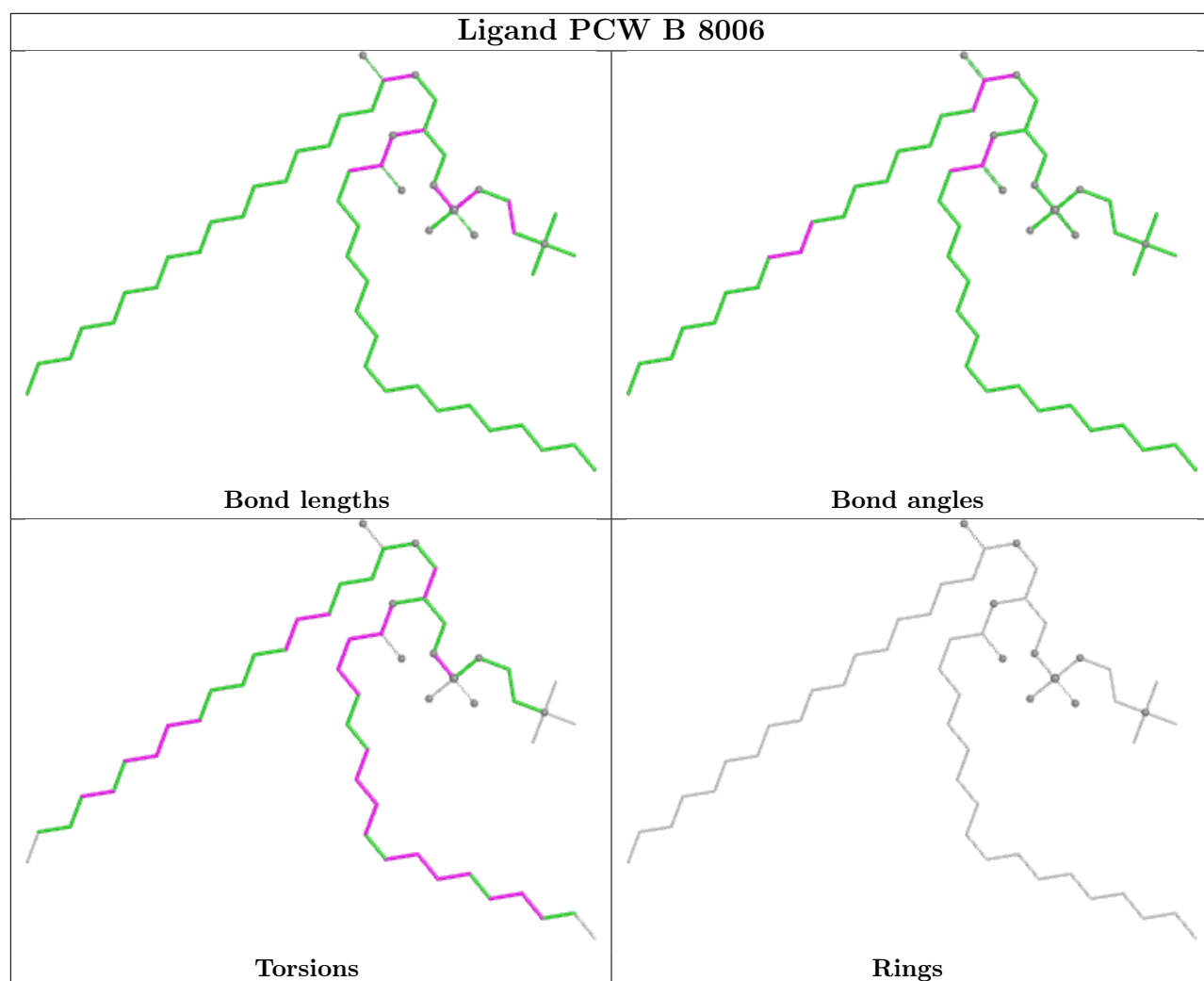


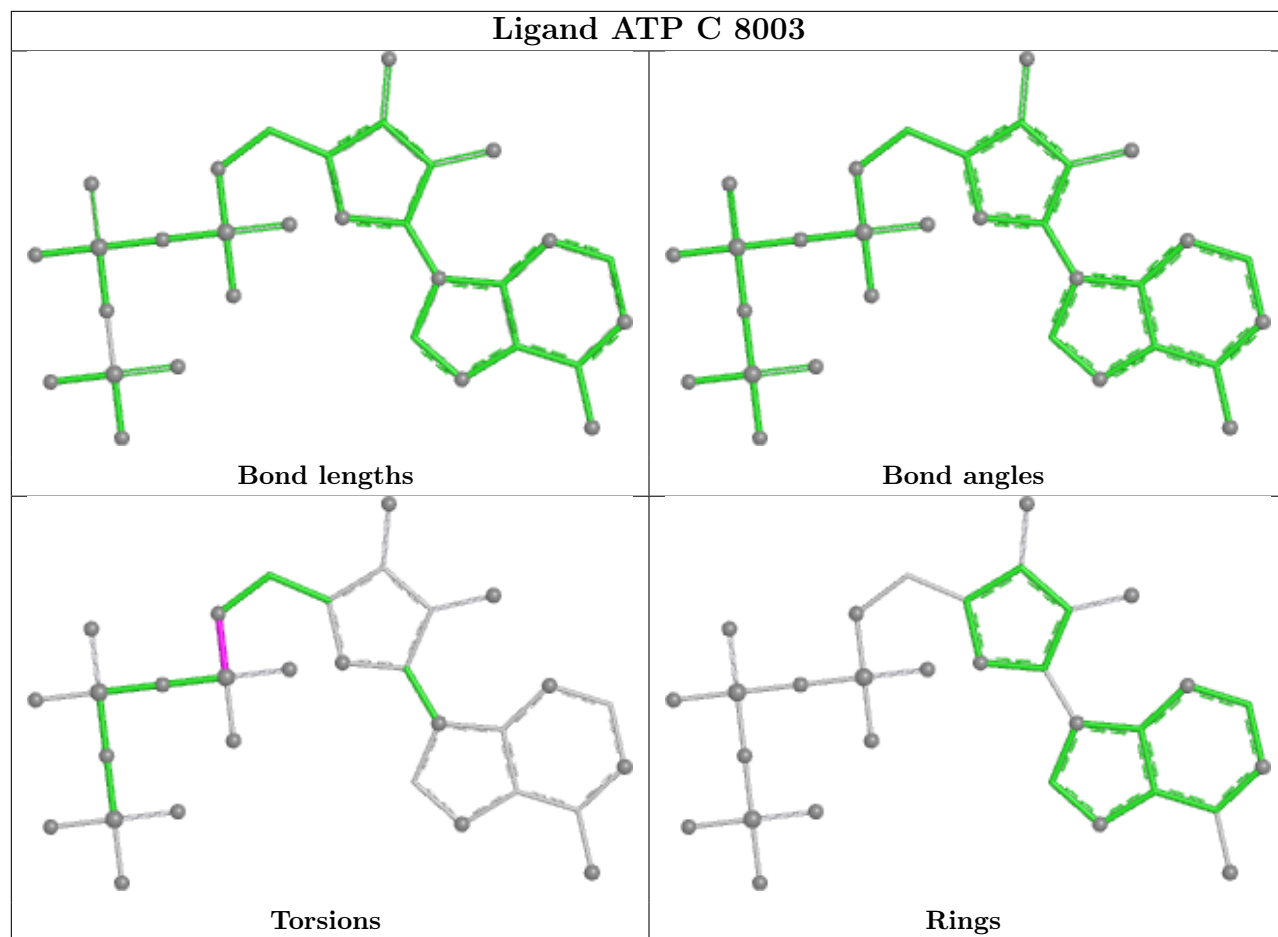


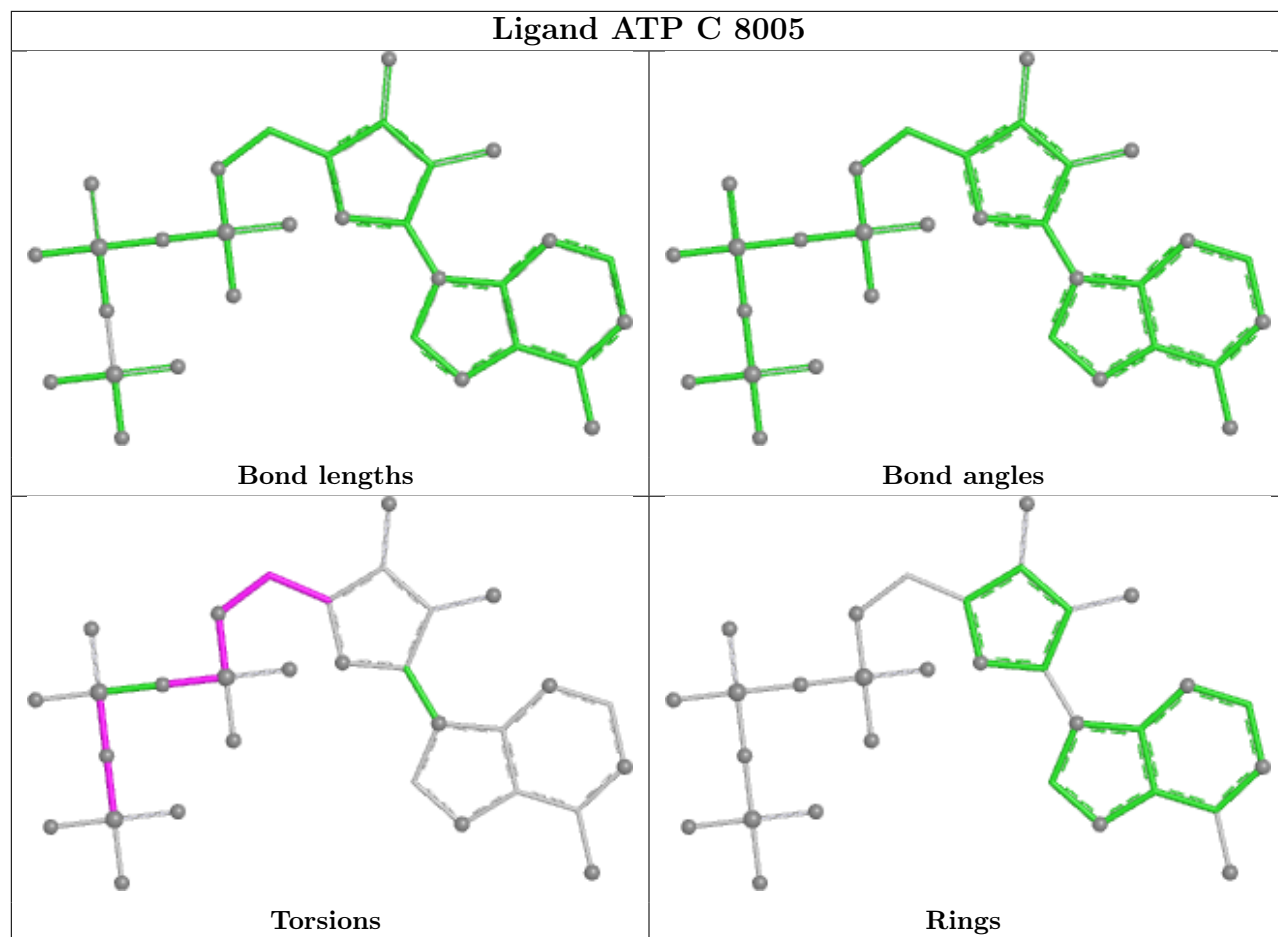


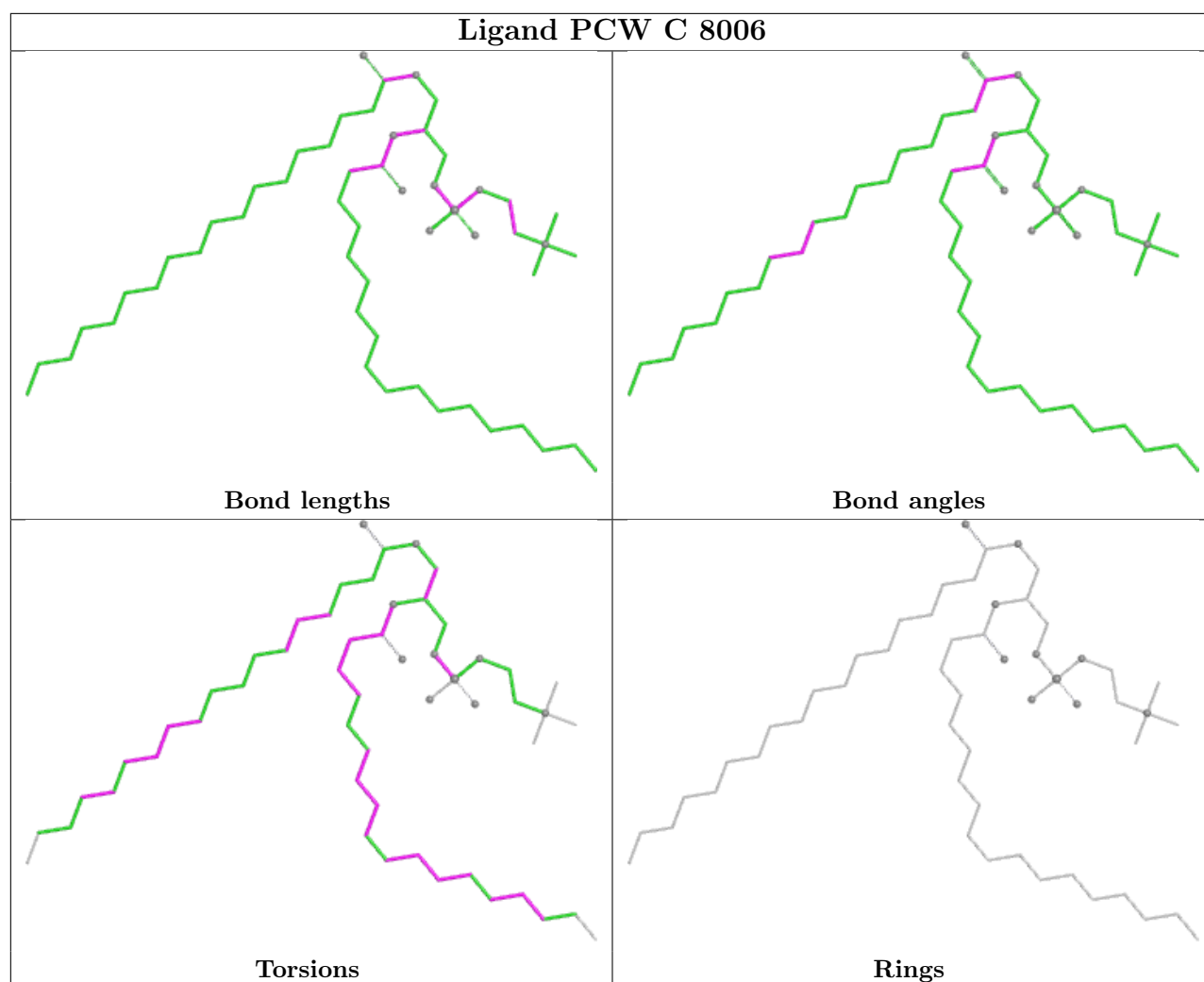


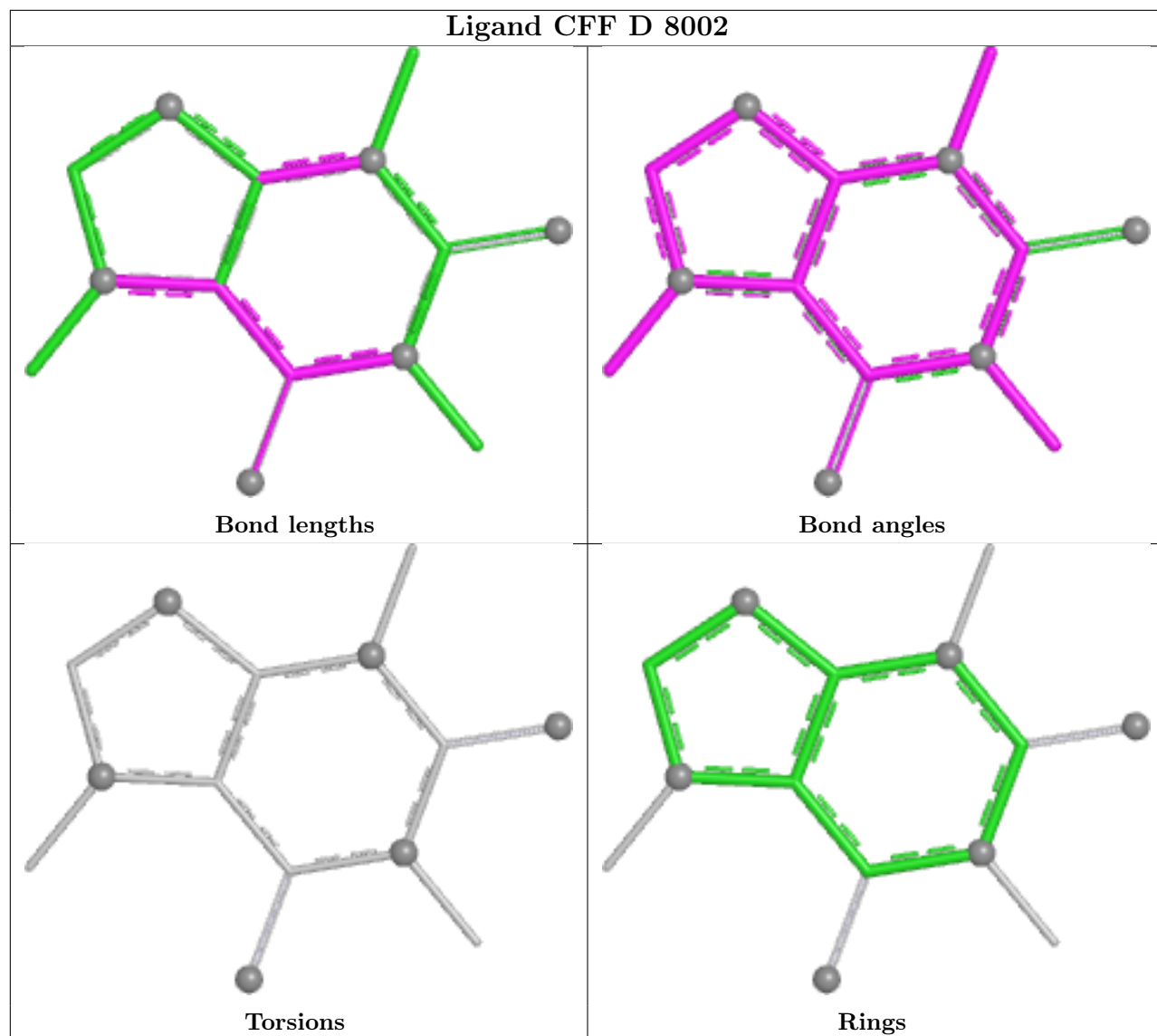


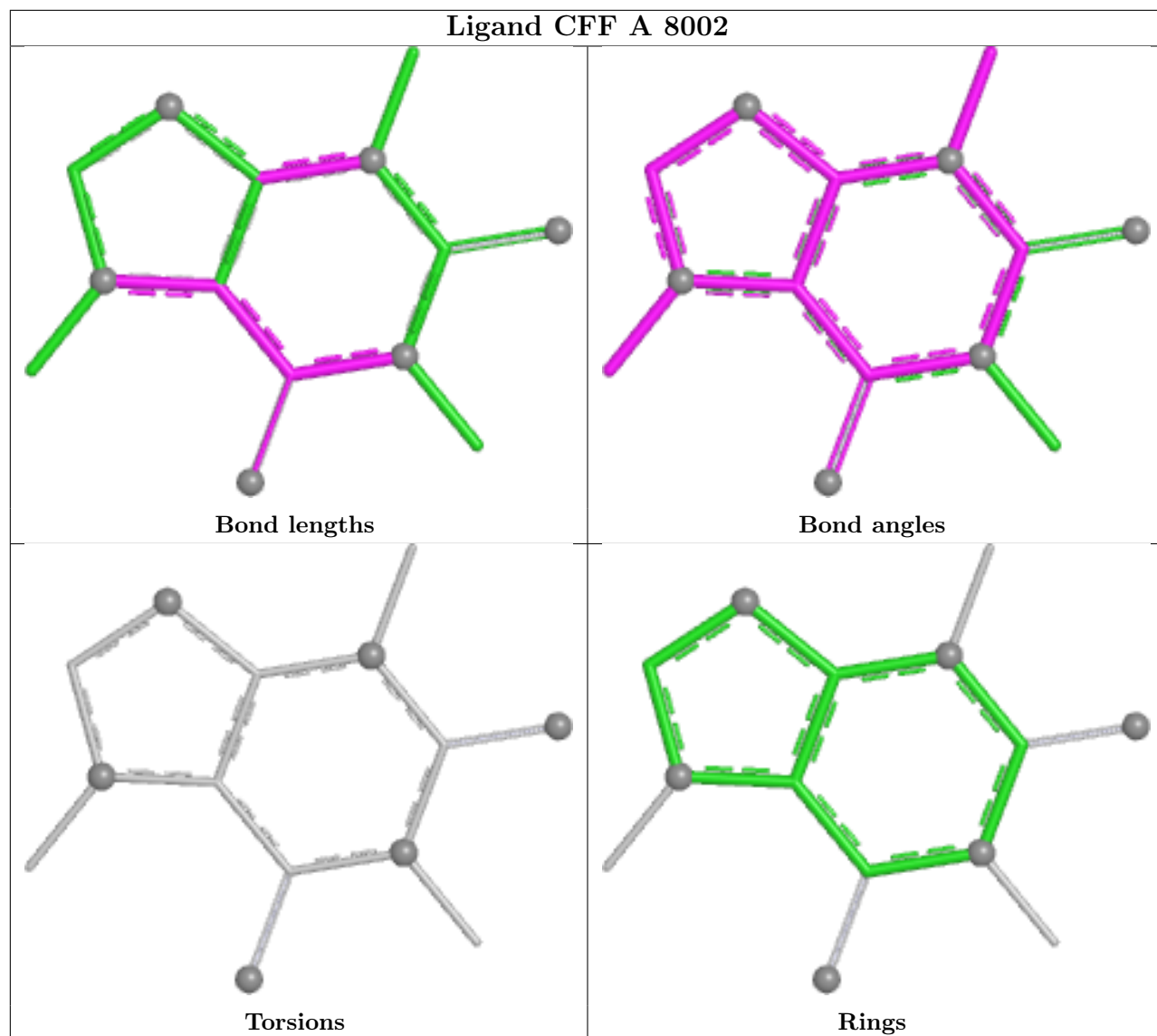


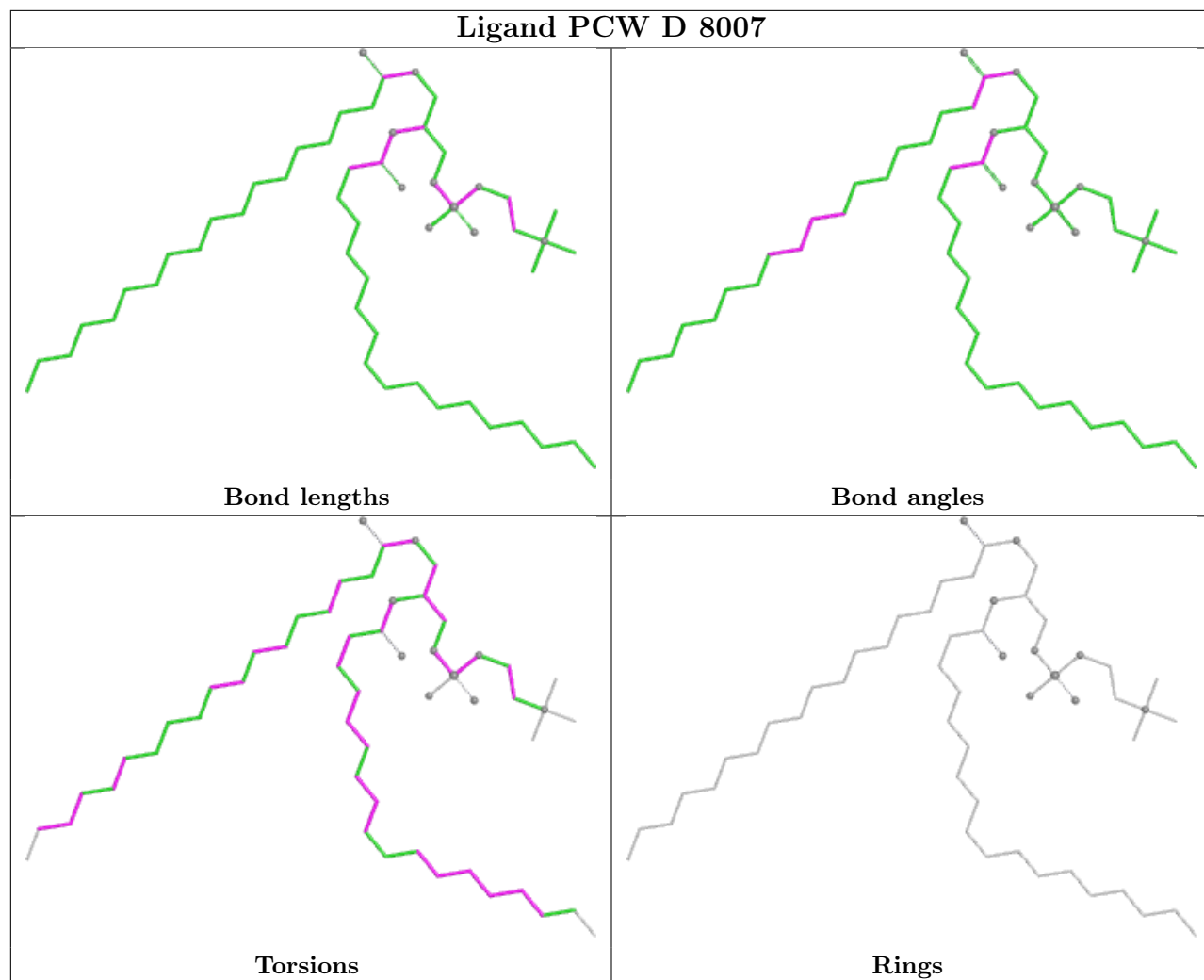


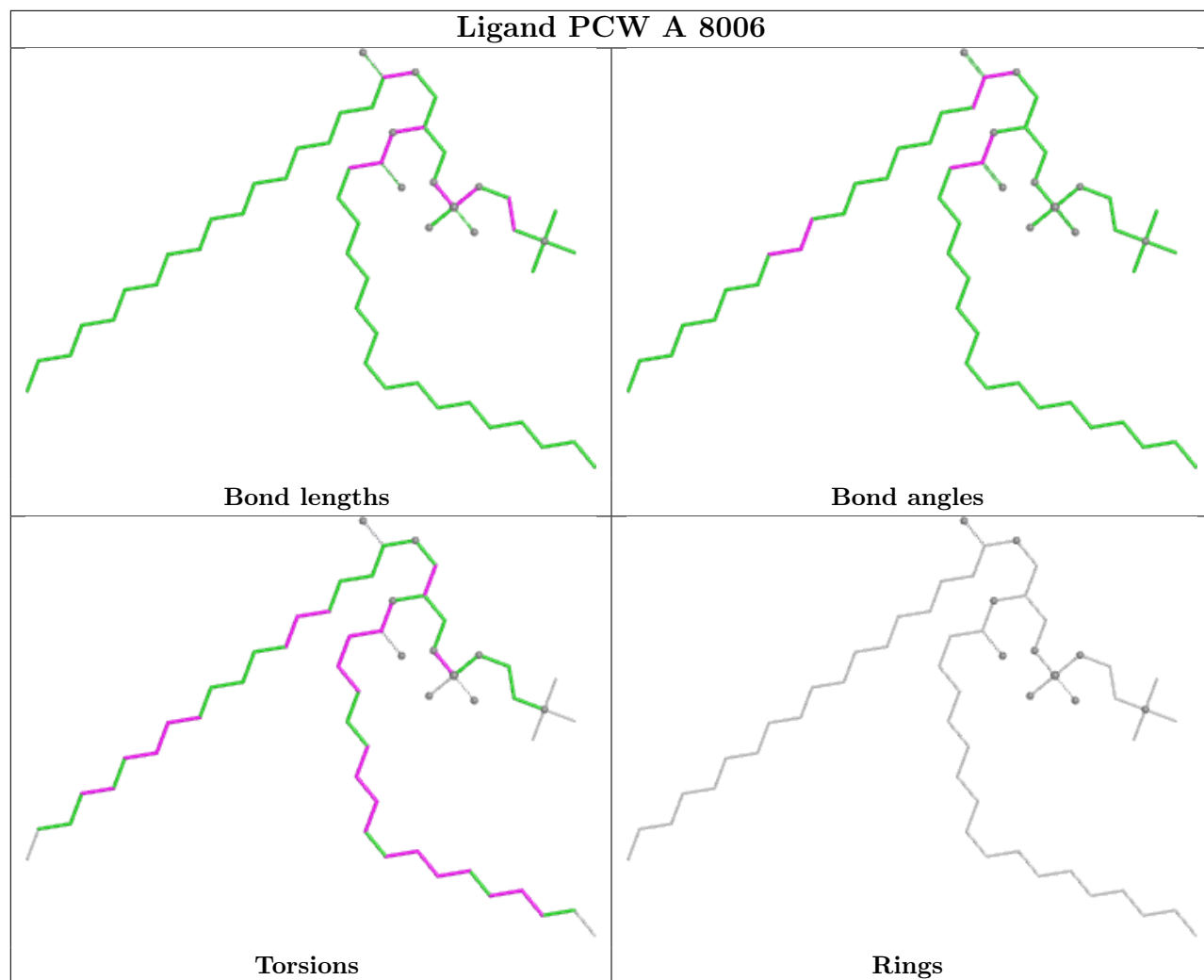


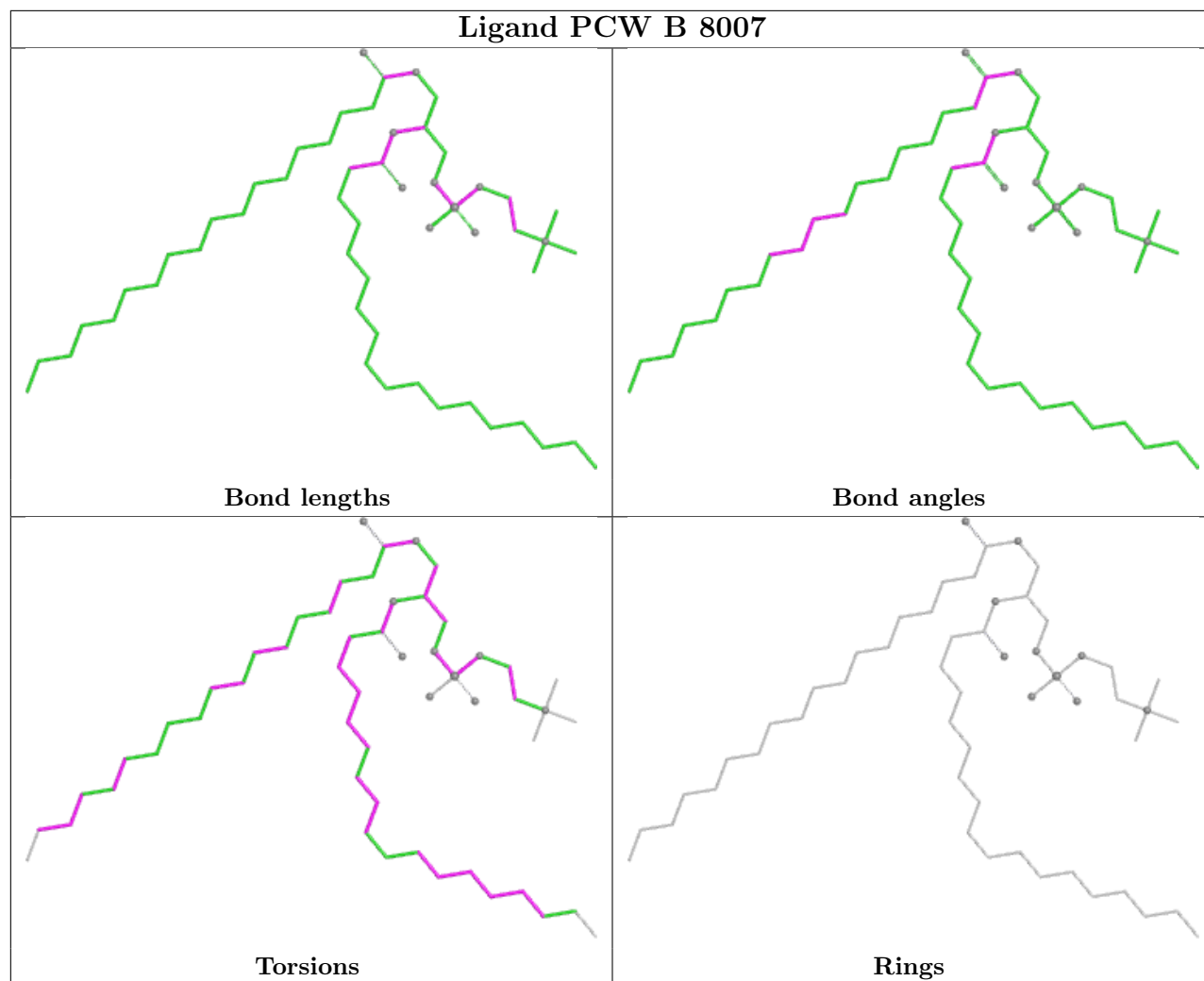


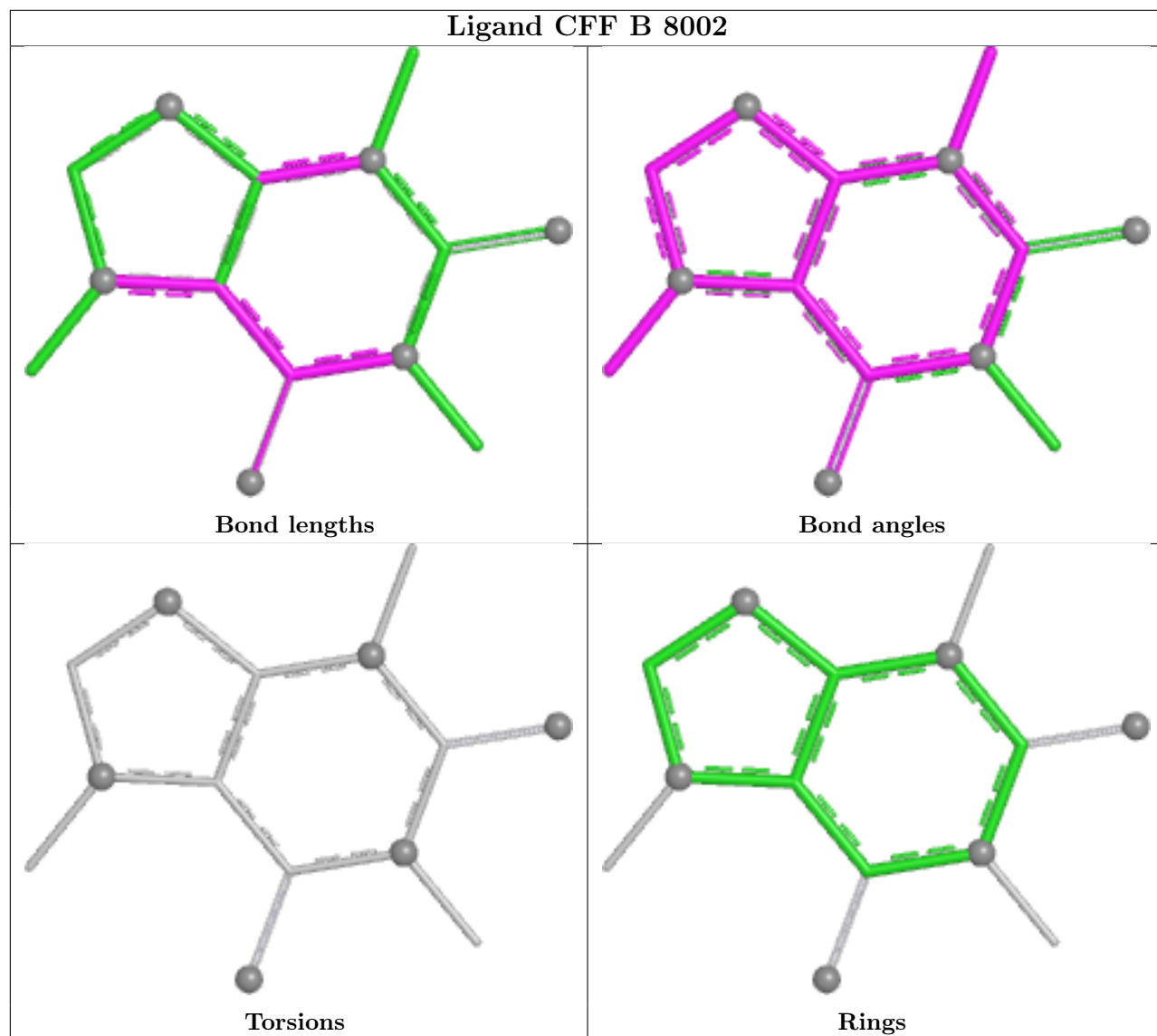


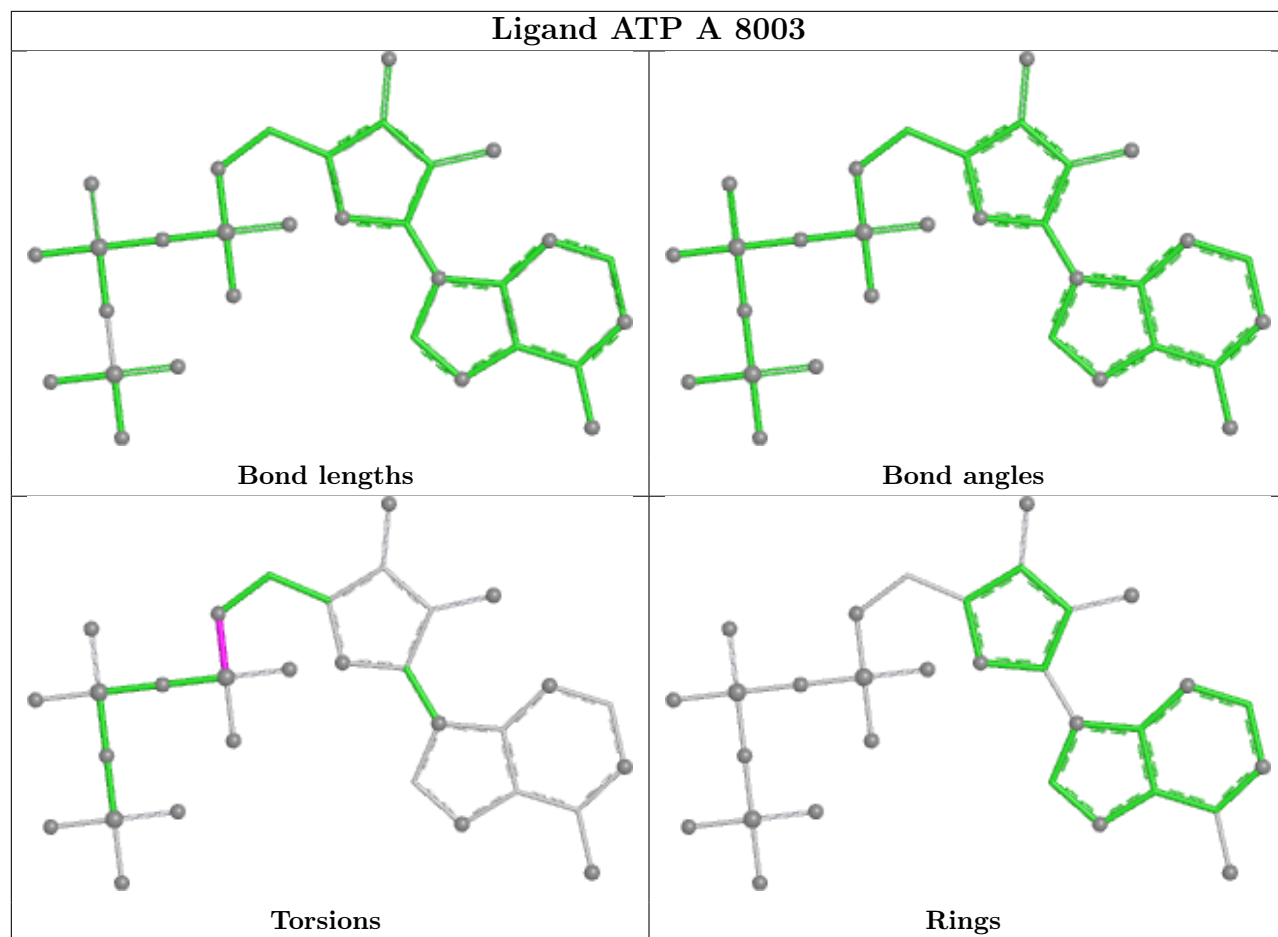


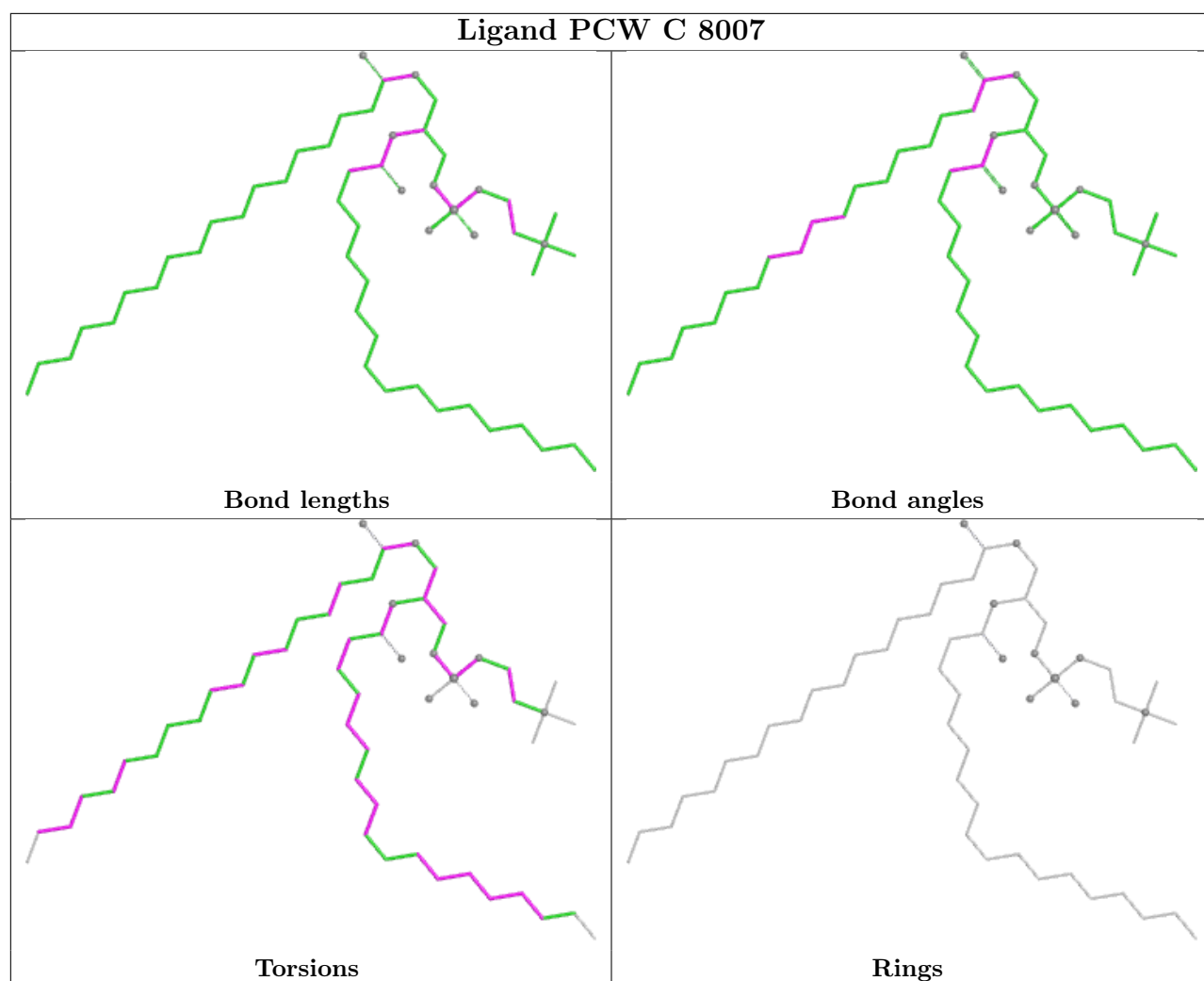


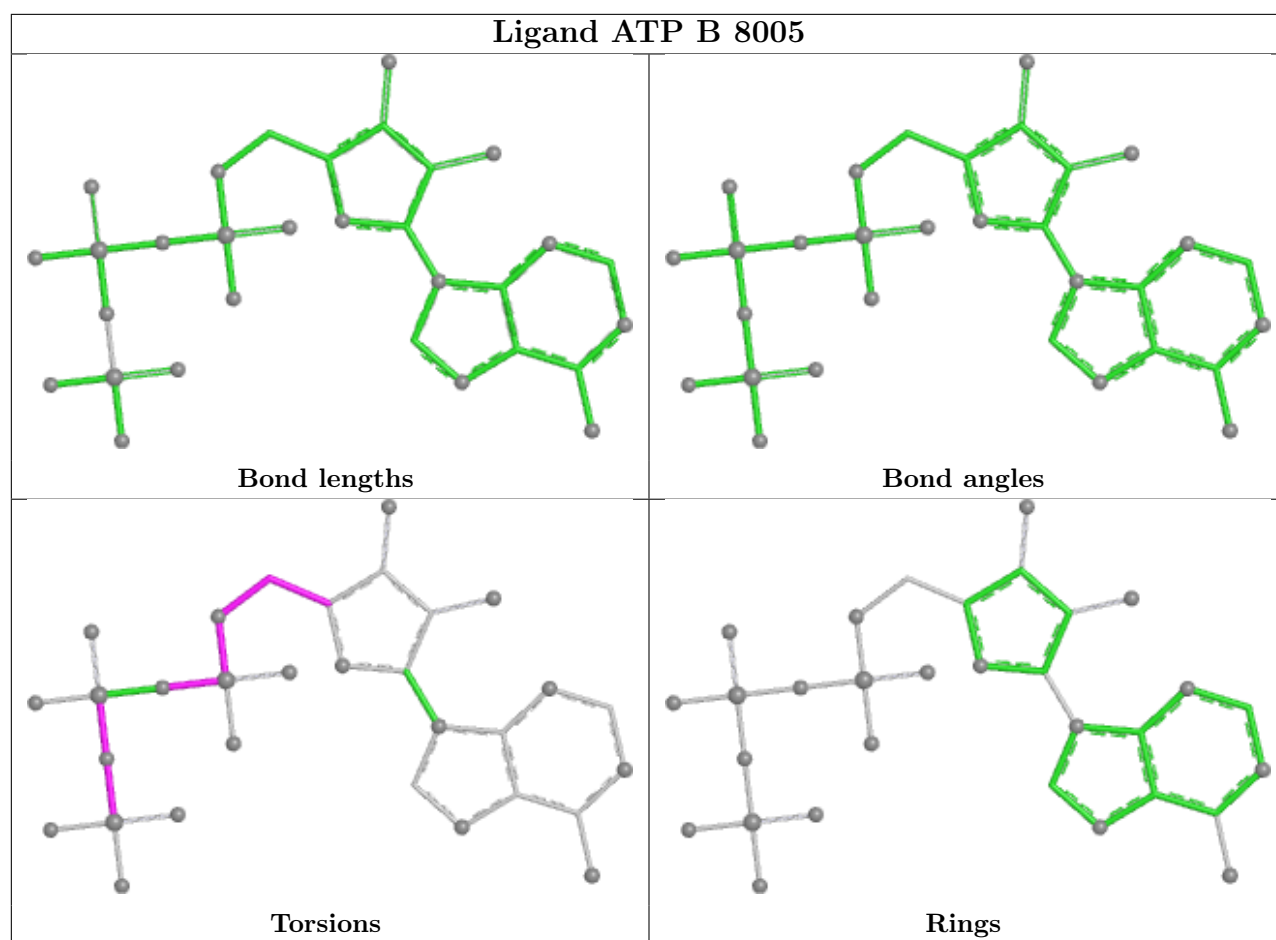












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

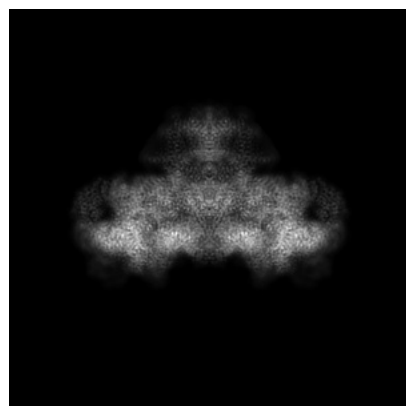
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49535. These allow visual inspection of the internal detail of the map and identification of artifacts.

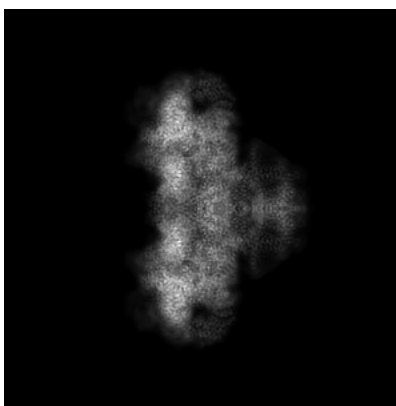
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

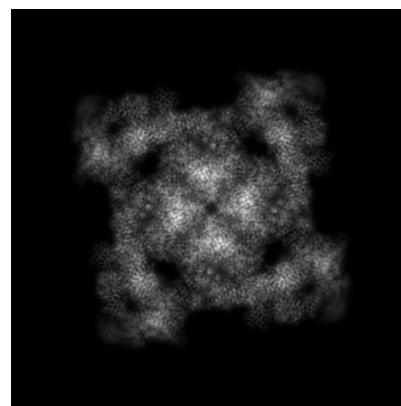
6.1.1 Primary map



X

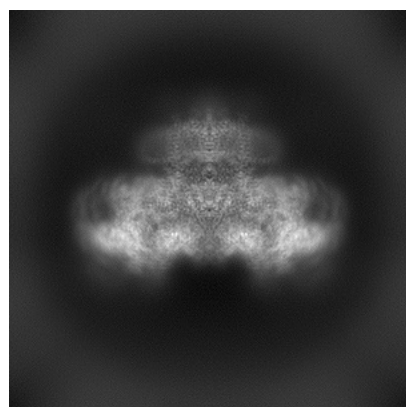


Y

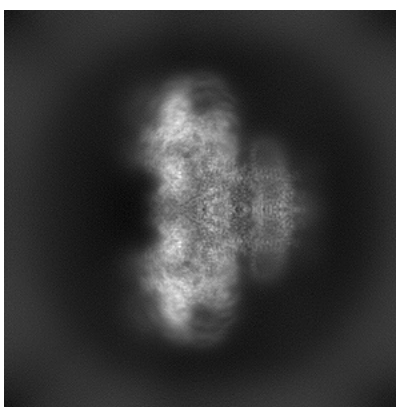


Z

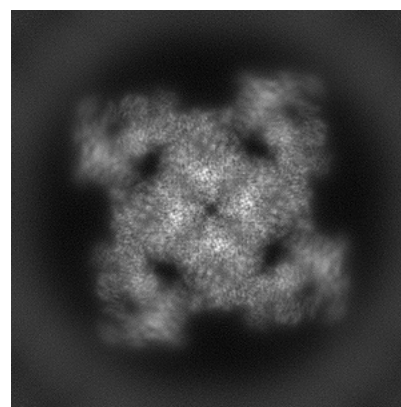
6.1.2 Raw map



X



Y

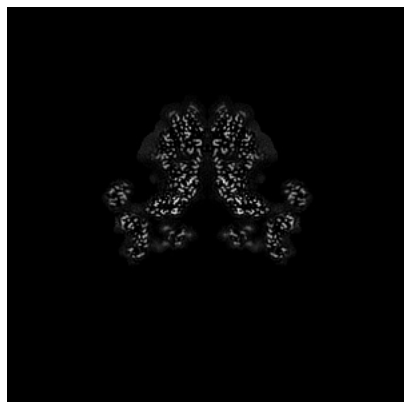


Z

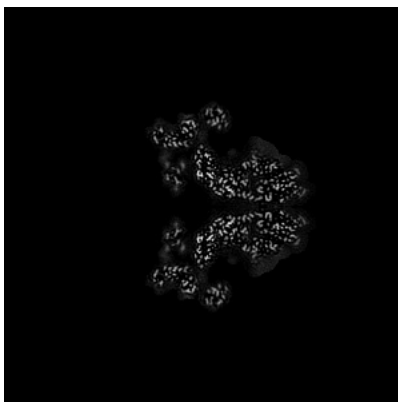
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

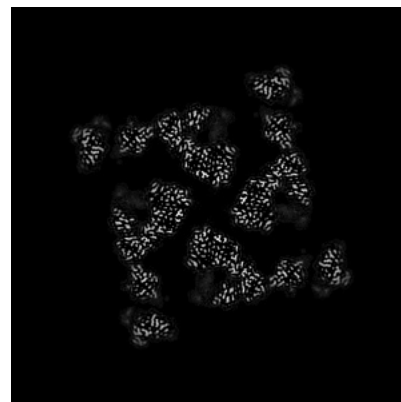
6.2.1 Primary map



X Index: 256

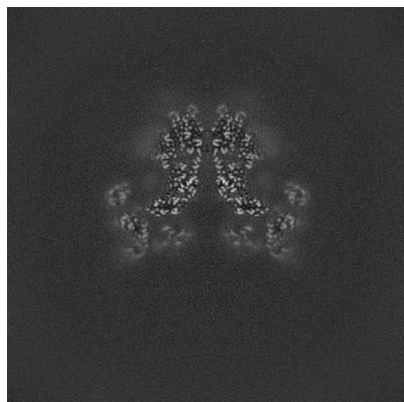


Y Index: 256

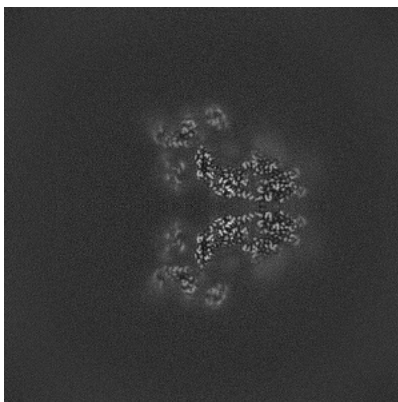


Z Index: 256

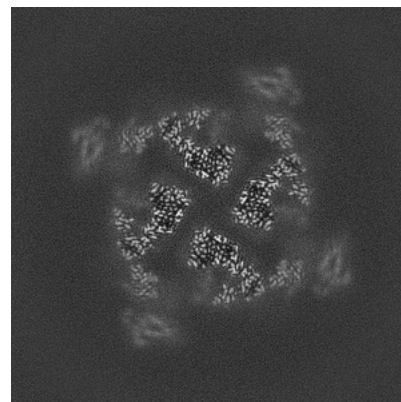
6.2.2 Raw map



X Index: 256



Y Index: 256

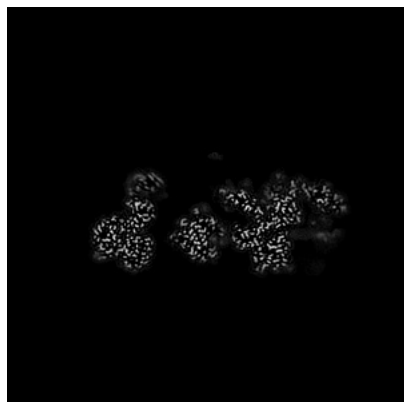


Z Index: 256

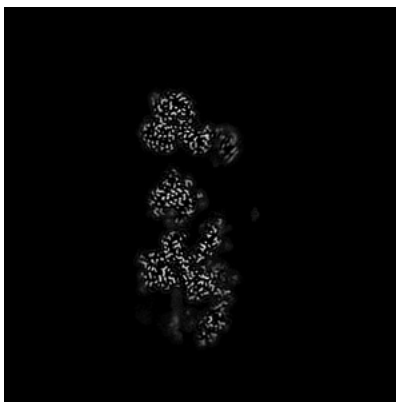
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

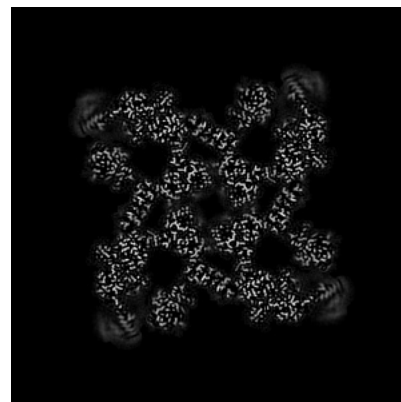
6.3.1 Primary map



X Index: 347

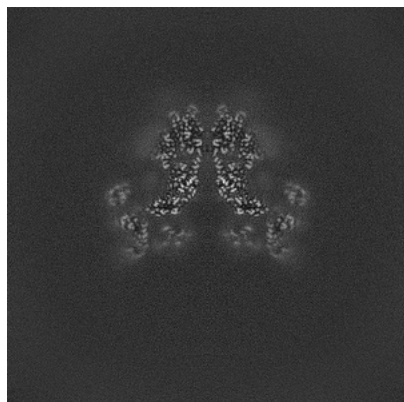


Y Index: 347

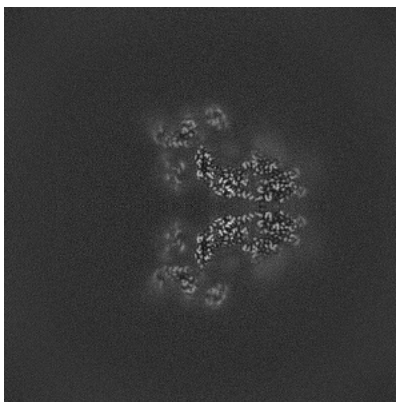


Z Index: 225

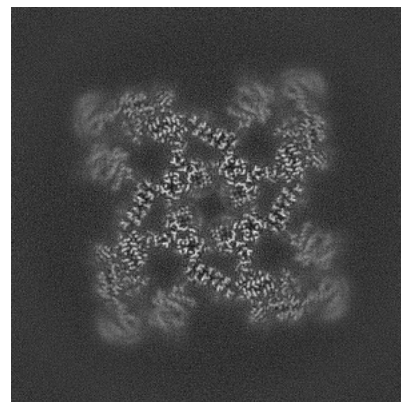
6.3.2 Raw map



X Index: 256



Y Index: 256

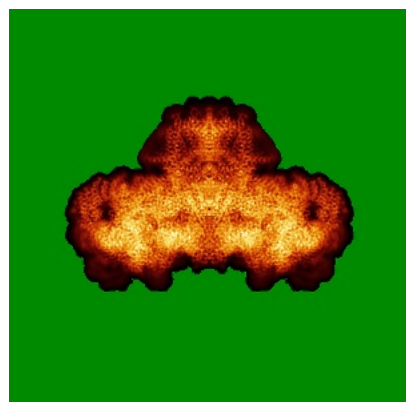


Z Index: 225

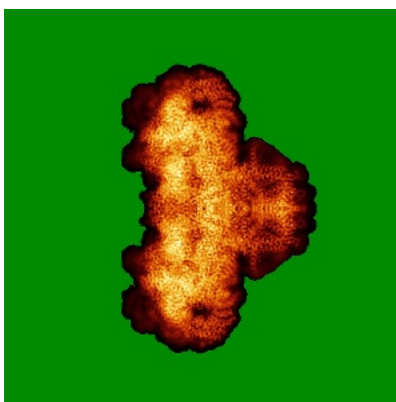
The images above show the largest variance slices of the map in three orthogonal directions.

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

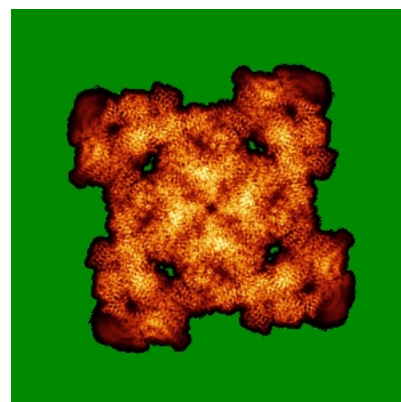
6.4.1 Primary map



X

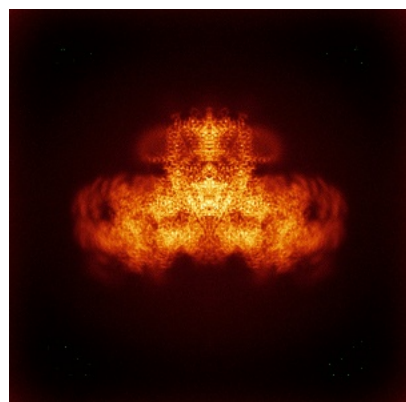


Y

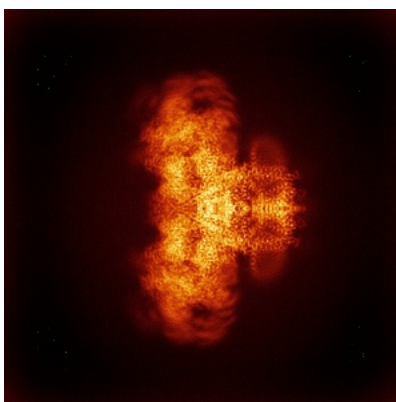


Z

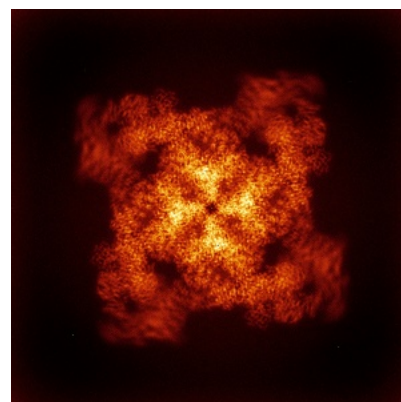
6.4.2 Raw map



X



Y

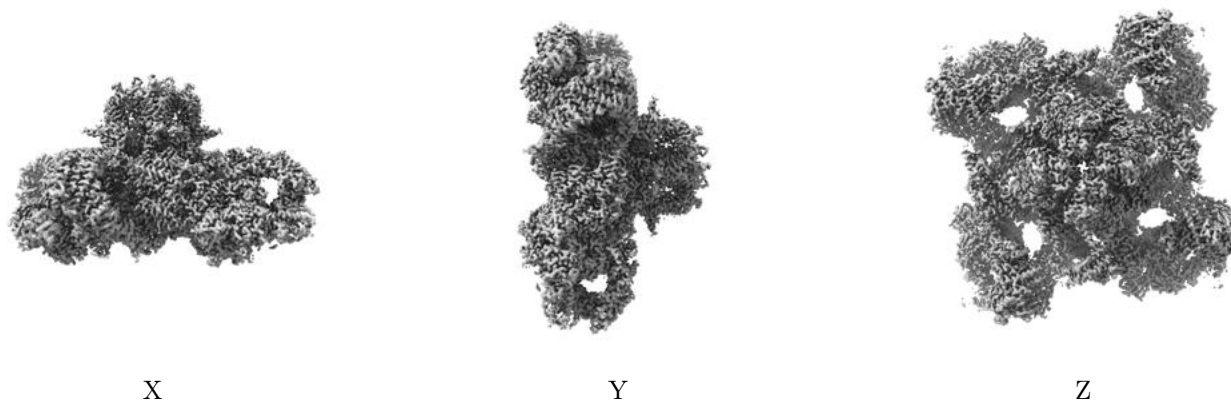


Z

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.

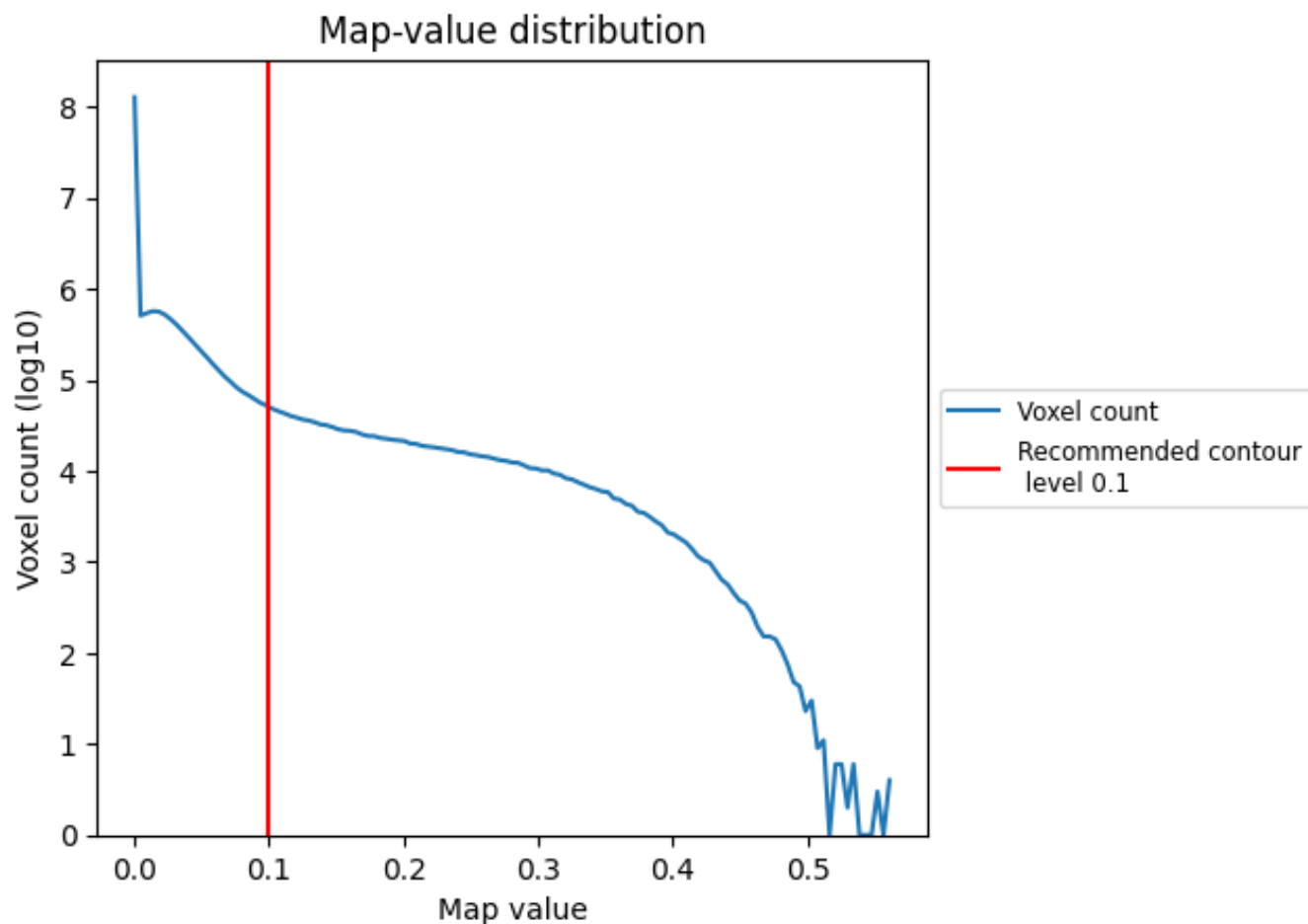
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

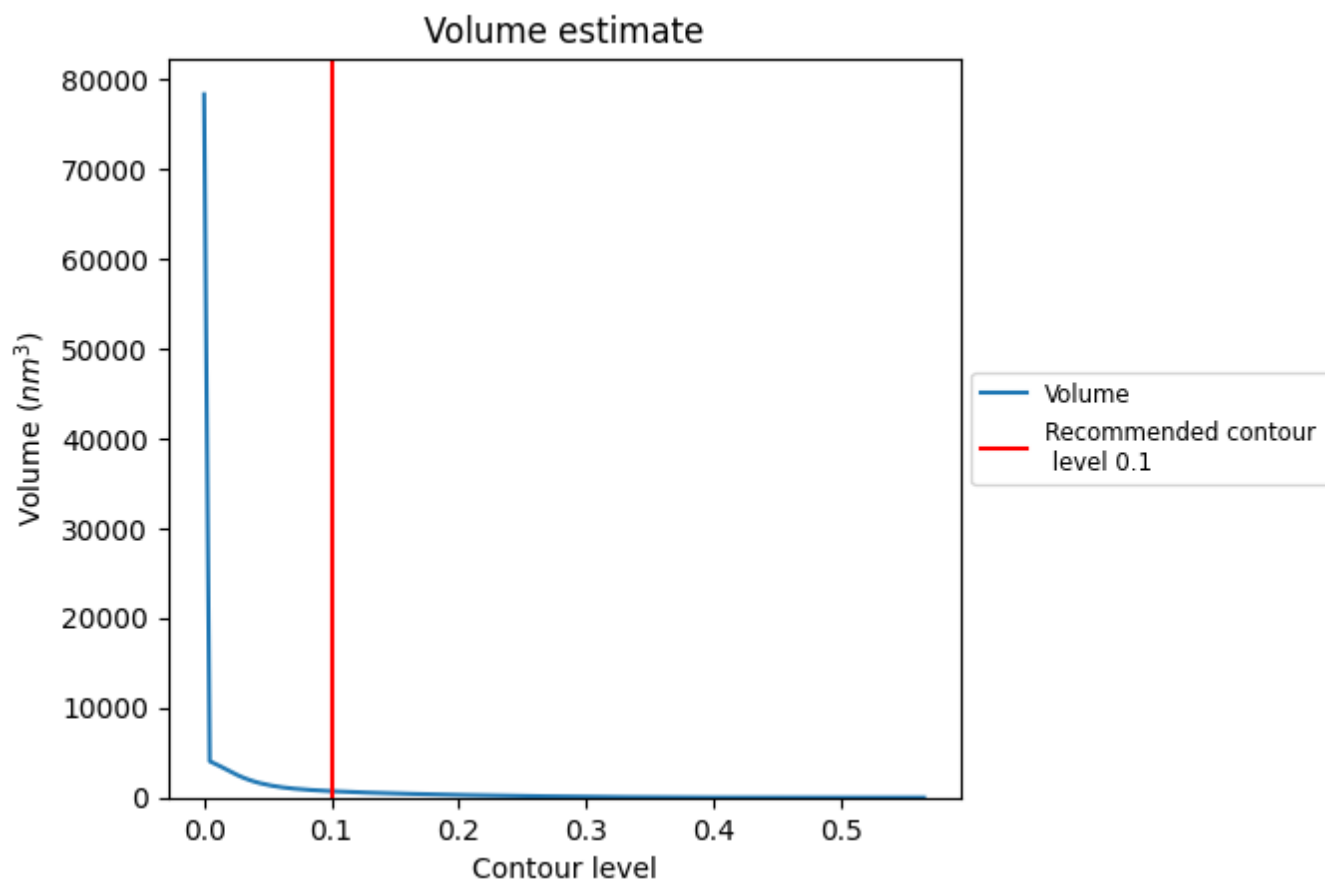
This section contains the results of statistical analysis of the map.

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.

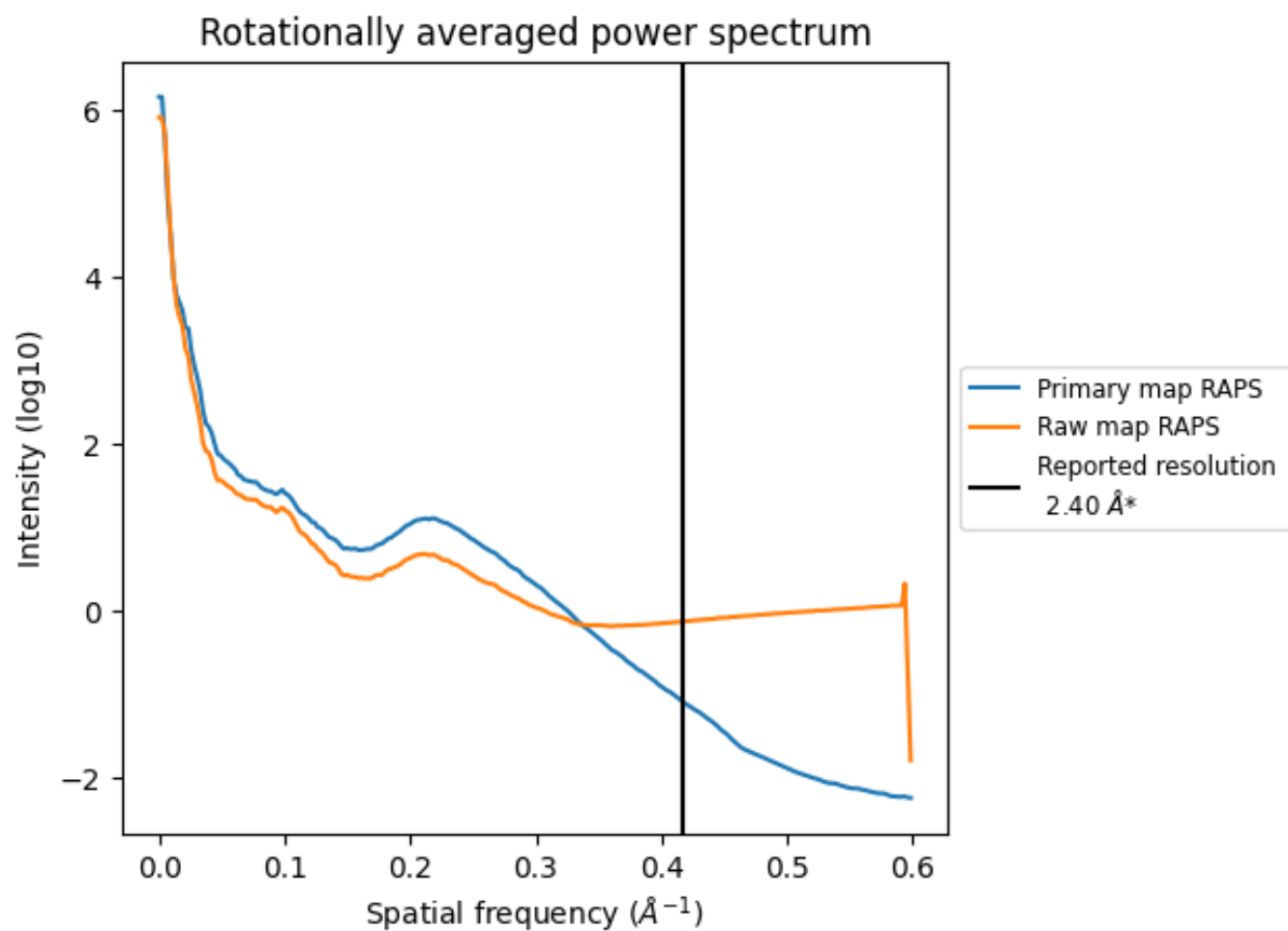
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 712 nm^3 ; this corresponds to an approximate mass of 643 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 ⓘ

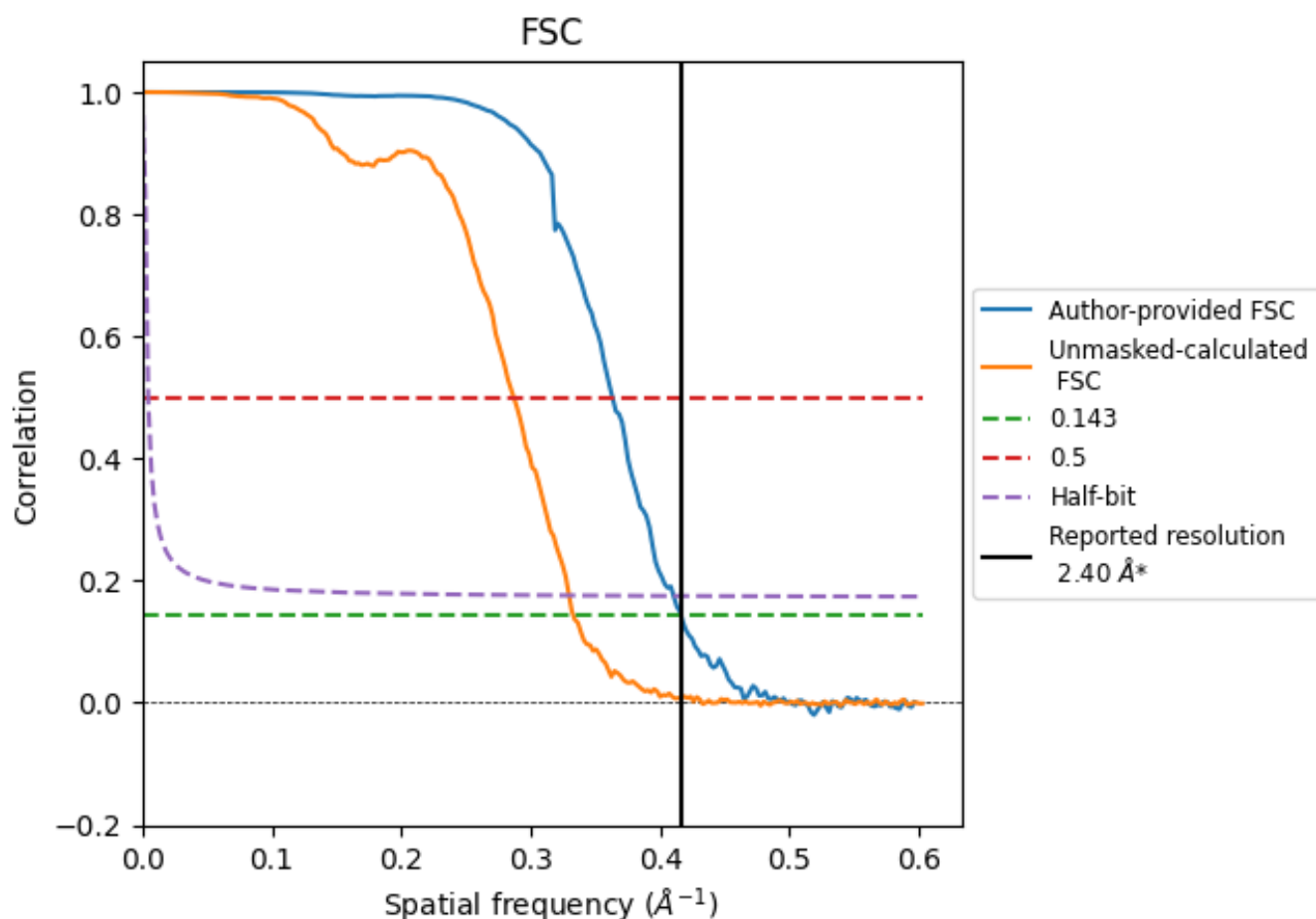


*Reported resolution corresponds to spatial frequency of 0.417 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 \AA^{-1}

8.2 Resolution estimates [i](#)

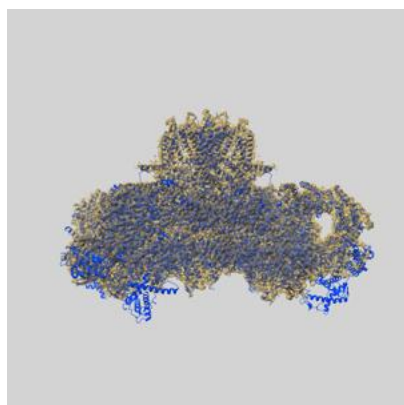
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.40	2.75	2.44
Unmasked-calculated*	3.00	3.48	3.03

*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 3.00 differs from the reported value 2.4 by more than 10 %

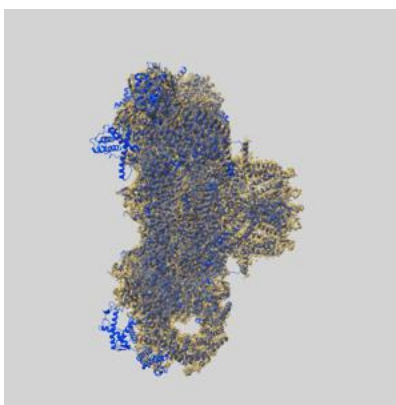
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49535 and PDB model 9NMO. Per-residue inclusion information can be found in section [3](#) on page [8](#).

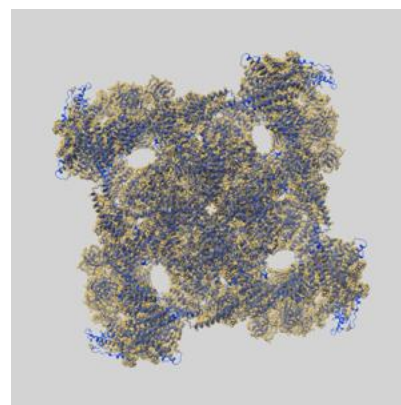
9.1 Map-model overlay [i](#)



X



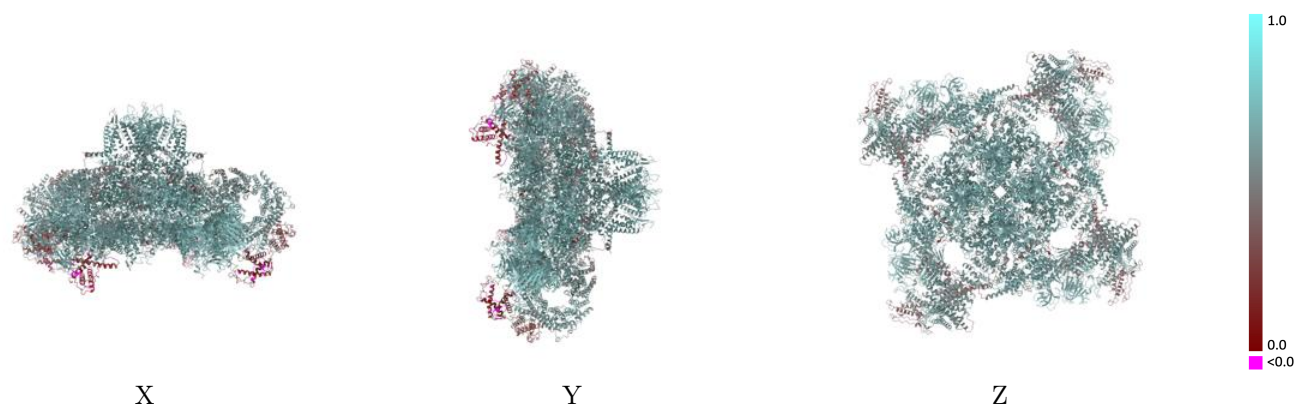
Y



Z

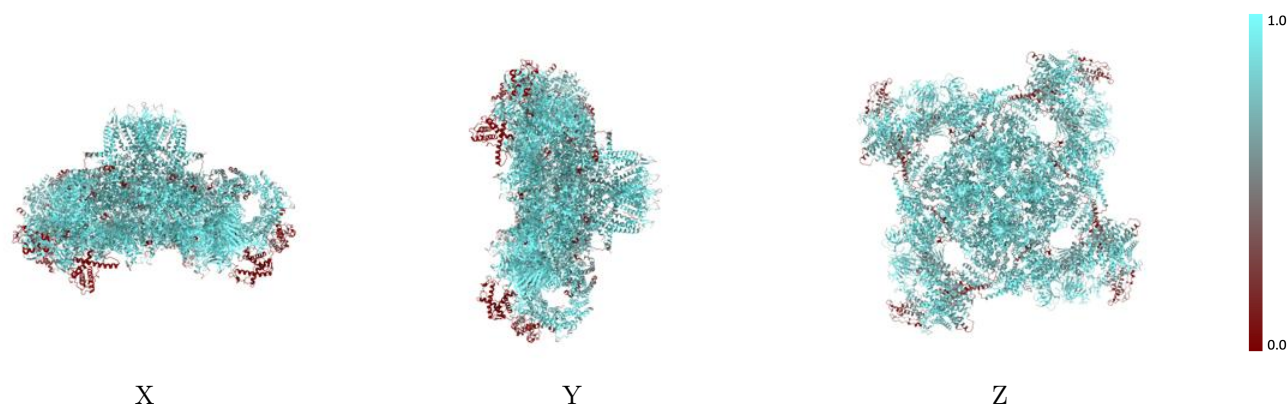
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



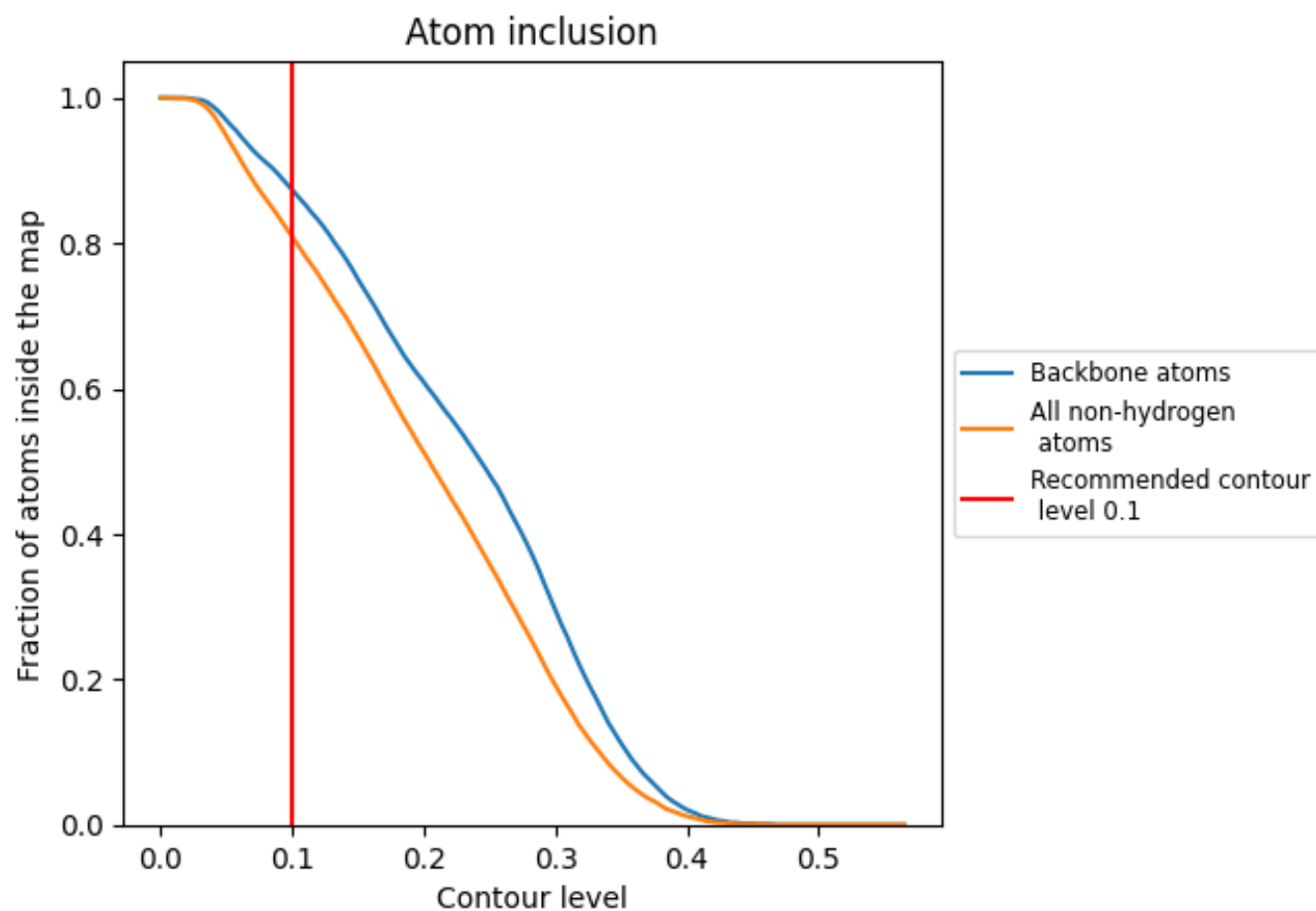
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 87% of all backbone atoms, 81% 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> 0.8090	<div></div> 0.5990
A	<div></div> 0.8060	<div></div> 0.5970
B	<div></div> 0.8060	<div></div> 0.5970
C	<div></div> 0.8060	<div></div> 0.5970
D	<div></div> 0.8060	<div></div> 0.5970
E	<div></div> 0.9240	<div></div> 0.6590
F	<div></div> 0.9240	<div></div> 0.6600
G	<div></div> 0.9240	<div></div> 0.6600
H	<div></div> 0.9240	<div></div> 0.6580

