



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:31 AM UTC

PDB ID : 2W6D / pdb_00002w6d
EMDB ID : EMD-1589
Title : BACTERIAL DYNAMIN-LIKE PROTEIN LIPID TUBE BOUND
Authors : Low, H.H.; Sachse, C.; Amos, L.A.; Lowe, J.
Deposited on : 2008-12-18
Resolution : 9.00 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

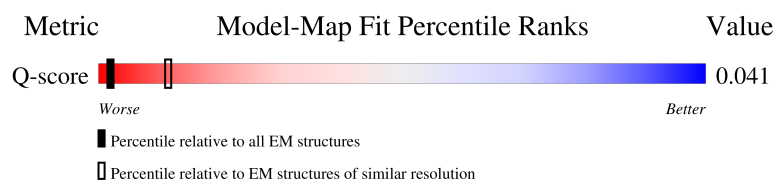
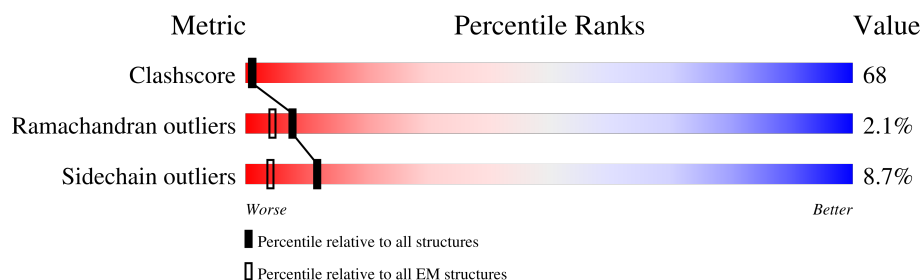
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.00 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	257 (8.50 - 9.50)

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	695	
1	B	695	

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
2	CPL	A	1697	-	-	X	-
2	CPL	A	1700	-	-	X	-
2	CPL	A	1701	-	-	X	-
2	CPL	A	1702	-	-	X	-
2	CPL	A	1703	-	-	X	-
2	CPL	A	1705	-	-	X	-
2	CPL	A	1707	-	-	X	-
2	CPL	A	1708	-	-	X	-
2	CPL	A	1709	-	-	X	-
2	CPL	A	1710	-	-	X	-
2	CPL	A	1718	-	-	X	-
2	CPL	A	3097	-	-	X	-
2	CPL	B	1696	-	-	X	-
2	CPL	B	1697	-	-	X	-
2	CPL	B	1700	-	-	X	-
2	CPL	B	1701	-	-	X	-
2	CPL	B	1703	-	-	X	-
2	CPL	B	1704	-	-	X	-
2	CPL	B	1705	-	-	X	-
2	CPL	B	1710	-	-	X	-
3	GDP	A	1696	-	-	X	-
3	GDP	B	1706	-	-	X	-

2 Entry composition [i](#)

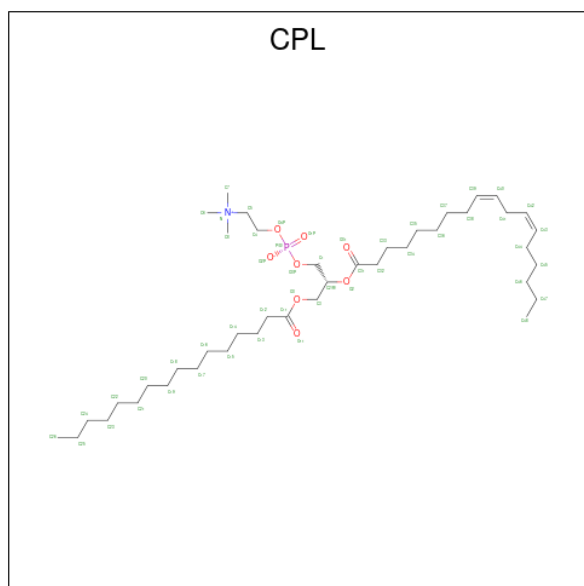
There are 3 unique types of molecules in this entry. The entry contains 13202 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DYNAMIN FAMILY PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	680	Total	C	N	O	S	0	0
			5429	3423	952	1043	11		
1	B	680	Total	C	N	O	S	0	0
			5429	3423	952	1043	11		

- Molecule 2 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: CPL) (formula: $C_{42}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	

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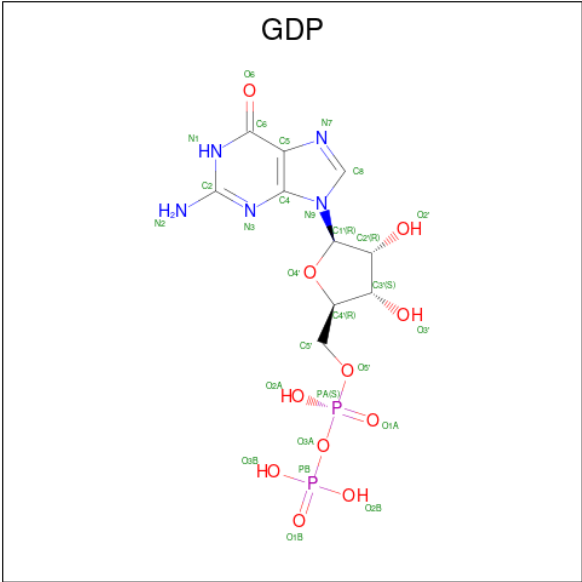
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

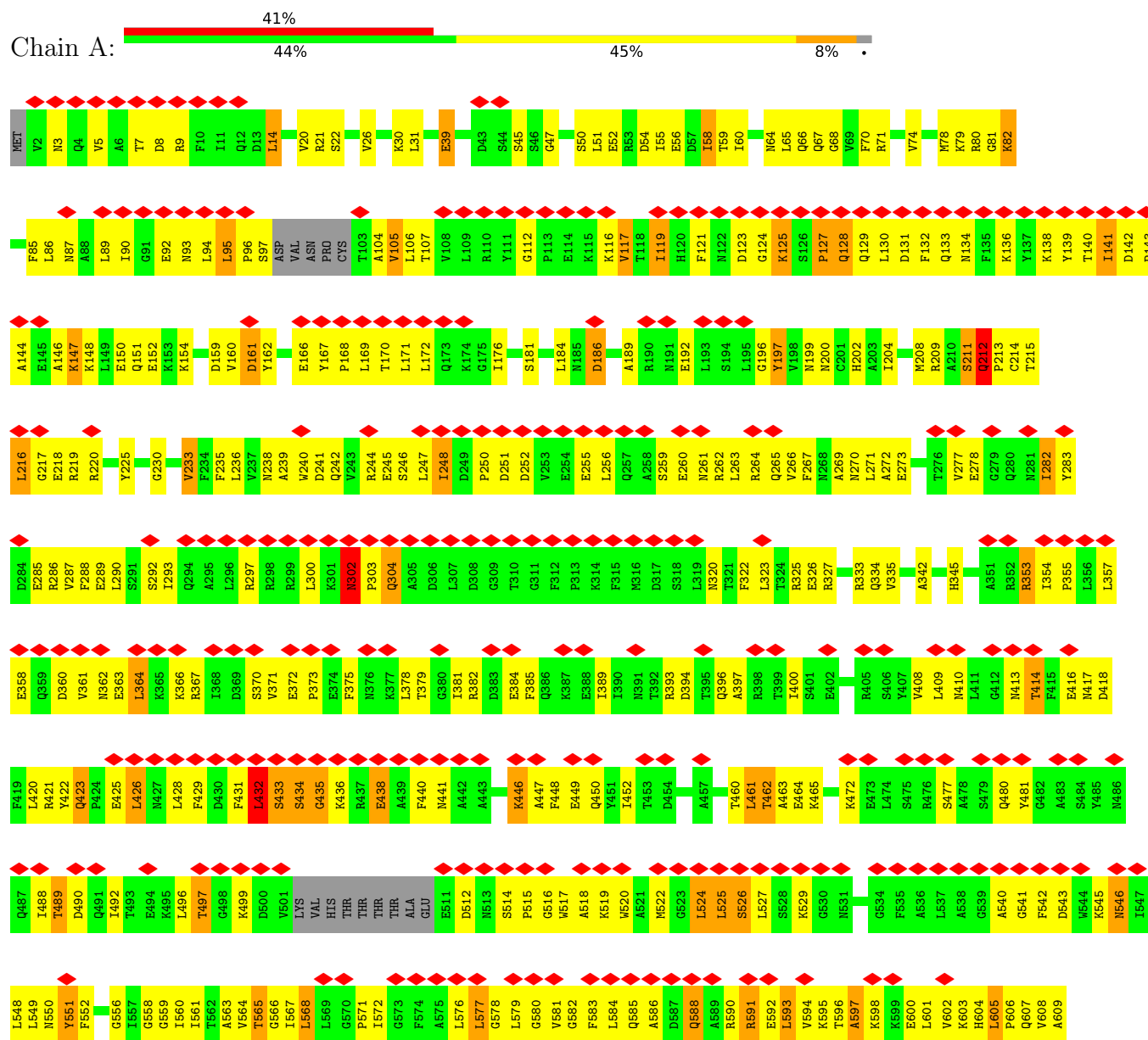


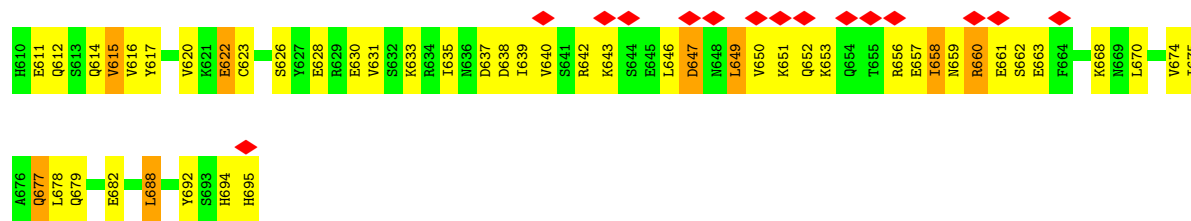
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

3 Residue-property plots

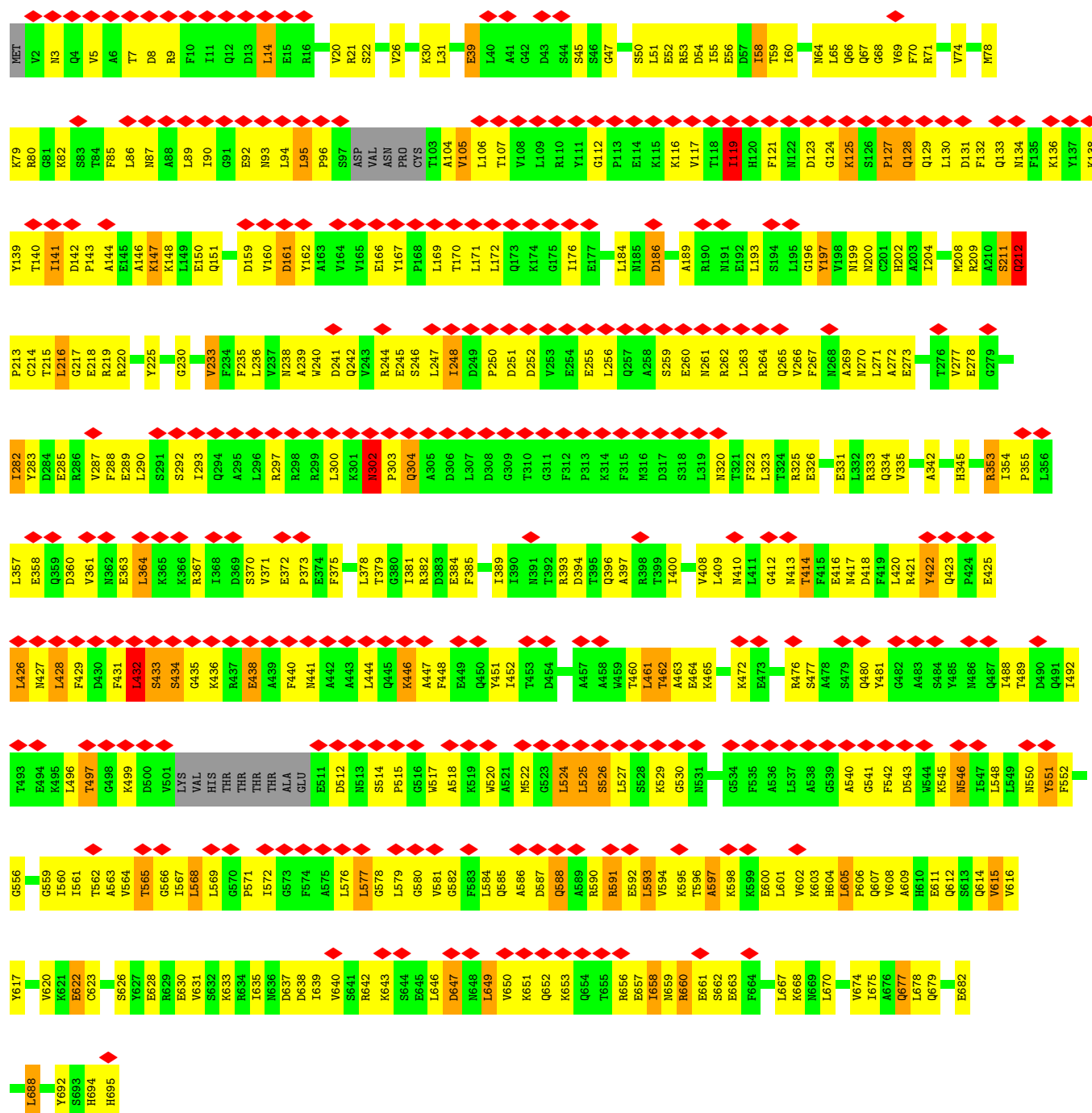
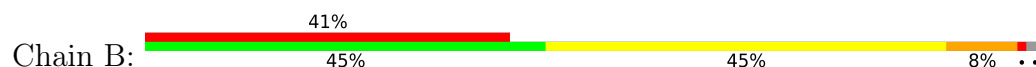
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: DYNAMIN FAMILY PROTEIN





• Molecule 1: DYNAMIN FAMILY PROTEIN



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	Not provided	
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	59000	Depositor
Image detector	GENERIC FILM	Depositor
Maximum map value	4.644	Depositor
Minimum map value	-3.495	Depositor
Average map value	0.006	Depositor
Map value standard deviation	1.001	Depositor
Recommended contour level	1.47	Depositor
Map size (Å)	671.213, 671.213, 671.213	wwPDB
Map dimensions	330, 330, 81	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.03398, 2.03398, 2.03398	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.49	0/5509	0.96	26/7428 (0.4%)
1	B	0.49	0/5509	0.96	27/7428 (0.4%)
All	All	0.49	0/11018	0.96	53/14856 (0.4%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	LEU	N-CA-C	-7.87	102.78	111.36
1	B	216	LEU	N-CA-C	-7.81	102.84	111.36
1	A	546	ASN	N-CA-C	-7.10	104.43	113.23
1	B	546	ASN	N-CA-C	-7.08	104.46	113.23
1	B	615	VAL	N-CA-C	-7.05	104.11	111.58
1	A	615	VAL	N-CA-C	-7.02	104.14	111.58
1	A	591	ARG	N-CA-C	-6.73	105.05	113.20
1	B	591	ARG	N-CA-C	-6.69	105.10	113.20
1	A	588	GLN	N-CA-C	-6.59	104.88	113.12
1	B	588	GLN	N-CA-C	-6.55	104.94	113.12
1	B	248	ILE	N-CA-C	-6.48	103.56	110.36
1	A	248	ILE	N-CA-C	-6.38	103.66	110.36
1	B	524	LEU	N-CA-C	-6.15	105.94	113.50
1	A	524	LEU	N-CA-C	-6.13	105.96	113.50
1	B	285	GLU	N-CA-C	-5.91	104.55	113.89
1	A	285	GLU	N-CA-C	-5.89	104.58	113.89
1	A	461	LEU	N-CA-C	-5.86	104.82	111.14
1	B	212	GLN	CA-C-N	5.86	126.77	119.98
1	B	212	GLN	C-N-CA	5.86	126.77	119.98
1	A	212	GLN	CA-C-N	5.82	126.73	119.98
1	A	212	GLN	C-N-CA	5.82	126.73	119.98
1	B	461	LEU	N-CA-C	-5.81	104.87	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	LYS	N-CA-C	-5.75	105.75	112.89
1	A	147	LYS	N-CA-C	-5.73	105.78	112.89
1	A	609	ALA	N-CA-C	-5.72	104.73	110.97
1	A	422	TYR	N-CA-C	-5.62	102.16	110.48
1	B	609	ALA	N-CA-C	-5.60	104.86	110.97
1	B	186	ASP	N-CA-C	5.59	118.31	111.82
1	B	422	TYR	N-CA-C	-5.59	102.21	110.48
1	A	186	ASP	N-CA-C	5.58	118.29	111.82
1	A	95	LEU	CA-C-N	5.56	126.79	119.84
1	A	95	LEU	C-N-CA	5.56	126.79	119.84
1	B	95	LEU	CA-C-N	5.44	126.64	119.84
1	B	95	LEU	C-N-CA	5.44	126.64	119.84
1	A	288	PHE	N-CA-C	5.39	117.18	108.34
1	B	288	PHE	N-CA-C	5.38	117.16	108.34
1	B	660	ARG	N-CA-C	5.37	117.83	111.33
1	B	626	SER	N-CA-C	-5.34	105.37	111.14
1	A	660	ARG	N-CA-C	5.32	117.77	111.33
1	A	626	SER	N-CA-C	-5.31	105.40	111.14
1	A	668	LYS	N-CA-C	-5.23	105.58	111.28
1	B	304	GLN	N-CA-C	-5.23	107.08	112.93
1	B	668	LYS	N-CA-C	-5.22	105.59	111.28
1	A	304	GLN	N-CA-C	-5.21	107.09	112.93
1	A	640	VAL	N-CA-C	5.11	116.45	110.62
1	B	323	LEU	N-CA-C	5.11	116.54	110.97
1	B	640	VAL	N-CA-C	5.09	116.43	110.62
1	A	353	ARG	N-CA-C	5.09	117.61	111.40
1	A	551	TYR	N-CA-C	-5.05	107.06	113.43
1	B	551	TYR	N-CA-C	-5.04	107.08	113.43
1	B	353	ARG	N-CA-C	5.04	117.55	111.40
1	A	323	LEU	N-CA-C	5.03	116.45	110.97
1	B	119	ILE	N-CA-C	5.01	115.06	107.75

There are no chirality outliers.

There are no planarity outliers.

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	5429	0	5411	998	0
1	B	5429	0	5407	986	0
2	A	1352	0	2047	454	0
2	B	936	0	1408	368	0
3	A	28	0	9	10	0
3	B	28	0	9	11	0
All	All	13202	0	14291	1863	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 68.

All (1863) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:LYS:CD	2:A:1708:CPL:HC72	1.26	1.65
1:B:585:GLN:CG	2:B:1696:CPL:H261	1.14	1.61
1:A:432:LEU:CB	2:A:1709:CPL:H322	1.14	1.61
1:B:581:VAL:CA	2:B:1699:CPL:H461	1.16	1.61
1:A:579:LEU:CD2	2:A:1705:CPL:H462	1.26	1.60
1:A:432:LEU:HB3	2:A:1709:CPL:C32	1.20	1.59
1:B:579:LEU:CD2	2:B:1697:CPL:H212	1.17	1.59
1:A:572:ILE:HD13	2:A:1705:CPL:C34	1.21	1.58
1:A:265:GLN:NE2	1:B:142:ASP:CA	1.67	1.57
1:A:429:PHE:CZ	2:A:1702:CPL:HC11	1.41	1.56
1:B:585:GLN:CB	2:B:1696:CPL:H261	1.29	1.55
1:A:150:GLU:CD	1:B:219:ARG:HD3	1.25	1.53
1:B:416:GLU:HB2	2:B:1704:CPL:P	1.46	1.53
1:B:591:ARG:CB	2:B:1703:CPL:H411	1.32	1.53
1:B:585:GLN:HG2	2:B:1696:CPL:C26	1.29	1.53
1:A:446:LYS:HE2	2:A:1708:CPL:C6	1.35	1.51
1:B:60:ILE:CG2	1:B:199:ASN:HB2	1.38	1.51
1:B:591:ARG:CG	2:B:1703:CPL:H411	1.39	1.51
1:A:577:LEU:HD11	2:A:1707:CPL:C41	1.08	1.50
1:A:581:VAL:CG2	2:A:1707:CPL:H452	1.03	1.50
1:B:579:LEU:CD2	2:B:1697:CPL:C21	1.85	1.50
1:A:219:ARG:HD3	1:B:150:GLU:CD	1.22	1.50
1:A:581:VAL:HG21	2:A:1707:CPL:C45	1.38	1.50
1:A:429:PHE:CE1	2:A:1702:CPL:C1	1.91	1.50
1:A:219:ARG:CD	1:B:150:GLU:CD	1.85	1.49
2:A:1697:CPL:H121	2:A:1700:CPL:C34	1.34	1.49
1:A:572:ILE:CD1	2:A:1705:CPL:H341	1.01	1.49
1:A:435:GLY:H	2:A:1709:CPL:C8	1.24	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:581:VAL:HA	2:B:1699:CPL:C46	1.41	1.48
1:B:586:ALA:HB2	2:B:1697:CPL:C46	1.43	1.47
1:A:97:SER:C	1:B:262:ARG:NE	1.73	1.47
1:B:579:LEU:HD23	2:B:1697:CPL:C20	1.40	1.46
1:A:581:VAL:CG2	2:A:1707:CPL:C45	1.89	1.46
1:A:60:ILE:CG2	1:A:199:ASN:HB3	1.45	1.46
1:B:598:LYS:NZ	2:B:1703:CPL:C2	1.79	1.46
1:A:150:GLU:CD	1:B:219:ARG:CD	1.88	1.45
1:A:278:GLU:CG	1:A:333:ARG:HH12	1.29	1.44
1:A:213:PRO:HG2	1:B:79:LYS:CB	1.48	1.44
1:B:586:ALA:CB	2:B:1697:CPL:H461	1.44	1.44
1:A:266:VAL:N	1:B:143:PRO:CB	1.69	1.44
1:B:585:GLN:CG	2:B:1696:CPL:C26	1.90	1.43
1:B:591:ARG:HB2	2:B:1703:CPL:C41	1.49	1.42
2:A:1704:CPL:H261	2:A:1714:CPL:C48	1.48	1.42
1:A:579:LEU:CD2	2:A:1705:CPL:C46	1.95	1.41
1:B:591:ARG:CB	2:B:1703:CPL:C41	1.99	1.40
1:A:147:LYS:CB	1:B:269:ALA:HB3	1.51	1.40
1:A:421:ARG:CD	2:B:1700:CPL:HC73	1.26	1.40
1:A:271:LEU:HG	1:B:147:LYS:NZ	1.34	1.39
1:A:429:PHE:HE1	2:A:1702:CPL:C1	1.27	1.39
1:A:577:LEU:CD1	2:A:1707:CPL:H412	1.47	1.39
1:B:565:THR:HA	2:B:1697:CPL:C4	1.39	1.38
1:A:79:LYS:CB	1:B:213:PRO:HG2	1.51	1.38
1:B:594:VAL:C	2:B:1703:CPL:C34	1.90	1.38
1:A:278:GLU:CG	1:A:333:ARG:NH1	1.86	1.37
1:A:446:LYS:CE	2:A:1708:CPL:HC63	1.53	1.37
1:B:595:LYS:N	2:B:1703:CPL:C34	1.86	1.37
2:A:1704:CPL:C26	2:A:1714:CPL:H481	1.54	1.37
1:A:250:PRO:HG3	1:B:297:ARG:NH2	1.40	1.37
2:A:1697:CPL:C12	2:A:1700:CPL:H342	1.53	1.37
1:A:147:LYS:NZ	1:B:271:LEU:HG	1.39	1.37
2:A:1698:CPL:C48	2:A:1707:CPL:H481	1.51	1.36
1:A:250:PRO:CG	1:B:297:ARG:NH2	1.88	1.36
1:A:265:GLN:NE2	1:B:142:ASP:HA	1.05	1.36
1:A:278:GLU:HG2	1:A:333:ARG:NH1	1.05	1.36
1:A:577:LEU:CD1	2:A:1707:CPL:C41	2.02	1.36
1:B:565:THR:C	2:B:1697:CPL:HC42	1.49	1.36
2:A:1718:CPL:H241	2:A:3097:CPL:C23	1.56	1.35
1:A:269:ALA:HB3	1:B:147:LYS:CB	1.55	1.35
1:A:143:PRO:CB	1:B:266:VAL:N	1.75	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ARG:NH2	1:B:250:PRO:CG	1.90	1.34
1:A:79:LYS:HB2	1:B:213:PRO:CG	1.56	1.34
1:A:213:PRO:CG	1:B:79:LYS:HB2	1.53	1.34
1:B:579:LEU:HD23	2:B:1697:CPL:C21	1.50	1.34
2:B:1697:CPL:H261	2:B:1714:CPL:C48	1.58	1.33
1:A:265:GLN:CD	1:B:142:ASP:CA	1.94	1.33
1:A:297:ARG:NH2	1:B:250:PRO:HG3	1.44	1.33
1:A:432:LEU:HG	2:A:1709:CPL:C34	1.59	1.33
1:A:579:LEU:HD23	2:A:1705:CPL:C45	1.57	1.32
2:A:1704:CPL:C25	2:A:1714:CPL:H481	1.57	1.32
1:A:446:LYS:HD3	2:A:1708:CPL:C7	1.60	1.32
1:A:421:ARG:CD	2:B:1700:CPL:C7	1.90	1.31
1:B:586:ALA:CB	2:B:1697:CPL:C46	2.01	1.31
1:A:269:ALA:CB	1:B:147:LYS:H	1.43	1.31
1:B:579:LEU:HD21	2:B:1697:CPL:C21	1.54	1.31
1:A:209:ARG:HB3	1:B:212:GLN:NE2	1.46	1.31
1:A:579:LEU:HD23	2:A:1705:CPL:C46	1.56	1.30
2:A:1701:CPL:O11	1:B:420:LEU:CD1	1.78	1.30
1:A:248:ILE:HD11	1:B:93:ASN:OD1	1.33	1.29
1:B:363:GLU:CB	1:B:660:ARG:HH12	1.44	1.29
1:A:147:LYS:HB3	1:B:269:ALA:CB	1.62	1.29
1:A:449:GLU:OE1	2:A:1708:CPL:HC61	1.13	1.29
1:A:143:PRO:CG	1:B:265:GLN:H	1.35	1.29
1:A:425:GLU:HB2	2:A:1708:CPL:O3P	1.13	1.28
1:B:565:THR:CA	2:B:1697:CPL:C4	2.01	1.28
1:B:587:ASP:O	2:B:1703:CPL:H452	1.25	1.28
2:B:1702:CPL:H481	2:B:1707:CPL:C26	1.62	1.28
1:B:594:VAL:C	2:B:1703:CPL:H342	0.95	1.28
1:A:653:LYS:NZ	1:A:657:GLU:OE2	1.66	1.27
1:B:278:GLU:HB2	1:B:333:ARG:NH1	1.48	1.27
1:A:212:GLN:NE2	1:B:209:ARG:HB3	1.47	1.27
1:A:93:ASN:OD1	1:B:248:ILE:HD11	1.33	1.27
1:B:595:LYS:N	2:B:1703:CPL:H342	1.40	1.27
1:A:273:GLU:CB	1:B:151:GLN:HE22	1.47	1.26
1:A:429:PHE:CE1	2:A:1702:CPL:HC11	1.57	1.26
2:A:1701:CPL:O11	1:B:420:LEU:HD11	1.14	1.26
1:A:572:ILE:CD1	2:A:1705:CPL:C34	1.87	1.26
1:A:414:THR:O	2:A:1701:CPL:HC41	1.15	1.25
1:A:421:ARG:HH21	2:B:1700:CPL:C7	1.46	1.25
1:B:579:LEU:CD2	2:B:1697:CPL:C20	2.11	1.25
1:A:147:LYS:H	1:B:269:ALA:CB	1.49	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:GLU:CB	2:B:1704:CPL:O1P	1.85	1.24
1:A:269:ALA:CB	1:B:147:LYS:HB3	1.67	1.24
1:A:414:THR:O	2:A:1701:CPL:C4	1.85	1.23
1:B:60:ILE:CG2	1:B:199:ASN:CB	2.16	1.23
1:A:248:ILE:HG23	1:B:300:LEU:CD1	1.69	1.23
1:A:450:GLN:OE1	2:A:1708:CPL:HC82	1.29	1.22
1:A:434:SER:O	2:A:1709:CPL:O4P	1.52	1.22
1:A:147:LYS:CB	1:B:269:ALA:CB	2.15	1.22
2:A:1704:CPL:H261	2:A:1714:CPL:C47	1.70	1.22
1:A:579:LEU:HD21	2:A:1705:CPL:C46	1.64	1.21
1:A:209:ARG:CB	1:B:212:GLN:HE21	1.53	1.21
1:A:212:GLN:HE21	1:B:209:ARG:CB	1.53	1.21
1:A:465:LYS:HZ3	1:B:465:LYS:CB	1.54	1.21
1:A:150:GLU:OE1	1:B:219:ARG:HD3	1.38	1.20
1:A:269:ALA:CB	1:B:147:LYS:CB	2.17	1.20
1:A:250:PRO:HG2	1:B:297:ARG:CZ	1.71	1.20
1:B:581:VAL:CB	2:B:1699:CPL:H461	1.55	1.20
2:B:1705:CPL:H261	2:B:1711:CPL:C48	1.71	1.20
1:B:587:ASP:O	2:B:1703:CPL:C45	1.88	1.20
2:A:3094:CPL:H262	2:A:3181:CPL:H462	1.21	1.20
1:A:558:GLY:O	2:A:1705:CPL:HC81	1.32	1.20
2:B:1697:CPL:C26	2:B:1698:CPL:H483	1.70	1.20
1:A:151:GLN:HE22	1:B:273:GLU:CB	1.54	1.19
1:A:219:ARG:HD3	1:B:150:GLU:OE1	1.38	1.19
2:B:1700:CPL:O31	2:B:1704:CPL:O11	1.59	1.19
1:A:429:PHE:CE1	2:A:1702:CPL:O3P	1.89	1.19
2:A:1701:CPL:O1P	1:B:421:ARG:HG2	1.19	1.19
1:B:565:THR:CA	2:B:1697:CPL:HC42	1.66	1.19
1:A:273:GLU:OE2	1:B:151:GLN:NE2	1.74	1.19
1:A:297:ARG:CZ	1:B:250:PRO:HG2	1.74	1.18
1:A:432:LEU:CG	2:A:1709:CPL:H342	1.71	1.18
1:B:565:THR:O	2:B:1697:CPL:HC42	1.42	1.18
1:A:147:LYS:HD2	1:B:266:VAL:O	1.44	1.18
1:B:585:GLN:CB	2:B:1696:CPL:C26	2.18	1.18
1:A:60:ILE:CG2	1:A:199:ASN:CB	2.22	1.18
1:A:60:ILE:HG21	1:A:199:ASN:CB	1.72	1.18
1:A:421:ARG:HD2	2:B:1700:CPL:C7	1.60	1.17
1:A:432:LEU:HB3	2:A:1709:CPL:C31	1.75	1.17
1:A:151:GLN:NE2	1:B:273:GLU:OE2	1.78	1.17
1:A:446:LYS:CE	2:A:1708:CPL:HC72	1.72	1.17
1:A:582:GLY:C	2:A:1707:CPL:H482	1.69	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:GLN:CD	1:B:142:ASP:HA	1.45	1.17
1:B:60:ILE:HG22	1:B:199:ASN:CB	1.73	1.17
1:B:425:GLU:HB3	2:B:1705:CPL:C2	1.74	1.17
1:B:593:LEU:CD1	2:B:1697:CPL:H351	1.75	1.17
1:A:143:PRO:HG3	1:B:265:GLN:H	1.07	1.17
1:B:598:LYS:NZ	2:B:1703:CPL:HC2	0.84	1.17
1:A:269:ALA:CB	1:B:147:LYS:N	2.08	1.16
1:A:97:SER:C	1:B:262:ARG:HE	1.38	1.16
1:A:363:GLU:N	1:A:660:ARG:HH12	1.42	1.15
3:A:1696:GDP:C2'	1:B:246:SER:HB3	1.77	1.15
1:A:143:PRO:O	1:B:266:VAL:HA	1.47	1.14
1:A:246:SER:HB2	3:B:1706:GDP:C4	1.82	1.14
1:B:425:GLU:CB	2:B:1705:CPL:C1	2.21	1.14
2:A:1701:CPL:HC42	1:B:421:ARG:CD	1.76	1.14
2:A:1718:CPL:H251	2:A:3097:CPL:C25	1.77	1.14
1:B:363:GLU:CB	1:B:660:ARG:NH1	2.10	1.14
1:B:363:GLU:HB2	1:B:660:ARG:NH1	1.62	1.14
1:A:64:ASN:OD1	1:A:200:ASN:HA	1.43	1.14
1:A:151:GLN:HE22	1:B:273:GLU:HB2	0.98	1.14
1:A:300:LEU:CD1	1:B:248:ILE:HG23	1.76	1.14
1:A:450:GLN:OE1	2:A:1708:CPL:C8	1.95	1.14
2:B:1705:CPL:C25	2:B:1711:CPL:H481	1.76	1.14
1:A:147:LYS:HB3	1:B:269:ALA:CA	1.56	1.13
1:B:447:ALA:HB2	2:B:1705:CPL:O1P	1.47	1.13
3:A:1696:GDP:C4	1:B:246:SER:HB2	1.82	1.13
1:A:432:LEU:CG	2:A:1709:CPL:H322	1.79	1.12
1:A:435:GLY:H	2:A:1709:CPL:HC83	1.08	1.12
1:B:585:GLN:HG2	2:B:1696:CPL:H263	1.18	1.12
1:A:425:GLU:HB2	2:A:1708:CPL:P	1.89	1.12
1:A:449:GLU:OE1	2:A:1708:CPL:C6	1.97	1.12
1:A:78:MET:O	1:B:213:PRO:HD2	1.48	1.12
1:A:269:ALA:HB1	1:B:147:LYS:N	1.62	1.12
2:B:1710:CPL:H251	2:B:1712:CPL:H462	1.15	1.12
1:A:143:PRO:CB	1:B:266:VAL:H	1.49	1.12
1:A:425:GLU:CB	2:A:1708:CPL:O3P	1.97	1.12
1:A:266:VAL:CA	1:B:143:PRO:O	1.94	1.11
1:A:446:LYS:CD	2:A:1708:CPL:C7	2.22	1.11
1:B:416:GLU:CB	2:B:1704:CPL:P	2.21	1.11
1:A:144:ALA:N	1:B:265:GLN:HB2	1.59	1.11
1:A:266:VAL:O	1:B:147:LYS:HD2	1.50	1.11
1:B:425:GLU:HB3	2:B:1705:CPL:C1	1.75	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:SER:HB3	2:A:1709:CPL:HC83	1.28	1.11
1:A:143:PRO:CG	1:B:265:GLN:N	1.80	1.11
1:A:363:GLU:H	1:A:660:ARG:NH1	1.48	1.11
1:A:434:SER:C	2:A:1709:CPL:HC51	1.67	1.11
1:A:577:LEU:HD11	2:A:1707:CPL:H411	1.28	1.11
1:A:213:PRO:HD2	1:B:78:MET:O	1.46	1.11
1:A:561:ILE:HD12	2:A:1705:CPL:C4	1.72	1.11
2:B:1702:CPL:C48	2:B:1707:CPL:H261	1.81	1.10
1:B:585:GLN:OE1	2:B:1696:CPL:H251	1.49	1.10
1:B:593:LEU:HD11	2:B:1697:CPL:H351	1.16	1.10
1:A:246:SER:HB3	3:B:1706:GDP:C2'	1.80	1.10
2:B:1701:CPL:H261	2:B:1710:CPL:C48	1.82	1.10
1:A:581:VAL:C	2:A:1707:CPL:H472	1.76	1.09
2:B:1697:CPL:H262	2:B:1698:CPL:H483	1.13	1.09
1:A:219:ARG:HD2	1:B:150:GLU:CG	1.82	1.09
1:A:429:PHE:CD1	2:A:1702:CPL:H331	1.87	1.09
1:A:561:ILE:CD1	2:A:1705:CPL:C4	2.12	1.09
1:B:590:ARG:O	2:B:1703:CPL:H371	1.52	1.09
1:A:147:LYS:N	1:B:269:ALA:CB	2.14	1.09
1:A:435:GLY:N	2:A:1709:CPL:C8	1.92	1.09
1:A:147:LYS:N	1:B:269:ALA:HB1	1.68	1.09
1:B:363:GLU:HB3	1:B:660:ARG:HH12	1.04	1.09
1:B:602:VAL:CG2	2:B:1703:CPL:HC51	1.82	1.09
1:B:104:ALA:HB2	1:B:141:ILE:HD12	1.30	1.09
1:A:362:ASN:HB2	1:A:660:ARG:NH1	1.67	1.08
2:A:3094:CPL:H241	2:A:3181:CPL:H451	1.35	1.08
1:B:602:VAL:HG22	2:B:1703:CPL:HC51	1.26	1.08
1:B:579:LEU:HD23	2:B:1697:CPL:H201	1.17	1.08
1:A:266:VAL:N	1:B:143:PRO:HB2	0.99	1.08
1:A:143:PRO:HB3	1:B:262:ARG:O	1.54	1.08
1:A:465:LYS:NZ	1:B:465:LYS:HA	1.66	1.08
2:A:3094:CPL:C26	2:A:3181:CPL:H462	1.83	1.08
1:A:104:ALA:HB2	1:A:141:ILE:HD12	1.30	1.08
1:A:362:ASN:HB2	1:A:660:ARG:HH11	0.91	1.08
1:B:591:ARG:HG3	2:B:1703:CPL:H411	1.15	1.07
1:A:421:ARG:HH21	2:B:1700:CPL:HC71	1.19	1.07
2:A:1697:CPL:H482	2:A:1705:CPL:H263	1.34	1.07
1:A:579:LEU:HD23	2:A:1705:CPL:H451	1.20	1.07
1:B:416:GLU:HB2	2:B:1704:CPL:O1P	0.92	1.07
1:B:598:LYS:HZ1	2:B:1703:CPL:C2	1.52	1.07
1:A:266:VAL:HA	1:B:143:PRO:O	1.50	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:PRO:HB2	1:B:266:VAL:N	1.02	1.06
1:A:147:LYS:HB2	1:B:269:ALA:HB3	1.32	1.06
2:A:1697:CPL:H141	2:A:1700:CPL:C36	1.84	1.06
1:A:97:SER:O	1:B:262:ARG:NE	1.71	1.06
1:A:269:ALA:CA	1:B:147:LYS:HB3	1.55	1.06
1:A:273:GLU:CB	1:B:151:GLN:NE2	2.18	1.06
1:A:273:GLU:HB2	1:B:151:GLN:HE22	0.95	1.06
1:B:586:ALA:HB1	2:B:1697:CPL:H461	1.12	1.06
1:B:598:LYS:HZ2	2:B:1703:CPL:C2	1.51	1.06
2:A:1697:CPL:H151	2:A:1700:CPL:C39	1.85	1.06
1:A:67:GLN:HE22	1:A:200:ASN:HB3	1.20	1.06
1:B:585:GLN:HB3	2:B:1696:CPL:H261	1.37	1.06
2:B:1701:CPL:C25	2:B:1710:CPL:H482	1.86	1.06
2:A:1701:CPL:HC42	1:B:421:ARG:HD3	1.27	1.06
2:A:1718:CPL:H251	2:A:3097:CPL:H251	1.33	1.06
1:A:265:GLN:NE2	1:B:142:ASP:C	2.02	1.05
1:A:271:LEU:CG	1:B:147:LYS:HZ1	1.69	1.05
1:B:68:GLY:HA2	1:B:202:HIS:CE1	1.91	1.05
1:B:582:GLY:HA3	2:B:1696:CPL:H481	1.37	1.05
1:B:595:LYS:N	2:B:1703:CPL:H341	1.62	1.05
1:A:269:ALA:HB3	1:B:147:LYS:HB2	1.34	1.05
1:B:581:VAL:HA	2:B:1699:CPL:C47	1.87	1.05
2:B:1705:CPL:H251	2:B:1711:CPL:H481	1.34	1.05
1:A:150:GLU:CG	1:B:219:ARG:HD2	1.85	1.05
1:B:581:VAL:CB	2:B:1699:CPL:C46	2.26	1.05
1:A:432:LEU:HG	2:A:1709:CPL:C33	1.84	1.05
1:A:581:VAL:HG23	2:A:1707:CPL:H452	1.10	1.05
2:A:1697:CPL:H141	2:A:1700:CPL:H361	1.08	1.05
1:A:265:GLN:HB2	1:B:144:ALA:N	1.62	1.05
1:A:436:LYS:HE3	2:A:1709:CPL:HC71	1.39	1.05
1:A:465:LYS:HG3	1:B:465:LYS:HG3	1.34	1.05
2:A:1697:CPL:H261	2:A:1710:CPL:H483	1.39	1.05
1:A:429:PHE:HD1	2:A:1702:CPL:H331	1.16	1.04
1:A:572:ILE:HD11	2:A:1705:CPL:H321	1.35	1.04
1:A:217:GLY:HA3	1:B:216:LEU:HB3	1.36	1.04
1:A:262:ARG:O	1:B:143:PRO:HB3	1.58	1.04
1:A:414:THR:CA	2:A:1701:CPL:HC51	1.82	1.04
1:A:144:ALA:H	1:B:265:GLN:HB2	0.89	1.03
1:A:266:VAL:O	1:B:147:LYS:HB2	1.58	1.03
2:A:1701:CPL:O11	1:B:420:LEU:CG	2.05	1.03
2:A:1718:CPL:C24	2:A:3097:CPL:C23	2.35	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:GLN:HB3	1:B:71:ARG:HH22	0.88	1.03
1:A:216:LEU:HB3	1:B:217:GLY:HA3	1.35	1.03
1:B:67:GLN:HB3	1:B:71:ARG:NH2	1.73	1.03
1:A:128:GLN:HG2	1:A:129:GLN:H	1.22	1.03
1:B:598:LYS:CE	2:B:1703:CPL:HC2	1.89	1.03
1:A:265:GLN:HB2	1:B:144:ALA:H	0.90	1.03
1:A:572:ILE:HG21	2:A:1705:CPL:H361	1.40	1.03
2:B:1702:CPL:C48	2:B:1707:CPL:C26	2.36	1.03
1:A:246:SER:HB3	3:B:1706:GDP:H2'	1.05	1.02
1:A:278:GLU:CD	1:A:333:ARG:HH12	1.67	1.02
1:A:429:PHE:HE1	2:A:1702:CPL:C2	1.70	1.02
1:B:278:GLU:CB	1:B:333:ARG:NH1	2.22	1.02
1:B:426:LEU:HA	2:B:1705:CPL:O1P	1.57	1.02
3:A:1696:GDP:H2'	1:B:246:SER:CB	1.89	1.02
1:B:579:LEU:HD22	2:B:1697:CPL:H192	1.39	1.02
1:A:147:LYS:HZ1	1:B:271:LEU:CG	1.72	1.02
1:B:414:THR:O	2:B:1700:CPL:C8	2.06	1.02
1:B:434:SER:HA	2:B:1701:CPL:HC41	1.35	1.02
1:A:147:LYS:HZ1	1:B:271:LEU:HG	0.99	1.01
1:A:211:SER:HA	1:B:209:ARG:NH1	1.74	1.01
1:A:579:LEU:CD2	2:A:1705:CPL:C45	2.33	1.01
1:A:216:LEU:HB3	1:B:217:GLY:CA	1.89	1.01
1:A:278:GLU:HB2	1:A:333:ARG:NH2	1.73	1.01
1:A:150:GLU:HG2	1:B:219:ARG:HD2	1.43	1.01
1:A:151:GLN:NE2	1:B:273:GLU:CB	2.23	1.01
2:A:1718:CPL:H241	2:A:3097:CPL:H232	1.03	1.01
1:B:360:ASP:OD2	1:B:363:GLU:OE2	1.76	1.01
1:B:418:ASP:N	2:B:1700:CPL:HC41	1.74	1.01
1:A:432:LEU:C	2:A:1709:CPL:O31	2.03	1.01
2:A:1697:CPL:C48	2:A:1705:CPL:H263	1.90	1.01
2:A:1718:CPL:HC62	2:A:3097:CPL:HC73	1.41	1.01
1:A:250:PRO:HG2	1:B:297:ARG:NH2	1.65	1.00
1:A:421:ARG:NH2	2:B:1700:CPL:HC73	1.76	1.00
1:A:429:PHE:HD1	2:A:1702:CPL:C33	1.74	1.00
2:A:1718:CPL:C24	2:A:3097:CPL:H232	1.91	1.00
1:A:217:GLY:CA	1:B:216:LEU:HB3	1.90	1.00
1:A:271:LEU:CG	1:B:147:LYS:NZ	2.21	1.00
1:A:585:GLN:HG3	2:A:1699:CPL:H262	1.44	1.00
2:A:1698:CPL:H482	2:A:1707:CPL:C48	1.90	1.00
1:B:230:GLY:O	1:B:334:GLN:NE2	1.92	1.00
1:B:591:ARG:HB2	2:B:1703:CPL:C42	1.91	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLY:HA2	1:A:202:HIS:NE2	1.75	1.00
1:A:250:PRO:CG	1:B:297:ARG:CZ	2.34	1.00
2:B:1697:CPL:H261	2:B:1714:CPL:H482	1.41	1.00
1:A:143:PRO:O	1:B:266:VAL:CA	1.94	1.00
1:A:147:LYS:HB2	1:B:266:VAL:O	1.60	1.00
1:B:128:GLN:HG2	1:B:129:GLN:H	1.22	1.00
1:A:429:PHE:CZ	2:A:1702:CPL:C1	2.28	0.99
1:B:434:SER:O	2:B:1701:CPL:O2P	1.80	0.99
3:A:1696:GDP:H2'	1:B:246:SER:HB3	1.02	0.99
2:A:1701:CPL:C11	1:B:420:LEU:HD11	1.92	0.99
2:A:1703:CPL:H261	2:A:1715:CPL:C48	1.91	0.99
2:B:1705:CPL:C26	2:B:1711:CPL:C48	2.40	0.99
2:A:1697:CPL:H261	2:A:1710:CPL:C48	1.91	0.99
2:B:1701:CPL:H481	2:B:1712:CPL:H483	1.45	0.99
1:B:60:ILE:HG21	1:B:199:ASN:CB	1.87	0.99
1:B:591:ARG:HB2	2:B:1703:CPL:C43	1.91	0.99
1:A:246:SER:CB	3:B:1706:GDP:H2'	1.92	0.99
1:A:432:LEU:HG	2:A:1709:CPL:H342	1.00	0.99
2:A:1698:CPL:H482	2:A:1707:CPL:H481	1.00	0.99
1:B:425:GLU:HB2	2:B:1705:CPL:HC11	1.43	0.99
1:A:421:ARG:HD2	2:B:1700:CPL:HC72	1.42	0.98
2:A:3094:CPL:H262	2:A:3181:CPL:C46	1.91	0.98
1:A:209:ARG:NH1	1:B:211:SER:HA	1.76	0.98
2:B:1701:CPL:C26	2:B:1710:CPL:H482	1.93	0.98
1:A:297:ARG:NH2	1:B:250:PRO:HG2	1.65	0.98
1:A:219:ARG:HD2	1:B:150:GLU:HG2	1.42	0.98
1:A:265:GLN:CB	1:B:144:ALA:H	1.76	0.98
1:A:572:ILE:HD11	2:A:1705:CPL:H341	1.46	0.98
1:A:421:ARG:NE	2:B:1700:CPL:HC73	1.79	0.98
1:A:144:ALA:H	1:B:265:GLN:CB	1.75	0.98
1:A:60:ILE:HG23	1:A:199:ASN:HB3	1.43	0.97
1:A:362:ASN:CB	1:A:660:ARG:HH11	1.77	0.97
1:A:216:LEU:HD12	1:B:217:GLY:HA2	1.45	0.97
1:A:219:ARG:HD2	1:B:150:GLU:CD	1.87	0.97
1:B:591:ARG:HG3	2:B:1703:CPL:C41	1.91	0.97
2:A:1697:CPL:H121	2:A:1700:CPL:H341	1.46	0.97
1:A:421:ARG:NH2	2:B:1700:CPL:C7	2.27	0.97
1:A:150:GLU:CD	1:B:219:ARG:HD2	1.89	0.97
2:A:1697:CPL:H132	2:A:1700:CPL:H362	1.44	0.97
1:B:602:VAL:HG22	2:B:1703:CPL:C5	1.94	0.97
2:B:1702:CPL:H481	2:B:1707:CPL:H263	1.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:PHE:O	1:B:147:LYS:HD3	1.65	0.96
2:A:1706:CPL:H482	2:A:1711:CPL:H263	1.45	0.96
1:B:585:GLN:HB3	2:B:1696:CPL:C26	1.88	0.96
1:B:591:ARG:CA	2:B:1703:CPL:H412	1.95	0.96
1:A:297:ARG:HH21	1:B:250:PRO:HG3	1.16	0.96
1:A:416:GLU:OE2	2:A:1701:CPL:C31	1.96	0.96
1:A:67:GLN:NE2	1:A:200:ASN:HB3	1.81	0.96
1:B:569:LEU:N	2:B:1697:CPL:O1P	1.98	0.96
1:B:586:ALA:HB2	2:B:1697:CPL:H462	0.99	0.96
1:A:68:GLY:CA	1:A:202:HIS:HE2	1.77	0.96
2:A:1698:CPL:C48	2:A:1707:CPL:C48	2.43	0.96
1:B:591:ARG:CA	2:B:1703:CPL:C41	2.42	0.96
1:A:269:ALA:CB	1:B:147:LYS:CA	2.44	0.96
1:A:449:GLU:CB	2:A:1708:CPL:HC71	1.94	0.96
2:A:1704:CPL:H251	2:A:1714:CPL:H481	1.48	0.96
1:A:248:ILE:HG23	1:B:300:LEU:HD13	1.44	0.95
2:B:1701:CPL:H261	2:B:1710:CPL:H482	1.46	0.95
2:A:1718:CPL:C24	2:A:3097:CPL:H231	1.96	0.95
1:A:147:LYS:NZ	1:B:271:LEU:CG	2.27	0.95
2:A:1704:CPL:C26	2:A:1714:CPL:C48	2.24	0.95
1:B:67:GLN:CB	1:B:71:ARG:HH22	1.79	0.95
1:B:565:THR:HA	2:B:1697:CPL:HC41	0.97	0.95
2:A:1700:CPL:H482	2:A:1710:CPL:C48	1.96	0.95
1:B:572:ILE:HD12	2:B:1697:CPL:O3P	1.65	0.95
2:B:1697:CPL:C26	2:B:1714:CPL:C48	2.44	0.95
1:A:250:PRO:HG3	1:B:297:ARG:HH21	1.13	0.95
1:A:147:LYS:HE3	1:B:214:CYS:SG	2.07	0.95
1:A:219:ARG:HD3	1:B:150:GLU:OE2	1.66	0.95
2:A:1700:CPL:O1P	2:A:1713:CPL:HC2	1.66	0.95
1:A:273:GLU:HB2	1:B:151:GLN:NE2	1.78	0.95
1:A:416:GLU:CD	2:A:1701:CPL:C32	2.36	0.95
1:B:591:ARG:CG	2:B:1703:CPL:C41	2.35	0.95
1:A:211:SER:O	1:B:209:ARG:CD	2.15	0.94
1:B:579:LEU:CD2	2:B:1697:CPL:C19	2.45	0.94
2:A:1697:CPL:C14	2:A:1700:CPL:H361	1.97	0.94
2:A:1704:CPL:H261	2:A:1714:CPL:H472	1.48	0.94
1:A:217:GLY:HA2	1:B:216:LEU:HD12	1.46	0.94
1:B:425:GLU:CB	2:B:1705:CPL:HC11	1.93	0.94
2:B:1705:CPL:C26	2:B:1711:CPL:H481	1.96	0.94
1:A:297:ARG:CZ	1:B:250:PRO:CG	2.38	0.94
1:A:465:LYS:HZ3	1:B:465:LYS:CA	1.79	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LYS:CA	1:B:269:ALA:CB	2.45	0.94
1:B:444:LEU:HD13	2:B:1697:CPL:HC51	1.47	0.94
1:A:151:GLN:NE2	1:B:273:GLU:HB2	1.81	0.94
1:B:572:ILE:CD1	2:B:1697:CPL:O3P	2.16	0.94
1:A:413:ASN:HA	2:A:1703:CPL:C4	1.98	0.93
1:A:414:THR:HA	2:A:1701:CPL:HC51	1.50	0.93
2:A:1697:CPL:H482	2:A:1705:CPL:C26	1.98	0.93
1:A:248:ILE:HG23	1:B:300:LEU:HD12	1.50	0.93
1:A:418:ASP:OD2	2:A:1701:CPL:C8	2.16	0.93
1:A:465:LYS:NZ	1:B:465:LYS:CA	2.31	0.93
2:B:1710:CPL:H251	2:B:1712:CPL:C46	1.99	0.93
1:A:214:CYS:SG	1:B:147:LYS:HE3	2.08	0.93
2:A:1711:CPL:C48	2:A:1716:CPL:H481	1.98	0.93
1:A:147:LYS:HD3	1:B:267:PHE:O	1.68	0.93
1:A:418:ASP:OD2	2:A:1701:CPL:HC82	1.68	0.93
1:B:60:ILE:HG21	1:B:199:ASN:HB2	0.94	0.93
1:A:60:ILE:HG21	1:A:199:ASN:CG	1.94	0.93
1:A:429:PHE:CD1	2:A:1702:CPL:C33	2.50	0.92
2:A:1701:CPL:C4	1:B:421:ARG:HD3	1.83	0.92
1:A:572:ILE:HD11	2:A:1705:CPL:C32	2.00	0.92
1:A:80:ARG:CZ	1:B:212:GLN:HG2	2.00	0.92
1:B:579:LEU:CD2	2:B:1697:CPL:H192	1.99	0.92
1:A:209:ARG:CD	1:B:211:SER:O	2.17	0.91
1:A:572:ILE:CD1	2:A:1705:CPL:C32	2.48	0.91
2:A:1703:CPL:C26	2:A:1715:CPL:C48	2.48	0.91
1:A:150:GLU:OE2	1:B:219:ARG:HD3	1.71	0.91
1:A:212:GLN:HG2	1:B:80:ARG:CZ	2.01	0.91
1:A:300:LEU:HD13	1:B:248:ILE:HG23	1.49	0.91
2:A:1700:CPL:C48	2:A:1710:CPL:C48	2.49	0.91
1:B:585:GLN:HB3	2:B:1696:CPL:C25	2.00	0.91
1:B:591:ARG:HA	2:B:1703:CPL:C38	1.99	0.91
1:A:434:SER:C	2:A:1709:CPL:C5	2.17	0.91
1:A:446:LYS:CE	2:A:1708:CPL:C7	2.45	0.91
1:A:212:GLN:HE21	1:B:209:ARG:HB3	0.74	0.90
1:A:577:LEU:HD11	2:A:1707:CPL:C42	2.00	0.90
2:A:1718:CPL:H241	2:A:3097:CPL:H231	1.49	0.90
1:A:219:ARG:CD	1:B:150:GLU:CG	2.46	0.90
1:A:363:GLU:HB2	1:A:660:ARG:HH22	1.34	0.90
1:A:421:ARG:HD2	2:B:1700:CPL:HC73	1.26	0.90
1:A:68:GLY:HA2	1:A:202:HIS:CE1	2.07	0.90
1:A:577:LEU:CG	2:A:1707:CPL:H411	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LYS:HZ3	1:B:465:LYS:HB2	1.34	0.90
1:B:568:LEU:C	2:B:1697:CPL:O1P	2.14	0.90
1:A:143:PRO:HB3	1:B:266:VAL:HG23	1.53	0.90
1:A:421:ARG:CZ	2:B:1700:CPL:HC73	2.02	0.90
1:A:425:GLU:HG3	2:A:1708:CPL:C31	2.02	0.89
1:A:581:VAL:HG23	2:A:1707:CPL:C46	2.03	0.89
1:A:585:GLN:HG2	2:A:1699:CPL:H263	1.54	0.89
1:B:591:ARG:CB	2:B:1703:CPL:H412	2.01	0.89
1:B:595:LYS:CA	2:B:1703:CPL:H341	2.02	0.89
2:B:1699:CPL:H483	2:B:1709:CPL:H261	1.53	0.89
1:A:581:VAL:O	2:A:1698:CPL:H482	1.73	0.89
1:A:273:GLU:HB3	1:B:151:GLN:NE2	1.87	0.89
1:A:581:VAL:O	2:A:1707:CPL:H472	1.73	0.89
1:A:429:PHE:HE1	2:A:1702:CPL:O3P	1.38	0.89
1:A:246:SER:CB	3:B:1706:GDP:C4	2.56	0.88
2:A:1698:CPL:H481	2:A:1707:CPL:H481	1.54	0.88
1:B:432:LEU:HB3	2:B:1701:CPL:H331	1.54	0.88
1:A:97:SER:C	1:B:262:ARG:CZ	2.46	0.88
3:A:1696:GDP:C4	1:B:246:SER:CB	2.57	0.88
1:A:271:LEU:HG	1:B:147:LYS:HZ3	1.34	0.88
2:A:1718:CPL:C26	2:A:3097:CPL:H252	2.03	0.88
1:A:278:GLU:HG2	1:A:333:ARG:HH11	1.33	0.88
1:A:581:VAL:HG23	2:A:1707:CPL:C45	1.74	0.88
1:B:447:ALA:HA	2:B:1705:CPL:O2P	1.73	0.88
2:B:1710:CPL:C25	2:B:1712:CPL:H462	2.02	0.88
1:B:585:GLN:H	1:B:588:GLN:NE2	1.71	0.88
1:B:591:ARG:HB2	2:B:1703:CPL:H412	1.55	0.88
1:A:425:GLU:O	2:A:1708:CPL:O1P	1.90	0.88
1:A:465:LYS:NZ	1:B:465:LYS:CB	2.35	0.88
1:B:413:ASN:ND2	2:B:1704:CPL:HC61	1.89	0.88
1:B:591:ARG:HA	2:B:1703:CPL:H382	1.54	0.88
1:A:266:VAL:HG23	1:B:143:PRO:HB3	1.55	0.88
2:A:1700:CPL:H482	2:A:1710:CPL:H482	1.55	0.88
1:B:68:GLY:HA2	1:B:202:HIS:HE1	1.36	0.87
1:A:434:SER:O	2:A:1709:CPL:P	2.32	0.87
1:A:421:ARG:HA	2:B:1700:CPL:HC12	1.54	0.87
2:A:1697:CPL:C14	2:A:1700:CPL:C36	2.52	0.87
1:B:278:GLU:HB2	1:B:333:ARG:HH11	1.33	0.87
1:B:447:ALA:CB	2:B:1705:CPL:O1P	2.22	0.87
1:A:585:GLN:H	1:A:588:GLN:NE2	1.72	0.87
1:A:209:ARG:HB3	1:B:212:GLN:HE21	0.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:PHE:O	1:B:147:LYS:CD	2.23	0.87
2:A:3097:CPL:H261	2:B:1700:CPL:H261	1.55	0.87
1:B:278:GLU:HB2	1:B:333:ARG:CZ	2.05	0.87
2:A:1697:CPL:C11	2:A:1700:CPL:H342	2.05	0.87
2:B:1702:CPL:H481	2:B:1707:CPL:H261	1.38	0.87
1:B:425:GLU:HB2	2:B:1705:CPL:C1	1.96	0.86
1:A:80:ARG:CZ	1:B:212:GLN:CG	2.53	0.86
1:A:93:ASN:OD1	1:B:248:ILE:CD1	2.21	0.86
1:A:585:GLN:CG	2:A:1699:CPL:H262	2.03	0.86
2:A:1697:CPL:C13	2:A:1700:CPL:H362	2.03	0.86
2:A:1704:CPL:C25	2:A:1714:CPL:C48	2.48	0.86
1:A:143:PRO:CB	1:B:265:GLN:N	2.37	0.86
2:A:1701:CPL:HC42	1:B:421:ARG:NE	1.91	0.86
1:A:144:ALA:N	1:B:265:GLN:CB	2.23	0.86
1:A:209:ARG:CB	1:B:212:GLN:NE2	2.22	0.86
1:A:572:ILE:CD1	2:A:1705:CPL:H321	2.03	0.86
1:A:300:LEU:HD12	1:B:248:ILE:HG23	1.58	0.86
1:A:572:ILE:CG2	2:A:1705:CPL:H361	2.05	0.86
1:A:265:GLN:OE1	1:B:142:ASP:OD1	1.94	0.85
1:A:418:ASP:H	2:A:1701:CPL:HC41	1.38	0.85
1:A:436:LYS:CE	2:A:1709:CPL:HC71	2.07	0.85
2:A:1702:CPL:H483	2:A:1708:CPL:H252	1.55	0.85
1:B:593:LEU:CD1	2:B:1697:CPL:C35	2.54	0.85
2:A:1697:CPL:C26	2:A:1710:CPL:C48	2.53	0.85
2:A:1699:CPL:H39	2:A:1699:CPL:H171	1.57	0.85
1:B:587:ASP:C	2:B:1703:CPL:H452	2.01	0.85
1:A:449:GLU:CD	2:A:1708:CPL:HC71	2.01	0.85
1:A:147:LYS:HZ3	1:B:271:LEU:HG	1.39	0.85
1:A:429:PHE:HZ	2:A:1702:CPL:HC11	1.11	0.85
2:B:1697:CPL:H261	2:B:1714:CPL:H483	1.58	0.85
1:A:215:THR:HB	1:A:218:GLU:HG3	1.57	0.85
2:B:1699:CPL:C48	2:B:1709:CPL:H261	2.06	0.85
1:A:429:PHE:CE1	2:A:1702:CPL:C2	2.52	0.85
1:A:434:SER:CB	2:A:1709:CPL:HC83	2.06	0.85
2:A:1711:CPL:H481	2:A:1716:CPL:H481	1.57	0.85
1:A:212:GLN:CG	1:B:80:ARG:CZ	2.54	0.85
2:A:1718:CPL:H251	2:A:3097:CPL:H252	1.56	0.85
1:B:375:PHE:HD2	1:B:643:LYS:HE2	1.41	0.85
1:A:60:ILE:HG21	1:A:199:ASN:HB3	1.30	0.85
1:A:572:ILE:CD1	2:A:1705:CPL:C33	2.54	0.85
1:B:94:LEU:HD22	1:B:95:LEU:HD12	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:VAL:HG13	2:B:1703:CPL:HC62	1.58	0.85
1:A:263:LEU:HD23	1:B:79:LYS:HG3	1.57	0.84
1:A:434:SER:O	2:A:1709:CPL:C4	2.08	0.84
2:A:1706:CPL:H482	2:A:1711:CPL:C26	2.07	0.84
1:A:465:LYS:NZ	1:B:465:LYS:HG3	1.92	0.84
1:A:94:LEU:HD22	1:A:95:LEU:HD12	1.59	0.84
1:A:68:GLY:CA	1:A:202:HIS:NE2	2.37	0.84
2:A:1700:CPL:C48	2:A:1710:CPL:H482	2.07	0.84
2:A:1697:CPL:C12	2:A:1700:CPL:C34	2.30	0.84
1:A:147:LYS:CA	1:B:269:ALA:HB3	2.06	0.84
1:A:212:GLN:NE2	1:B:209:ARG:CB	2.22	0.84
1:A:269:ALA:HB3	1:B:147:LYS:CA	2.06	0.84
1:B:580:GLY:O	2:B:1698:CPL:H451	1.76	0.84
1:A:363:GLU:N	1:A:660:ARG:NH1	2.12	0.84
2:A:1700:CPL:H462	2:A:1713:CPL:H472	1.60	0.84
2:B:1701:CPL:C26	2:B:1710:CPL:C48	2.52	0.84
1:B:572:ILE:HD13	2:B:1697:CPL:O3	1.76	0.84
1:A:143:PRO:CB	1:B:262:ARG:O	2.25	0.84
1:A:150:GLU:CG	1:B:219:ARG:CD	2.48	0.84
1:B:215:THR:HB	1:B:218:GLU:HG3	1.57	0.84
1:B:581:VAL:CA	2:B:1699:CPL:C46	2.11	0.84
1:A:147:LYS:CD	1:B:266:VAL:O	2.26	0.83
1:B:60:ILE:HG22	1:B:199:ASN:HB3	1.57	0.83
1:B:425:GLU:HB3	2:B:1705:CPL:O2	1.29	0.83
2:B:1701:CPL:H252	2:B:1710:CPL:H482	1.60	0.83
1:A:465:LYS:HZ1	1:B:465:LYS:HA	1.38	0.83
1:A:579:LEU:CD2	2:A:1705:CPL:H451	2.03	0.83
1:B:594:VAL:O	2:B:1703:CPL:H342	1.77	0.83
1:A:147:LYS:H	1:B:269:ALA:HB1	1.30	0.83
1:A:269:ALA:HB1	1:B:147:LYS:CA	2.08	0.83
1:A:585:GLN:HG2	2:A:1699:CPL:C26	2.07	0.83
1:A:142:ASP:OD1	1:B:265:GLN:OE1	1.97	0.83
1:A:147:LYS:HZ2	1:B:267:PHE:HA	1.44	0.83
1:A:375:PHE:HD2	1:A:643:LYS:HE2	1.41	0.83
1:A:446:LYS:HD3	2:A:1708:CPL:HC72	0.84	0.83
1:A:151:GLN:NE2	1:B:273:GLU:HB3	1.94	0.83
1:A:465:LYS:CG	1:B:465:LYS:HG3	2.09	0.82
2:A:1718:CPL:C25	2:A:3097:CPL:H252	2.09	0.82
1:A:147:LYS:CD	1:B:267:PHE:O	2.26	0.82
1:A:248:ILE:CD1	1:B:93:ASN:OD1	2.23	0.82
1:B:416:GLU:HB3	2:B:1700:CPL:O2	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1718:CPL:C25	2:A:3097:CPL:C25	2.57	0.82
2:B:1705:CPL:H261	2:B:1711:CPL:H483	1.60	0.82
1:A:270:ASN:C	1:B:147:LYS:HE2	2.04	0.82
2:A:1703:CPL:H483	2:A:1715:CPL:H261	1.59	0.82
1:A:262:ARG:HB3	1:B:79:LYS:HZ3	1.45	0.82
1:B:591:ARG:CA	2:B:1703:CPL:H411	2.08	0.82
2:B:1699:CPL:C48	2:B:1709:CPL:C26	2.58	0.82
1:A:64:ASN:OD1	1:A:200:ASN:CA	2.07	0.82
1:A:263:LEU:HA	1:B:79:LYS:HE3	1.61	0.82
1:A:583:PHE:N	2:A:1707:CPL:H482	1.93	0.82
2:A:1718:CPL:C6	2:A:3097:CPL:HC73	2.08	0.82
1:A:446:LYS:HE2	2:A:1708:CPL:C7	2.09	0.82
1:A:590:ARG:NH1	2:A:1705:CPL:H182	1.94	0.82
1:B:425:GLU:CB	2:B:1705:CPL:O2	2.15	0.82
1:A:147:LYS:CA	1:B:269:ALA:HB1	2.09	0.82
2:B:1701:CPL:C25	2:B:1710:CPL:C48	2.57	0.81
1:A:147:LYS:HE2	1:B:270:ASN:C	2.04	0.81
1:A:265:GLN:OE1	1:B:142:ASP:CB	2.28	0.81
1:A:79:LYS:HG3	1:B:263:LEU:HD23	1.61	0.81
1:A:273:GLU:HB3	1:B:151:GLN:HE22	1.45	0.81
1:A:432:LEU:CB	2:A:1709:CPL:C32	2.06	0.81
1:B:429:PHE:CE1	2:B:1702:CPL:H322	2.14	0.81
1:A:265:GLN:CB	1:B:144:ALA:N	2.26	0.81
2:B:1710:CPL:H232	2:B:1712:CPL:H442	1.62	0.81
1:A:67:GLN:HE22	1:A:200:ASN:CB	1.94	0.81
1:A:269:ALA:HB3	1:B:147:LYS:H	1.37	0.81
1:B:409:LEU:HD21	1:B:606:PRO:HA	1.62	0.81
1:B:579:LEU:CG	2:B:1697:CPL:H212	2.11	0.81
1:A:265:GLN:CD	1:B:142:ASP:CB	2.53	0.81
2:A:1701:CPL:C11	1:B:420:LEU:CD1	2.54	0.81
1:B:416:GLU:HB3	2:B:1700:CPL:C2	2.10	0.81
1:A:409:LEU:HD21	1:A:606:PRO:HA	1.62	0.81
1:A:147:LYS:H	1:B:269:ALA:HB3	1.42	0.80
1:A:148:LYS:N	1:B:269:ALA:HB1	1.95	0.80
1:A:425:GLU:HB3	2:A:1708:CPL:C11	2.10	0.80
1:A:302:ASN:ND2	1:A:304:GLN:H	1.80	0.80
2:A:1703:CPL:H252	2:A:1704:CPL:H472	1.62	0.80
1:B:586:ALA:HB1	2:B:1697:CPL:C46	1.89	0.80
1:A:269:ALA:HB1	1:B:148:LYS:N	1.96	0.80
1:A:150:GLU:OE2	1:B:219:ARG:CD	2.27	0.80
1:A:219:ARG:CD	1:B:150:GLU:OE2	2.24	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:LEU:CD1	2:A:1707:CPL:H411	1.90	0.80
1:A:585:GLN:CG	2:A:1699:CPL:C26	2.60	0.80
2:A:1717:CPL:H171	2:A:1717:CPL:H39	1.64	0.80
1:B:413:ASN:HD22	2:B:1704:CPL:HC61	1.46	0.80
1:B:591:ARG:HA	2:B:1703:CPL:C37	2.11	0.80
2:A:1710:CPL:H39	2:A:1710:CPL:H171	1.64	0.80
2:B:1699:CPL:H481	2:B:1709:CPL:C26	2.11	0.80
1:B:447:ALA:HA	2:B:1705:CPL:P	2.22	0.80
2:B:1710:CPL:H39	2:B:1710:CPL:H171	1.64	0.80
2:B:1712:CPL:H263	2:B:1714:CPL:H251	1.64	0.80
1:A:449:GLU:OE1	2:A:1708:CPL:HC81	1.80	0.79
1:B:432:LEU:HD23	2:B:1701:CPL:H341	1.63	0.79
1:A:262:ARG:O	1:B:143:PRO:CB	2.30	0.79
1:A:446:LYS:CE	2:A:1708:CPL:C6	2.31	0.79
1:A:271:LEU:HG	1:B:147:LYS:HZ1	0.98	0.79
1:A:432:LEU:CD2	2:A:1709:CPL:H342	2.13	0.79
2:B:1701:CPL:H39	2:B:1701:CPL:H171	1.64	0.79
2:A:1697:CPL:HC31	2:A:1700:CPL:H322	1.64	0.79
2:A:1703:CPL:H171	2:A:1703:CPL:H39	1.65	0.79
1:B:90:ILE:HD12	1:B:169:LEU:HD13	1.64	0.79
2:A:1708:CPL:H39	2:A:1708:CPL:H171	1.65	0.79
1:A:418:ASP:CG	2:A:1701:CPL:HC82	2.07	0.79
1:B:598:LYS:HZ1	2:B:1703:CPL:HC2	0.96	0.79
1:A:367:ARG:O	1:A:370:SER:HB3	1.83	0.79
1:A:269:ALA:HB1	1:B:148:LYS:H	1.47	0.79
1:A:277:VAL:HG22	1:A:282:ILE:HD12	1.65	0.79
1:A:414:THR:O	2:A:1701:CPL:C5	2.30	0.79
1:A:520:TRP:HH2	1:A:527:LEU:HG	1.47	0.79
1:B:520:TRP:HH2	1:B:527:LEU:HG	1.47	0.79
1:B:591:ARG:HA	2:B:1703:CPL:H371	1.64	0.79
1:A:90:ILE:HD12	1:A:169:LEU:HD13	1.64	0.79
1:A:269:ALA:HB3	1:B:147:LYS:N	1.89	0.79
1:B:367:ARG:O	1:B:370:SER:HB3	1.83	0.79
1:B:598:LYS:NZ	2:B:1703:CPL:C1	2.46	0.79
1:A:421:ARG:HD3	2:B:1700:CPL:C7	1.51	0.78
1:A:465:LYS:NZ	1:B:465:LYS:CG	2.46	0.78
2:A:1700:CPL:C48	2:A:1710:CPL:H481	2.12	0.78
1:A:434:SER:CA	2:A:1709:CPL:HC51	2.12	0.78
2:A:1703:CPL:C26	2:A:1715:CPL:H481	2.14	0.78
1:B:444:LEU:HD13	2:B:1697:CPL:C5	2.13	0.78
1:B:302:ASN:ND2	1:B:304:GLN:H	1.80	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:LEU:HD21	2:A:1707:CPL:H411	1.64	0.78
1:B:414:THR:O	2:B:1700:CPL:HC82	1.80	0.78
1:A:432:LEU:CG	2:A:1709:CPL:C34	2.45	0.78
2:A:1698:CPL:HC73	2:A:1700:CPL:HC62	1.62	0.78
2:B:1696:CPL:H171	2:B:1696:CPL:H39	1.64	0.78
1:A:413:ASN:HA	2:A:1703:CPL:HC41	1.64	0.78
1:B:230:GLY:O	1:B:334:GLN:CG	2.31	0.78
1:A:123:ASP:OD2	1:A:125:LYS:HE3	1.83	0.78
1:A:265:GLN:OE1	1:B:142:ASP:HA	1.84	0.78
2:A:1697:CPL:C48	2:A:1705:CPL:C26	2.60	0.78
1:B:123:ASP:OD2	1:B:125:LYS:HE3	1.83	0.78
1:B:277:VAL:HG22	1:B:282:ILE:HD12	1.65	0.78
1:A:148:LYS:H	1:B:269:ALA:HB1	1.49	0.78
1:B:598:LYS:HZ1	2:B:1703:CPL:C3	1.97	0.78
1:A:607:GLN:O	1:A:611:GLU:HG3	1.84	0.77
2:B:1701:CPL:H481	2:B:1712:CPL:C48	2.12	0.77
2:A:1702:CPL:H171	2:A:1702:CPL:H39	1.65	0.77
2:A:1703:CPL:H252	2:A:1704:CPL:C47	2.15	0.77
1:B:427:ASN:HA	2:B:1705:CPL:HC31	1.66	0.77
1:B:591:ARG:HA	2:B:1703:CPL:C41	2.13	0.77
2:A:1703:CPL:C48	2:A:1715:CPL:H261	2.14	0.77
2:B:1712:CPL:H39	2:B:1712:CPL:H171	1.64	0.77
1:A:576:LEU:HD21	2:A:1705:CPL:H412	1.67	0.77
1:A:142:ASP:CB	1:B:265:GLN:OE1	2.26	0.76
1:A:79:LYS:HE3	1:B:263:LEU:HA	1.66	0.76
1:A:572:ILE:HD13	2:A:1705:CPL:C35	2.14	0.76
1:B:586:ALA:CB	2:B:1697:CPL:H462	1.86	0.76
1:B:564:VAL:HG13	1:B:601:LEU:HD11	1.67	0.76
1:A:31:LEU:HD11	1:A:674:VAL:HG13	1.68	0.76
1:A:577:LEU:CD2	2:A:1707:CPL:H411	2.15	0.76
1:B:607:GLN:O	1:B:611:GLU:HG3	1.84	0.76
1:B:31:LEU:HD11	1:B:674:VAL:HG13	1.68	0.76
1:A:60:ILE:HG22	1:A:199:ASN:HB3	1.64	0.76
1:A:278:GLU:HB2	1:A:333:ARG:HH22	1.49	0.76
2:B:1698:CPL:H171	2:B:1698:CPL:H39	1.65	0.76
1:A:435:GLY:C	2:A:1709:CPL:HC73	2.11	0.76
2:A:1697:CPL:C15	2:A:1700:CPL:C39	2.64	0.76
1:B:416:GLU:N	2:B:1704:CPL:O2P	2.14	0.76
1:A:266:VAL:O	1:B:147:LYS:CD	2.32	0.76
1:A:267:PHE:HA	1:B:147:LYS:HZ2	1.49	0.76
1:A:269:ALA:CA	1:B:147:LYS:CB	2.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:PRO:HG3	1:B:261:ASN:O	1.85	0.76
1:A:652:GLN:HE22	1:A:656:ARG:NH2	1.84	0.76
2:A:1697:CPL:H263	2:A:1710:CPL:H481	1.68	0.76
1:B:278:GLU:CG	1:B:333:ARG:HH11	1.99	0.76
1:A:449:GLU:CB	2:A:1708:CPL:C7	2.64	0.76
2:A:1703:CPL:H261	2:A:1715:CPL:H482	1.67	0.76
1:A:564:VAL:HG13	1:A:601:LEU:HD11	1.67	0.75
1:A:590:ARG:CZ	2:A:1705:CPL:H182	2.16	0.75
1:B:53:ARG:HH12	1:B:193:LEU:HD21	1.49	0.75
1:A:97:SER:C	1:B:262:ARG:CD	2.58	0.75
1:B:585:GLN:HB3	2:B:1696:CPL:H252	1.69	0.75
1:A:436:LYS:HE2	1:A:436:LYS:HA	1.68	0.75
1:A:581:VAL:O	2:A:1698:CPL:C48	2.34	0.75
1:A:416:GLU:CD	2:A:1701:CPL:H322	2.11	0.75
1:A:572:ILE:HD12	2:A:1705:CPL:C34	2.08	0.75
1:B:278:GLU:CB	1:B:333:ARG:HH11	1.91	0.75
1:B:447:ALA:N	2:B:1705:CPL:HC42	2.02	0.75
2:B:1697:CPL:H261	2:B:1714:CPL:H481	1.68	0.75
1:B:230:GLY:O	1:B:334:GLN:HG2	1.86	0.75
2:B:1697:CPL:C26	2:B:1698:CPL:C48	2.59	0.75
1:A:265:GLN:HE21	1:B:142:ASP:C	1.93	0.75
2:A:1697:CPL:H121	2:A:1700:CPL:H342	0.76	0.75
1:B:581:VAL:HA	2:B:1699:CPL:H461	0.75	0.75
1:A:263:LEU:CD2	1:B:79:LYS:HG3	2.17	0.74
1:A:446:LYS:HE2	2:A:1708:CPL:N	2.02	0.74
1:B:591:ARG:HB2	2:B:1703:CPL:H43	1.67	0.74
1:A:261:ASN:O	1:B:143:PRO:HG3	1.86	0.74
1:A:375:PHE:CD2	1:A:643:LYS:HE2	2.21	0.74
1:A:465:LYS:HG3	1:B:465:LYS:CG	2.17	0.74
1:B:363:GLU:HB2	1:B:660:ARG:CZ	2.16	0.74
1:B:375:PHE:CD2	1:B:643:LYS:HE2	2.21	0.74
1:A:265:GLN:OE1	1:B:142:ASP:CA	2.36	0.74
2:A:1703:CPL:H262	2:A:1715:CPL:H481	1.67	0.74
1:B:652:GLN:HE22	1:B:656:ARG:NH2	1.84	0.74
1:A:393:ARG:HG3	1:A:394:ASP:N	2.02	0.74
1:B:68:GLY:CA	1:B:202:HIS:CE1	2.70	0.74
1:B:129:GLN:C	1:B:130:LEU:HD12	2.13	0.74
1:B:393:ARG:HG3	1:B:394:ASP:N	2.02	0.74
1:B:585:GLN:OE1	2:B:1696:CPL:C25	2.34	0.74
2:A:1701:CPL:C5	1:B:421:ARG:HD3	2.17	0.74
1:B:202:HIS:HB3	1:B:331:GLU:CD	2.13	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:GLU:OE1	2:A:1708:CPL:HC71	1.87	0.74
1:A:449:GLU:HB3	2:A:1708:CPL:C7	2.18	0.74
1:A:79:LYS:HZ3	1:B:262:ARG:HB3	1.52	0.74
1:A:418:ASP:OD2	2:A:1701:CPL:HC81	1.88	0.74
1:A:143:PRO:CB	1:B:266:VAL:HG23	2.17	0.74
1:A:418:ASP:H	2:A:1701:CPL:C4	2.02	0.73
1:B:593:LEU:HD12	2:B:1697:CPL:C36	2.18	0.73
2:B:1701:CPL:H481	2:B:1710:CPL:H261	1.70	0.73
2:A:1700:CPL:H482	2:A:1710:CPL:H481	1.69	0.73
1:A:418:ASP:N	2:A:1701:CPL:C4	2.50	0.73
1:B:436:LYS:HA	1:B:436:LYS:HE2	1.68	0.73
1:A:129:GLN:C	1:A:130:LEU:HD12	2.12	0.73
1:A:465:LYS:HZ2	1:B:465:LYS:HG3	1.52	0.73
1:A:581:VAL:HG21	2:A:1707:CPL:H452	0.74	0.73
1:A:150:GLU:OE1	1:B:219:ARG:CD	2.19	0.73
1:A:449:GLU:HB3	2:A:1708:CPL:HC71	1.71	0.73
1:A:262:ARG:HB3	1:B:79:LYS:NZ	2.04	0.72
1:A:653:LYS:CE	1:A:657:GLU:OE2	2.36	0.72
1:A:266:VAL:O	1:B:147:LYS:CB	2.36	0.72
1:A:271:LEU:HG	1:B:147:LYS:CE	2.17	0.72
1:B:167:TYR:CD2	1:B:169:LEU:HG	2.24	0.72
1:A:429:PHE:HA	2:A:1702:CPL:H331	1.69	0.72
1:A:79:LYS:HG3	1:B:263:LEU:CD2	2.19	0.72
1:B:585:GLN:CA	2:B:1696:CPL:H261	2.16	0.72
1:A:167:TYR:CD2	1:A:169:LEU:HG	2.24	0.72
1:B:595:LYS:CA	2:B:1703:CPL:C34	2.65	0.72
1:A:583:PHE:CE2	2:A:1707:CPL:C48	2.40	0.72
1:B:128:GLN:HG2	1:B:129:GLN:N	2.03	0.72
2:A:3094:CPL:C25	2:A:3181:CPL:H462	2.19	0.72
1:A:246:SER:HB2	3:B:1706:GDP:N3	2.05	0.72
1:B:578:GLY:O	1:B:584:LEU:HB2	1.90	0.72
1:B:579:LEU:HD21	2:B:1697:CPL:H212	0.73	0.72
1:A:558:GLY:O	2:A:1705:CPL:C8	2.26	0.71
2:A:1708:CPL:H261	2:A:1716:CPL:C26	2.20	0.71
1:A:432:LEU:HB3	2:A:1709:CPL:O31	1.90	0.71
1:A:581:VAL:O	2:A:1707:CPL:C47	2.37	0.71
2:A:1701:CPL:H263	2:A:1712:CPL:C48	2.20	0.71
1:B:568:LEU:HB2	2:B:1697:CPL:O2P	1.90	0.71
1:A:105:VAL:O	1:A:107:THR:HG23	1.90	0.71
1:A:432:LEU:CG	2:A:1709:CPL:C33	2.68	0.71
3:A:1696:GDP:N3	1:B:246:SER:HB2	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LYS:CB	1:B:266:VAL:O	2.36	0.71
1:B:278:GLU:CD	1:B:333:ARG:NH1	2.49	0.71
1:A:278:GLU:HB2	1:A:333:ARG:CZ	2.20	0.71
1:A:450:GLN:CD	2:A:1708:CPL:C8	2.62	0.71
1:B:167:TYR:HD2	1:B:169:LEU:HG	1.55	0.71
1:A:582:GLY:C	2:A:1707:CPL:C48	2.59	0.71
1:A:647:ASP:O	1:A:651:LYS:HG2	1.91	0.71
1:A:432:LEU:HG	2:A:1709:CPL:C32	2.20	0.71
1:B:416:GLU:HB3	2:B:1700:CPL:C31	2.20	0.71
1:A:413:ASN:HA	2:A:1703:CPL:HC42	1.72	0.70
1:A:143:PRO:HG2	1:B:265:GLN:N	1.32	0.70
1:A:266:VAL:HG23	1:B:143:PRO:CB	2.20	0.70
2:A:1718:CPL:C6	2:A:3097:CPL:C7	2.69	0.70
1:B:426:LEU:CA	2:B:1705:CPL:O1P	2.35	0.70
1:A:79:LYS:NZ	1:B:262:ARG:HB3	2.06	0.70
1:A:432:LEU:CG	2:A:1709:CPL:C32	2.55	0.70
2:A:1697:CPL:C13	2:A:1700:CPL:C36	2.70	0.70
1:B:572:ILE:HD12	2:B:1697:CPL:P	2.31	0.70
1:B:585:GLN:H	1:B:588:GLN:HE21	1.39	0.70
1:A:167:TYR:HD2	1:A:169:LEU:HG	1.55	0.70
1:A:578:GLY:O	1:A:584:LEU:HB2	1.90	0.70
1:B:446:LYS:C	2:B:1705:CPL:C7	2.54	0.70
1:B:587:ASP:O	2:B:1703:CPL:C43	2.39	0.70
1:A:273:GLU:OE2	1:B:151:GLN:CD	2.34	0.70
1:A:432:LEU:HB2	2:A:1709:CPL:H322	1.62	0.70
1:A:21:ARG:HG3	1:A:65:LEU:CD2	2.22	0.70
1:A:147:LYS:NZ	1:B:267:PHE:O	2.25	0.69
2:A:1697:CPL:C26	2:A:1710:CPL:H481	2.20	0.69
1:B:105:VAL:O	1:B:107:THR:HG23	1.90	0.69
1:B:21:ARG:HG3	1:B:65:LEU:CD2	2.22	0.69
1:A:147:LYS:CE	1:B:271:LEU:HG	2.22	0.69
2:A:1697:CPL:H151	2:A:1700:CPL:H39	1.74	0.69
1:A:60:ILE:HG23	1:A:199:ASN:CB	2.10	0.69
1:A:213:PRO:CD	1:B:79:LYS:HB2	2.22	0.69
2:A:1697:CPL:C14	2:A:1700:CPL:H362	2.21	0.69
1:A:579:LEU:HD23	2:A:1705:CPL:C47	2.21	0.69
1:B:363:GLU:HB3	1:B:660:ARG:NH1	1.89	0.69
1:A:465:LYS:HZ3	1:B:465:LYS:CG	2.04	0.69
1:B:432:LEU:HB3	2:B:1701:CPL:C33	2.22	0.69
1:B:647:ASP:O	1:B:651:LYS:HG2	1.91	0.69
1:A:68:GLY:C	1:A:202:HIS:HE2	2.01	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:GLU:HB2	2:A:1708:CPL:HC71	1.72	0.69
1:A:572:ILE:HG21	2:A:1705:CPL:C36	2.20	0.69
2:A:3094:CPL:H241	2:A:3181:CPL:C45	2.19	0.69
1:B:591:ARG:CA	2:B:1703:CPL:H382	2.22	0.69
2:B:1702:CPL:H483	2:B:1707:CPL:H261	1.74	0.69
1:A:147:LYS:N	1:B:269:ALA:HB3	1.93	0.69
1:A:216:LEU:HB3	1:B:217:GLY:HA2	1.74	0.69
1:B:586:ALA:HA	2:B:1697:CPL:H442	1.73	0.68
1:A:572:ILE:HD11	2:A:1705:CPL:C33	2.21	0.68
1:A:652:GLN:OE1	1:A:656:ARG:HD2	1.93	0.68
1:A:128:GLN:HG2	1:A:129:GLN:N	2.03	0.68
1:B:412:GLY:O	2:B:1704:CPL:HC82	1.93	0.68
1:B:586:ALA:HB1	2:B:1697:CPL:H441	1.74	0.68
2:B:1697:CPL:C25	2:B:1714:CPL:H481	2.24	0.68
2:B:1712:CPL:HC73	2:B:1714:CPL:HC62	1.74	0.68
1:A:242:GLN:HG3	1:B:245:GLU:OE1	1.94	0.68
1:B:594:VAL:O	2:B:1703:CPL:H322	1.94	0.68
1:A:259:SER:HB3	3:B:1706:GDP:O3'	1.93	0.68
1:A:425:GLU:CG	2:A:1708:CPL:C31	2.71	0.68
1:A:449:GLU:OE1	2:A:1708:CPL:C8	2.42	0.68
1:B:591:ARG:CG	2:B:1703:CPL:H382	2.24	0.68
1:B:416:GLU:HG3	2:B:1704:CPL:O2P	1.93	0.68
1:B:602:VAL:HG21	2:B:1703:CPL:HC51	1.73	0.68
1:A:65:LEU:HD11	1:A:335:VAL:HG21	1.76	0.68
1:A:147:LYS:NZ	1:B:267:PHE:HA	2.08	0.68
2:A:1718:CPL:H263	2:A:3097:CPL:H252	1.76	0.68
1:B:87:ASN:HB3	1:B:92:GLU:O	1.94	0.68
1:B:65:LEU:HD11	1:B:335:VAL:HG21	1.76	0.68
1:B:278:GLU:CD	1:B:333:ARG:HH11	2.02	0.67
1:B:572:ILE:CD1	2:B:1697:CPL:O3	2.42	0.67
1:B:585:GLN:CD	2:B:1696:CPL:C26	2.66	0.67
1:A:131:ASP:OD2	1:A:133:GLN:HB2	1.94	0.67
1:A:278:GLU:CB	1:A:333:ARG:NH1	2.57	0.67
1:A:585:GLN:H	1:A:588:GLN:HE21	1.40	0.67
2:A:1700:CPL:H481	2:A:1710:CPL:C48	2.23	0.67
1:B:652:GLN:OE1	1:B:656:ARG:HD2	1.93	0.67
1:A:217:GLY:HA2	1:B:216:LEU:HB3	1.74	0.67
1:A:87:ASN:HB3	1:A:92:GLU:O	1.94	0.67
1:A:245:GLU:OE1	1:B:242:GLN:HG3	1.95	0.67
1:A:577:LEU:HD11	2:A:1707:CPL:H412	0.67	0.67
2:A:1706:CPL:C48	2:A:1711:CPL:H263	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LEU:CD1	1:B:217:GLY:HA2	2.24	0.67
1:A:579:LEU:CD2	2:A:1705:CPL:C47	2.71	0.67
1:A:579:LEU:HD21	2:A:1705:CPL:H462	0.68	0.67
1:B:96:PRO:HB3	1:B:136:LYS:HE3	1.77	0.67
1:A:212:GLN:HG3	1:B:80:ARG:CZ	2.25	0.67
1:A:267:PHE:O	1:B:147:LYS:NZ	2.28	0.67
1:B:131:ASP:OD2	1:B:133:GLN:HB2	1.94	0.67
1:A:96:PRO:HB3	1:A:136:LYS:HE3	1.77	0.67
1:A:417:ASN:C	1:B:421:ARG:HG2	2.19	0.67
1:A:79:LYS:HB2	1:B:213:PRO:CD	2.23	0.66
1:B:586:ALA:HA	2:B:1697:CPL:C44	2.25	0.66
1:A:265:GLN:OE1	1:B:142:ASP:CG	2.38	0.66
1:A:576:LEU:HD21	2:A:1705:CPL:C41	2.25	0.66
1:B:230:GLY:O	1:B:334:GLN:CD	2.38	0.66
2:A:1706:CPL:H461	2:A:1711:CPL:H263	1.78	0.66
1:B:425:GLU:N	2:B:1705:CPL:O2P	2.28	0.66
1:B:595:LYS:HA	2:B:1703:CPL:H341	1.76	0.66
1:A:219:ARG:NE	1:B:150:GLU:OE2	2.28	0.66
1:B:21:ARG:HG3	1:B:65:LEU:HD22	1.78	0.66
1:B:428:LEU:HD22	2:B:1705:CPL:H141	1.78	0.66
1:A:80:ARG:CZ	1:B:212:GLN:HG3	2.24	0.66
1:A:143:PRO:CG	1:B:262:ARG:O	2.44	0.66
1:A:278:GLU:CB	1:A:333:ARG:CZ	2.74	0.66
1:A:429:PHE:CE1	2:A:1702:CPL:P	2.89	0.66
1:B:68:GLY:C	1:B:69:VAL:O	2.39	0.66
1:A:142:ASP:CG	1:B:265:GLN:OE1	2.39	0.66
1:A:572:ILE:HD12	2:A:1705:CPL:C32	2.25	0.66
2:A:1704:CPL:C26	2:A:1714:CPL:C47	2.63	0.66
2:A:3077:CPL:H462	2:A:1697:CPL:H462	1.78	0.66
1:B:413:ASN:CG	2:B:1704:CPL:HC81	1.75	0.66
1:B:551:TYR:HD1	1:B:552:PHE:HD1	1.44	0.66
1:B:581:VAL:HB	2:B:1699:CPL:C46	2.25	0.66
1:B:602:VAL:HG22	2:B:1703:CPL:HC83	1.77	0.66
1:A:141:ILE:H	1:A:141:ILE:HD13	1.62	0.65
1:A:563:ALA:O	1:A:567:ILE:HG12	1.96	0.65
1:B:563:ALA:O	1:B:567:ILE:HG12	1.96	0.65
1:A:150:GLU:OE2	1:B:219:ARG:NE	2.29	0.65
2:A:1704:CPL:H252	2:A:1714:CPL:H481	1.74	0.65
1:B:436:LYS:C	1:B:438:GLU:H	2.04	0.65
1:B:426:LEU:HB3	2:B:1705:CPL:O11	1.96	0.65
1:A:363:GLU:H	1:A:660:ARG:HH12	0.70	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:SER:OG	2:A:1702:CPL:HC73	1.95	0.65
1:A:436:LYS:HG2	2:A:1709:CPL:C8	2.26	0.65
1:A:436:LYS:C	1:A:438:GLU:H	2.04	0.65
1:B:230:GLY:C	1:B:334:GLN:HG2	2.22	0.65
1:B:363:GLU:H	1:B:660:ARG:HH11	1.44	0.65
1:A:497:THR:HG23	1:A:499:LYS:H	1.61	0.65
1:B:565:THR:O	2:B:1697:CPL:C4	2.33	0.65
1:B:569:LEU:CA	2:B:1697:CPL:O1P	2.44	0.65
1:A:209:ARG:CG	1:B:212:GLN:HE21	2.10	0.65
2:A:3077:CPL:H262	2:A:1709:CPL:H483	1.78	0.65
3:A:1696:GDP:O3'	1:B:259:SER:HB3	1.97	0.65
1:A:79:LYS:HB2	1:B:213:PRO:HG2	0.70	0.65
1:A:21:ARG:HG3	1:A:65:LEU:HD22	1.78	0.64
1:A:416:GLU:HB2	2:A:1701:CPL:HC11	1.79	0.64
1:B:141:ILE:HD13	1:B:141:ILE:H	1.62	0.64
1:A:68:GLY:CA	1:A:202:HIS:CE1	2.80	0.64
1:A:414:THR:CA	2:A:1701:CPL:C5	2.62	0.64
1:B:565:THR:C	2:B:1697:CPL:C4	2.39	0.64
1:B:581:VAL:HA	2:B:1699:CPL:C48	2.28	0.64
1:A:260:GLU:O	1:A:264:ARG:HG3	1.98	0.64
1:A:426:LEU:N	2:A:1708:CPL:O11	2.31	0.64
2:A:3077:CPL:H262	2:A:1709:CPL:C48	2.27	0.64
1:B:579:LEU:HD22	2:B:1697:CPL:C19	2.14	0.64
1:A:151:GLN:CD	1:B:273:GLU:OE2	2.40	0.64
1:A:211:SER:HA	1:B:209:ARG:HH11	1.62	0.64
1:A:217:GLY:HA2	1:B:216:LEU:CD1	2.26	0.64
1:A:576:LEU:CD2	2:A:1705:CPL:H43	2.28	0.64
2:A:1701:CPL:O11	1:B:420:LEU:HG	1.92	0.64
1:B:497:THR:HG23	1:B:499:LYS:H	1.61	0.64
1:A:302:ASN:ND2	1:A:302:ASN:C	2.56	0.64
2:A:1698:CPL:H481	2:A:1707:CPL:C48	2.21	0.63
1:B:260:GLU:O	1:B:264:ARG:HG3	1.98	0.63
1:A:143:PRO:HB2	1:B:265:GLN:N	2.11	0.63
1:A:230:GLY:C	1:A:334:GLN:NE2	2.55	0.63
1:B:202:HIS:HB3	1:B:331:GLU:OE1	1.99	0.63
1:B:587:ASP:O	2:B:1703:CPL:C44	2.46	0.63
2:A:1711:CPL:C48	2:A:1716:CPL:C48	2.74	0.63
1:B:60:ILE:HG13	1:B:196:GLY:HA2	1.80	0.63
1:A:236:LEU:HD22	1:A:290:LEU:HD11	1.79	0.63
1:A:446:LYS:HE2	2:A:1708:CPL:HC63	0.65	0.63
2:A:1701:CPL:O11	1:B:420:LEU:CD2	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:PHE:CE2	2:A:1707:CPL:H483	2.08	0.63
1:B:593:LEU:CD1	2:B:1697:CPL:C36	2.76	0.63
2:B:1701:CPL:H261	2:B:1710:CPL:H481	1.78	0.63
1:A:413:ASN:CA	2:A:1703:CPL:HC42	2.29	0.63
1:A:212:GLN:HE21	1:B:209:ARG:CG	2.10	0.63
1:A:213:PRO:HG2	1:B:79:LYS:CG	2.27	0.63
1:A:267:PHE:HA	1:B:147:LYS:NZ	2.13	0.63
1:A:375:PHE:CE1	1:A:492:ILE:HD13	2.34	0.63
1:B:432:LEU:HG	2:B:1701:CPL:H342	1.80	0.62
1:B:593:LEU:HD12	2:B:1697:CPL:H362	1.79	0.62
2:A:1698:CPL:H321	2:A:1699:CPL:C11	2.29	0.62
1:B:372:GLU:N	1:B:373:PRO:HD2	2.14	0.62
2:B:1697:CPL:C26	2:B:1714:CPL:H481	2.23	0.62
2:A:1708:CPL:H261	2:A:1716:CPL:H263	1.80	0.62
1:B:236:LEU:HD22	1:B:290:LEU:HD11	1.79	0.62
1:B:418:ASP:H	2:B:1700:CPL:HC41	1.59	0.62
1:A:551:TYR:HD1	1:A:552:PHE:HD1	1.44	0.62
2:A:1718:CPL:H242	2:A:3097:CPL:H231	1.78	0.62
1:A:450:GLN:HE22	2:A:1708:CPL:HC81	1.64	0.62
1:A:581:VAL:HG23	2:A:1707:CPL:C47	2.29	0.62
1:B:375:PHE:CE1	1:B:492:ILE:HD13	2.34	0.62
1:B:602:VAL:HG22	2:B:1703:CPL:C8	2.28	0.62
1:B:595:LYS:HA	2:B:1703:CPL:H321	1.82	0.62
2:B:1705:CPL:H261	2:B:1711:CPL:H482	1.77	0.62
1:A:68:GLY:C	1:A:202:HIS:NE2	2.58	0.62
1:A:372:GLU:N	1:A:373:PRO:HD2	2.14	0.62
1:A:449:GLU:OE1	2:A:1708:CPL:C7	2.47	0.62
1:B:543:ASP:OD2	1:B:545:LYS:HG2	1.99	0.62
1:A:543:ASP:OD2	1:A:545:LYS:HG2	1.99	0.62
1:A:633:LYS:O	1:A:637:ASP:HB2	2.00	0.62
1:B:302:ASN:ND2	1:B:302:ASN:C	2.55	0.62
1:A:147:LYS:CD	1:B:267:PHE:C	2.73	0.61
1:B:595:LYS:C	1:B:595:LYS:HD3	2.25	0.61
2:A:1697:CPL:H151	2:A:1700:CPL:C40	2.29	0.61
1:B:678:LEU:HD13	1:B:682:GLU:HG3	1.83	0.61
1:A:245:GLU:HG3	1:B:293:ILE:HG21	1.81	0.61
1:A:262:ARG:O	1:B:143:PRO:CG	2.49	0.61
1:A:413:ASN:CA	2:A:1703:CPL:C4	2.77	0.61
1:A:561:ILE:HD12	2:A:1705:CPL:O4P	2.01	0.61
1:A:293:ILE:HG21	1:B:245:GLU:HG3	1.81	0.61
1:A:586:ALA:O	2:A:1699:CPL:H481	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:GLU:H	1:B:660:ARG:NH1	1.97	0.61
1:A:267:PHE:C	1:B:147:LYS:CD	2.73	0.61
1:A:414:THR:C	2:A:1701:CPL:HC51	2.25	0.61
1:B:590:ARG:O	2:B:1703:CPL:C37	2.39	0.61
1:B:633:LYS:O	1:B:637:ASP:HB2	2.00	0.61
1:B:581:VAL:C	2:B:1699:CPL:H482	2.26	0.61
1:A:568:LEU:HD11	1:A:601:LEU:HD21	1.83	0.61
1:A:581:VAL:HG23	2:A:1707:CPL:H472	1.82	0.61
1:B:60:ILE:HG23	1:B:200:ASN:ND2	2.16	0.61
1:B:432:LEU:HB3	2:B:1701:CPL:C34	2.31	0.61
1:B:590:ARG:NH1	2:B:1697:CPL:H182	2.16	0.61
1:B:605:LEU:HA	1:B:608:VAL:HG22	1.83	0.61
2:B:1697:CPL:H251	2:B:1714:CPL:H481	1.83	0.61
2:B:1705:CPL:H261	2:B:1711:CPL:H481	1.62	0.61
1:B:576:LEU:HA	2:B:1697:CPL:C17	2.31	0.61
1:A:270:ASN:ND2	1:B:147:LYS:HA	2.15	0.60
1:B:85:PHE:CZ	1:B:236:LEU:HD13	2.37	0.60
1:B:364:LEU:HD13	1:B:650:VAL:HG22	1.83	0.60
1:B:520:TRP:CH2	1:B:527:LEU:HG	2.35	0.60
1:B:675:ILE:O	1:B:679:GLN:HG3	2.01	0.60
1:A:270:ASN:OD1	1:B:150:GLU:HB3	2.01	0.60
1:A:423:GLN:OE1	2:B:1700:CPL:H121	2.00	0.60
1:A:421:ARG:NH2	2:B:1700:CPL:HC71	2.03	0.60
1:A:675:ILE:O	1:A:679:GLN:HG3	2.01	0.60
2:A:1697:CPL:C3	2:A:1700:CPL:H322	2.29	0.60
1:B:302:ASN:HD21	1:B:304:GLN:H	1.49	0.60
1:B:427:ASN:CA	2:B:1705:CPL:HC31	2.30	0.60
1:B:568:LEU:HD11	1:B:601:LEU:HD21	1.83	0.60
1:A:79:LYS:CB	1:B:213:PRO:CG	2.43	0.60
1:A:265:GLN:N	1:B:143:PRO:CB	2.32	0.60
1:B:579:LEU:CD2	2:B:1697:CPL:H201	2.05	0.60
1:A:418:ASP:HA	1:B:421:ARG:HH11	1.67	0.60
1:B:9:ARG:HB3	1:B:9:ARG:CZ	2.32	0.60
1:A:529:LYS:HG3	1:A:540:ALA:HB2	1.84	0.60
1:A:230:GLY:O	1:A:334:GLN:NE2	2.35	0.60
1:A:271:LEU:CD1	1:B:147:LYS:HZ1	2.15	0.60
1:A:364:LEU:HD13	1:A:650:VAL:HG22	1.84	0.60
1:A:514:SER:HB2	1:A:515:PRO:HD2	1.84	0.60
1:A:595:LYS:HD3	1:A:595:LYS:C	2.25	0.60
1:B:580:GLY:O	2:B:1699:CPL:H472	2.01	0.60
1:A:678:LEU:HD13	1:A:682:GLU:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1702:CPL:H40	2:A:1702:CPL:H191	1.84	0.59
2:B:1698:CPL:H40	2:B:1698:CPL:H191	1.84	0.59
1:A:80:ARG:NH2	1:B:212:GLN:HG2	2.17	0.59
1:A:302:ASN:HD21	1:A:304:GLN:H	1.50	0.59
1:A:432:LEU:HD13	1:A:432:LEU:N	2.17	0.59
1:B:514:SER:HB2	1:B:515:PRO:HD2	1.84	0.59
1:A:363:GLU:HB2	1:A:660:ARG:NH2	2.12	0.59
1:A:85:PHE:CZ	1:A:236:LEU:HD13	2.36	0.59
1:B:60:ILE:HG22	1:B:199:ASN:C	2.26	0.59
1:A:211:SER:HG	1:B:211:SER:CB	2.14	0.59
1:B:586:ALA:CB	2:B:1697:CPL:H441	2.32	0.59
2:B:1696:CPL:H483	2:B:1709:CPL:H262	1.83	0.59
1:A:79:LYS:CG	1:B:213:PRO:HG2	2.28	0.59
1:A:605:LEU:HA	1:A:608:VAL:HG22	1.83	0.59
1:B:416:GLU:HB3	2:B:1700:CPL:HC2	1.84	0.59
1:B:432:LEU:HD13	1:B:432:LEU:N	2.17	0.59
1:A:212:GLN:NE2	1:B:209:ARG:CG	2.66	0.59
2:A:1708:CPL:H40	2:A:1708:CPL:H191	1.84	0.59
1:B:560:ILE:O	1:B:564:VAL:HG23	2.03	0.59
1:A:9:ARG:CZ	1:A:9:ARG:HB3	2.32	0.59
1:A:142:ASP:HB3	1:B:265:GLN:OE1	2.03	0.59
2:A:1703:CPL:H40	2:A:1703:CPL:H191	1.85	0.59
1:A:147:LYS:HA	1:B:270:ASN:ND2	2.18	0.58
1:A:9:ARG:HH22	1:A:320:ASN:HD22	1.51	0.58
1:A:560:ILE:O	1:A:564:VAL:HG23	2.03	0.58
1:B:569:LEU:HA	2:B:1697:CPL:O1P	2.02	0.58
1:A:90:ILE:HD12	1:A:169:LEU:CD1	2.33	0.58
1:B:53:ARG:NH1	1:B:193:LEU:HD21	2.18	0.58
1:B:215:THR:HG22	1:B:216:LEU:N	2.18	0.58
1:B:447:ALA:HA	2:B:1705:CPL:C4	2.33	0.58
2:B:1697:CPL:C26	2:B:1714:CPL:H482	2.22	0.58
2:B:1701:CPL:H40	2:B:1701:CPL:H191	1.85	0.58
1:A:212:GLN:HG2	1:B:80:ARG:NH2	2.18	0.58
1:A:435:GLY:C	2:A:1709:CPL:C7	2.76	0.58
1:B:434:SER:CA	2:B:1701:CPL:HC41	2.23	0.58
1:A:68:GLY:C	1:A:202:HIS:CE1	2.82	0.58
1:A:215:THR:HG22	1:A:216:LEU:N	2.18	0.58
1:A:416:GLU:OE2	2:A:1701:CPL:C32	2.46	0.58
3:A:1696:GDP:N9	1:B:246:SER:CB	2.66	0.58
1:B:413:ASN:ND2	2:B:1704:CPL:C6	2.64	0.58
2:B:1696:CPL:H40	2:B:1696:CPL:H191	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1701:CPL:C48	2:B:1712:CPL:C48	2.81	0.58
2:B:1710:CPL:H40	2:B:1710:CPL:H191	1.85	0.58
2:B:1712:CPL:H39	2:B:1712:CPL:C17	2.33	0.58
1:A:213:PRO:HG2	1:B:79:LYS:HB2	0.66	0.58
1:A:267:PHE:C	1:B:147:LYS:HD2	2.29	0.58
1:A:435:GLY:N	2:A:1709:CPL:HC83	1.90	0.58
1:A:278:GLU:CG	1:A:333:ARG:CZ	2.75	0.58
1:A:421:ARG:HD3	2:B:1700:CPL:HC73	1.14	0.58
1:B:93:ASN:HD22	1:B:93:ASN:C	2.12	0.58
1:B:551:TYR:HD1	1:B:552:PHE:CD1	2.22	0.58
1:B:591:ARG:HG2	2:B:1703:CPL:H382	1.86	0.58
1:A:141:ILE:HD13	1:A:141:ILE:N	2.18	0.58
1:A:267:PHE:CA	1:B:147:LYS:HD2	2.34	0.58
1:A:273:GLU:CD	1:B:151:GLN:NE2	2.59	0.58
1:A:556:GLY:O	1:A:560:ILE:HG12	2.04	0.58
1:A:577:LEU:CD1	2:A:1707:CPL:H43	2.34	0.58
2:A:1701:CPL:C7	1:B:421:ARG:CD	2.81	0.58
2:A:1717:CPL:H40	2:A:1717:CPL:H191	1.86	0.58
1:B:593:LEU:CD1	2:B:1697:CPL:H362	2.34	0.58
1:A:517:TRP:CG	1:A:635:ILE:HG12	2.39	0.58
2:B:1701:CPL:H261	2:B:1710:CPL:C47	2.32	0.58
1:A:209:ARG:CG	1:B:212:GLN:NE2	2.66	0.57
1:A:213:PRO:CG	1:B:79:LYS:CB	2.40	0.57
1:A:612:GLN:C	1:A:614:GLN:H	2.12	0.57
2:A:1703:CPL:C26	2:A:1715:CPL:H482	2.30	0.57
1:B:364:LEU:HD11	1:B:649:LEU:HD13	1.86	0.57
1:B:381:ILE:HG23	1:B:481:TYR:HD2	1.69	0.57
2:B:1710:CPL:C25	2:B:1712:CPL:H483	2.34	0.57
2:B:1712:CPL:H40	2:B:1712:CPL:H191	1.86	0.57
1:A:147:LYS:C	1:B:269:ALA:HB1	2.28	0.57
1:A:465:LYS:HZ2	1:B:465:LYS:CG	2.14	0.57
1:B:141:ILE:HD13	1:B:141:ILE:N	2.18	0.57
1:A:269:ALA:C	1:B:147:LYS:C	2.72	0.57
1:A:381:ILE:HG23	1:A:481:TYR:HD2	1.69	0.57
1:A:421:ARG:HD3	2:B:1700:CPL:C8	2.11	0.57
1:A:577:LEU:HD13	2:A:1707:CPL:H43	1.87	0.57
2:A:1708:CPL:H39	2:A:1708:CPL:C17	2.33	0.57
1:B:517:TRP:CG	1:B:635:ILE:HG12	2.39	0.57
1:A:150:GLU:CD	1:B:219:ARG:NE	2.60	0.57
1:A:150:GLU:HB3	1:B:270:ASN:OD1	2.04	0.57
1:A:219:ARG:CD	1:B:150:GLU:OE1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ARG:HH22	1:B:320:ASN:HD22	1.51	0.57
2:B:1710:CPL:H39	2:B:1710:CPL:C17	2.33	0.57
1:A:211:SER:O	1:B:209:ARG:HD2	2.03	0.57
1:A:246:SER:CB	3:B:1706:GDP:N9	2.67	0.57
1:B:302:ASN:C	1:B:302:ASN:HD22	2.12	0.57
1:B:529:LYS:HG3	1:B:540:ALA:HB2	1.84	0.57
2:B:1696:CPL:H39	2:B:1696:CPL:C17	2.33	0.57
1:A:520:TRP:CH2	1:A:527:LEU:HG	2.35	0.57
2:A:1717:CPL:H39	2:A:1717:CPL:C17	2.33	0.57
1:B:556:GLY:O	1:B:560:ILE:HG12	2.04	0.57
1:B:591:ARG:N	2:B:1703:CPL:H412	2.19	0.57
1:B:612:GLN:C	1:B:614:GLN:H	2.12	0.57
1:A:449:GLU:OE1	2:A:1708:CPL:N	2.38	0.57
1:A:515:PRO:HG2	1:A:518:ALA:HB2	1.87	0.57
1:B:90:ILE:HD12	1:B:169:LEU:CD1	2.34	0.57
1:A:209:ARG:HH11	1:B:211:SER:HA	1.64	0.57
1:A:263:LEU:CA	1:B:79:LYS:HE3	2.33	0.57
1:A:429:PHE:CB	2:A:1702:CPL:H331	2.35	0.57
1:A:433:SER:N	2:A:1709:CPL:O31	2.37	0.57
2:A:1710:CPL:H39	2:A:1710:CPL:C17	2.33	0.57
2:B:1701:CPL:H251	2:B:1710:CPL:C48	2.32	0.57
1:A:147:LYS:CB	1:B:269:ALA:CA	2.51	0.57
1:A:271:LEU:CG	1:B:147:LYS:HZ3	2.04	0.57
1:A:429:PHE:CA	2:A:1702:CPL:H331	2.35	0.57
1:A:434:SER:HB3	2:A:1709:CPL:C8	2.19	0.57
1:A:657:GLU:HG3	1:A:657:GLU:O	2.05	0.57
2:A:1701:CPL:O11	1:B:420:LEU:HD21	2.05	0.57
1:B:515:PRO:HG2	1:B:518:ALA:HB2	1.87	0.57
1:A:80:ARG:NE	1:B:212:GLN:HG3	2.20	0.56
1:A:449:GLU:CG	2:A:1708:CPL:HC71	2.35	0.56
1:A:551:TYR:HD1	1:A:552:PHE:CD1	2.22	0.56
1:A:590:ARG:HH12	2:A:1705:CPL:C42	2.18	0.56
1:B:591:ARG:HA	2:B:1703:CPL:H412	1.76	0.56
1:A:112:GLY:HA3	1:A:166:GLU:HB3	1.88	0.56
1:A:302:ASN:C	1:A:302:ASN:HD22	2.12	0.56
1:A:577:LEU:HD11	2:A:1707:CPL:C43	2.35	0.56
2:A:1710:CPL:H40	2:A:1710:CPL:H191	1.85	0.56
1:B:378:LEU:HB3	1:B:639:ILE:HD11	1.88	0.56
1:B:591:ARG:HG3	2:B:1703:CPL:C40	2.35	0.56
1:B:657:GLU:HG3	1:B:657:GLU:O	2.05	0.56
2:B:1701:CPL:H39	2:B:1701:CPL:C17	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ASN:C	2:A:1703:CPL:HC73	1.85	0.56
1:B:134:ASN:OD1	1:B:138:LYS:HE3	2.05	0.56
2:A:1697:CPL:C26	2:A:1700:CPL:H482	2.35	0.56
1:B:384:GLU:HB3	1:B:481:TYR:HE2	1.70	0.56
1:B:434:SER:C	2:B:1701:CPL:O2P	2.49	0.56
1:A:93:ASN:C	1:A:93:ASN:HD22	2.12	0.56
2:A:1703:CPL:H39	2:A:1703:CPL:C17	2.33	0.56
1:B:576:LEU:HA	2:B:1697:CPL:H172	1.86	0.56
1:B:595:LYS:HA	2:B:1703:CPL:C32	2.35	0.56
1:A:134:ASN:OD1	1:A:138:LYS:HE3	2.05	0.56
1:A:212:GLN:NE2	1:B:209:ARG:C	2.63	0.56
1:A:364:LEU:HD11	1:A:649:LEU:HD13	1.86	0.56
2:A:1708:CPL:H261	2:A:1716:CPL:H261	1.87	0.56
1:B:497:THR:HG23	1:B:499:LYS:N	2.21	0.56
1:A:147:LYS:HD2	1:B:267:PHE:CA	2.35	0.56
1:A:271:LEU:CD1	1:B:147:LYS:NZ	2.68	0.56
1:A:432:LEU:CA	2:A:1709:CPL:O31	2.54	0.56
1:B:446:LYS:HB3	2:B:1705:CPL:HC42	1.87	0.56
1:A:269:ALA:HB1	1:B:147:LYS:C	2.30	0.56
2:A:1703:CPL:H261	2:A:1715:CPL:H483	1.86	0.56
1:B:586:ALA:CB	2:B:1697:CPL:C44	2.84	0.56
1:A:147:LYS:CE	1:B:270:ASN:C	2.78	0.55
1:A:265:GLN:N	1:B:143:PRO:HB2	2.08	0.55
1:A:384:GLU:HB3	1:A:481:TYR:HE2	1.70	0.55
2:A:1703:CPL:H262	2:A:1715:CPL:C48	2.28	0.55
2:A:1703:CPL:C25	2:A:1704:CPL:H472	2.35	0.55
1:A:577:LEU:CD1	2:A:1707:CPL:C43	2.84	0.55
1:B:447:ALA:CA	2:B:1705:CPL:P	2.93	0.55
1:A:147:LYS:HD2	1:B:267:PHE:C	2.31	0.55
1:A:209:ARG:C	1:B:212:GLN:NE2	2.64	0.55
1:A:212:GLN:HG3	1:B:80:ARG:NE	2.21	0.55
1:A:362:ASN:CB	1:A:660:ARG:NH1	2.52	0.55
1:A:450:GLN:NE2	2:A:1708:CPL:C8	2.69	0.55
1:B:67:GLN:HE21	1:B:71:ARG:NH1	2.04	0.55
1:B:375:PHE:CE2	1:B:643:LYS:HG3	2.41	0.55
1:B:591:ARG:HG2	1:B:591:ARG:HH21	1.71	0.55
1:A:64:ASN:HD21	1:A:199:ASN:HB3	1.71	0.55
1:A:449:GLU:HB2	2:A:1708:CPL:C7	2.33	0.55
1:A:591:ARG:HG2	1:A:591:ARG:HH21	1.71	0.55
2:A:1699:CPL:H39	2:A:1699:CPL:C17	2.32	0.55
1:A:429:PHE:CD1	2:A:1702:CPL:C32	2.62	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1703:CPL:C48	2:A:1715:CPL:C26	2.84	0.55
1:A:209:ARG:HD2	1:B:211:SER:O	2.05	0.55
1:A:282:ILE:HD13	1:A:282:ILE:H	1.71	0.55
1:B:112:GLY:HA3	1:B:166:GLU:HB3	1.87	0.55
2:B:1696:CPL:H483	2:B:1709:CPL:C26	2.36	0.55
1:A:147:LYS:CE	1:B:214:CYS:SG	2.90	0.55
1:A:432:LEU:CB	2:A:1709:CPL:C31	2.67	0.55
2:B:1705:CPL:C26	2:B:1711:CPL:H482	2.36	0.55
1:A:375:PHE:CE2	1:A:643:LYS:HG3	2.41	0.55
2:A:1701:CPL:C7	1:B:421:ARG:HD3	2.37	0.55
2:A:1702:CPL:H39	2:A:1702:CPL:C17	2.34	0.55
1:B:389:ILE:HG21	1:B:628:GLU:HB2	1.89	0.55
1:B:565:THR:HG22	1:B:566:GLY:N	2.22	0.55
2:B:1698:CPL:H39	2:B:1698:CPL:C17	2.34	0.55
1:A:147:LYS:HZ1	1:B:271:LEU:CD1	2.19	0.55
1:A:450:GLN:NE2	2:A:1708:CPL:HC81	2.21	0.55
1:A:497:THR:HG23	1:A:499:LYS:N	2.21	0.55
1:B:428:LEU:HD22	2:B:1705:CPL:C14	2.37	0.55
2:B:1707:CPL:HC11	2:B:1708:CPL:O1P	2.06	0.55
1:A:214:CYS:SG	1:B:147:LYS:CE	2.91	0.55
1:A:577:LEU:HD12	2:A:1707:CPL:H412	1.74	0.55
1:A:238:ASN:ND2	1:A:239:ALA:H	2.05	0.54
1:A:465:LYS:CD	1:B:465:LYS:HG3	2.36	0.54
1:A:565:THR:HG22	1:A:566:GLY:N	2.22	0.54
1:B:652:GLN:NE2	1:B:656:ARG:NH2	2.55	0.54
1:A:397:ALA:O	1:A:617:TYR:CD1	2.60	0.54
1:B:397:ALA:O	1:B:617:TYR:CD1	2.60	0.54
1:A:378:LEU:HB3	1:A:639:ILE:HD11	1.88	0.54
1:B:238:ASN:ND2	1:B:239:ALA:H	2.05	0.54
1:B:282:ILE:HD13	1:B:282:ILE:H	1.71	0.54
1:B:688:LEU:O	1:B:688:LEU:HD22	2.07	0.54
1:A:67:GLN:NE2	1:A:200:ASN:CB	2.61	0.54
1:A:215:THR:HG22	1:A:217:GLY:H	1.73	0.54
1:A:270:ASN:C	1:B:147:LYS:CE	2.76	0.54
1:A:431:PHE:HB3	1:A:432:LEU:HD13	1.90	0.54
1:A:432:LEU:CB	2:A:1709:CPL:O31	2.55	0.54
1:A:577:LEU:HG	2:A:1707:CPL:H381	1.89	0.54
1:B:216:LEU:HA	1:B:219:ARG:NH2	2.23	0.54
1:A:212:GLN:HE22	1:B:209:ARG:C	2.16	0.54
1:A:216:LEU:HA	1:A:219:ARG:NH2	2.22	0.54
1:B:60:ILE:O	1:B:200:ASN:OD1	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLU:OE1	1:A:39:GLU:HA	2.08	0.54
1:A:688:LEU:O	1:A:688:LEU:HD22	2.07	0.54
2:B:1710:CPL:H251	2:B:1712:CPL:H483	1.88	0.54
1:B:413:ASN:HD22	2:B:1704:CPL:C6	2.17	0.54
1:B:568:LEU:CB	2:B:1697:CPL:O2P	2.55	0.54
1:A:80:ARG:HD2	1:B:211:SER:O	2.08	0.54
1:A:265:GLN:NE2	1:B:141:ILE:O	2.41	0.54
1:A:525:LEU:O	1:A:526:SER:HB3	2.08	0.54
2:A:1701:CPL:H263	2:A:1712:CPL:H482	1.90	0.54
1:B:586:ALA:CA	2:B:1697:CPL:H441	2.38	0.54
1:A:211:SER:O	1:B:80:ARG:HD2	2.08	0.54
1:A:389:ILE:HG21	1:A:628:GLU:HB2	1.89	0.54
1:A:414:THR:C	2:A:1701:CPL:C5	2.80	0.54
1:B:60:ILE:HG22	1:B:199:ASN:CA	2.36	0.54
1:B:431:PHE:HB3	1:B:432:LEU:HD13	1.90	0.54
1:A:31:LEU:CD1	1:A:674:VAL:HG13	2.38	0.53
1:B:694:HIS:C	1:B:695:HIS:ND1	2.67	0.53
1:A:450:GLN:HE22	2:A:1708:CPL:C8	2.20	0.53
1:A:694:HIS:C	1:A:695:HIS:ND1	2.67	0.53
1:B:39:GLU:OE1	1:B:39:GLU:HA	2.08	0.53
1:B:447:ALA:CB	2:B:1705:CPL:P	2.97	0.53
1:B:579:LEU:HD23	2:B:1697:CPL:C22	2.33	0.53
1:A:435:GLY:HA2	2:A:1709:CPL:O2P	2.08	0.53
2:A:1697:CPL:H172	2:A:1700:CPL:H40	1.91	0.53
1:B:186:ASP:OD1	1:B:220:ARG:NH2	2.40	0.53
1:B:215:THR:HG22	1:B:217:GLY:H	1.73	0.53
1:B:379:THR:HG23	1:B:382:ARG:HH11	1.73	0.53
1:A:379:THR:HG23	1:A:382:ARG:HH11	1.73	0.53
1:A:147:LYS:C	1:B:269:ALA:C	2.77	0.53
1:B:591:ARG:CA	2:B:1703:CPL:H371	2.37	0.53
1:A:421:ARG:HD3	2:B:1700:CPL:HC82	1.89	0.53
1:A:212:GLN:HA	1:B:80:ARG:NE	2.24	0.53
2:A:1697:CPL:C15	2:A:1700:CPL:C40	2.86	0.53
1:B:598:LYS:HZ1	2:B:1703:CPL:C1	2.13	0.53
1:A:264:ARG:HD3	1:A:289:GLU:OE1	2.09	0.53
2:A:1698:CPL:C7	2:A:1700:CPL:HC62	2.36	0.53
1:B:264:ARG:HD3	1:B:289:GLU:OE1	2.09	0.53
1:A:209:ARG:C	1:B:212:GLN:HE22	2.16	0.53
1:A:256:LEU:O	1:A:260:GLU:HG3	2.09	0.53
1:A:418:ASP:N	2:A:1701:CPL:HC42	2.24	0.53
3:A:1696:GDP:C2'	1:B:246:SER:CB	2.68	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ARG:NE	1:B:212:GLN:HA	2.24	0.53
1:A:413:ASN:O	2:A:1703:CPL:HC42	2.09	0.53
1:B:427:ASN:HA	2:B:1705:CPL:C3	2.37	0.53
1:A:265:GLN:OE1	1:B:142:ASP:HB3	2.09	0.52
1:B:602:VAL:HA	2:B:1703:CPL:HC83	1.90	0.52
1:A:141:ILE:HG12	1:A:146:ALA:HB2	1.91	0.52
1:A:414:THR:O	2:A:1701:CPL:C8	2.57	0.52
1:A:568:LEU:C	1:A:571:PRO:HD2	2.35	0.52
1:A:582:GLY:O	2:A:1707:CPL:H482	2.05	0.52
1:B:67:GLN:HB2	1:B:71:ARG:HH12	1.75	0.52
1:B:141:ILE:HG12	1:B:146:ALA:HB2	1.91	0.52
1:B:233:VAL:HG22	1:B:235:PHE:CZ	2.44	0.52
1:B:525:LEU:O	1:B:526:SER:HB3	2.08	0.52
1:A:128:GLN:CG	1:A:129:GLN:H	1.99	0.52
1:B:60:ILE:CG2	1:B:199:ASN:CA	2.84	0.52
1:A:360:ASP:OD2	1:A:366:LYS:CG	2.52	0.52
1:A:385:PHE:HE2	1:A:631:VAL:HG11	1.75	0.52
1:A:429:PHE:CG	2:A:1702:CPL:H331	2.39	0.52
1:B:568:LEU:C	1:B:571:PRO:HD2	2.35	0.52
1:A:148:LYS:C	1:A:150:GLU:H	2.17	0.52
1:A:652:GLN:NE2	1:A:656:ARG:NH2	2.55	0.52
3:A:1696:GDP:C8	1:B:246:SER:OG	2.63	0.52
1:B:413:ASN:CG	2:B:1704:CPL:C8	2.49	0.52
1:B:282:ILE:HD13	1:B:282:ILE:N	2.25	0.52
1:B:302:ASN:ND2	1:B:304:GLN:N	2.55	0.52
1:A:104:ALA:HB2	1:A:141:ILE:CD1	2.22	0.52
1:A:143:PRO:CA	1:B:266:VAL:CA	2.81	0.52
2:A:1707:CPL:O31	2:A:1710:CPL:O1P	2.28	0.52
1:B:30:LYS:HD2	1:B:677:GLN:OE1	2.09	0.52
1:B:148:LYS:C	1:B:150:GLU:H	2.17	0.52
1:B:588:GLN:HA	2:B:1703:CPL:H451	1.91	0.52
1:A:30:LYS:HD2	1:A:677:GLN:OE1	2.09	0.52
1:A:302:ASN:ND2	1:A:304:GLN:N	2.56	0.52
1:A:590:ARG:N	1:A:590:ARG:HD2	2.25	0.52
2:A:1700:CPL:H481	2:A:1710:CPL:H481	1.85	0.52
2:A:1700:CPL:H251	2:A:1710:CPL:H261	1.91	0.52
1:B:204:ILE:HB	1:B:233:VAL:HB	1.92	0.52
1:B:432:LEU:CD2	2:B:1701:CPL:H341	2.38	0.52
1:A:147:LYS:NZ	1:B:271:LEU:CD1	2.73	0.51
1:A:204:ILE:HB	1:A:233:VAL:HB	1.93	0.51
1:A:233:VAL:HG22	1:A:235:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LEU:CD1	1:B:674:VAL:HG13	2.38	0.51
1:B:598:LYS:HZ2	2:B:1703:CPL:HC2	0.70	0.51
1:A:248:ILE:CG2	1:B:300:LEU:HD13	2.29	0.51
1:A:576:LEU:HD23	2:A:1705:CPL:H43	1.92	0.51
1:B:256:LEU:O	1:B:260:GLU:HG3	2.09	0.51
1:B:571:PRO:HB3	1:B:596:THR:HG21	1.92	0.51
1:A:266:VAL:CA	1:B:143:PRO:CB	2.81	0.51
1:A:663:GLU:OE1	1:A:663:GLU:HA	2.10	0.51
2:A:3077:CPL:C26	2:A:1709:CPL:H483	2.39	0.51
1:B:132:PHE:HE1	1:B:136:LYS:HD2	1.76	0.51
1:B:593:LEU:HD12	2:B:1697:CPL:H371	1.92	0.51
1:A:302:ASN:HD21	1:A:304:GLN:HB2	1.76	0.51
1:A:605:LEU:N	1:A:606:PRO:HD2	2.25	0.51
1:A:658:ILE:HD13	1:A:658:ILE:O	2.11	0.51
1:B:119:ILE:HD11	1:B:160:VAL:HG22	1.93	0.51
1:B:385:PHE:HE2	1:B:631:VAL:HG11	1.75	0.51
1:A:238:ASN:HD21	1:A:292:SER:H	1.59	0.51
2:B:1697:CPL:H481	2:B:1714:CPL:H261	1.91	0.51
1:A:119:ILE:HD11	1:A:160:VAL:HG22	1.93	0.51
1:A:590:ARG:NH1	2:A:1705:CPL:C42	2.73	0.51
2:A:1704:CPL:C26	2:A:1714:CPL:H472	2.30	0.51
2:A:1711:CPL:H483	2:A:1716:CPL:C48	2.41	0.51
1:B:432:LEU:N	1:B:432:LEU:CD1	2.73	0.51
1:B:586:ALA:HB1	2:B:1697:CPL:C44	2.39	0.51
1:A:74:VAL:HG21	1:A:86:LEU:HD21	1.93	0.51
1:A:252:ASP:OD2	1:A:252:ASP:C	2.54	0.51
1:A:266:VAL:C	1:B:143:PRO:O	2.50	0.51
1:A:282:ILE:HD13	1:A:282:ILE:N	2.25	0.51
1:A:515:PRO:HG2	1:A:518:ALA:CB	2.41	0.51
1:A:590:ARG:CZ	2:A:1705:CPL:C18	2.83	0.51
1:B:283:TYR:CE1	1:B:287:VAL:HG21	2.46	0.51
1:A:209:ARG:O	1:B:212:GLN:NE2	2.44	0.51
1:A:432:LEU:N	1:A:432:LEU:CD1	2.73	0.51
1:A:571:PRO:HB3	1:A:596:THR:HG21	1.92	0.51
1:B:238:ASN:HD21	1:B:292:SER:H	1.59	0.51
1:B:585:GLN:CG	2:B:1696:CPL:C25	2.83	0.51
1:A:143:PRO:O	1:B:266:VAL:C	2.54	0.50
1:A:266:VAL:CA	1:B:143:PRO:CA	2.77	0.50
1:A:590:ARG:NH1	2:A:1705:CPL:C18	2.70	0.50
1:A:128:GLN:CG	1:A:129:GLN:N	2.68	0.50
1:A:132:PHE:HE1	1:A:136:LYS:HD2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:SER:OG	3:B:1706:GDP:C8	2.64	0.50
1:A:269:ALA:O	1:B:147:LYS:C	2.53	0.50
1:B:215:THR:CB	1:B:218:GLU:HG3	2.37	0.50
1:B:605:LEU:N	1:B:606:PRO:HD2	2.26	0.50
1:A:212:GLN:NE2	1:B:209:ARG:O	2.43	0.50
1:A:583:PHE:N	2:A:1707:CPL:C46	2.70	0.50
1:A:583:PHE:N	2:A:1707:CPL:C48	2.71	0.50
1:B:74:VAL:HG21	1:B:86:LEU:HD21	1.93	0.50
1:B:432:LEU:CB	2:B:1701:CPL:C34	2.89	0.50
1:A:577:LEU:O	1:A:581:VAL:HG22	2.11	0.50
1:B:577:LEU:O	1:B:581:VAL:HG22	2.11	0.50
1:A:147:LYS:NZ	1:B:267:PHE:CA	2.74	0.50
1:A:353:ARG:O	1:A:354:ILE:C	2.54	0.50
1:A:393:ARG:CG	1:A:394:ASP:N	2.73	0.50
1:A:283:TYR:CE1	1:A:287:VAL:HG21	2.45	0.50
2:B:1701:CPL:C26	2:B:1710:CPL:H481	2.38	0.50
2:A:1699:CPL:H40	2:A:1699:CPL:H191	1.93	0.50
1:B:302:ASN:HD21	1:B:304:GLN:HB2	1.76	0.50
1:B:586:ALA:CA	2:B:1697:CPL:C44	2.89	0.50
1:B:658:ILE:O	1:B:658:ILE:HD13	2.11	0.50
1:A:371:VAL:C	1:A:373:PRO:HD2	2.37	0.50
1:A:529:LYS:HB3	1:A:542:PHE:CD1	2.47	0.50
1:B:529:LYS:HB3	1:B:542:PHE:CD1	2.47	0.50
1:A:267:PHE:CA	1:B:147:LYS:HZ2	2.23	0.50
1:B:360:ASP:OD2	1:B:363:GLU:CD	2.52	0.50
1:B:515:PRO:HG2	1:B:518:ALA:CB	2.41	0.50
1:B:520:TRP:CZ3	1:B:526:SER:HA	2.47	0.50
1:A:418:ASP:HA	1:B:421:ARG:NH1	2.26	0.49
1:A:518:ALA:HB1	1:A:522:MET:HE2	1.94	0.49
1:B:9:ARG:HB3	1:B:9:ARG:NH2	2.28	0.49
1:B:22:SER:O	1:B:26:VAL:HG23	2.12	0.49
1:B:480:GLN:HG3	1:B:481:TYR:N	2.28	0.49
1:B:518:ALA:HB1	1:B:522:MET:HE2	1.94	0.49
1:B:590:ARG:HD2	1:B:590:ARG:N	2.26	0.49
1:A:186:ASP:OD1	1:A:220:ARG:NH2	2.40	0.49
1:A:271:LEU:N	1:B:147:LYS:HD3	2.27	0.49
1:A:358:GLU:OE2	1:A:660:ARG:HD2	2.12	0.49
1:A:435:GLY:CA	2:A:1709:CPL:HC73	2.39	0.49
1:B:252:ASP:C	1:B:252:ASP:OD2	2.54	0.49
1:B:663:GLU:HA	1:B:663:GLU:OE1	2.10	0.49
1:A:67:GLN:HB3	1:A:71:ARG:HH12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:H	1:B:147:LYS:HD3	1.77	0.49
1:A:520:TRP:CZ3	1:A:526:SER:HA	2.47	0.49
1:A:22:SER:O	1:A:26:VAL:HG23	2.12	0.49
1:A:480:GLN:HG3	1:A:481:TYR:N	2.28	0.49
1:A:105:VAL:O	1:A:106:LEU:C	2.56	0.49
1:A:267:PHE:HA	1:B:147:LYS:HD2	1.95	0.49
1:A:449:GLU:CD	2:A:1708:CPL:HC61	2.19	0.49
1:B:105:VAL:O	1:B:106:LEU:C	2.56	0.49
1:B:371:VAL:C	1:B:373:PRO:HD2	2.37	0.49
1:A:361:VAL:HG22	1:A:653:LYS:HB3	1.94	0.49
1:A:552:PHE:HD2	1:A:615:VAL:HG12	1.78	0.49
1:B:393:ARG:CG	1:B:394:ASP:N	2.73	0.49
1:B:400:ILE:HD12	1:B:620:VAL:HG11	1.95	0.49
1:B:446:LYS:C	2:B:1705:CPL:HC42	2.38	0.49
1:A:477:SER:O	1:A:480:GLN:HG2	2.12	0.49
1:B:477:SER:O	1:B:480:GLN:HG2	2.12	0.49
1:B:598:LYS:NZ	2:B:1703:CPL:C3	2.61	0.49
1:A:9:ARG:HB3	1:A:9:ARG:NH2	2.28	0.48
1:A:598:LYS:O	1:A:602:VAL:HG23	2.13	0.48
1:B:358:GLU:OE2	1:B:660:ARG:HD2	2.12	0.48
1:B:416:GLU:CB	2:B:1704:CPL:O2P	2.58	0.48
1:B:416:GLU:H	2:B:1704:CPL:P	2.31	0.48
1:A:147:LYS:HZ2	1:B:267:PHE:CA	2.19	0.48
2:A:1703:CPL:H482	2:A:1715:CPL:C25	2.43	0.48
1:B:21:ARG:HG3	1:B:65:LEU:HD23	1.95	0.48
1:B:353:ARG:O	1:B:354:ILE:C	2.54	0.48
1:A:378:LEU:HB3	1:A:639:ILE:CD1	2.44	0.48
2:A:1698:CPL:H341	2:A:1699:CPL:H132	1.96	0.48
2:A:1718:CPL:HC32	2:A:3097:CPL:O11	2.13	0.48
1:B:196:GLY:HA3	1:B:200:ASN:HD22	1.78	0.48
1:B:378:LEU:HB3	1:B:639:ILE:CD1	2.44	0.48
1:B:460:THR:OG1	1:B:550:ASN:ND2	2.47	0.48
1:B:581:VAL:HA	2:B:1699:CPL:H482	1.95	0.48
1:A:151:GLN:NE2	1:B:273:GLU:CD	2.64	0.48
2:A:1703:CPL:C48	2:A:1715:CPL:C25	2.92	0.48
1:A:196:GLY:HA3	1:A:200:ASN:HD22	1.78	0.48
1:A:414:THR:O	2:A:1701:CPL:HC51	2.10	0.48
1:A:446:LYS:NZ	2:A:1708:CPL:HC63	2.21	0.48
1:A:460:THR:OG1	1:A:550:ASN:ND2	2.47	0.48
1:B:244:ARG:HB3	1:B:256:LEU:HD13	1.95	0.48
1:B:598:LYS:O	1:B:602:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ARG:NH1	1:A:327:ARG:HH12	2.11	0.48
1:A:432:LEU:CD2	2:A:1709:CPL:C34	2.86	0.48
1:A:568:LEU:HD11	1:A:601:LEU:CD2	2.44	0.48
1:A:576:LEU:CD2	2:A:1705:CPL:H412	2.39	0.48
2:A:1697:CPL:H263	2:A:1700:CPL:H482	1.96	0.48
2:A:1708:CPL:H483	2:B:1704:CPL:H263	1.95	0.48
1:B:361:VAL:HG22	1:B:653:LYS:HB3	1.94	0.48
1:B:590:ARG:CB	2:B:1704:CPL:H412	2.44	0.48
1:B:561:ILE:O	2:B:1697:CPL:HC81	2.14	0.48
2:A:1718:CPL:H221	2:A:3097:CPL:H212	1.95	0.48
1:A:141:ILE:O	1:B:265:GLN:NE2	2.46	0.47
1:A:322:PHE:O	1:A:326:GLU:HB2	2.14	0.47
1:A:551:TYR:CD1	1:A:552:PHE:CD1	3.02	0.47
1:A:612:GLN:C	1:A:614:GLN:N	2.72	0.47
1:B:593:LEU:HD12	2:B:1697:CPL:C37	2.44	0.47
1:A:265:GLN:CD	1:B:142:ASP:HB3	2.35	0.47
2:A:1704:CPL:H482	2:A:1714:CPL:H261	1.96	0.47
1:B:552:PHE:HD2	1:B:615:VAL:HG12	1.78	0.47
1:A:421:ARG:HG2	1:B:417:ASN:C	1.81	0.47
1:B:447:ALA:CA	2:B:1705:CPL:O2P	2.54	0.47
1:A:580:GLY:O	2:A:1710:CPL:H42	2.14	0.47
1:A:79:LYS:HE3	1:B:263:LEU:CA	2.38	0.47
1:A:244:ARG:HB3	1:A:256:LEU:HD13	1.95	0.47
1:A:278:GLU:OE2	1:A:333:ARG:NH1	2.47	0.47
1:A:416:GLU:CD	2:A:1701:CPL:H321	2.33	0.47
1:A:604:HIS:C	1:A:606:PRO:HD2	2.40	0.47
1:B:604:HIS:C	1:B:606:PRO:HD2	2.40	0.47
1:A:248:ILE:CG2	1:B:300:LEU:HD12	2.34	0.47
2:B:1710:CPL:H251	2:B:1712:CPL:C48	2.44	0.47
1:A:209:ARG:HD3	1:B:211:SER:O	1.59	0.47
1:A:436:LYS:HE3	2:A:1709:CPL:C7	2.27	0.47
1:B:104:ALA:HB2	1:B:141:ILE:CD1	2.22	0.47
1:B:433:SER:HA	2:B:1701:CPL:O31	2.15	0.47
1:B:563:ALA:C	1:B:565:THR:N	2.71	0.47
1:B:591:ARG:HG2	1:B:591:ARG:NH2	2.29	0.47
1:A:400:ILE:HD12	1:A:620:VAL:HG11	1.95	0.47
1:B:514:SER:OG	1:B:522:MET:HE1	2.15	0.47
1:B:581:VAL:O	2:B:1699:CPL:H482	2.14	0.47
1:A:563:ALA:C	1:A:565:THR:H	2.23	0.47
1:B:123:ASP:OD1	1:B:125:LYS:HG3	2.15	0.47
1:A:561:ILE:CD1	2:A:1705:CPL:O4P	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1702:CPL:H483	2:A:1708:CPL:C25	2.37	0.47
2:A:1706:CPL:H461	2:A:1711:CPL:C26	2.43	0.47
1:B:60:ILE:CB	1:B:199:ASN:HB2	2.32	0.47
1:B:67:GLN:HE21	1:B:71:ARG:CZ	2.28	0.47
1:B:302:ASN:HD22	1:B:303:PRO:N	2.13	0.47
1:B:416:GLU:OE1	2:B:1704:CPL:H331	2.15	0.47
1:A:579:LEU:HD12	1:A:584:LEU:O	2.15	0.46
1:A:147:LYS:HD2	1:B:267:PHE:HA	1.97	0.46
1:A:147:LYS:HZ3	1:B:271:LEU:CG	2.11	0.46
1:A:591:ARG:HG2	1:A:591:ARG:NH2	2.29	0.46
2:A:1697:CPL:HC63	2:A:1700:CPL:C8	2.45	0.46
1:B:420:LEU:HD22	2:B:1700:CPL:O11	2.07	0.46
1:B:579:LEU:HD12	1:B:584:LEU:O	2.15	0.46
1:A:147:LYS:CG	1:B:266:VAL:O	2.63	0.46
1:A:267:PHE:CA	1:B:147:LYS:NZ	2.79	0.46
1:A:448:PHE:O	1:A:452:ILE:HG13	2.16	0.46
1:A:525:LEU:CD2	1:A:526:SER:H	2.28	0.46
1:A:552:PHE:CD2	1:A:615:VAL:HG12	2.50	0.46
1:A:563:ALA:C	1:A:565:THR:N	2.71	0.46
1:A:577:LEU:C	1:A:579:LEU:H	2.23	0.46
2:A:1701:CPL:C11	1:B:420:LEU:HG	2.45	0.46
1:B:525:LEU:CD2	1:B:526:SER:H	2.28	0.46
1:A:219:ARG:NE	1:B:150:GLU:CD	2.60	0.46
2:A:3094:CPL:H252	2:A:3181:CPL:H462	1.96	0.46
1:B:552:PHE:CD2	1:B:615:VAL:HG12	2.50	0.46
1:A:67:GLN:HE22	1:A:200:ASN:CG	2.23	0.46
1:A:129:GLN:O	1:A:130:LEU:HD12	2.15	0.46
1:A:302:ASN:HD22	1:A:303:PRO:N	2.13	0.46
1:A:496:LEU:HD11	1:A:646:LEU:HD11	1.97	0.46
1:B:54:ASP:OD1	1:B:345:HIS:HD2	1.98	0.46
1:B:416:GLU:CB	2:B:1700:CPL:C2	2.90	0.46
1:A:54:ASP:OD1	1:A:345:HIS:HD2	1.98	0.46
1:A:300:LEU:HD13	1:B:248:ILE:CG2	2.35	0.46
1:A:436:LYS:HG2	2:A:1709:CPL:HC61	1.97	0.46
1:A:447:ALA:HA	2:A:1708:CPL:O1P	2.14	0.46
1:B:448:PHE:O	1:B:452:ILE:HG13	2.16	0.46
1:B:587:ASP:O	2:B:1703:CPL:H451	2.00	0.46
2:A:1701:CPL:C11	1:B:420:LEU:CG	2.90	0.46
1:B:597:ALA:O	1:B:598:LYS:C	2.59	0.46
1:B:416:GLU:OE1	2:B:1704:CPL:C33	2.58	0.46
1:B:425:GLU:HB3	2:B:1705:CPL:HC11	1.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:ILE:HB	1:A:355:PRO:CD	2.46	0.46
2:A:1704:CPL:H252	2:A:1714:CPL:C48	2.40	0.46
2:A:1718:CPL:C25	2:A:3097:CPL:C23	2.93	0.46
1:B:322:PHE:O	1:B:326:GLU:HB2	2.15	0.46
1:B:496:LEU:HD11	1:B:646:LEU:HD11	1.97	0.46
2:B:1701:CPL:H481	2:B:1710:CPL:C26	2.43	0.46
1:A:144:ALA:C	1:A:146:ALA:H	2.24	0.46
1:A:215:THR:CB	1:A:218:GLU:HG3	2.37	0.46
1:A:514:SER:OG	1:A:522:MET:HE1	2.15	0.46
1:A:572:ILE:CD1	2:A:1705:CPL:H342	2.21	0.46
1:B:551:TYR:CD1	1:B:552:PHE:CD1	3.02	0.46
1:A:212:GLN:CG	1:B:80:ARG:NE	2.79	0.45
1:A:240:TRP:HZ2	1:A:260:GLU:HB3	1.81	0.45
1:A:450:GLN:OE1	2:A:1708:CPL:HC81	2.06	0.45
2:A:1714:CPL:H461	2:B:1708:CPL:H262	1.97	0.45
1:B:70:PHE:HB2	1:B:176:ILE:HD13	1.98	0.45
1:B:568:LEU:HD11	1:B:601:LEU:CD2	2.44	0.45
1:A:141:ILE:N	1:A:141:ILE:CD1	2.79	0.45
1:A:147:LYS:C	1:B:269:ALA:O	2.59	0.45
1:A:414:THR:O	2:A:1701:CPL:HC82	2.15	0.45
1:A:433:SER:O	2:A:1709:CPL:HC11	2.16	0.45
1:B:432:LEU:CG	2:B:1701:CPL:C34	2.94	0.45
1:B:581:VAL:CA	2:B:1699:CPL:H482	2.46	0.45
1:A:123:ASP:OD1	1:A:125:LYS:HG3	2.15	0.45
1:A:147:LYS:HD2	1:B:266:VAL:C	2.33	0.45
1:A:246:SER:HB2	3:B:1706:GDP:C5	2.46	0.45
1:A:408:VAL:HG11	1:A:560:ILE:CD1	2.47	0.45
1:B:147:LYS:O	1:B:150:GLU:HB3	2.17	0.45
1:B:278:GLU:CG	1:B:333:ARG:NH1	2.66	0.45
1:B:354:ILE:HB	1:B:355:PRO:CD	2.46	0.45
1:B:408:VAL:HG11	1:B:560:ILE:CD1	2.47	0.45
1:B:416:GLU:O	2:B:1700:CPL:O3P	2.31	0.45
1:B:432:LEU:O	1:B:433:SER:C	2.59	0.45
1:A:143:PRO:HG3	1:B:262:ARG:O	2.14	0.45
1:A:372:GLU:N	1:A:373:PRO:CD	2.80	0.45
1:A:410:ASN:ND2	1:A:410:ASN:O	2.49	0.45
1:A:413:ASN:N	2:A:1703:CPL:HC82	2.14	0.45
1:A:420:LEU:HD23	1:B:420:LEU:HB3	1.11	0.45
2:A:1700:CPL:O1P	2:A:1713:CPL:C2	2.50	0.45
2:A:1706:CPL:C48	2:A:1711:CPL:C26	2.88	0.45
1:B:240:TRP:HZ2	1:B:260:GLU:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:GLU:HA	2:B:1705:CPL:H322	1.97	0.45
1:B:577:LEU:O	1:B:577:LEU:HD22	2.16	0.45
1:A:21:ARG:HG3	1:A:65:LEU:HD23	1.95	0.45
1:A:212:GLN:N	1:A:213:PRO:HD3	2.31	0.45
1:B:594:VAL:C	2:B:1703:CPL:C33	2.78	0.45
2:B:1697:CPL:H481	2:B:1714:CPL:C26	2.46	0.45
1:A:581:VAL:CB	2:A:1707:CPL:H472	2.47	0.45
1:A:582:GLY:O	2:A:1699:CPL:C25	2.64	0.45
2:A:3077:CPL:HC2	2:A:1697:CPL:O1P	2.17	0.45
2:A:1701:CPL:C13	1:B:420:LEU:HD11	2.47	0.45
1:B:104:ALA:O	1:B:105:VAL:HB	2.15	0.45
1:B:144:ALA:C	1:B:146:ALA:H	2.24	0.45
1:B:233:VAL:HG22	1:B:235:PHE:CE1	2.52	0.45
1:B:240:TRP:NE1	1:B:260:GLU:OE1	2.50	0.45
1:B:638:ASP:O	1:B:642:ARG:HG3	2.17	0.45
1:B:128:GLN:CG	1:B:129:GLN:H	1.99	0.45
1:B:591:ARG:NE	2:B:1703:CPL:H182	2.31	0.45
1:A:104:ALA:O	1:A:105:VAL:HB	2.15	0.45
1:A:432:LEU:O	1:A:433:SER:C	2.59	0.45
2:A:1718:CPL:C48	2:B:1704:CPL:H481	2.46	0.45
1:B:325:ARG:HG2	1:B:692:TYR:CE1	2.52	0.45
1:B:436:LYS:C	1:B:438:GLU:N	2.71	0.45
1:B:563:ALA:C	1:B:565:THR:H	2.23	0.45
1:A:212:GLN:NE2	1:B:209:ARG:HG2	2.30	0.45
1:A:240:TRP:NE1	1:A:260:GLU:OE1	2.50	0.45
1:A:638:ASP:O	1:A:642:ARG:HG3	2.17	0.45
1:B:585:GLN:CG	2:B:1696:CPL:H263	2.02	0.45
2:B:1701:CPL:C48	2:B:1710:CPL:H261	2.42	0.45
1:A:209:ARG:HG2	1:B:212:GLN:NE2	2.31	0.45
1:A:604:HIS:O	1:A:605:LEU:C	2.59	0.45
1:B:141:ILE:N	1:B:141:ILE:CD1	2.79	0.45
1:A:60:ILE:HG22	1:A:64:ASN:ND2	2.31	0.44
1:A:116:LYS:HG3	1:A:129:GLN:HE22	1.82	0.44
1:A:409:LEU:HD21	1:A:606:PRO:CA	2.42	0.44
1:A:413:ASN:HA	2:A:1703:CPL:HC82	1.44	0.44
1:A:577:LEU:O	1:A:577:LEU:HD22	2.16	0.44
2:A:1703:CPL:C48	2:A:1715:CPL:H252	2.47	0.44
1:B:212:GLN:N	1:B:213:PRO:HD3	2.31	0.44
1:B:577:LEU:C	1:B:579:LEU:H	2.23	0.44
1:A:147:LYS:O	1:A:150:GLU:HB3	2.17	0.44
1:A:325:ARG:HG2	1:A:692:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1698:CPL:H321	2:A:1699:CPL:C12	2.47	0.44
1:B:410:ASN:O	1:B:410:ASN:ND2	2.49	0.44
1:B:432:LEU:CG	2:B:1701:CPL:H342	2.45	0.44
1:B:541:GLY:O	1:B:542:PHE:C	2.60	0.44
1:A:265:GLN:HB2	1:B:142:ASP:HB3	1.98	0.44
1:B:60:ILE:HG22	1:B:64:ASN:ND2	2.31	0.44
1:B:124:GLY:O	1:B:125:LYS:C	2.60	0.44
1:B:129:GLN:O	1:B:130:LEU:HD12	2.15	0.44
1:B:409:LEU:HD21	1:B:606:PRO:CA	2.42	0.44
1:B:594:VAL:O	1:B:595:LYS:C	2.61	0.44
1:B:604:HIS:O	1:B:605:LEU:C	2.59	0.44
1:A:435:GLY:HA3	2:A:1709:CPL:HC73	1.98	0.44
1:B:121:PHE:HD1	1:B:159:ASP:O	2.01	0.44
1:B:215:THR:HG22	1:B:216:LEU:H	1.82	0.44
1:B:417:ASN:HB2	2:B:1700:CPL:HC12	1.62	0.44
1:A:124:GLY:O	1:A:125:LYS:C	2.60	0.44
1:A:417:ASN:HB2	2:A:1701:CPL:HC12	1.63	0.44
1:A:418:ASP:CG	2:A:1701:CPL:C8	2.80	0.44
1:A:425:GLU:HB3	2:A:1708:CPL:O3	2.17	0.44
1:B:106:LEU:HD21	1:B:197:TYR:CE1	2.53	0.44
1:B:562:THR:C	2:B:1697:CPL:HC71	2.43	0.44
1:B:595:LYS:H	2:B:1703:CPL:H361	1.83	0.44
1:A:541:GLY:O	1:A:542:PHE:C	2.60	0.44
1:A:572:ILE:HD12	2:A:1705:CPL:H322	1.97	0.44
2:A:1718:CPL:H482	2:B:1704:CPL:C48	2.48	0.44
1:B:66:GLN:C	1:B:68:GLY:H	2.26	0.44
1:B:208:MET:HE2	1:B:218:GLU:OE1	2.18	0.44
1:A:80:ARG:CD	1:B:212:GLN:HG3	2.48	0.44
1:B:601:LEU:C	1:B:603:LYS:N	2.75	0.44
1:A:66:GLN:C	1:A:68:GLY:H	2.26	0.44
1:A:250:PRO:HG2	1:B:297:ARG:NH1	2.26	0.44
1:A:357:LEU:O	1:A:660:ARG:HD3	2.18	0.44
1:A:449:GLU:HB3	2:A:1708:CPL:HC73	1.97	0.44
1:A:578:GLY:HA3	1:A:584:LEU:HD12	2.00	0.44
1:A:597:ALA:O	1:A:598:LYS:C	2.59	0.44
1:A:80:ARG:NE	1:B:212:GLN:CG	2.78	0.44
1:A:147:LYS:CE	1:B:267:PHE:O	2.66	0.44
1:A:558:GLY:HA2	2:A:1705:CPL:HC71	2.00	0.44
1:B:116:LYS:HG3	1:B:129:GLN:HE22	1.82	0.44
1:B:444:LEU:HD13	2:B:1697:CPL:HC62	2.00	0.44
1:A:121:PHE:HD1	1:A:159:ASP:O	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LYS:HD3	1:B:271:LEU:N	2.33	0.43
1:A:233:VAL:HG22	1:A:235:PHE:CE1	2.52	0.43
1:A:605:LEU:HA	1:A:608:VAL:CG2	2.48	0.43
2:A:1697:CPL:C26	2:A:1710:CPL:H483	2.22	0.43
1:B:605:LEU:HA	1:B:608:VAL:CG2	2.48	0.43
1:A:70:PHE:HB2	1:A:176:ILE:HD13	1.98	0.43
1:A:212:GLN:HG3	1:B:80:ARG:CD	2.49	0.43
1:A:267:PHE:O	1:B:147:LYS:CE	2.66	0.43
2:B:1703:CPL:O11	2:B:1704:CPL:O31	2.36	0.43
1:A:9:ARG:NH2	1:A:9:ARG:CB	2.81	0.43
1:A:525:LEU:HD22	1:A:526:SER:H	1.83	0.43
1:B:9:ARG:NH2	1:B:9:ARG:CB	2.81	0.43
1:A:434:SER:O	2:A:1709:CPL:HC11	2.19	0.43
1:A:462:THR:HG22	1:A:463:ALA:N	2.33	0.43
1:B:414:THR:HA	2:B:1704:CPL:C4	2.47	0.43
1:A:266:VAL:O	1:B:147:LYS:CG	2.66	0.43
1:A:601:LEU:C	1:A:603:LYS:H	2.26	0.43
1:B:45:SER:C	1:B:47:GLY:H	2.27	0.43
1:B:60:ILE:CG2	1:B:199:ASN:C	2.90	0.43
1:B:85:PHE:CE1	1:B:236:LEU:HD13	2.54	0.43
1:B:441:ASN:HD22	1:B:441:ASN:HA	1.63	0.43
1:B:659:ASN:HD22	1:B:662:SER:CB	2.31	0.43
1:A:14:LEU:HD12	1:A:14:LEU:HA	1.81	0.43
1:A:208:MET:HE2	1:A:218:GLU:OE1	2.18	0.43
1:A:420:LEU:HD21	1:B:420:LEU:HB2	1.40	0.43
1:A:659:ASN:HD22	1:A:662:SER:CB	2.31	0.43
1:B:20:VAL:HG21	1:B:688:LEU:HG	2.00	0.43
1:B:68:GLY:CA	1:B:202:HIS:NE2	2.81	0.43
1:B:372:GLU:N	1:B:373:PRO:CD	2.80	0.43
1:B:462:THR:HG22	1:B:463:ALA:N	2.33	0.43
1:B:517:TRP:CD2	1:B:635:ILE:HG12	2.54	0.43
1:A:147:LYS:HD3	1:B:271:LEU:H	1.83	0.43
1:A:246:SER:CB	3:B:1706:GDP:C2'	2.71	0.43
1:A:581:VAL:CG2	2:A:1707:CPL:H472	2.48	0.43
1:A:80:ARG:HD2	1:B:212:GLN:HG3	2.01	0.43
1:A:106:LEU:HD21	1:A:197:TYR:CE1	2.53	0.43
1:A:423:GLN:HE21	1:A:423:GLN:HB3	1.65	0.43
1:B:379:THR:CG2	1:B:382:ARG:HH11	2.32	0.43
1:B:525:LEU:HD22	1:B:526:SER:H	1.83	0.43
1:B:590:ARG:CG	2:B:1704:CPL:H412	2.49	0.43
1:A:45:SER:C	1:A:47:GLY:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLU:O	1:A:56:GLU:HG3	2.19	0.43
1:B:52:GLU:O	1:B:56:GLU:HG3	2.19	0.43
1:A:244:ARG:C	1:A:246:SER:H	2.27	0.43
2:A:1698:CPL:P	2:A:1700:CPL:HC2	2.59	0.43
2:A:1702:CPL:H481	2:A:1717:CPL:H481	2.00	0.43
2:A:1712:CPL:O11	2:A:3097:CPL:H321	2.19	0.43
1:B:548:LEU:HD13	1:B:548:LEU:C	2.44	0.43
1:A:464:GLU:OE1	1:A:546:ASN:OD1	2.37	0.42
1:A:548:LEU:C	1:A:548:LEU:HD13	2.44	0.42
1:A:603:LYS:HE3	1:A:604:HIS:NE2	2.34	0.42
1:B:244:ARG:C	1:B:246:SER:H	2.27	0.42
2:B:1712:CPL:C26	2:B:1714:CPL:H251	2.42	0.42
1:A:230:GLY:C	1:A:334:GLN:HE22	2.27	0.42
1:A:517:TRP:CD2	1:A:635:ILE:HG12	2.54	0.42
2:A:1718:CPL:C25	2:A:3097:CPL:H232	2.47	0.42
1:B:357:LEU:O	1:B:660:ARG:HD3	2.18	0.42
1:B:559:GLY:O	1:B:563:ALA:N	2.51	0.42
1:B:561:ILE:C	1:B:563:ALA:N	2.77	0.42
1:B:569:LEU:HA	1:B:569:LEU:HD23	1.87	0.42
1:B:582:GLY:HA3	2:B:1696:CPL:C48	2.27	0.42
1:B:594:VAL:HG21	2:B:1703:CPL:H372	1.59	0.42
1:A:20:VAL:HG21	1:A:688:LEU:HG	2.00	0.42
1:A:211:SER:O	1:B:209:ARG:HD3	1.58	0.42
1:A:385:PHE:CE2	1:A:389:ILE:HD11	2.54	0.42
1:A:460:THR:HG21	1:A:550:ASN:HA	2.01	0.42
1:A:472:LYS:HE2	1:B:472:LYS:HE2	1.41	0.42
1:A:516:GLY:O	1:A:519:LYS:N	2.51	0.42
1:A:590:ARG:NH1	2:A:1705:CPL:C19	2.82	0.42
1:B:169:LEU:HB2	1:B:172:LEU:HG	2.01	0.42
1:B:196:GLY:CA	1:B:200:ASN:HD22	2.32	0.42
1:B:385:PHE:CE2	1:B:389:ILE:HD11	2.54	0.42
1:B:578:GLY:HA3	1:B:584:LEU:HD12	2.00	0.42
1:B:601:LEU:C	1:B:603:LYS:H	2.26	0.42
2:B:1697:CPL:H481	2:B:1714:CPL:H252	2.02	0.42
1:A:132:PHE:CE1	1:A:136:LYS:HD2	2.54	0.42
1:A:212:GLN:HG3	1:B:80:ARG:HD2	2.01	0.42
1:A:270:ASN:HB3	1:B:147:LYS:HE2	1.55	0.42
1:A:441:ASN:HD22	1:A:441:ASN:HA	1.63	0.42
1:A:450:GLN:CD	2:A:1708:CPL:HC81	2.42	0.42
1:A:580:GLY:O	2:A:1710:CPL:C42	2.67	0.42
2:A:1701:CPL:HC52	1:B:421:ARG:HD3	1.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:GLU:N	1:B:660:ARG:NH1	2.65	0.42
1:B:565:THR:HA	2:B:1697:CPL:HC82	1.80	0.42
1:A:85:PHE:CE1	1:A:236:LEU:HD13	2.54	0.42
1:A:92:GLU:HG3	1:A:169:LEU:HD21	2.02	0.42
1:A:429:PHE:O	1:A:433:SER:HB2	2.20	0.42
1:B:5:VAL:O	1:B:8:ASP:HB2	2.20	0.42
1:A:261:ASN:HD22	1:A:264:ARG:HE	1.68	0.42
1:A:413:ASN:O	2:A:1703:CPL:HC73	2.15	0.42
1:A:576:LEU:CD2	2:A:1705:CPL:C41	2.96	0.42
2:A:1718:CPL:HC62	2:A:3097:CPL:C7	2.23	0.42
1:B:408:VAL:HG11	1:B:560:ILE:HD12	2.02	0.42
1:B:464:GLU:OE1	1:B:546:ASN:OD1	2.37	0.42
1:B:647:ASP:HB3	1:B:651:LYS:HE2	2.02	0.42
2:B:1712:CPL:HC73	2:B:1714:CPL:C6	2.46	0.42
1:A:5:VAL:O	1:A:8:ASP:HB2	2.20	0.42
1:A:123:ASP:CG	1:A:125:LYS:HE3	2.45	0.42
1:A:414:THR:HG22	2:A:1701:CPL:HC52	1.70	0.42
1:B:261:ASN:HD22	1:B:264:ARG:HE	1.68	0.42
1:B:603:LYS:HE3	1:B:604:HIS:NE2	2.35	0.42
1:A:248:ILE:HD12	1:B:300:LEU:HD11	2.02	0.42
1:A:446:LYS:HD2	2:A:1708:CPL:HC52	2.00	0.42
2:A:1701:CPL:C26	2:A:1712:CPL:H482	2.49	0.42
1:B:189:ALA:HB1	1:B:225:TYR:CZ	2.55	0.42
2:A:3077:CPL:H262	2:A:1709:CPL:H481	2.00	0.42
1:B:14:LEU:HD12	1:B:14:LEU:HA	1.81	0.42
1:B:105:VAL:HG21	1:B:160:VAL:HG11	2.01	0.42
2:B:1710:CPL:C23	2:B:1712:CPL:H442	2.40	0.42
1:A:161:ASP:O	1:A:162:TYR:HB3	2.20	0.42
1:A:169:LEU:HB2	1:A:172:LEU:HG	2.01	0.42
1:A:196:GLY:CA	1:A:200:ASN:HD22	2.32	0.42
1:A:212:GLN:CG	1:B:80:ARG:NH1	2.83	0.42
1:A:278:GLU:CB	1:A:333:ARG:NH2	2.61	0.42
2:A:1703:CPL:H252	2:A:1704:CPL:H471	1.96	0.42
1:B:585:GLN:CD	2:B:1696:CPL:H251	2.35	0.42
1:B:590:ARG:HG2	2:B:1704:CPL:H412	2.02	0.42
1:B:602:VAL:HG22	2:B:1703:CPL:C4	2.47	0.42
1:B:612:GLN:C	1:B:614:GLN:N	2.73	0.42
1:A:262:ARG:O	1:B:143:PRO:HG3	2.20	0.41
1:A:360:ASP:OD2	1:A:366:LYS:HG2	2.18	0.41
1:A:432:LEU:HG	2:A:1709:CPL:H331	1.90	0.41
1:A:559:GLY:O	1:A:563:ALA:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PHE:CZ	1:A:236:LEU:CD1	3.03	0.41
1:A:278:GLU:OE1	1:A:278:GLU:HA	2.20	0.41
1:A:592:GLU:O	1:A:593:LEU:C	2.61	0.41
1:A:594:VAL:O	1:A:595:LYS:C	2.61	0.41
1:A:601:LEU:C	1:A:603:LYS:N	2.75	0.41
1:B:94:LEU:HD23	1:B:94:LEU:C	2.45	0.41
1:B:277:VAL:HG23	1:B:277:VAL:O	2.20	0.41
1:B:385:PHE:CE2	1:B:631:VAL:HG11	2.54	0.41
1:B:592:GLU:O	1:B:593:LEU:C	2.61	0.41
2:B:1701:CPL:H261	2:B:1710:CPL:H472	2.00	0.41
1:A:94:LEU:HD23	1:A:94:LEU:C	2.45	0.41
1:A:379:THR:CG2	1:A:382:ARG:HH11	2.32	0.41
1:A:413:ASN:N	2:A:1703:CPL:C8	2.74	0.41
1:B:213:PRO:O	1:B:214:CYS:C	2.63	0.41
1:B:622:GLU:O	1:B:623:CYS:C	2.63	0.41
1:A:143:PRO:HA	1:B:266:VAL:CG2	2.50	0.41
1:A:230:GLY:C	1:A:334:GLN:HE21	2.28	0.41
1:A:240:TRP:CZ2	1:A:260:GLU:HB3	2.55	0.41
1:A:488:ILE:O	1:A:492:ILE:HG13	2.20	0.41
1:A:489:THR:HG22	1:A:490:ASP:N	2.36	0.41
1:A:577:LEU:HD13	2:A:1707:CPL:C43	2.48	0.41
1:B:518:ALA:O	1:B:522:MET:HE3	2.20	0.41
1:B:586:ALA:HB1	2:B:1697:CPL:C45	2.47	0.41
1:A:60:ILE:HG22	1:A:64:ASN:HD21	1.86	0.41
1:A:269:ALA:H	1:B:144:ALA:HA	1.85	0.41
1:A:358:GLU:CD	1:A:660:ARG:HD2	2.45	0.41
1:A:418:ASP:N	2:A:1701:CPL:HC41	2.11	0.41
2:A:1698:CPL:H321	2:A:1699:CPL:H121	2.02	0.41
2:B:1700:CPL:O31	2:B:1704:CPL:C11	2.53	0.41
1:A:58:ILE:HD11	1:A:342:ALA:CB	2.51	0.41
1:A:81:GLY:O	1:A:82:LYS:C	2.63	0.41
1:A:213:PRO:O	1:A:214:CYS:C	2.63	0.41
1:A:241:ASP:OD2	1:B:245:GLU:OE1	2.15	0.41
1:A:245:GLU:OE1	1:B:241:ASP:OD2	2.15	0.41
1:A:271:LEU:O	1:A:272:ALA:C	2.63	0.41
1:B:58:ILE:HD11	1:B:342:ALA:CB	2.51	0.41
1:B:123:ASP:CG	1:B:125:LYS:HE3	2.45	0.41
1:B:132:PHE:CE1	1:B:136:LYS:HD2	2.55	0.41
1:B:271:LEU:O	1:B:272:ALA:C	2.63	0.41
1:B:434:SER:CA	2:B:1701:CPL:O2P	2.69	0.41
1:B:667:LEU:HA	1:B:667:LEU:HD23	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:O	1:A:55:ILE:HG13	2.21	0.41
1:A:141:ILE:CG1	1:A:146:ALA:HB2	2.50	0.41
1:A:189:ALA:HB1	1:A:225:TYR:CZ	2.55	0.41
1:A:215:THR:HG22	1:A:216:LEU:H	1.82	0.41
1:A:248:ILE:CD1	1:B:300:LEU:HD11	2.50	0.41
1:A:277:VAL:HG23	1:A:277:VAL:O	2.20	0.41
1:A:561:ILE:C	1:A:563:ALA:N	2.77	0.41
1:A:647:ASP:HB3	1:A:651:LYS:HE2	2.02	0.41
1:B:39:GLU:OE2	1:B:50:SER:N	2.54	0.41
1:B:92:GLU:HG3	1:B:169:LEU:HD21	2.02	0.41
1:B:141:ILE:CG1	1:B:146:ALA:HB2	2.50	0.41
1:B:247:LEU:O	1:B:248:ILE:C	2.63	0.41
1:B:429:PHE:O	1:B:433:SER:HB2	2.20	0.41
1:B:488:ILE:O	1:B:492:ILE:HG13	2.20	0.41
1:A:105:VAL:HG21	1:A:160:VAL:HG11	2.01	0.41
1:A:121:PHE:HE2	1:A:128:GLN:HB2	1.86	0.41
1:A:436:LYS:O	1:A:438:GLU:N	2.50	0.41
1:A:622:GLU:O	1:A:623:CYS:C	2.63	0.41
1:B:240:TRP:CZ2	1:B:260:GLU:HB3	2.56	0.41
1:B:446:LYS:HE2	2:B:1705:CPL:HC81	1.44	0.41
1:B:460:THR:HG21	1:B:550:ASN:HA	2.01	0.41
1:A:80:ARG:NH1	1:B:212:GLN:CG	2.82	0.41
1:A:247:LEU:HB3	1:A:255:GLU:CD	2.46	0.41
1:A:518:ALA:O	1:A:522:MET:HE3	2.20	0.41
1:A:600:GLU:O	1:A:603:LYS:HB3	2.21	0.41
1:B:30:LYS:HE3	1:B:30:LYS:HB2	1.92	0.41
1:B:247:LEU:HB3	1:B:255:GLU:CD	2.46	0.41
1:B:600:GLU:O	1:B:603:LYS:HB3	2.21	0.41
1:A:39:GLU:OE2	1:A:50:SER:N	2.54	0.41
1:A:80:ARG:CD	1:B:211:SER:O	2.68	0.41
1:A:211:SER:O	1:B:80:ARG:CD	2.69	0.41
1:A:248:ILE:HD12	1:B:300:LEU:CD1	2.51	0.41
1:A:263:LEU:CD2	1:B:79:LYS:CG	2.95	0.41
1:A:581:VAL:O	2:A:1707:CPL:C48	2.68	0.41
1:B:432:LEU:HD13	1:B:432:LEU:H	1.86	0.41
1:B:565:THR:HG21	2:B:1697:CPL:HC63	0.92	0.41
1:B:585:GLN:CB	2:B:1696:CPL:C25	2.76	0.41
1:A:167:TYR:HA	1:A:168:PRO:HD3	1.93	0.40
1:A:472:LYS:HE3	1:B:476:ARG:NH1	2.36	0.40
1:A:604:HIS:O	1:A:607:GLN:N	2.54	0.40
2:A:1701:CPL:HC42	1:B:421:ARG:CZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:GLU:OE1	1:B:278:GLU:HA	2.20	0.40
1:B:440:PHE:CD1	1:B:440:PHE:C	2.99	0.40
1:B:587:ASP:O	2:B:1703:CPL:H43	2.18	0.40
1:A:139:TYR:O	1:A:140:THR:HG23	2.21	0.40
1:A:143:PRO:CB	1:B:266:VAL:CG2	2.96	0.40
1:A:592:GLU:HA	1:A:595:LYS:HB3	2.04	0.40
2:A:1700:CPL:H442	2:A:1713:CPL:H452	2.03	0.40
1:B:358:GLU:CD	1:B:660:ARG:HD2	2.46	0.40
1:B:447:ALA:HA	2:B:1705:CPL:HC41	2.02	0.40
1:A:152:GLU:OE2	1:A:154:LYS:HD2	2.22	0.40
1:A:181:SER:OG	1:A:192:GLU:OE2	2.38	0.40
1:A:266:VAL:CG2	1:B:143:PRO:HA	2.51	0.40
1:A:408:VAL:HG11	1:A:560:ILE:HD12	2.02	0.40
1:A:434:SER:O	2:A:1709:CPL:O2P	2.40	0.40
1:A:446:LYS:O	2:A:1708:CPL:HC73	2.20	0.40
1:A:116:LYS:C	1:A:117:VAL:HG23	2.47	0.40
1:A:247:LEU:O	1:A:248:ILE:C	2.63	0.40
1:A:266:VAL:HA	1:B:143:PRO:CA	2.51	0.40
1:A:381:ILE:CG2	1:A:481:TYR:HD2	2.34	0.40
1:A:583:PHE:HE1	2:A:1707:CPL:H42	1.85	0.40
1:B:585:GLN:CD	2:B:1696:CPL:C25	2.93	0.40
1:A:143:PRO:CB	1:B:266:VAL:CA	2.84	0.40
1:A:440:PHE:CD1	1:A:440:PHE:C	2.99	0.40
1:A:549:LEU:C	1:A:551:TYR:H	2.29	0.40
1:A:571:PRO:HB3	1:A:596:THR:CG2	2.51	0.40
1:B:51:LEU:O	1:B:55:ILE:HG13	2.21	0.40
1:B:128:GLN:CG	1:B:129:GLN:N	2.67	0.40
1:B:139:TYR:O	1:B:140:THR:HG23	2.21	0.40
1:B:161:ASP:O	1:B:162:TYR:HB3	2.20	0.40
1:B:422:TYR:CE1	1:B:451:TYR:HA	2.57	0.40
1:B:530:GLY:HA3	1:B:542:PHE:HB2	2.04	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	666/695 (96%)	571 (86%)	81 (12%)	14 (2%)	5	30
1	B	666/695 (96%)	570 (86%)	82 (12%)	14 (2%)	5	30
All	All	1332/1390 (96%)	1141 (86%)	163 (12%)	28 (2%)	8	30

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	197	TYR
1	B	128	GLN
1	B	197	TYR
1	A	125	LYS
1	A	433	SER
1	A	434	SER
1	A	597	ALA
1	B	125	LYS
1	B	433	SER
1	B	434	SER
1	B	597	ALA
1	A	127	PRO
1	A	435	GLY
1	A	526	SER
1	B	127	PRO
1	B	435	GLY
1	B	526	SER
1	A	432	LEU
1	B	432	LEU
1	A	3	ASN
1	B	3	ASN
1	A	105	VAL
1	B	105	VAL
1	A	117	VAL
1	A	302	ASN
1	B	117	VAL
1	B	302	ASN

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	587/601 (98%)	536 (91%)	51 (9%)	9	29
1	B	587/601 (98%)	536 (91%)	51 (9%)	9	29
All	All	1174/1202 (98%)	1072 (91%)	102 (9%)	12	29

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	14	LEU
1	A	39	GLU
1	A	58	ILE
1	A	59	THR
1	A	82	LYS
1	A	89	LEU
1	A	119	ILE
1	A	127	PRO
1	A	141	ILE
1	A	161	ASP
1	A	170	THR
1	A	171	LEU
1	A	184	LEU
1	A	211	SER
1	A	212	GLN
1	A	233	VAL
1	A	251	ASP
1	A	282	ILE
1	A	302	ASN
1	A	364	LEU
1	A	396	GLN
1	A	414	THR
1	A	423	GLN
1	A	426	LEU
1	A	428	LEU
1	A	432	LEU

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Mol	Chain	Res	Type
1	A	438	GLU
1	A	446	LYS
1	A	461	LEU
1	A	462	THR
1	A	489	THR
1	A	497	THR
1	A	512	ASP
1	A	524	LEU
1	A	525	LEU
1	A	565	THR
1	A	568	LEU
1	A	577	LEU
1	A	593	LEU
1	A	605	LEU
1	A	616	VAL
1	A	622	GLU
1	A	630	GLU
1	A	647	ASP
1	A	649	LEU
1	A	658	ILE
1	A	661	GLU
1	A	670	LEU
1	A	677	GLN
1	A	688	LEU
1	B	7	THR
1	B	14	LEU
1	B	39	GLU
1	B	58	ILE
1	B	59	THR
1	B	82	LYS
1	B	89	LEU
1	B	119	ILE
1	B	127	PRO
1	B	141	ILE
1	B	161	ASP
1	B	170	THR
1	B	171	LEU
1	B	184	LEU
1	B	211	SER
1	B	212	GLN
1	B	233	VAL
1	B	251	ASP

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Mol	Chain	Res	Type
1	B	282	ILE
1	B	302	ASN
1	B	364	LEU
1	B	396	GLN
1	B	414	THR
1	B	423	GLN
1	B	426	LEU
1	B	428	LEU
1	B	432	LEU
1	B	438	GLU
1	B	446	LYS
1	B	461	LEU
1	B	462	THR
1	B	489	THR
1	B	497	THR
1	B	512	ASP
1	B	524	LEU
1	B	525	LEU
1	B	565	THR
1	B	568	LEU
1	B	577	LEU
1	B	593	LEU
1	B	605	LEU
1	B	616	VAL
1	B	622	GLU
1	B	630	GLU
1	B	647	ASP
1	B	649	LEU
1	B	658	ILE
1	B	661	GLU
1	B	670	LEU
1	B	677	GLN
1	B	688	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	19	GLN
1	A	67	GLN
1	A	122	ASN
1	A	128	GLN

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Mol	Chain	Res	Type
1	A	151	GLN
1	A	199	ASN
1	A	200	ASN
1	A	212	GLN
1	A	238	ASN
1	A	261	ASN
1	A	294	GLN
1	A	302	ASN
1	A	320	ASN
1	A	334	GLN
1	A	345	HIS
1	A	386	GLN
1	A	396	GLN
1	A	410	ASN
1	A	423	GLN
1	A	441	ASN
1	A	486	ASN
1	A	546	ASN
1	A	550	ASN
1	A	588	GLN
1	A	607	GLN
1	A	618	ASN
1	A	659	ASN
1	A	671	GLN
1	A	687	ASN
1	B	12	GLN
1	B	19	GLN
1	B	67	GLN
1	B	122	ASN
1	B	128	GLN
1	B	151	GLN
1	B	199	ASN
1	B	212	GLN
1	B	238	ASN
1	B	261	ASN
1	B	294	GLN
1	B	302	ASN
1	B	320	ASN
1	B	345	HIS
1	B	386	GLN
1	B	396	GLN
1	B	410	ASN

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Mol	Chain	Res	Type
1	B	413	ASN
1	B	423	GLN
1	B	441	ASN
1	B	486	ASN
1	B	546	ASN
1	B	550	ASN
1	B	588	GLN
1	B	607	GLN
1	B	618	ASN
1	B	659	ASN
1	B	671	GLN
1	B	687	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

46 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CPL	A	3077	-	51,51,51	0.84	2 (3%)	57,59,59	0.89	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CPL	A	1707	-	51,51,51	0.86	4 (7%)	57,59,59	0.85	2 (3%)
2	CPL	B	1713	-	51,51,51	0.90	3 (5%)	57,59,59	0.92	2 (3%)
2	CPL	B	1711	-	51,51,51	0.86	3 (5%)	57,59,59	0.78	1 (1%)
2	CPL	B	1712	-	51,51,51	0.85	3 (5%)	57,59,59	0.99	2 (3%)
2	CPL	A	1715	-	51,51,51	0.86	3 (5%)	57,59,59	0.75	1 (1%)
2	CPL	A	1718	-	51,51,51	0.86	3 (5%)	57,59,59	0.78	1 (1%)
2	CPL	A	3097	-	51,51,51	0.84	3 (5%)	57,59,59	0.89	3 (5%)
2	CPL	B	1699	-	51,51,51	0.90	3 (5%)	57,59,59	0.90	2 (3%)
2	CPL	A	1703	-	51,51,51	0.86	3 (5%)	57,59,59	0.99	2 (3%)
2	CPL	B	1701	-	51,51,51	0.86	3 (5%)	57,59,59	0.98	2 (3%)
2	CPL	B	1708	-	51,51,51	0.90	3 (5%)	57,59,59	0.89	2 (3%)
3	GDP	B	1706	-	29,30,30	1.00	1 (3%)	45,47,47	1.79	12 (26%)
2	CPL	A	1701	-	51,51,51	0.88	3 (5%)	57,59,59	1.01	2 (3%)
2	CPL	A	1709	-	51,51,51	0.87	3 (5%)	57,59,59	1.03	2 (3%)
2	CPL	A	3181	-	51,51,51	0.88	4 (7%)	57,59,59	1.02	2 (3%)
2	CPL	A	1698	-	51,51,51	0.86	3 (5%)	57,59,59	0.85	2 (3%)
2	CPL	B	1700	-	51,51,51	0.90	3 (5%)	57,59,59	0.90	2 (3%)
2	CPL	B	1698	-	51,51,51	0.86	3 (5%)	57,59,59	0.99	2 (3%)
2	CPL	B	1703	-	51,51,51	0.88	4 (7%)	57,59,59	1.01	2 (3%)
2	CPL	B	1707	-	51,51,51	0.88	3 (5%)	57,59,59	1.01	2 (3%)
2	CPL	A	1706	-	51,51,51	0.90	3 (5%)	57,59,59	0.90	2 (3%)
2	CPL	A	1697	-	51,51,51	0.86	3 (5%)	57,59,59	0.78	1 (1%)
2	CPL	B	1709	-	51,51,51	0.87	3 (5%)	57,59,59	1.03	2 (3%)
2	CPL	B	1702	-	51,51,51	0.86	3 (5%)	57,59,59	0.78	1 (1%)
2	CPL	A	1702	-	51,51,51	0.86	3 (5%)	57,59,59	0.99	2 (3%)
2	CPL	A	1716	-	51,51,51	0.88	4 (7%)	57,59,59	1.02	2 (3%)
2	CPL	A	1711	-	51,51,51	0.86	3 (5%)	57,59,59	0.78	1 (1%)
2	CPL	A	1712	-	51,51,51	0.90	3 (5%)	57,59,59	0.89	2 (3%)
2	CPL	A	1704	-	51,51,51	0.88	3 (5%)	57,59,59	1.01	2 (3%)
2	CPL	B	1697	-	51,51,51	0.90	3 (5%)	57,59,59	0.90	2 (3%)
2	CPL	A	1705	-	51,51,51	0.88	3 (5%)	57,59,59	1.01	2 (3%)
2	CPL	A	1699	-	51,51,51	0.85	3 (5%)	57,59,59	0.84	2 (3%)
2	CPL	A	1710	-	51,51,51	0.86	3 (5%)	57,59,59	0.99	2 (3%)
2	CPL	A	1708	-	51,51,51	0.86	3 (5%)	57,59,59	0.99	2 (3%)
2	CPL	A	1700	-	51,51,51	0.90	3 (5%)	57,59,59	0.91	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CPL	B	1705	-	51,51,51	0.86	3 (5%)	57,59,59	0.86	2 (3%)
2	CPL	B	1714	-	51,51,51	0.86	3 (5%)	57,59,59	0.77	1 (1%)
2	CPL	A	1713	-	51,51,51	0.90	3 (5%)	57,59,59	0.92	2 (3%)
2	CPL	A	1714	-	51,51,51	0.86	3 (5%)	57,59,59	0.85	1 (1%)
2	CPL	B	1704	-	51,51,51	0.89	4 (7%)	57,59,59	0.90	2 (3%)
2	CPL	B	1696	-	51,51,51	0.85	3 (5%)	57,59,59	0.98	2 (3%)
2	CPL	B	1710	-	51,51,51	0.85	3 (5%)	57,59,59	0.99	2 (3%)
3	GDP	A	1696	-	29,30,30	1.00	1 (3%)	45,47,47	1.78	12 (26%)
2	CPL	A	3094	-	51,51,51	0.90	3 (5%)	57,59,59	0.91	2 (3%)
2	CPL	A	1717	-	51,51,51	0.86	3 (5%)	57,59,59	0.99	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CPL	A	3077	-	-	13/55/55/55	-
2	CPL	A	1707	-	-	11/55/55/55	-
2	CPL	B	1713	-	-	14/55/55/55	-
2	CPL	B	1711	-	-	11/55/55/55	-
2	CPL	B	1712	-	-	14/55/55/55	-
2	CPL	A	1715	-	-	11/55/55/55	-
2	CPL	A	1718	-	-	11/55/55/55	-
2	CPL	A	3097	-	-	12/55/55/55	-
2	CPL	B	1699	-	-	14/55/55/55	-
2	CPL	A	1703	-	-	14/55/55/55	-
2	CPL	B	1701	-	-	14/55/55/55	-
2	CPL	B	1708	-	-	15/55/55/55	-
3	GDP	B	1706	-	-	0/16/32/32	0/3/3/3
2	CPL	A	1701	-	-	11/55/55/55	-
2	CPL	A	1709	-	-	12/55/55/55	-
2	CPL	A	3181	-	-	12/55/55/55	-
2	CPL	A	1698	-	-	12/55/55/55	-
2	CPL	B	1700	-	-	15/55/55/55	-
2	CPL	B	1698	-	-	14/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CPL	B	1703	-	-	11/55/55/55	-
2	CPL	B	1707	-	-	11/55/55/55	-
2	CPL	A	1706	-	-	15/55/55/55	-
2	CPL	A	1697	-	-	10/55/55/55	-
2	CPL	B	1709	-	-	12/55/55/55	-
2	CPL	B	1702	-	-	11/55/55/55	-
2	CPL	A	1702	-	-	14/55/55/55	-
2	CPL	A	1716	-	-	12/55/55/55	-
2	CPL	A	1711	-	-	11/55/55/55	-
2	CPL	A	1712	-	-	15/55/55/55	-
2	CPL	A	1704	-	-	11/55/55/55	-
2	CPL	B	1697	-	-	15/55/55/55	-
2	CPL	A	1705	-	-	11/55/55/55	-
2	CPL	A	1699	-	-	11/55/55/55	-
2	CPL	A	1710	-	-	14/55/55/55	-
2	CPL	A	1708	-	-	14/55/55/55	-
2	CPL	A	1700	-	-	15/55/55/55	-
2	CPL	B	1705	-	-	11/55/55/55	-
2	CPL	B	1714	-	-	11/55/55/55	-
2	CPL	A	1713	-	-	14/55/55/55	-
2	CPL	A	1714	-	-	11/55/55/55	-
2	CPL	B	1704	-	-	14/55/55/55	-
2	CPL	B	1696	-	-	14/55/55/55	-
2	CPL	B	1710	-	-	14/55/55/55	-
3	GDP	A	1696	-	-	0/16/32/32	0/3/3/3
2	CPL	A	3094	-	-	15/55/55/55	-
2	CPL	A	1717	-	-	14/55/55/55	-

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1708	CPL	C43-C42	3.50	1.51	1.31
2	A	1715	CPL	C43-C42	3.48	1.51	1.31
2	A	3077	CPL	C43-C42	3.47	1.51	1.31
2	A	1712	CPL	C43-C42	3.47	1.51	1.31
2	A	3097	CPL	C43-C42	3.45	1.51	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1713	CPL	C43-C42	3.44	1.51	1.31
2	B	1699	CPL	C43-C42	3.44	1.51	1.31
2	A	1706	CPL	C43-C42	3.44	1.51	1.31
2	B	1714	CPL	C43-C42	3.44	1.51	1.31
2	B	1713	CPL	C43-C42	3.43	1.51	1.31
2	A	1711	CPL	C43-C42	3.43	1.51	1.31
2	A	1697	CPL	C43-C42	3.43	1.51	1.31
2	B	1704	CPL	C43-C42	3.43	1.51	1.31
2	B	1702	CPL	C43-C42	3.43	1.51	1.31
2	B	1711	CPL	C43-C42	3.42	1.51	1.31
2	A	1718	CPL	C43-C42	3.42	1.51	1.31
2	A	3094	CPL	C43-C42	3.42	1.51	1.31
2	A	1698	CPL	C43-C42	3.42	1.51	1.31
2	A	1700	CPL	C43-C42	3.41	1.51	1.31
2	B	1697	CPL	C43-C42	3.41	1.51	1.31
2	B	1700	CPL	C43-C42	3.40	1.51	1.31
2	A	1716	CPL	C43-C42	3.38	1.50	1.31
2	B	1709	CPL	C43-C42	3.37	1.50	1.31
2	A	1705	CPL	C43-C42	3.37	1.50	1.31
2	B	1703	CPL	C43-C42	3.36	1.50	1.31
2	B	1707	CPL	C43-C42	3.35	1.50	1.31
2	A	1701	CPL	C43-C42	3.35	1.50	1.31
2	A	1709	CPL	C43-C42	3.35	1.50	1.31
2	A	1699	CPL	C43-C42	3.34	1.50	1.31
2	A	3181	CPL	C43-C42	3.34	1.50	1.31
2	A	1704	CPL	C43-C42	3.33	1.50	1.31
2	A	1707	CPL	C43-C42	3.32	1.50	1.31
2	A	1714	CPL	C43-C42	3.30	1.50	1.31
2	B	1705	CPL	C43-C42	3.30	1.50	1.31
2	A	1702	CPL	C43-C42	3.28	1.50	1.31
2	A	1717	CPL	C43-C42	3.28	1.50	1.31
2	B	1698	CPL	C43-C42	3.27	1.50	1.31
2	A	1703	CPL	C43-C42	3.27	1.50	1.31
2	B	1710	CPL	C43-C42	3.27	1.50	1.31
2	A	1708	CPL	C43-C42	3.27	1.50	1.31
2	B	1701	CPL	C43-C42	3.27	1.50	1.31
2	B	1696	CPL	C43-C42	3.25	1.50	1.31
2	B	1712	CPL	C43-C42	3.25	1.50	1.31
2	A	1710	CPL	C43-C42	3.24	1.50	1.31
3	B	1706	GDP	PA-O3A	2.88	1.62	1.59
3	A	1696	GDP	PA-O3A	2.88	1.62	1.59
2	B	1699	CPL	C5-N	-2.26	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1710	CPL	P-O2P	-2.25	1.44	1.55
2	B	1701	CPL	P-O2P	-2.24	1.45	1.55
2	B	1713	CPL	C5-N	-2.24	1.44	1.51
2	A	1713	CPL	C5-N	-2.24	1.44	1.51
2	A	1712	CPL	C5-N	-2.22	1.44	1.51
2	A	1717	CPL	P-O2P	-2.22	1.45	1.55
2	B	1698	CPL	P-O2P	-2.22	1.45	1.55
2	A	1708	CPL	P-O2P	-2.22	1.45	1.55
2	A	3094	CPL	C5-N	-2.22	1.44	1.51
2	A	1710	CPL	P-O2P	-2.21	1.45	1.55
2	A	1706	CPL	C5-N	-2.21	1.44	1.51
2	B	1696	CPL	P-O2P	-2.21	1.45	1.55
2	B	1707	CPL	P-O2P	-2.21	1.45	1.55
2	B	1700	CPL	C5-N	-2.21	1.44	1.51
2	B	1708	CPL	C5-N	-2.20	1.44	1.51
2	A	3181	CPL	P-O2P	-2.20	1.45	1.55
2	B	1697	CPL	C5-N	-2.20	1.44	1.51
2	A	1701	CPL	P-O2P	-2.19	1.45	1.55
2	B	1703	CPL	P-O2P	-2.19	1.45	1.55
2	A	1700	CPL	C5-N	-2.19	1.44	1.51
2	A	1704	CPL	P-O2P	-2.18	1.45	1.55
2	A	1716	CPL	P-O2P	-2.18	1.45	1.55
2	A	1702	CPL	P-O2P	-2.18	1.45	1.55
2	B	1697	CPL	P-O2P	-2.17	1.45	1.55
2	B	1713	CPL	P-O2P	-2.16	1.45	1.55
2	A	1705	CPL	P-O2P	-2.16	1.45	1.55
2	B	1704	CPL	C5-N	-2.16	1.44	1.51
2	A	1709	CPL	P-O2P	-2.16	1.45	1.55
2	B	1712	CPL	P-O2P	-2.16	1.45	1.55
2	B	1709	CPL	P-O2P	-2.16	1.45	1.55
2	A	3094	CPL	P-O2P	-2.16	1.45	1.55
2	A	1713	CPL	P-O2P	-2.16	1.45	1.55
2	A	1703	CPL	P-O2P	-2.15	1.45	1.55
2	A	1697	CPL	C5-N	-2.15	1.44	1.51
2	B	1704	CPL	P-O2P	-2.15	1.45	1.55
2	A	1712	CPL	P-O2P	-2.15	1.45	1.55
2	B	1708	CPL	P-O2P	-2.14	1.45	1.55
2	A	3077	CPL	P-O2P	-2.14	1.45	1.55
2	A	1699	CPL	P-O2P	-2.14	1.45	1.55
2	B	1702	CPL	C5-N	-2.14	1.45	1.51
2	A	1706	CPL	P-O2P	-2.14	1.45	1.55
2	A	1697	CPL	P-O2P	-2.14	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1700	CPL	P-O2P	-2.14	1.45	1.55
2	A	3097	CPL	P-O2P	-2.14	1.45	1.55
2	B	1702	CPL	P-O2P	-2.14	1.45	1.55
2	B	1714	CPL	P-O2P	-2.14	1.45	1.55
2	A	1718	CPL	P-O2P	-2.13	1.45	1.55
2	B	1711	CPL	C5-N	-2.13	1.45	1.51
2	A	1714	CPL	P-O2P	-2.13	1.45	1.55
2	A	1700	CPL	P-O2P	-2.13	1.45	1.55
2	A	1715	CPL	P-O2P	-2.12	1.45	1.55
2	B	1703	CPL	C6-N	-2.12	1.43	1.50
2	B	1705	CPL	P-O2P	-2.12	1.45	1.55
2	A	1711	CPL	C5-N	-2.12	1.45	1.51
2	B	1714	CPL	C5-N	-2.12	1.45	1.51
2	A	1707	CPL	P-O2P	-2.12	1.45	1.55
2	B	1711	CPL	P-O2P	-2.12	1.45	1.55
2	B	1699	CPL	P-O2P	-2.11	1.45	1.55
2	A	1698	CPL	P-O2P	-2.11	1.45	1.55
2	A	1705	CPL	C6-N	-2.11	1.43	1.50
2	A	1699	CPL	C5-N	-2.10	1.45	1.51
2	A	1715	CPL	C5-N	-2.10	1.45	1.51
2	A	1711	CPL	P-O2P	-2.09	1.45	1.55
2	A	1710	CPL	C6-N	-2.09	1.43	1.50
2	A	1701	CPL	C6-N	-2.07	1.44	1.50
2	A	1708	CPL	C6-N	-2.07	1.44	1.50
2	A	1714	CPL	C5-N	-2.07	1.45	1.51
2	B	1701	CPL	C6-N	-2.06	1.44	1.50
2	B	1698	CPL	C6-N	-2.06	1.44	1.50
2	A	1717	CPL	C6-N	-2.06	1.44	1.50
2	A	1718	CPL	C5-N	-2.06	1.45	1.51
2	B	1705	CPL	C5-N	-2.06	1.45	1.51
2	A	3181	CPL	C6-N	-2.05	1.44	1.50
2	A	1716	CPL	C6-N	-2.05	1.44	1.50
2	A	1707	CPL	C5-N	-2.04	1.45	1.51
2	A	1704	CPL	C6-N	-2.04	1.44	1.50
2	B	1712	CPL	C6-N	-2.04	1.44	1.50
2	B	1707	CPL	C6-N	-2.04	1.44	1.50
2	A	3181	CPL	C5-N	-2.04	1.45	1.51
2	A	1709	CPL	C6-N	-2.04	1.44	1.50
2	A	1707	CPL	C6-N	-2.03	1.44	1.50
2	B	1696	CPL	C6-N	-2.03	1.44	1.50
2	B	1703	CPL	C5-N	-2.02	1.45	1.51
2	A	1703	CPL	C6-N	-2.02	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1698	CPL	C5-N	-2.02	1.45	1.51
2	B	1709	CPL	C5-N	-2.01	1.45	1.51
2	B	1704	CPL	C6-N	-2.01	1.44	1.50
2	A	1716	CPL	C5-N	-2.01	1.45	1.51
2	A	1702	CPL	C6-N	-2.01	1.44	1.50
2	A	3097	CPL	C5-N	-2.01	1.45	1.51
2	B	1710	CPL	C6-N	-2.00	1.44	1.50

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1706	GDP	C2-N3-C4	5.45	121.69	112.30
3	A	1696	GDP	C2-N3-C4	5.41	121.63	112.30
3	B	1706	GDP	C5-C4-N3	-4.85	120.67	128.39
3	A	1696	GDP	C5-C4-N3	-4.82	120.72	128.39
2	A	1709	CPL	C2-O2-C31	4.26	127.99	117.80
2	A	1701	CPL	C2-O2-C31	4.24	127.93	117.80
2	A	1705	CPL	C2-O2-C31	4.23	127.92	117.80
2	B	1703	CPL	C2-O2-C31	4.22	127.91	117.80
2	B	1709	CPL	C2-O2-C31	4.21	127.87	117.80
2	A	1716	CPL	C2-O2-C31	4.21	127.87	117.80
2	B	1707	CPL	C2-O2-C31	4.18	127.81	117.80
2	A	3181	CPL	C2-O2-C31	4.17	127.78	117.80
2	A	1704	CPL	C2-O2-C31	4.15	127.73	117.80
3	B	1706	GDP	N9-C4-N3	3.63	133.20	125.95
3	A	1696	GDP	N9-C4-N3	3.56	133.08	125.95
2	A	1702	CPL	C2-O2-C31	3.42	125.99	117.80
2	B	1698	CPL	C2-O2-C31	3.41	125.95	117.80
2	A	1708	CPL	C2-O2-C31	3.39	125.92	117.80
2	A	1703	CPL	C2-O2-C31	3.36	125.85	117.80
2	A	1717	CPL	C2-O2-C31	3.35	125.80	117.80
2	B	1710	CPL	C2-O2-C31	3.33	125.77	117.80
2	A	1710	CPL	C2-O2-C31	3.33	125.77	117.80
2	B	1712	CPL	C2-O2-C31	3.32	125.75	117.80
2	B	1701	CPL	C2-O2-C31	3.31	125.72	117.80
2	B	1696	CPL	C2-O2-C31	3.31	125.71	117.80
2	A	3077	CPL	C2-O2-C31	3.21	125.47	117.80
2	A	3097	CPL	C2-O2-C31	3.18	125.41	117.80
2	A	1713	CPL	C2-O2-C31	3.09	125.20	117.80
2	B	1713	CPL	C2-O2-C31	3.03	125.04	117.80
3	A	1696	GDP	O4'-C4'-C3'	3.02	111.14	105.15
2	A	1700	CPL	C2-O2-C31	3.00	124.98	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1706	GDP	O4'-C4'-C3'	3.00	111.11	105.15
2	A	3094	CPL	C2-O2-C31	3.00	124.97	117.80
2	B	1697	CPL	C2-O2-C31	2.99	124.95	117.80
2	A	1706	CPL	C2-O2-C31	2.97	124.90	117.80
2	B	1700	CPL	C2-O2-C31	2.97	124.90	117.80
2	B	1699	CPL	C2-O2-C31	2.96	124.88	117.80
2	B	1704	CPL	C2-O2-C31	2.96	124.88	117.80
2	B	1708	CPL	C2-O2-C31	2.93	124.81	117.80
2	A	1712	CPL	C2-O2-C31	2.88	124.69	117.80
2	A	3097	CPL	C3-O3-C11	2.78	127.27	117.12
2	A	3077	CPL	C3-O3-C11	2.78	127.27	117.12
2	A	1699	CPL	C3-O3-C11	2.71	127.01	117.12
3	B	1706	GDP	C6-C5-N7	2.62	135.05	130.29
3	B	1706	GDP	C8-N7-C5	2.60	108.90	104.26
3	A	1696	GDP	C8-N7-C5	2.59	108.88	104.26
3	A	1696	GDP	C6-C5-N7	2.58	134.99	130.29
2	A	1709	CPL	C3-O3-C11	2.54	126.41	117.12
2	A	1716	CPL	C3-O3-C11	2.54	126.41	117.12
2	B	1709	CPL	C3-O3-C11	2.54	126.39	117.12
2	A	3181	CPL	C3-O3-C11	2.53	126.37	117.12
2	A	1704	CPL	C3-O3-C11	2.49	126.23	117.12
2	A	1705	CPL	C3-O3-C11	2.49	126.20	117.12
2	B	1707	CPL	C3-O3-C11	2.49	126.20	117.12
2	B	1703	CPL	C3-O3-C11	2.47	126.15	117.12
2	A	1701	CPL	C3-O3-C11	2.47	126.14	117.12
2	B	1710	CPL	C3-O3-C11	2.47	126.13	117.12
2	A	1708	CPL	C3-O3-C11	2.46	126.13	117.12
2	A	1703	CPL	C3-O3-C11	2.46	126.12	117.12
2	B	1698	CPL	C3-O3-C11	2.46	126.12	117.12
2	A	1710	CPL	C3-O3-C11	2.46	126.11	117.12
2	B	1701	CPL	C3-O3-C11	2.45	126.06	117.12
2	A	1717	CPL	C3-O3-C11	2.45	126.06	117.12
2	B	1696	CPL	C3-O3-C11	2.44	126.05	117.12
2	B	1712	CPL	C3-O3-C11	2.44	126.04	117.12
2	A	1702	CPL	C3-O3-C11	2.42	125.96	117.12
2	A	1707	CPL	C3-O3-C11	2.42	125.95	117.12
2	A	1714	CPL	C3-O3-C11	2.41	125.92	117.12
2	B	1699	CPL	C33-C32-C31	-2.40	104.90	113.69
2	A	1711	CPL	C3-O3-C11	2.39	125.86	117.12
2	A	1706	CPL	C33-C32-C31	-2.39	104.94	113.69
2	A	1700	CPL	C33-C32-C31	-2.39	104.94	113.69
2	B	1705	CPL	C3-O3-C11	2.39	125.85	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1713	CPL	C33-C32-C31	-2.39	104.95	113.69
2	B	1704	CPL	C33-C32-C31	-2.38	104.97	113.69
2	A	1697	CPL	C3-O3-C11	2.38	125.82	117.12
2	B	1697	CPL	C33-C32-C31	-2.38	104.99	113.69
2	B	1714	CPL	C3-O3-C11	2.38	125.80	117.12
2	A	1698	CPL	C3-O3-C11	2.37	125.80	117.12
2	B	1700	CPL	C33-C32-C31	-2.37	104.99	113.69
2	A	1713	CPL	C33-C32-C31	-2.37	105.01	113.69
2	B	1702	CPL	C3-O3-C11	2.37	125.77	117.12
2	B	1711	CPL	C3-O3-C11	2.36	125.76	117.12
2	A	3094	CPL	C33-C32-C31	-2.36	105.04	113.69
3	A	1696	GDP	PA-O5'-C5'	-2.36	107.84	121.35
3	B	1706	GDP	PA-O5'-C5'	-2.35	107.90	121.35
2	A	1712	CPL	C33-C32-C31	-2.35	105.09	113.69
2	A	1718	CPL	C3-O3-C11	2.34	125.66	117.12
3	B	1706	GDP	C2-N1-C6	-2.34	120.88	125.11
2	A	1715	CPL	C3-O3-C11	2.31	125.58	117.12
2	B	1708	CPL	C33-C32-C31	-2.31	105.22	113.69
2	A	1699	CPL	C2-O2-C31	2.29	123.27	117.80
3	A	1696	GDP	C2-N1-C6	-2.28	120.98	125.11
2	A	1698	CPL	O2-C31-C32	2.21	116.27	111.48
3	A	1696	GDP	C5'-C4'-C3'	-2.19	107.34	115.21
3	B	1706	GDP	C5'-C4'-C3'	-2.19	107.35	115.21
2	A	3097	CPL	O2-C31-C32	2.17	116.19	111.48
3	B	1706	GDP	C4-C5-N7	-2.12	107.30	110.67
2	A	3077	CPL	O2-C31-C32	2.11	116.05	111.48
3	A	1696	GDP	C4-C5-N7	-2.09	107.36	110.67
3	A	1696	GDP	O6-C6-C5	-2.09	121.03	126.53
3	B	1706	GDP	O6-C6-C5	-2.07	121.06	126.53
2	B	1705	CPL	O2-C31-C32	2.07	115.95	111.48
3	A	1696	GDP	C3'-C2'-C1'	2.06	105.36	101.46
3	B	1706	GDP	C3'-C2'-C1'	2.05	105.35	101.46
2	A	1707	CPL	O2-C31-C32	2.01	115.83	111.48

There are no chirality outliers.

All (561) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3077	CPL	C12-C11-O3-C3
2	A	3077	CPL	O11-C11-O3-C3
2	A	3077	CPL	C1-O3P-P-O1P
2	A	3077	CPL	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
2	A	3077	CPL	C1-O3P-P-O4P
2	A	3077	CPL	C4-O4P-P-O1P
2	A	1697	CPL	C12-C11-O3-C3
2	A	1697	CPL	O11-C11-O3-C3
2	A	1697	CPL	C1-O3P-P-O1P
2	A	1697	CPL	C1-O3P-P-O2P
2	A	1697	CPL	C1-O3P-P-O4P
2	A	1697	CPL	C4-O4P-P-O1P
2	A	1698	CPL	C12-C11-O3-C3
2	A	1698	CPL	O11-C11-O3-C3
2	A	1698	CPL	C1-O3P-P-O1P
2	A	1698	CPL	C1-O3P-P-O2P
2	A	1698	CPL	C1-O3P-P-O4P
2	A	1698	CPL	C4-O4P-P-O1P
2	A	1698	CPL	C4-O4P-P-O3P
2	A	1699	CPL	C12-C11-O3-C3
2	A	1699	CPL	O11-C11-O3-C3
2	A	1699	CPL	C1-O3P-P-O1P
2	A	1699	CPL	C1-O3P-P-O2P
2	A	1700	CPL	C12-C11-O3-C3
2	A	1700	CPL	O11-C11-O3-C3
2	A	1700	CPL	C1-O3P-P-O1P
2	A	1700	CPL	C1-O3P-P-O2P
2	A	1700	CPL	C4-O4P-P-O3P
2	A	1701	CPL	C12-C11-O3-C3
2	A	1701	CPL	O11-C11-O3-C3
2	A	1701	CPL	C40-C41-C42-C43
2	A	1701	CPL	C1-O3P-P-O1P
2	A	1701	CPL	C1-O3P-P-O2P
2	A	1701	CPL	C1-O3P-P-O4P
2	A	1701	CPL	C4-O4P-P-O1P
2	A	1702	CPL	C12-C11-O3-C3
2	A	1702	CPL	O11-C11-O3-C3
2	A	1702	CPL	C1-O3P-P-O1P
2	A	1702	CPL	C1-O3P-P-O2P
2	A	1702	CPL	C4-O4P-P-O1P
2	A	1703	CPL	C12-C11-O3-C3
2	A	1703	CPL	O11-C11-O3-C3
2	A	1703	CPL	C1-O3P-P-O1P
2	A	1703	CPL	C1-O3P-P-O2P
2	A	1703	CPL	C4-O4P-P-O1P
2	A	1704	CPL	C12-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
2	A	1704	CPL	O11-C11-O3-C3
2	A	1704	CPL	C40-C41-C42-C43
2	A	1704	CPL	C1-O3P-P-O1P
2	A	1704	CPL	C1-O3P-P-O2P
2	A	1704	CPL	C1-O3P-P-O4P
2	A	1704	CPL	C4-O4P-P-O1P
2	A	1705	CPL	C12-C11-O3-C3
2	A	1705	CPL	O11-C11-O3-C3
2	A	1705	CPL	C40-C41-C42-C43
2	A	1705	CPL	C1-O3P-P-O1P
2	A	1705	CPL	C1-O3P-P-O2P
2	A	1705	CPL	C1-O3P-P-O4P
2	A	1705	CPL	C4-O4P-P-O1P
2	A	1706	CPL	C12-C11-O3-C3
2	A	1706	CPL	O11-C11-O3-C3
2	A	1706	CPL	C1-O3P-P-O1P
2	A	1706	CPL	C1-O3P-P-O2P
2	A	1706	CPL	C4-O4P-P-O3P
2	A	1707	CPL	C12-C11-O3-C3
2	A	1707	CPL	O11-C11-O3-C3
2	A	1707	CPL	C1-O3P-P-O1P
2	A	1707	CPL	C1-O3P-P-O2P
2	A	1707	CPL	C1-O3P-P-O4P
2	A	1707	CPL	C4-O4P-P-O1P
2	A	1708	CPL	C12-C11-O3-C3
2	A	1708	CPL	O11-C11-O3-C3
2	A	1708	CPL	C1-O3P-P-O1P
2	A	1708	CPL	C1-O3P-P-O2P
2	A	1708	CPL	C4-O4P-P-O1P
2	A	1709	CPL	C12-C11-O3-C3
2	A	1709	CPL	O11-C11-O3-C3
2	A	1709	CPL	C1-O3P-P-O1P
2	A	1709	CPL	C1-O3P-P-O2P
2	A	1709	CPL	C1-O3P-P-O4P
2	A	1709	CPL	C4-O4P-P-O1P
2	A	1710	CPL	C12-C11-O3-C3
2	A	1710	CPL	O11-C11-O3-C3
2	A	1710	CPL	C1-O3P-P-O1P
2	A	1710	CPL	C1-O3P-P-O2P
2	A	1710	CPL	C4-O4P-P-O1P
2	A	1711	CPL	C12-C11-O3-C3
2	A	1711	CPL	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
2	A	1711	CPL	C1-O3P-P-O1P
2	A	1711	CPL	C1-O3P-P-O2P
2	A	1711	CPL	C1-O3P-P-O4P
2	A	1711	CPL	C4-O4P-P-O1P
2	A	1712	CPL	C12-C11-O3-C3
2	A	1712	CPL	O11-C11-O3-C3
2	A	1712	CPL	C40-C41-C42-C43
2	A	1712	CPL	C1-O3P-P-O1P
2	A	1712	CPL	C1-O3P-P-O2P
2	A	1712	CPL	C1-O3P-P-O4P
2	A	1712	CPL	C4-O4P-P-O3P
2	A	1713	CPL	C12-C11-O3-C3
2	A	1713	CPL	O11-C11-O3-C3
2	A	1713	CPL	C1-O3P-P-O1P
2	A	1713	CPL	C1-O3P-P-O2P
2	A	1713	CPL	C4-O4P-P-O3P
2	A	1714	CPL	C12-C11-O3-C3
2	A	1714	CPL	O11-C11-O3-C3
2	A	1714	CPL	C1-O3P-P-O1P
2	A	1714	CPL	C1-O3P-P-O2P
2	A	1714	CPL	C1-O3P-P-O4P
2	A	1714	CPL	C4-O4P-P-O1P
2	A	1715	CPL	C12-C11-O3-C3
2	A	1715	CPL	O11-C11-O3-C3
2	A	1715	CPL	C1-O3P-P-O1P
2	A	1715	CPL	C1-O3P-P-O2P
2	A	1715	CPL	C1-O3P-P-O4P
2	A	1715	CPL	C4-O4P-P-O1P
2	A	1716	CPL	C12-C11-O3-C3
2	A	1716	CPL	O11-C11-O3-C3
2	A	1716	CPL	C1-O3P-P-O1P
2	A	1716	CPL	C1-O3P-P-O2P
2	A	1716	CPL	C1-O3P-P-O4P
2	A	1716	CPL	C4-O4P-P-O1P
2	A	1717	CPL	C12-C11-O3-C3
2	A	1717	CPL	O11-C11-O3-C3
2	A	1717	CPL	C1-O3P-P-O1P
2	A	1717	CPL	C1-O3P-P-O2P
2	A	1717	CPL	C4-O4P-P-O1P
2	A	1718	CPL	C12-C11-O3-C3
2	A	1718	CPL	O11-C11-O3-C3
2	A	1718	CPL	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
2	A	1718	CPL	C1-O3P-P-O2P
2	A	1718	CPL	C1-O3P-P-O4P
2	A	1718	CPL	C4-O4P-P-O1P
2	A	3094	CPL	C12-C11-O3-C3
2	A	3094	CPL	O11-C11-O3-C3
2	A	3094	CPL	C1-O3P-P-O1P
2	A	3094	CPL	C1-O3P-P-O2P
2	A	3094	CPL	C4-O4P-P-O3P
2	A	3097	CPL	C12-C11-O3-C3
2	A	3097	CPL	O11-C11-O3-C3
2	A	3097	CPL	C1-O3P-P-O1P
2	A	3097	CPL	C1-O3P-P-O2P
2	A	3097	CPL	C1-O3P-P-O4P
2	A	3097	CPL	C4-O4P-P-O1P
2	A	3181	CPL	C12-C11-O3-C3
2	A	3181	CPL	O11-C11-O3-C3
2	A	3181	CPL	C1-O3P-P-O1P
2	A	3181	CPL	C1-O3P-P-O2P
2	A	3181	CPL	C1-O3P-P-O4P
2	A	3181	CPL	C4-O4P-P-O1P
2	B	1696	CPL	C12-C11-O3-C3
2	B	1696	CPL	O11-C11-O3-C3
2	B	1696	CPL	C1-O3P-P-O1P
2	B	1696	CPL	C1-O3P-P-O2P
2	B	1696	CPL	C4-O4P-P-O1P
2	B	1697	CPL	C12-C11-O3-C3
2	B	1697	CPL	O11-C11-O3-C3
2	B	1697	CPL	C1-O3P-P-O1P
2	B	1697	CPL	C1-O3P-P-O2P
2	B	1697	CPL	C4-O4P-P-O3P
2	B	1698	CPL	C12-C11-O3-C3
2	B	1698	CPL	O11-C11-O3-C3
2	B	1698	CPL	C1-O3P-P-O1P
2	B	1698	CPL	C1-O3P-P-O2P
2	B	1698	CPL	C4-O4P-P-O1P
2	B	1699	CPL	C12-C11-O3-C3
2	B	1699	CPL	O11-C11-O3-C3
2	B	1699	CPL	C1-O3P-P-O1P
2	B	1699	CPL	C1-O3P-P-O2P
2	B	1699	CPL	C4-O4P-P-O3P
2	B	1700	CPL	C12-C11-O3-C3
2	B	1700	CPL	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
2	B	1700	CPL	C1-O3P-P-O1P
2	B	1700	CPL	C1-O3P-P-O2P
2	B	1700	CPL	C4-O4P-P-O3P
2	B	1701	CPL	C12-C11-O3-C3
2	B	1701	CPL	O11-C11-O3-C3
2	B	1701	CPL	C1-O3P-P-O1P
2	B	1701	CPL	C1-O3P-P-O2P
2	B	1701	CPL	C4-O4P-P-O1P
2	B	1702	CPL	C12-C11-O3-C3
2	B	1702	CPL	O11-C11-O3-C3
2	B	1702	CPL	C1-O3P-P-O1P
2	B	1702	CPL	C1-O3P-P-O2P
2	B	1702	CPL	C1-O3P-P-O4P
2	B	1702	CPL	C4-O4P-P-O1P
2	B	1703	CPL	C12-C11-O3-C3
2	B	1703	CPL	O11-C11-O3-C3
2	B	1703	CPL	C40-C41-C42-C43
2	B	1703	CPL	C1-O3P-P-O1P
2	B	1703	CPL	C1-O3P-P-O2P
2	B	1703	CPL	C1-O3P-P-O4P
2	B	1703	CPL	C4-O4P-P-O1P
2	B	1704	CPL	C12-C11-O3-C3
2	B	1704	CPL	O11-C11-O3-C3
2	B	1704	CPL	C1-O3P-P-O1P
2	B	1704	CPL	C1-O3P-P-O2P
2	B	1704	CPL	C4-O4P-P-O3P
2	B	1705	CPL	C12-C11-O3-C3
2	B	1705	CPL	O11-C11-O3-C3
2	B	1705	CPL	C1-O3P-P-O1P
2	B	1705	CPL	C1-O3P-P-O2P
2	B	1705	CPL	C1-O3P-P-O4P
2	B	1705	CPL	C4-O4P-P-O1P
2	B	1707	CPL	C12-C11-O3-C3
2	B	1707	CPL	O11-C11-O3-C3
2	B	1707	CPL	C40-C41-C42-C43
2	B	1707	CPL	C1-O3P-P-O1P
2	B	1707	CPL	C1-O3P-P-O2P
2	B	1707	CPL	C1-O3P-P-O4P
2	B	1707	CPL	C4-O4P-P-O1P
2	B	1708	CPL	C12-C11-O3-C3
2	B	1708	CPL	O11-C11-O3-C3
2	B	1708	CPL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
2	B	1708	CPL	C1-O3P-P-O1P
2	B	1708	CPL	C1-O3P-P-O2P
2	B	1708	CPL	C1-O3P-P-O4P
2	B	1708	CPL	C4-O4P-P-O3P
2	B	1709	CPL	C12-C11-O3-C3
2	B	1709	CPL	O11-C11-O3-C3
2	B	1709	CPL	C1-O3P-P-O1P
2	B	1709	CPL	C1-O3P-P-O2P
2	B	1709	CPL	C1-O3P-P-O4P
2	B	1709	CPL	C4-O4P-P-O1P
2	B	1710	CPL	C12-C11-O3-C3
2	B	1710	CPL	O11-C11-O3-C3
2	B	1710	CPL	C1-O3P-P-O1P
2	B	1710	CPL	C1-O3P-P-O2P
2	B	1710	CPL	C4-O4P-P-O1P
2	B	1711	CPL	C12-C11-O3-C3
2	B	1711	CPL	O11-C11-O3-C3
2	B	1711	CPL	C1-O3P-P-O1P
2	B	1711	CPL	C1-O3P-P-O2P
2	B	1711	CPL	C1-O3P-P-O4P
2	B	1711	CPL	C4-O4P-P-O1P
2	B	1712	CPL	C12-C11-O3-C3
2	B	1712	CPL	O11-C11-O3-C3
2	B	1712	CPL	C1-O3P-P-O1P
2	B	1712	CPL	C1-O3P-P-O2P
2	B	1712	CPL	C4-O4P-P-O1P
2	B	1713	CPL	C12-C11-O3-C3
2	B	1713	CPL	O11-C11-O3-C3
2	B	1713	CPL	C1-O3P-P-O1P
2	B	1713	CPL	C1-O3P-P-O2P
2	B	1713	CPL	C4-O4P-P-O3P
2	B	1714	CPL	C12-C11-O3-C3
2	B	1714	CPL	O11-C11-O3-C3
2	B	1714	CPL	C1-O3P-P-O1P
2	B	1714	CPL	C1-O3P-P-O2P
2	B	1714	CPL	C1-O3P-P-O4P
2	B	1714	CPL	C4-O4P-P-O1P
2	A	3077	CPL	C44-C45-C46-C47
2	A	1716	CPL	C44-C45-C46-C47
2	A	3181	CPL	C44-C45-C46-C47
2	A	1709	CPL	C44-C45-C46-C47
2	B	1709	CPL	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
2	A	3077	CPL	C39-C40-C41-C42
2	A	3077	CPL	C40-C41-C42-C43
2	A	1697	CPL	C39-C40-C41-C42
2	A	1697	CPL	C40-C41-C42-C43
2	A	1698	CPL	C39-C40-C41-C42
2	A	1699	CPL	C39-C40-C41-C42
2	A	1699	CPL	C40-C41-C42-C43
2	A	1700	CPL	C40-C41-C42-C43
2	A	1701	CPL	C39-C40-C41-C42
2	A	1702	CPL	C39-C40-C41-C42
2	A	1702	CPL	C40-C41-C42-C43
2	A	1703	CPL	C39-C40-C41-C42
2	A	1703	CPL	C40-C41-C42-C43
2	A	1704	CPL	C39-C40-C41-C42
2	A	1705	CPL	C39-C40-C41-C42
2	A	1706	CPL	C40-C41-C42-C43
2	A	1707	CPL	C39-C40-C41-C42
2	A	1708	CPL	C39-C40-C41-C42
2	A	1708	CPL	C40-C41-C42-C43
2	A	1709	CPL	C39-C40-C41-C42
2	A	1709	CPL	C40-C41-C42-C43
2	A	1710	CPL	C39-C40-C41-C42
2	A	1710	CPL	C40-C41-C42-C43
2	A	1711	CPL	C39-C40-C41-C42
2	A	1711	CPL	C40-C41-C42-C43
2	A	1713	CPL	C40-C41-C42-C43
2	A	1714	CPL	C39-C40-C41-C42
2	A	1715	CPL	C39-C40-C41-C42
2	A	1715	CPL	C40-C41-C42-C43
2	A	1716	CPL	C39-C40-C41-C42
2	A	1716	CPL	C40-C41-C42-C43
2	A	1717	CPL	C39-C40-C41-C42
2	A	1717	CPL	C40-C41-C42-C43
2	A	1718	CPL	C39-C40-C41-C42
2	A	1718	CPL	C40-C41-C42-C43
2	A	3094	CPL	C40-C41-C42-C43
2	A	3097	CPL	C39-C40-C41-C42
2	A	3097	CPL	C40-C41-C42-C43
2	A	3181	CPL	C39-C40-C41-C42
2	A	3181	CPL	C40-C41-C42-C43
2	B	1696	CPL	C39-C40-C41-C42
2	B	1696	CPL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
2	B	1697	CPL	C40-C41-C42-C43
2	B	1698	CPL	C39-C40-C41-C42
2	B	1698	CPL	C40-C41-C42-C43
2	B	1699	CPL	C40-C41-C42-C43
2	B	1700	CPL	C40-C41-C42-C43
2	B	1701	CPL	C39-C40-C41-C42
2	B	1701	CPL	C40-C41-C42-C43
2	B	1702	CPL	C39-C40-C41-C42
2	B	1702	CPL	C40-C41-C42-C43
2	B	1703	CPL	C39-C40-C41-C42
2	B	1704	CPL	C40-C41-C42-C43
2	B	1705	CPL	C39-C40-C41-C42
2	B	1707	CPL	C39-C40-C41-C42
2	B	1709	CPL	C39-C40-C41-C42
2	B	1709	CPL	C40-C41-C42-C43
2	B	1710	CPL	C39-C40-C41-C42
2	B	1710	CPL	C40-C41-C42-C43
2	B	1711	CPL	C39-C40-C41-C42
2	B	1711	CPL	C40-C41-C42-C43
2	B	1712	CPL	C39-C40-C41-C42
2	B	1712	CPL	C40-C41-C42-C43
2	B	1713	CPL	C40-C41-C42-C43
2	B	1714	CPL	C39-C40-C41-C42
2	B	1714	CPL	C40-C41-C42-C43
2	A	1707	CPL	C36-C37-C38-C39
2	A	1714	CPL	C36-C37-C38-C39
2	B	1705	CPL	C36-C37-C38-C39
2	A	3077	CPL	O4P-C4-C5-N
2	A	1697	CPL	O4P-C4-C5-N
2	A	1698	CPL	O4P-C4-C5-N
2	A	1699	CPL	O4P-C4-C5-N
2	A	1700	CPL	O4P-C4-C5-N
2	A	1701	CPL	O4P-C4-C5-N
2	A	1702	CPL	O4P-C4-C5-N
2	A	1703	CPL	O4P-C4-C5-N
2	A	1704	CPL	O4P-C4-C5-N
2	A	1705	CPL	O4P-C4-C5-N
2	A	1706	CPL	O4P-C4-C5-N
2	A	1707	CPL	O4P-C4-C5-N
2	A	1708	CPL	O4P-C4-C5-N
2	A	1709	CPL	O4P-C4-C5-N
2	A	1710	CPL	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
2	A	1711	CPL	O4P-C4-C5-N
2	A	1712	CPL	O4P-C4-C5-N
2	A	1713	CPL	O4P-C4-C5-N
2	A	1714	CPL	O4P-C4-C5-N
2	A	1715	CPL	O4P-C4-C5-N
2	A	1716	CPL	O4P-C4-C5-N
2	A	1717	CPL	O4P-C4-C5-N
2	A	1718	CPL	O4P-C4-C5-N
2	A	3094	CPL	O4P-C4-C5-N
2	A	3097	CPL	O4P-C4-C5-N
2	A	3181	CPL	O4P-C4-C5-N
2	B	1696	CPL	O4P-C4-C5-N
2	B	1697	CPL	O4P-C4-C5-N
2	B	1698	CPL	O4P-C4-C5-N
2	B	1699	CPL	O4P-C4-C5-N
2	B	1700	CPL	O4P-C4-C5-N
2	B	1701	CPL	O4P-C4-C5-N
2	B	1702	CPL	O4P-C4-C5-N
2	B	1703	CPL	O4P-C4-C5-N
2	B	1704	CPL	O4P-C4-C5-N
2	B	1705	CPL	O4P-C4-C5-N
2	B	1707	CPL	O4P-C4-C5-N
2	B	1708	CPL	O4P-C4-C5-N
2	B	1709	CPL	O4P-C4-C5-N
2	B	1710	CPL	O4P-C4-C5-N
2	B	1711	CPL	O4P-C4-C5-N
2	B	1712	CPL	O4P-C4-C5-N
2	B	1713	CPL	O4P-C4-C5-N
2	B	1714	CPL	O4P-C4-C5-N
2	A	1699	CPL	C42-C43-C44-C45
2	A	1702	CPL	C37-C38-C39-C40
2	A	1703	CPL	C37-C38-C39-C40
2	A	1708	CPL	C37-C38-C39-C40
2	A	1710	CPL	C37-C38-C39-C40
2	A	1717	CPL	C37-C38-C39-C40
2	A	3097	CPL	C42-C43-C44-C45
2	B	1696	CPL	C37-C38-C39-C40
2	B	1698	CPL	C37-C38-C39-C40
2	B	1701	CPL	C37-C38-C39-C40
2	B	1710	CPL	C37-C38-C39-C40
2	B	1712	CPL	C37-C38-C39-C40
2	A	1698	CPL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
2	A	1699	CPL	C1-O3P-P-O4P
2	A	1699	CPL	C4-O4P-P-O1P
2	A	1700	CPL	C1-O3P-P-O4P
2	A	1700	CPL	C4-O4P-P-O1P
2	A	1702	CPL	C1-O3P-P-O4P
2	A	1703	CPL	C1-O3P-P-O4P
2	A	1706	CPL	C1-O3P-P-O4P
2	A	1706	CPL	C4-O4P-P-O1P
2	A	1707	CPL	C4-O4P-P-O3P
2	A	1708	CPL	C1-O3P-P-O4P
2	A	1710	CPL	C1-O3P-P-O4P
2	A	1711	CPL	C4-O4P-P-O3P
2	A	1712	CPL	C4-O4P-P-O1P
2	A	1713	CPL	C1-O3P-P-O4P
2	A	1713	CPL	C4-O4P-P-O1P
2	A	1714	CPL	C4-O4P-P-O3P
2	A	1715	CPL	C4-O4P-P-O3P
2	A	1717	CPL	C1-O3P-P-O4P
2	A	1718	CPL	C4-O4P-P-O3P
2	A	3094	CPL	C1-O3P-P-O4P
2	A	3094	CPL	C4-O4P-P-O1P
2	B	1696	CPL	C1-O3P-P-O4P
2	B	1697	CPL	C1-O3P-P-O4P
2	B	1697	CPL	C4-O4P-P-O1P
2	B	1698	CPL	C1-O3P-P-O4P
2	B	1699	CPL	C1-O3P-P-O4P
2	B	1699	CPL	C4-O4P-P-O1P
2	B	1700	CPL	C1-O3P-P-O4P
2	B	1700	CPL	C4-O4P-P-O1P
2	B	1701	CPL	C1-O3P-P-O4P
2	B	1702	CPL	C4-O4P-P-O3P
2	B	1704	CPL	C1-O3P-P-O4P
2	B	1704	CPL	C4-O4P-P-O1P
2	B	1705	CPL	C4-O4P-P-O3P
2	B	1708	CPL	C4-O4P-P-O1P
2	B	1710	CPL	C1-O3P-P-O4P
2	B	1711	CPL	C4-O4P-P-O3P
2	B	1712	CPL	C1-O3P-P-O4P
2	B	1713	CPL	C1-O3P-P-O4P
2	B	1713	CPL	C4-O4P-P-O1P
2	B	1714	CPL	C4-O4P-P-O3P
2	A	3077	CPL	C1-C2-O2-C31

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Mol	Chain	Res	Type	Atoms
2	A	3077	CPL	C3-C2-O2-C31
2	A	1701	CPL	C1-C2-O2-C31
2	A	1702	CPL	C1-C2-O2-C31
2	A	1703	CPL	C1-C2-O2-C31
2	A	1704	CPL	C1-C2-O2-C31
2	A	1705	CPL	C1-C2-O2-C31
2	A	1708	CPL	C1-C2-O2-C31
2	A	1709	CPL	C1-C2-O2-C31
2	A	1710	CPL	C1-C2-O2-C31
2	A	1716	CPL	C1-C2-O2-C31
2	A	1717	CPL	C1-C2-O2-C31
2	A	3097	CPL	C1-C2-O2-C31
2	A	3097	CPL	C3-C2-O2-C31
2	A	3181	CPL	C1-C2-O2-C31
2	B	1696	CPL	C1-C2-O2-C31
2	B	1698	CPL	C1-C2-O2-C31
2	B	1701	CPL	C1-C2-O2-C31
2	B	1703	CPL	C1-C2-O2-C31
2	B	1707	CPL	C1-C2-O2-C31
2	B	1709	CPL	C1-C2-O2-C31
2	B	1710	CPL	C1-C2-O2-C31
2	B	1712	CPL	C1-C2-O2-C31
2	B	1697	CPL	C42-C43-C44-C45
2	B	1713	CPL	C42-C43-C44-C45
2	A	1700	CPL	C42-C43-C44-C45
2	A	1706	CPL	C42-C43-C44-C45
2	A	1713	CPL	C42-C43-C44-C45
2	A	3094	CPL	C42-C43-C44-C45
2	B	1699	CPL	C42-C43-C44-C45
2	B	1700	CPL	C42-C43-C44-C45
2	B	1704	CPL	C42-C43-C44-C45
2	B	1709	CPL	C42-C43-C44-C45
2	A	1698	CPL	C36-C37-C38-C39
2	A	1709	CPL	C42-C43-C44-C45
2	A	1712	CPL	C42-C43-C44-C45
2	A	1716	CPL	C42-C43-C44-C45
2	A	3181	CPL	C42-C43-C44-C45
2	B	1708	CPL	C42-C43-C44-C45
2	A	1707	CPL	C42-C43-C44-C45
2	A	1711	CPL	C42-C43-C44-C45
2	A	1714	CPL	C42-C43-C44-C45
2	A	1715	CPL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
2	B	1702	CPL	C42-C43-C44-C45
2	B	1705	CPL	C42-C43-C44-C45
2	A	1697	CPL	C42-C43-C44-C45
2	A	1699	CPL	C37-C38-C39-C40
2	A	1718	CPL	C42-C43-C44-C45
2	B	1711	CPL	C42-C43-C44-C45
2	B	1714	CPL	C42-C43-C44-C45
2	A	1702	CPL	C42-C43-C44-C45
2	A	1703	CPL	C42-C43-C44-C45
2	A	1708	CPL	C42-C43-C44-C45
2	A	1710	CPL	C42-C43-C44-C45
2	A	1717	CPL	C42-C43-C44-C45
2	B	1696	CPL	C42-C43-C44-C45
2	B	1698	CPL	C42-C43-C44-C45
2	B	1701	CPL	C42-C43-C44-C45
2	B	1710	CPL	C42-C43-C44-C45
2	B	1712	CPL	C42-C43-C44-C45
2	A	1712	CPL	C37-C38-C39-C40
2	B	1708	CPL	C37-C38-C39-C40
2	A	1698	CPL	C40-C41-C42-C43
2	A	1700	CPL	C37-C38-C39-C40
2	A	1706	CPL	C37-C38-C39-C40
2	A	1713	CPL	C37-C38-C39-C40
2	A	3094	CPL	C37-C38-C39-C40
2	B	1697	CPL	C37-C38-C39-C40
2	B	1699	CPL	C37-C38-C39-C40
2	B	1700	CPL	C37-C38-C39-C40
2	B	1704	CPL	C37-C38-C39-C40
2	B	1713	CPL	C37-C38-C39-C40
2	A	3077	CPL	C42-C43-C44-C45
2	A	1702	CPL	C3-C2-O2-C31
2	A	1703	CPL	C3-C2-O2-C31
2	A	1708	CPL	C3-C2-O2-C31
2	A	1710	CPL	C3-C2-O2-C31
2	A	1717	CPL	C3-C2-O2-C31
2	B	1696	CPL	C3-C2-O2-C31
2	B	1698	CPL	C3-C2-O2-C31
2	B	1701	CPL	C3-C2-O2-C31
2	B	1710	CPL	C3-C2-O2-C31
2	B	1712	CPL	C3-C2-O2-C31
2	A	1701	CPL	C42-C43-C44-C45
2	A	1705	CPL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
2	B	1707	CPL	C42-C43-C44-C45
2	A	1706	CPL	C13-C14-C15-C16
2	B	1699	CPL	C13-C14-C15-C16
2	A	1700	CPL	C13-C14-C15-C16
2	B	1697	CPL	C13-C14-C15-C16
2	B	1704	CPL	C13-C14-C15-C16
2	B	1700	CPL	C13-C14-C15-C16
2	B	1713	CPL	C13-C14-C15-C16
2	A	1713	CPL	C13-C14-C15-C16
2	B	1708	CPL	C13-C14-C15-C16
2	A	1704	CPL	C42-C43-C44-C45
2	B	1703	CPL	C42-C43-C44-C45
2	A	3094	CPL	C13-C14-C15-C16
2	A	1712	CPL	C13-C14-C15-C16
2	A	1700	CPL	C3-C2-O2-C31
2	A	1706	CPL	C3-C2-O2-C31
2	A	1712	CPL	C3-C2-O2-C31
2	A	1713	CPL	C3-C2-O2-C31
2	A	3094	CPL	C3-C2-O2-C31
2	B	1697	CPL	C3-C2-O2-C31
2	B	1699	CPL	C3-C2-O2-C31
2	B	1700	CPL	C3-C2-O2-C31
2	B	1704	CPL	C3-C2-O2-C31
2	B	1708	CPL	C3-C2-O2-C31
2	B	1713	CPL	C3-C2-O2-C31
2	A	1703	CPL	O2-C31-C32-C33
2	A	1712	CPL	O2-C31-C32-C33
2	B	1708	CPL	O2-C31-C32-C33
2	A	1700	CPL	O2-C31-C32-C33
2	A	1702	CPL	O2-C31-C32-C33
2	A	1706	CPL	O2-C31-C32-C33
2	A	1708	CPL	O2-C31-C32-C33
2	A	3094	CPL	O2-C31-C32-C33
2	B	1697	CPL	O2-C31-C32-C33
2	B	1699	CPL	O2-C31-C32-C33
2	B	1700	CPL	O2-C31-C32-C33
2	B	1704	CPL	O2-C31-C32-C33
2	B	1713	CPL	O2-C31-C32-C33
2	A	1713	CPL	O2-C31-C32-C33
2	B	1698	CPL	O2-C31-C32-C33
2	B	1696	CPL	O2-C31-C32-C33
2	B	1712	CPL	O2-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
2	B	1710	CPL	O2-C31-C32-C33
2	A	1712	CPL	O31-C31-C32-C33
2	B	1708	CPL	O31-C31-C32-C33
2	A	1710	CPL	O2-C31-C32-C33
2	A	1717	CPL	O2-C31-C32-C33
2	B	1701	CPL	O2-C31-C32-C33
2	A	1700	CPL	O31-C31-C32-C33
2	A	1706	CPL	O31-C31-C32-C33
2	A	3094	CPL	O31-C31-C32-C33
2	B	1697	CPL	O31-C31-C32-C33
2	B	1700	CPL	O31-C31-C32-C33

There are no ring outliers.

45 monomers are involved in 838 short contacts:

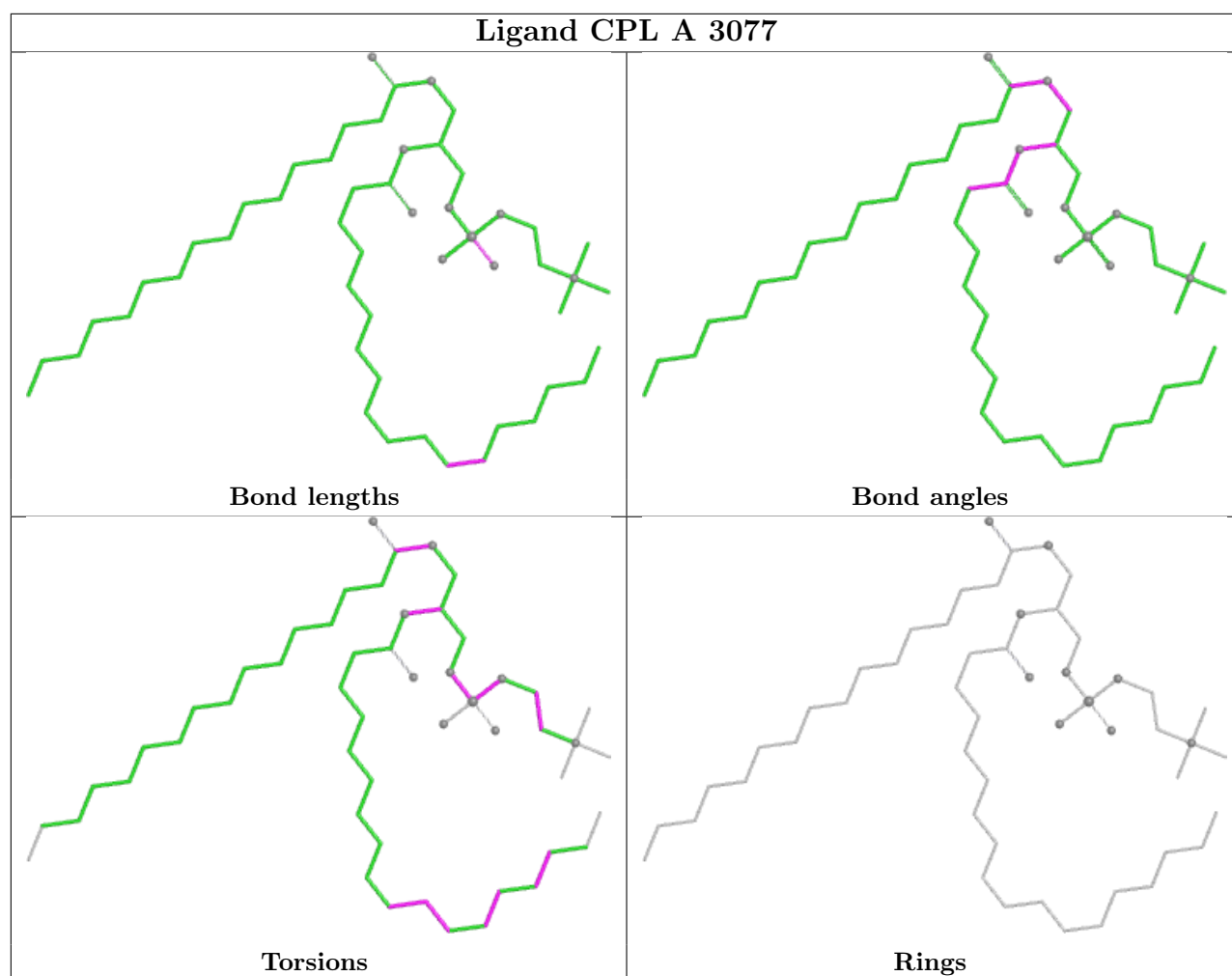
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3077	CPL	6	0
2	A	1707	CPL	48	0
2	B	1711	CPL	9	0
2	B	1712	CPL	18	0
2	A	1715	CPL	14	0
2	A	1718	CPL	24	0
2	A	3097	CPL	24	0
2	B	1699	CPL	18	0
2	A	1703	CPL	32	0
2	B	1701	CPL	36	0
2	B	1708	CPL	2	0
3	B	1706	GDP	11	0
2	A	1701	CPL	53	0
2	A	1709	CPL	53	0
2	A	3181	CPL	7	0
2	A	1698	CPL	15	0
2	B	1700	CPL	33	0
2	B	1698	CPL	7	0
2	B	1703	CPL	74	0
2	B	1707	CPL	7	0
2	A	1706	CPL	6	0
2	A	1697	CPL	37	0
2	B	1709	CPL	6	0
2	B	1702	CPL	7	0
2	A	1702	CPL	27	0
2	A	1716	CPL	7	0

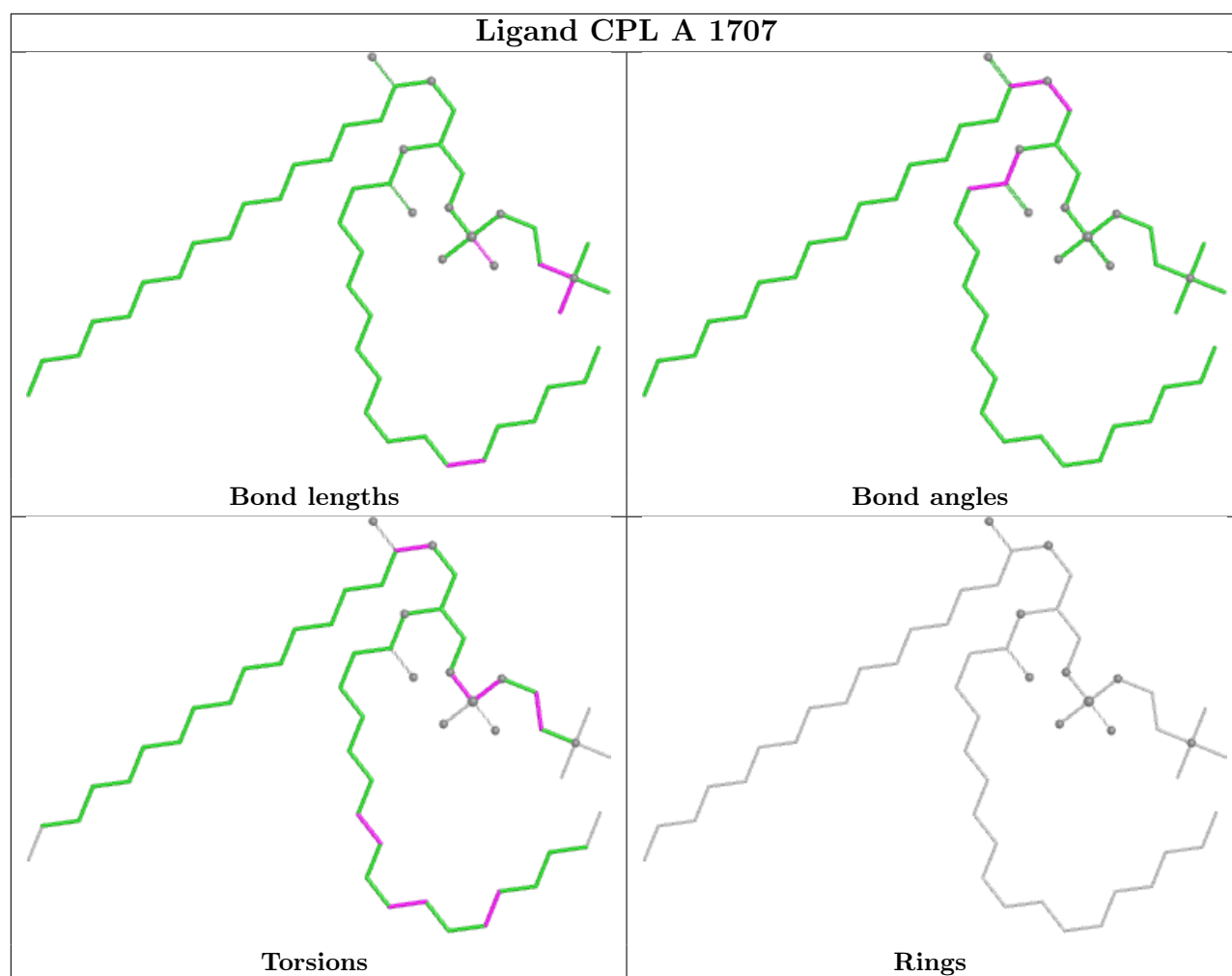
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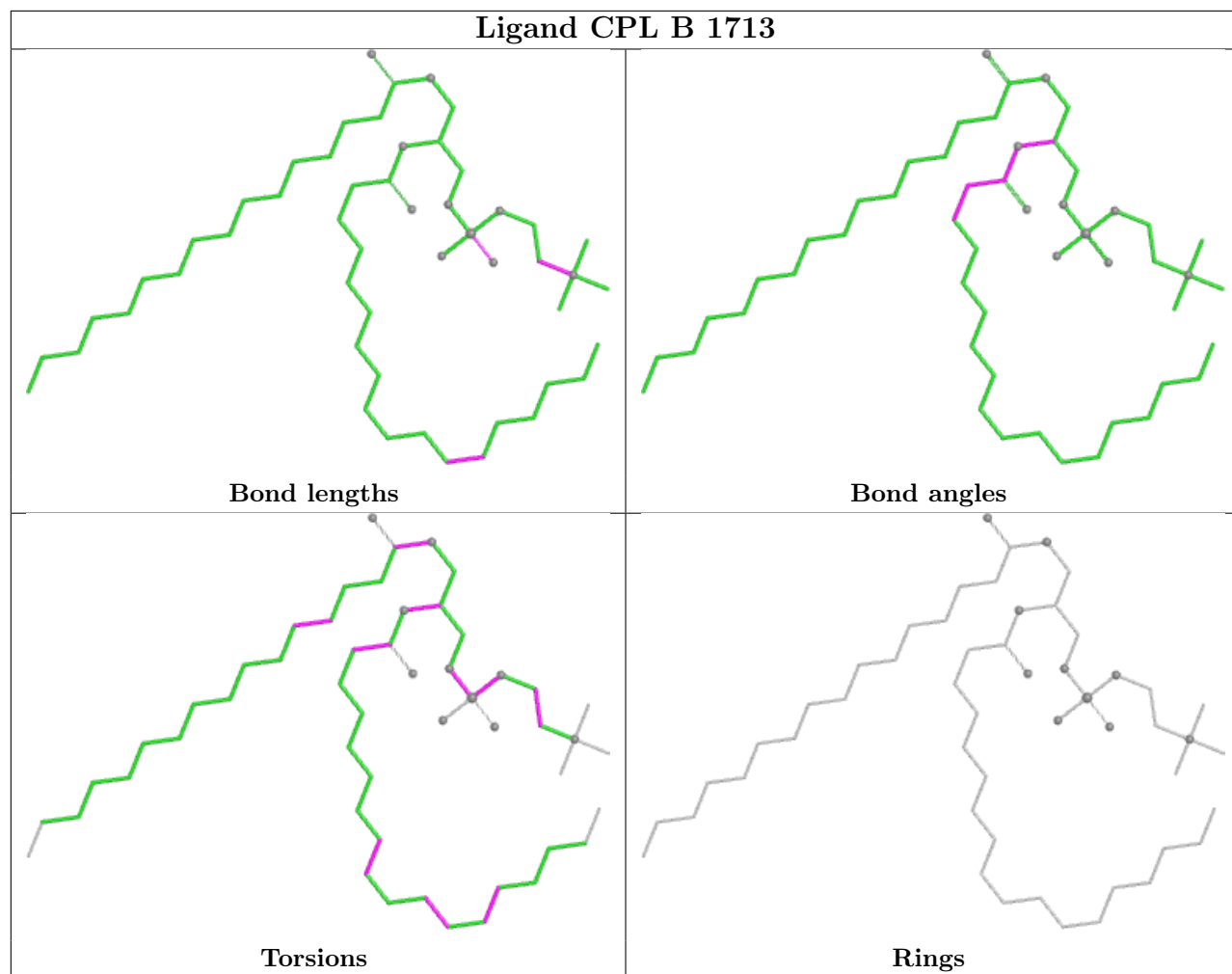
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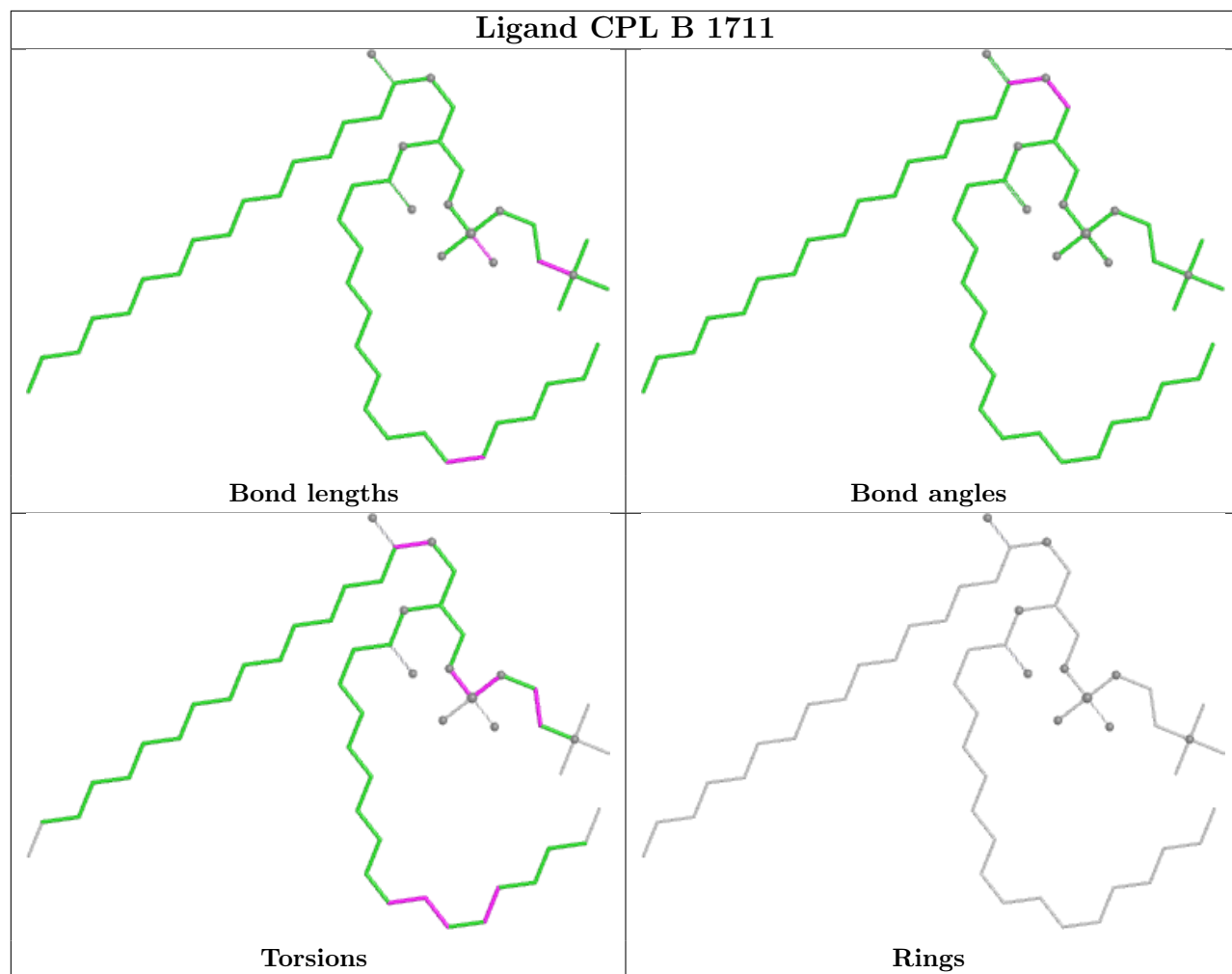
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1711	CPL	10	0
2	A	1712	CPL	4	0
2	A	1704	CPL	17	0
2	B	1697	CPL	84	0
2	A	1705	CPL	53	0
2	A	1699	CPL	14	0
2	A	1710	CPL	21	0
2	A	1708	CPL	60	0
2	A	1700	CPL	41	0
2	B	1705	CPL	42	0
2	B	1714	CPL	16	0
2	A	1713	CPL	4	0
2	A	1714	CPL	14	0
2	B	1704	CPL	27	0
2	B	1696	CPL	26	0
2	B	1710	CPL	26	0
3	A	1696	GDP	10	0
2	A	3094	CPL	7	0
2	A	1717	CPL	4	0

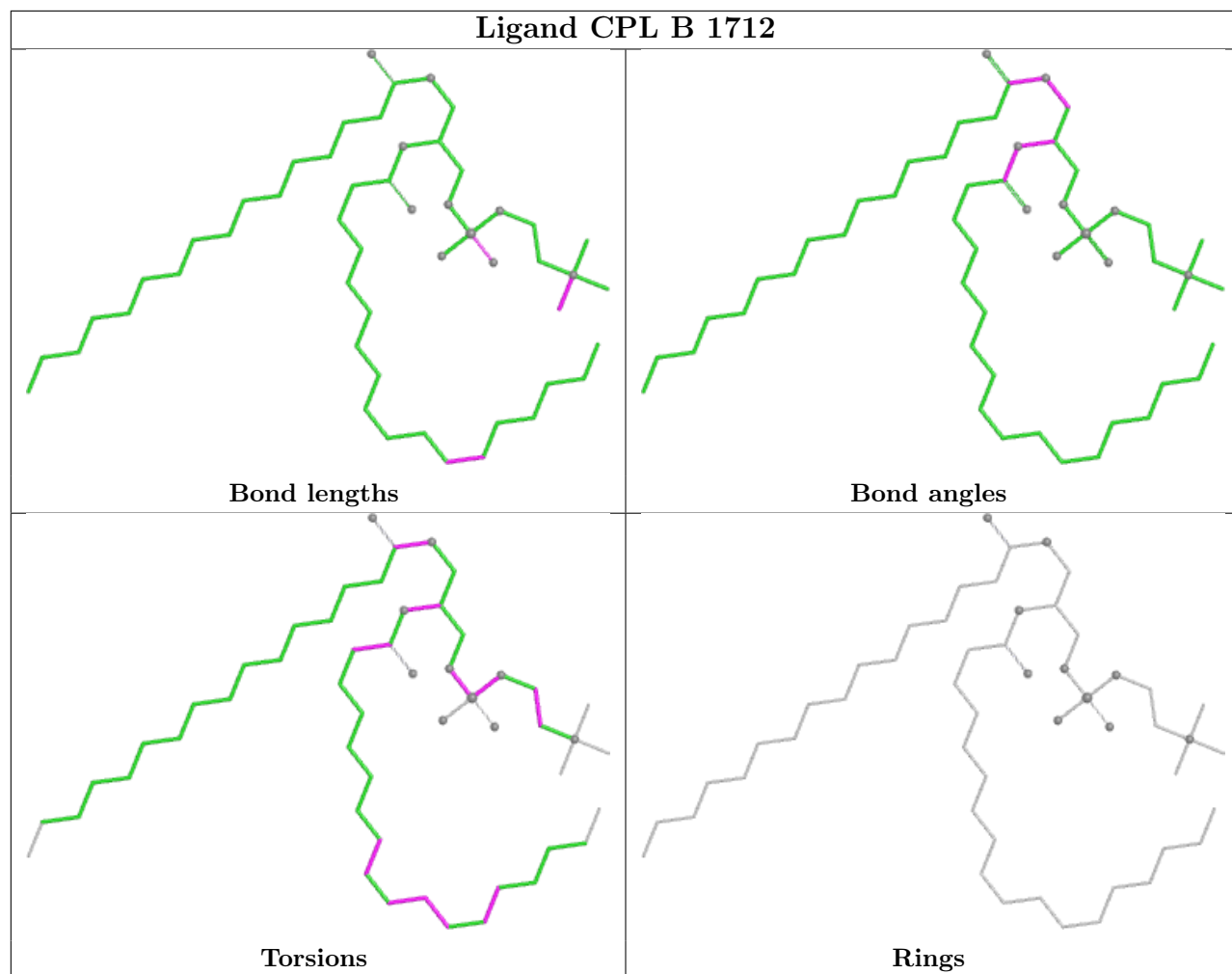
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

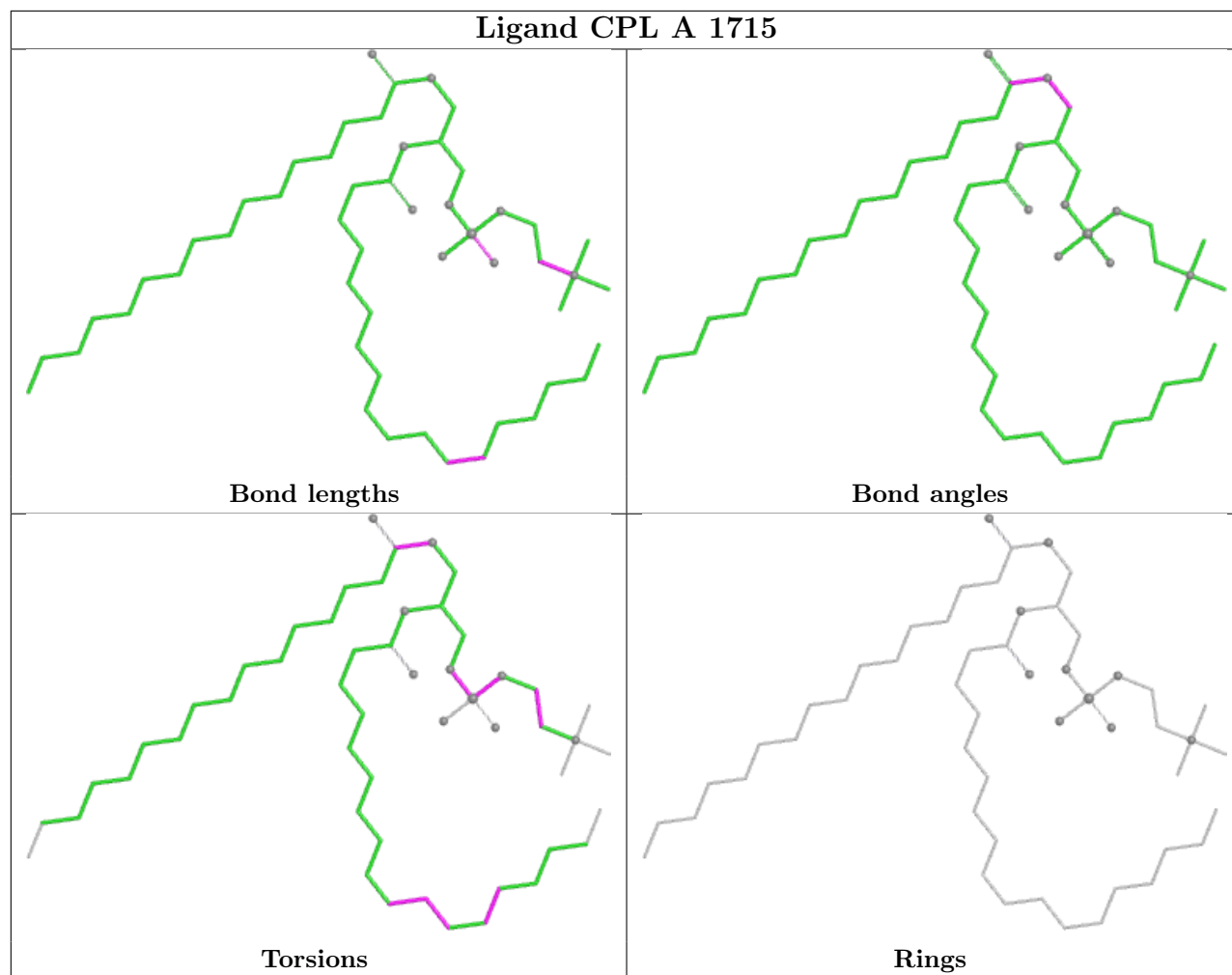


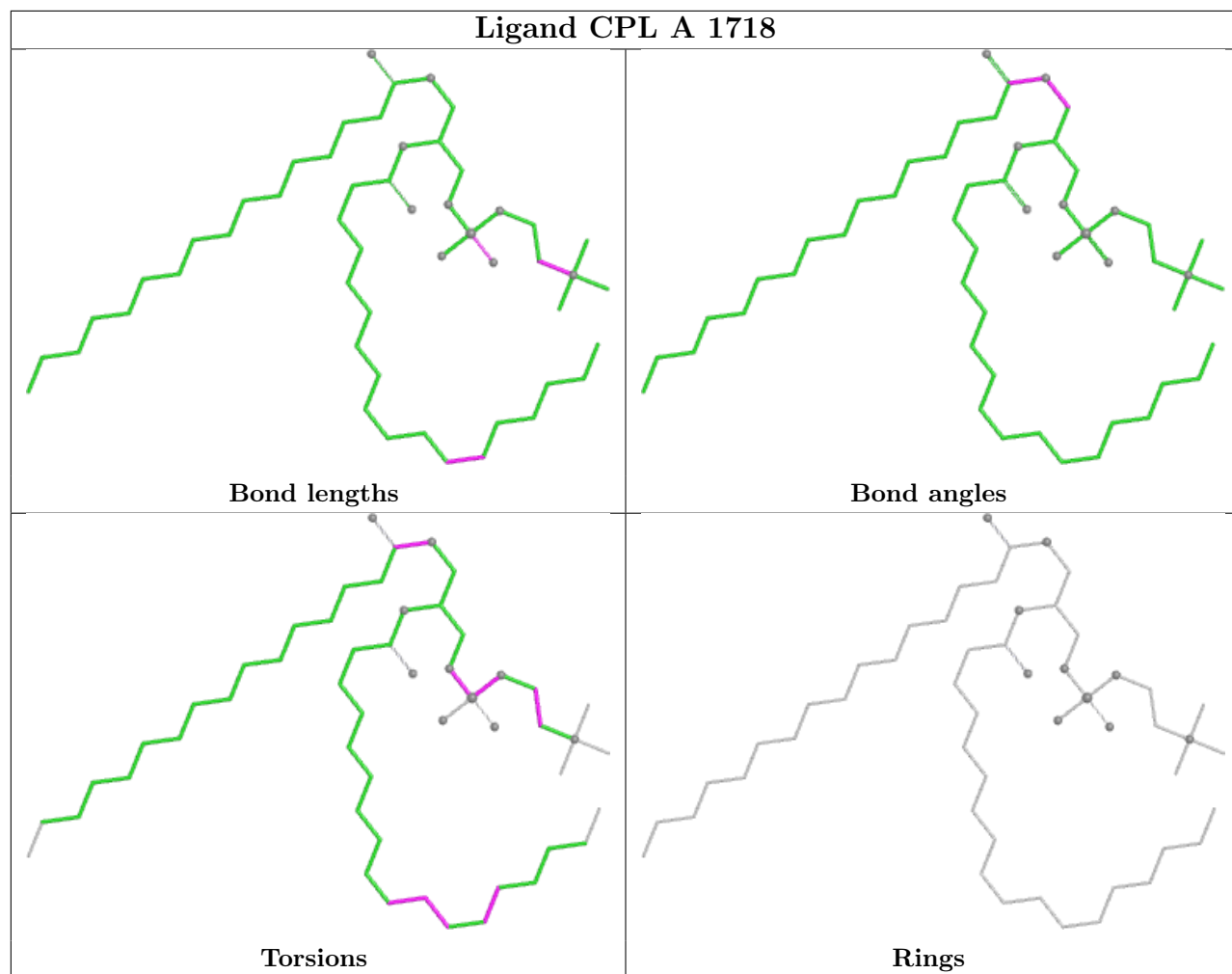


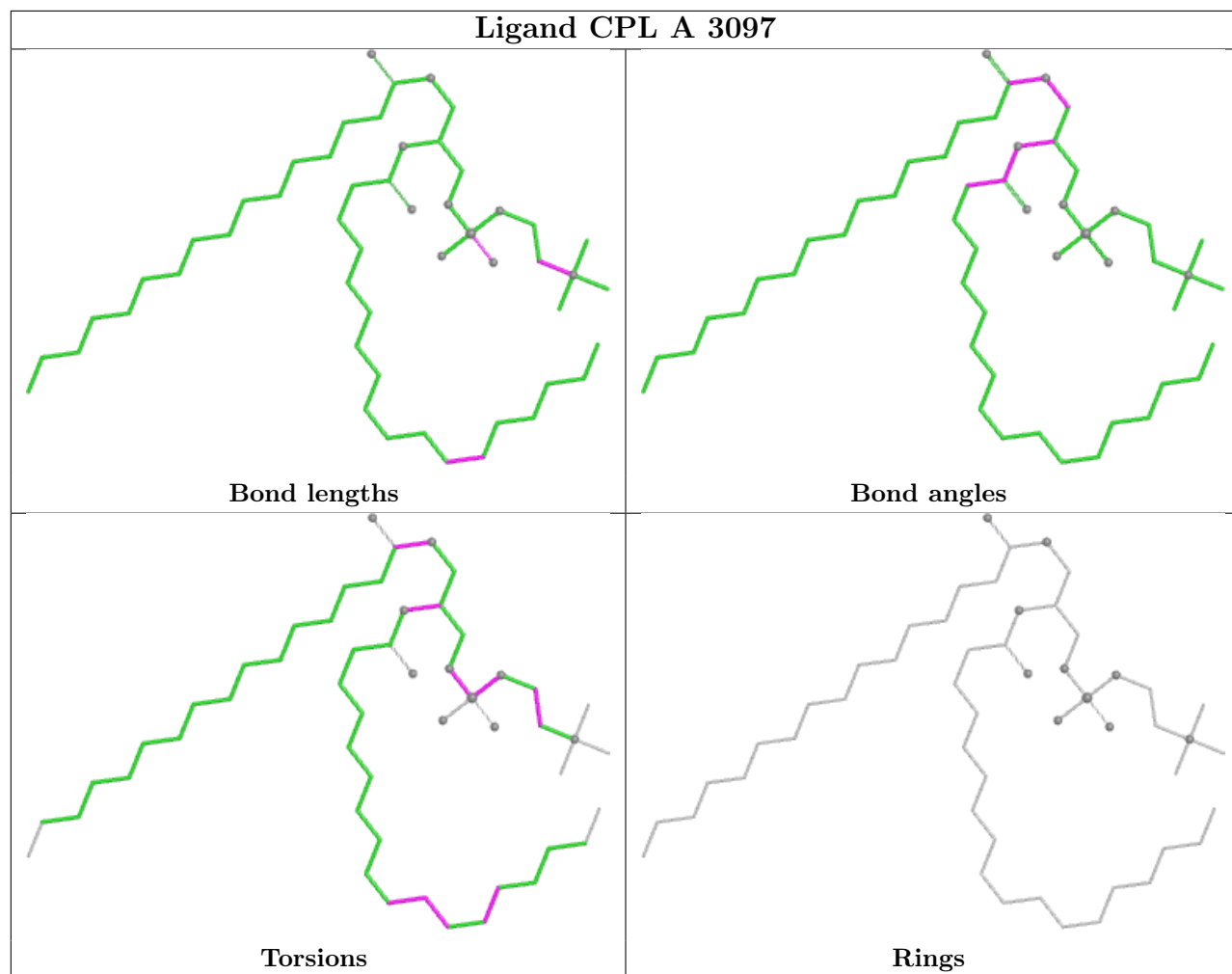


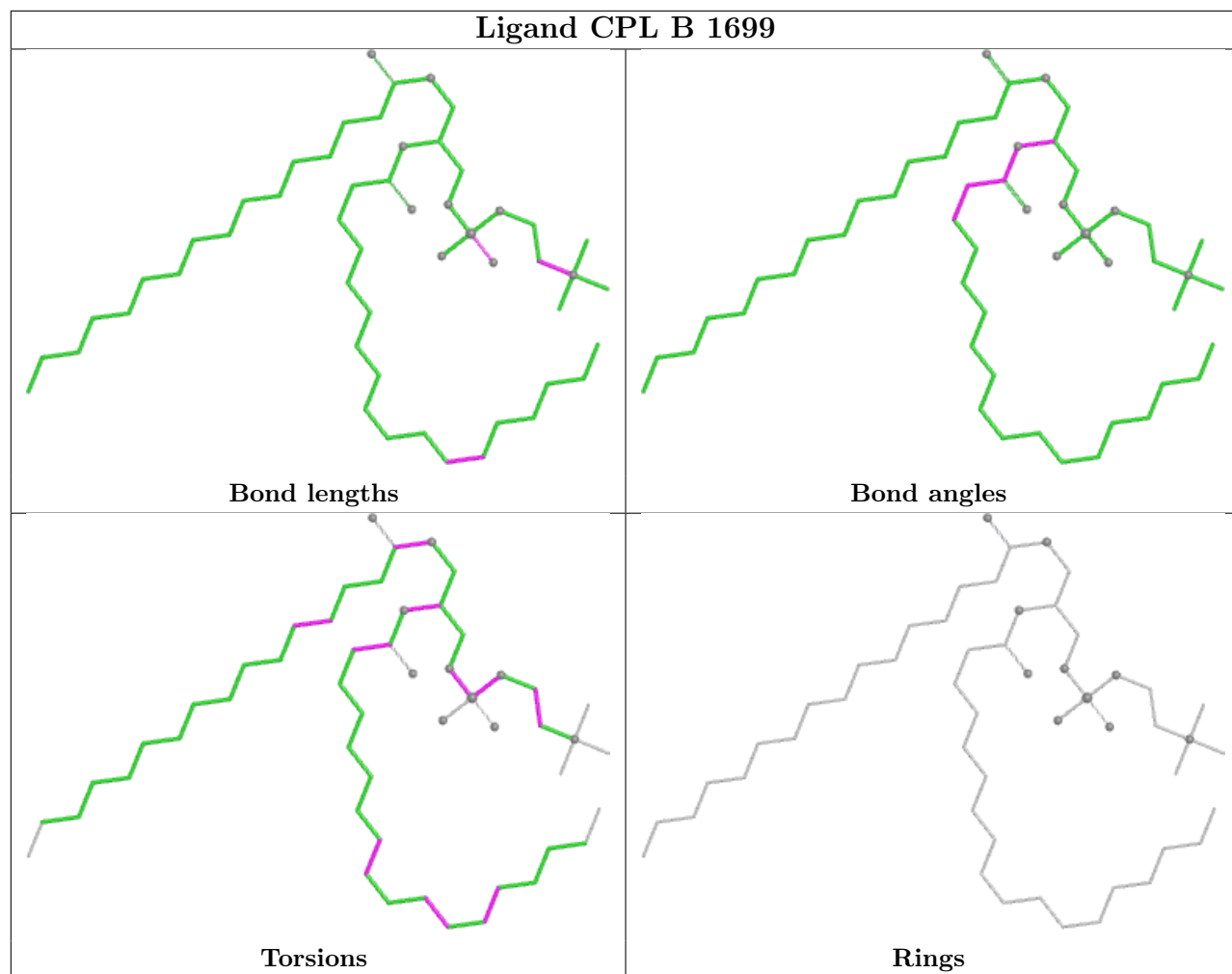


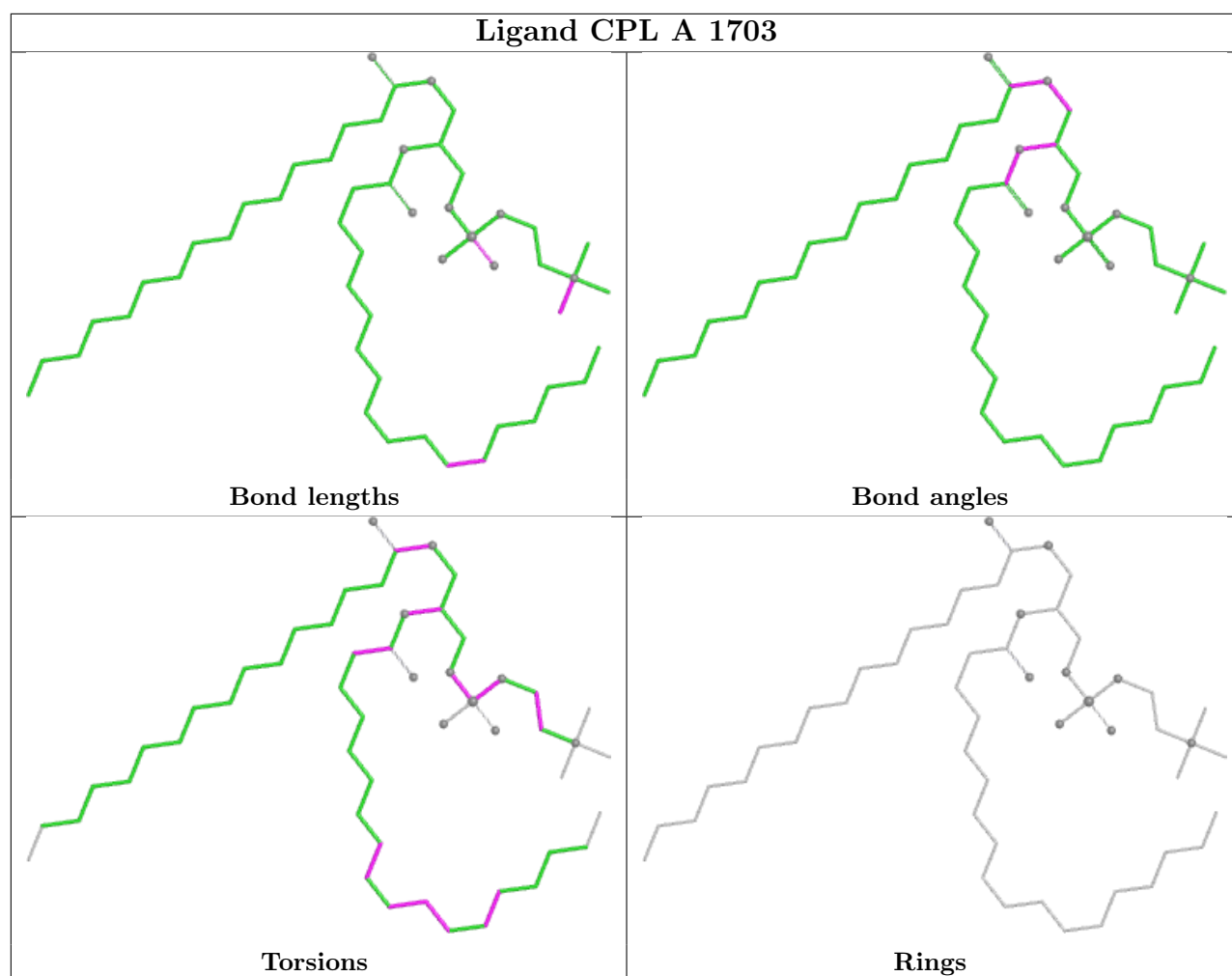


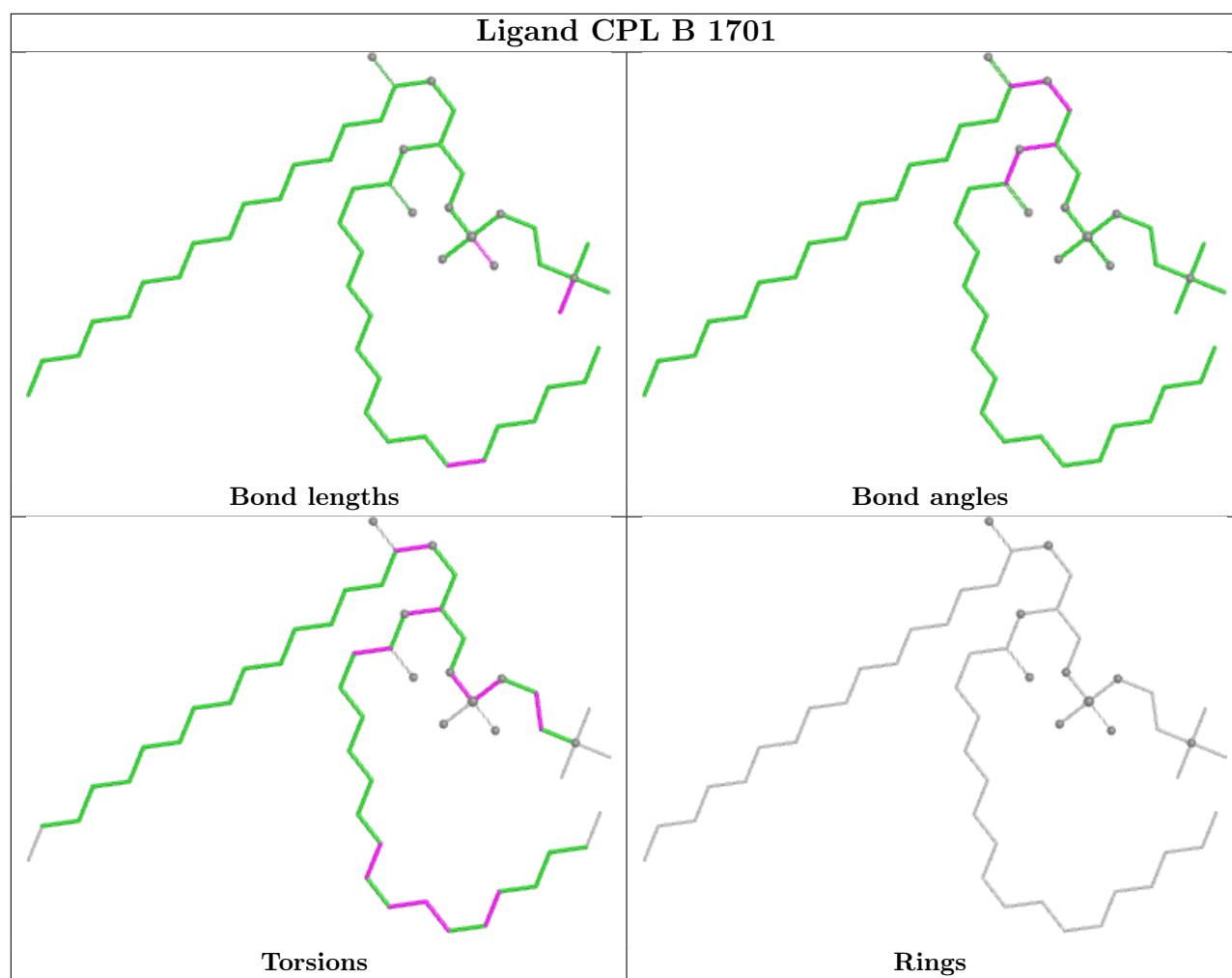


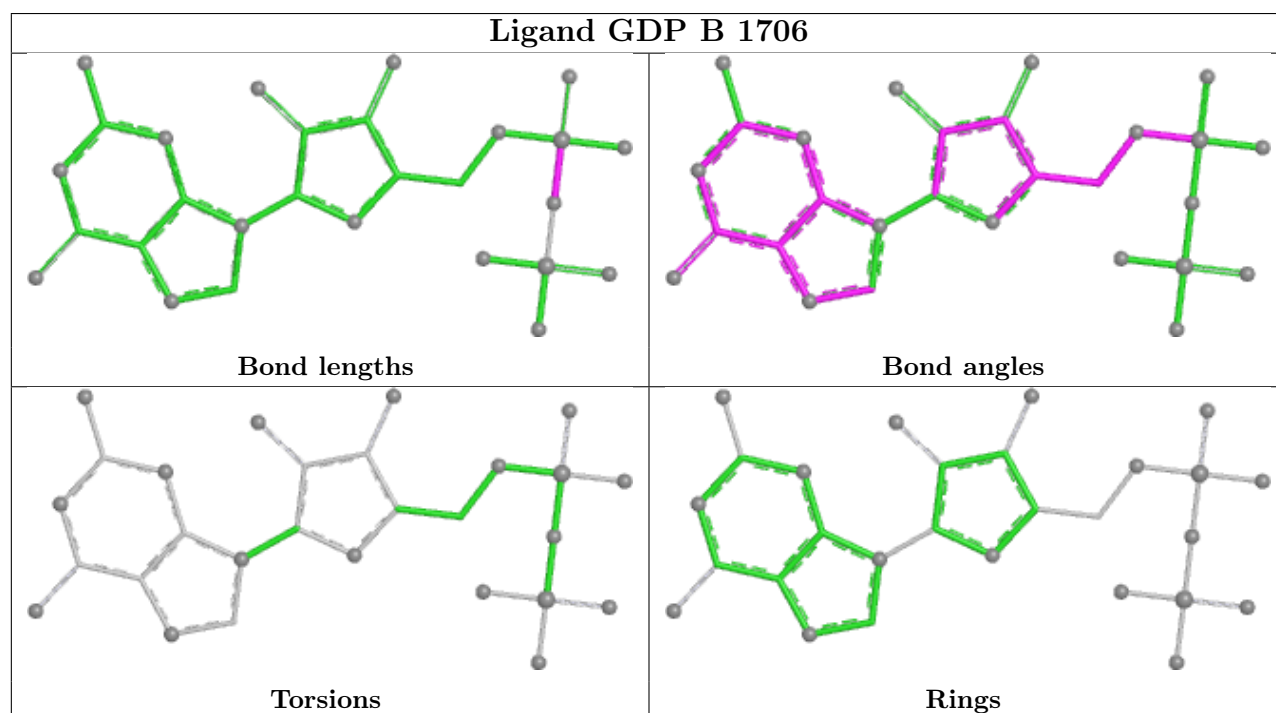
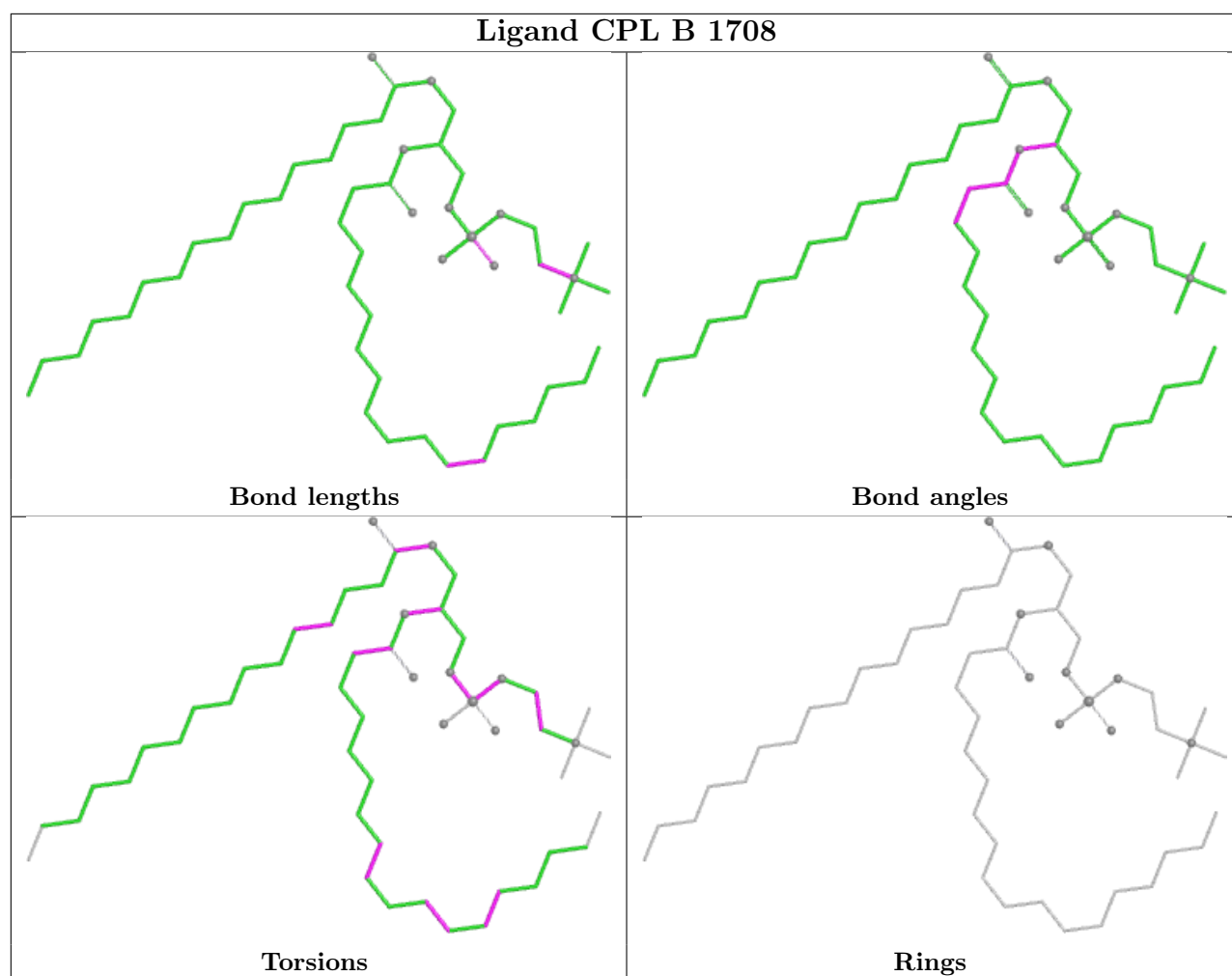


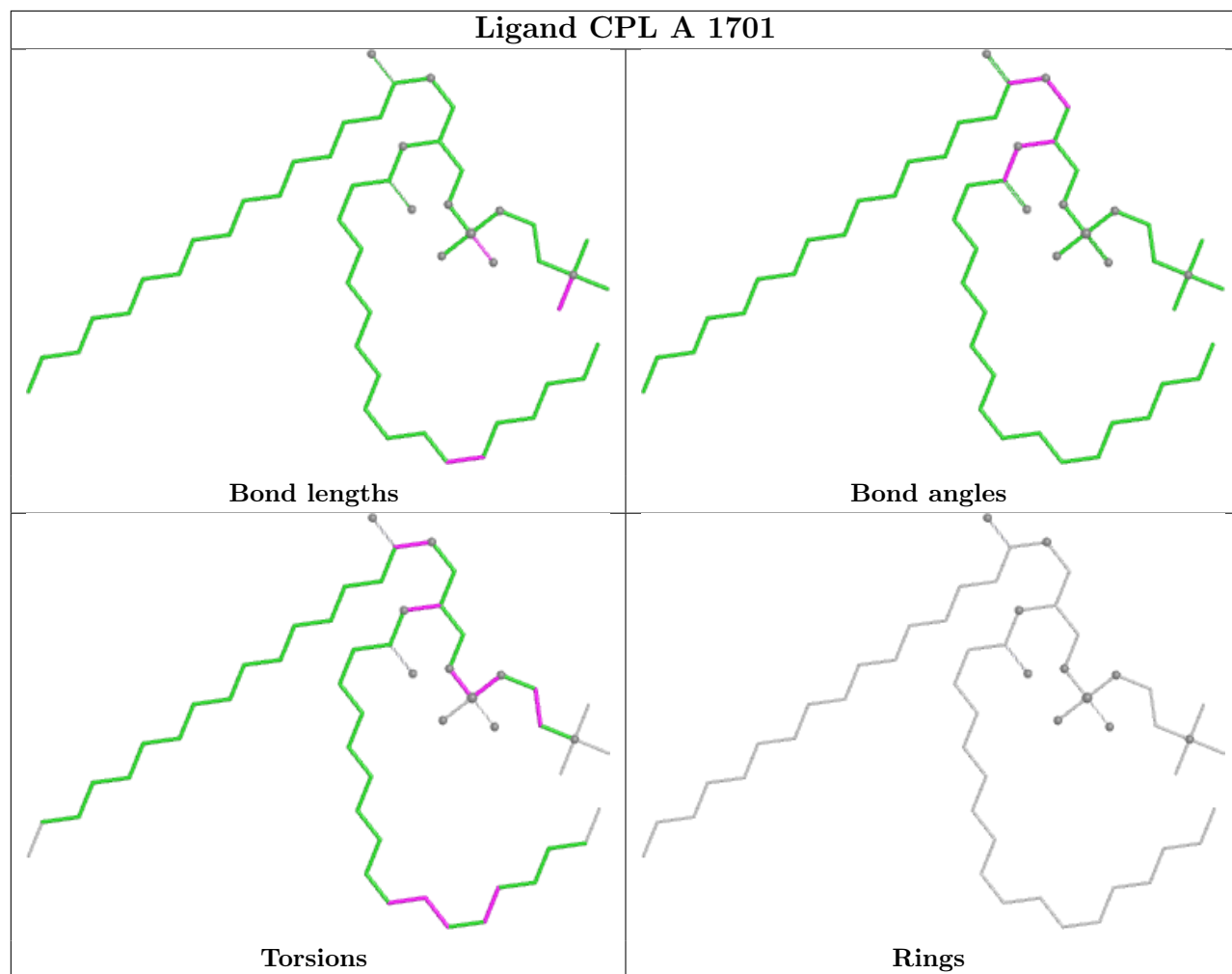


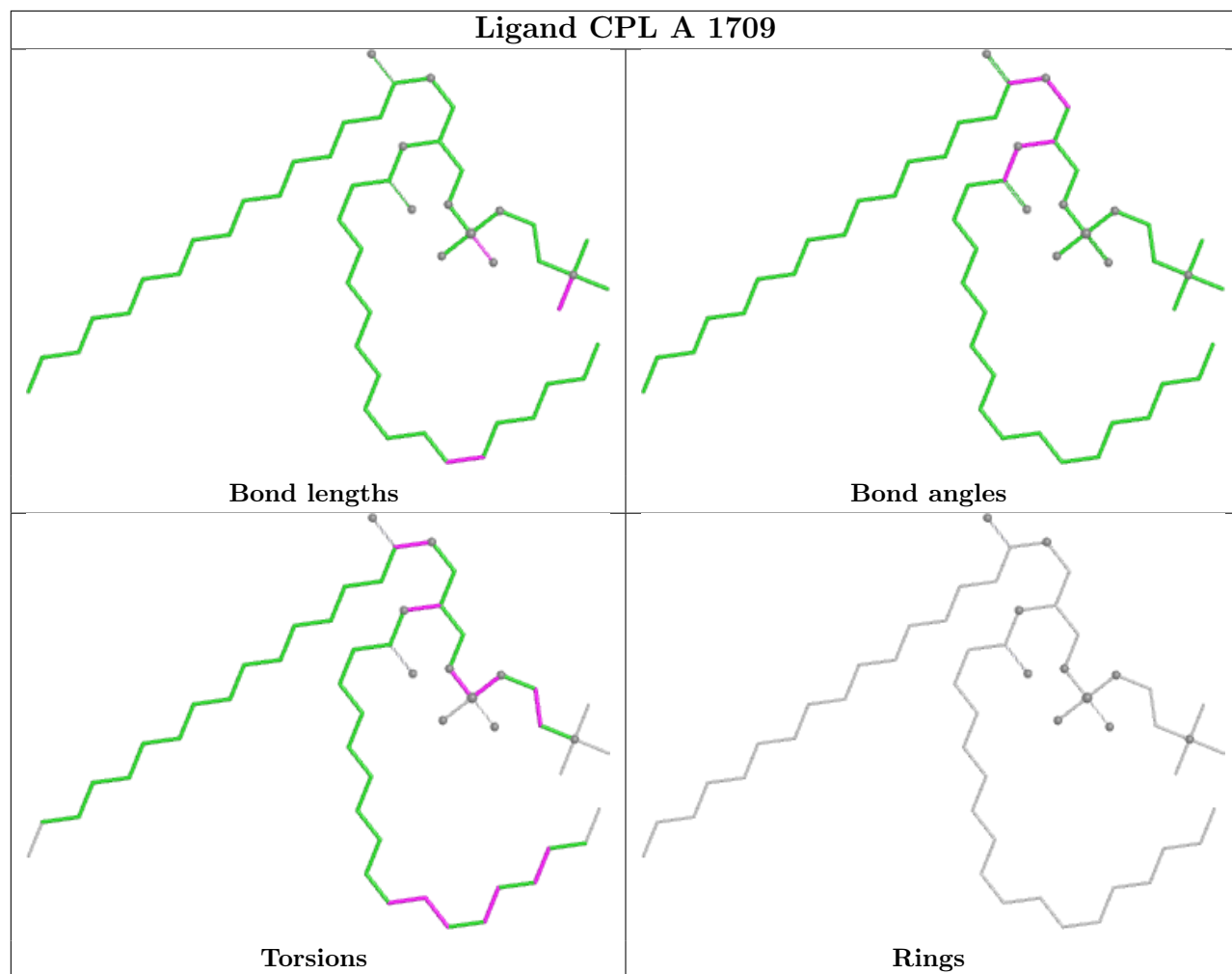


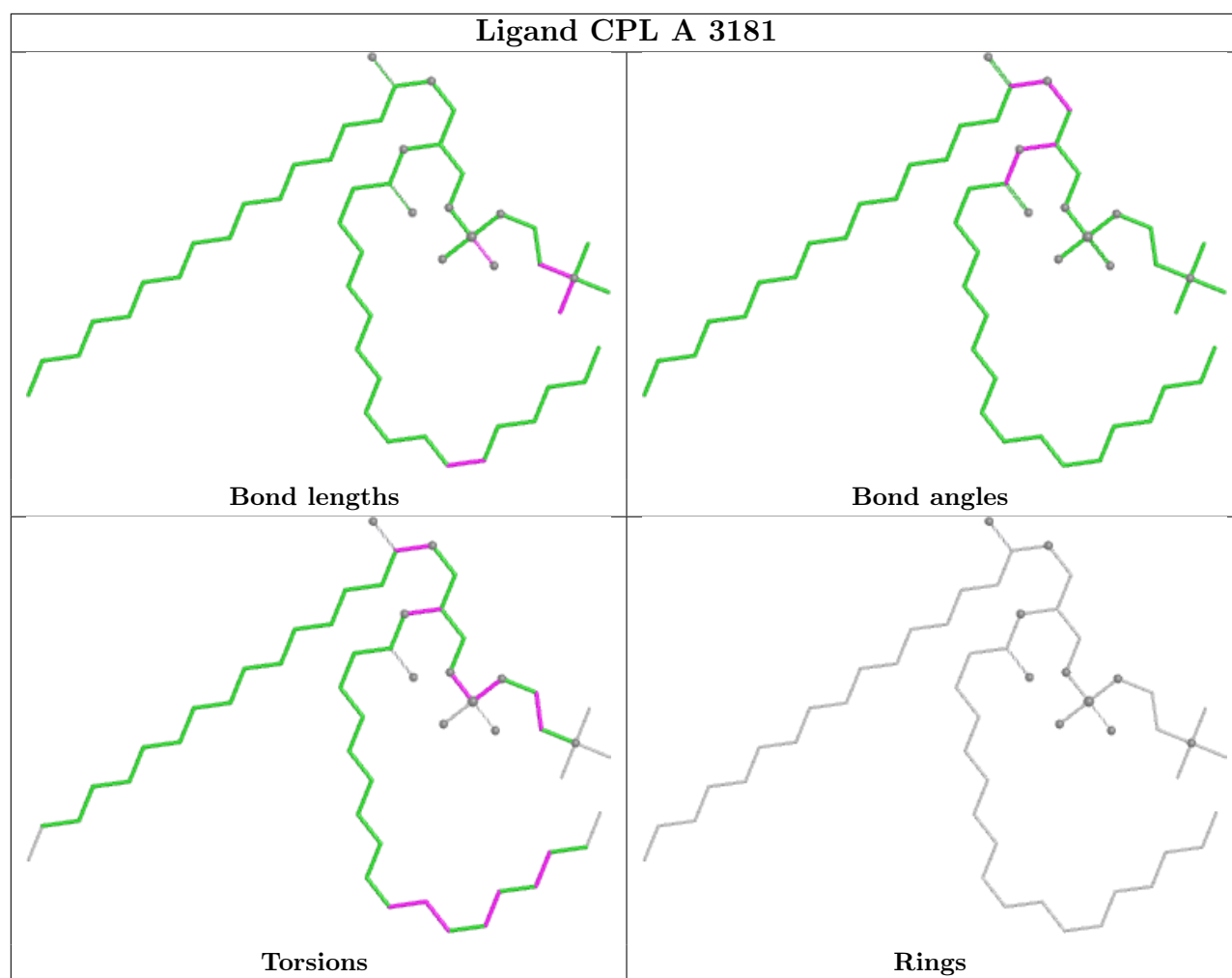


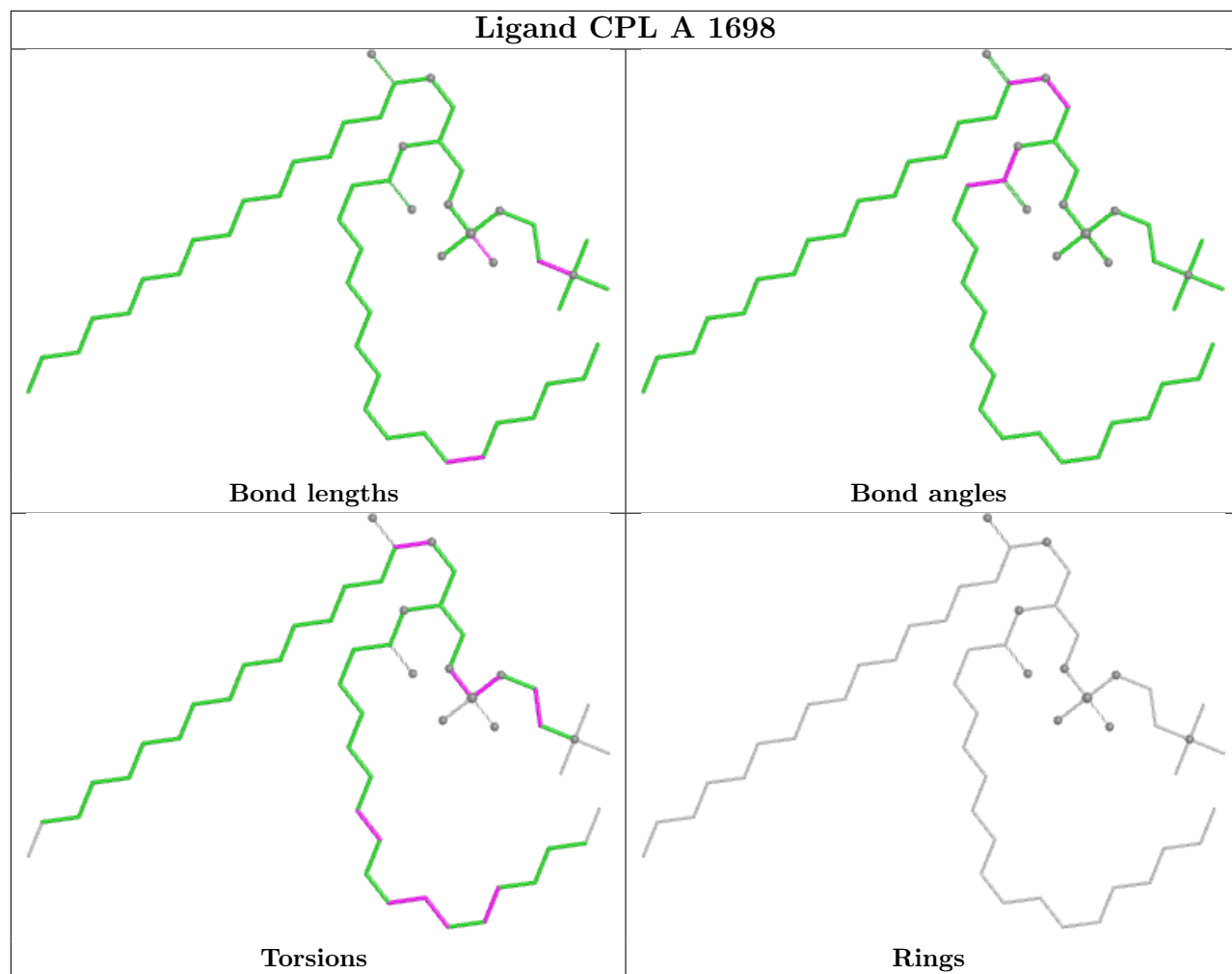


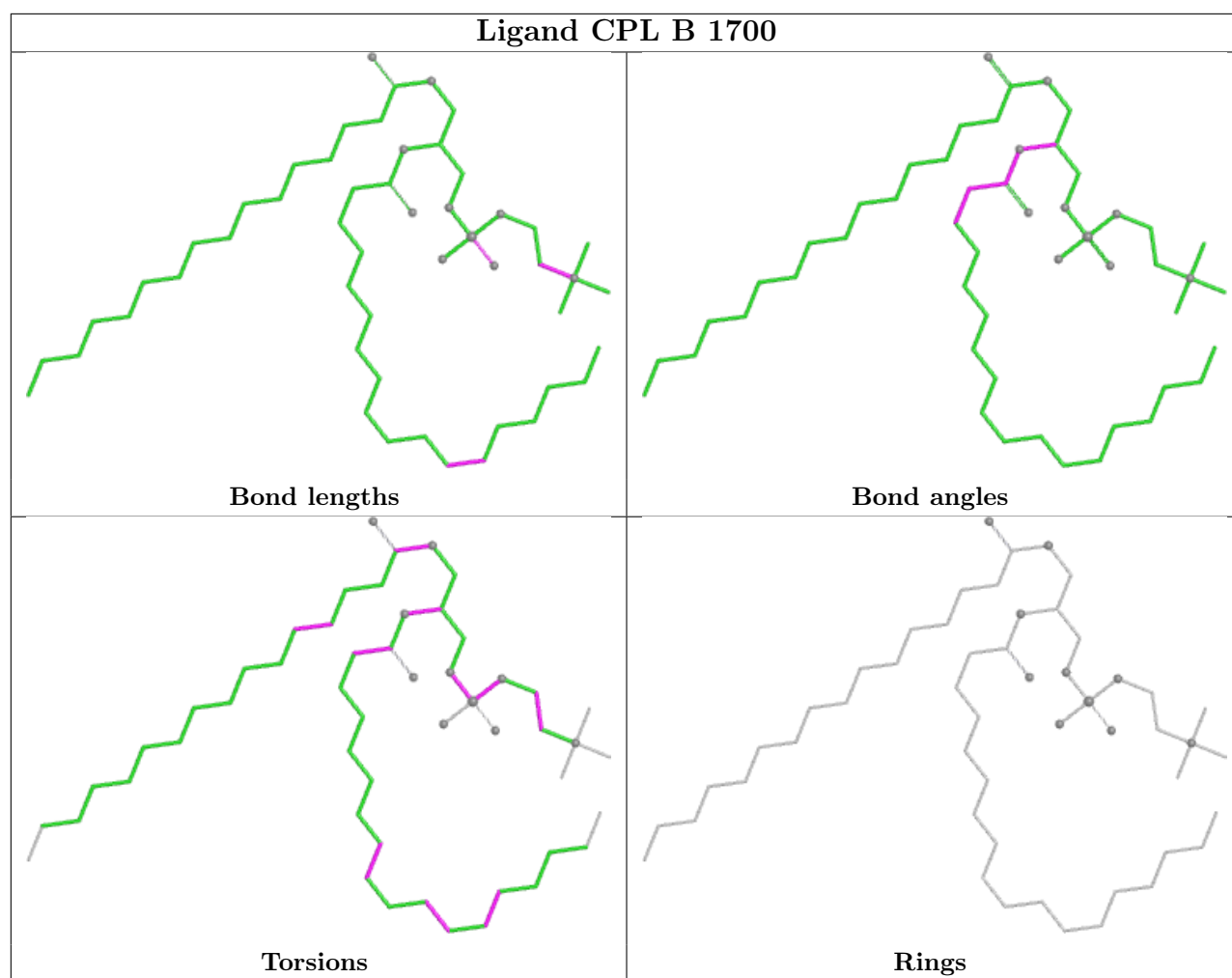


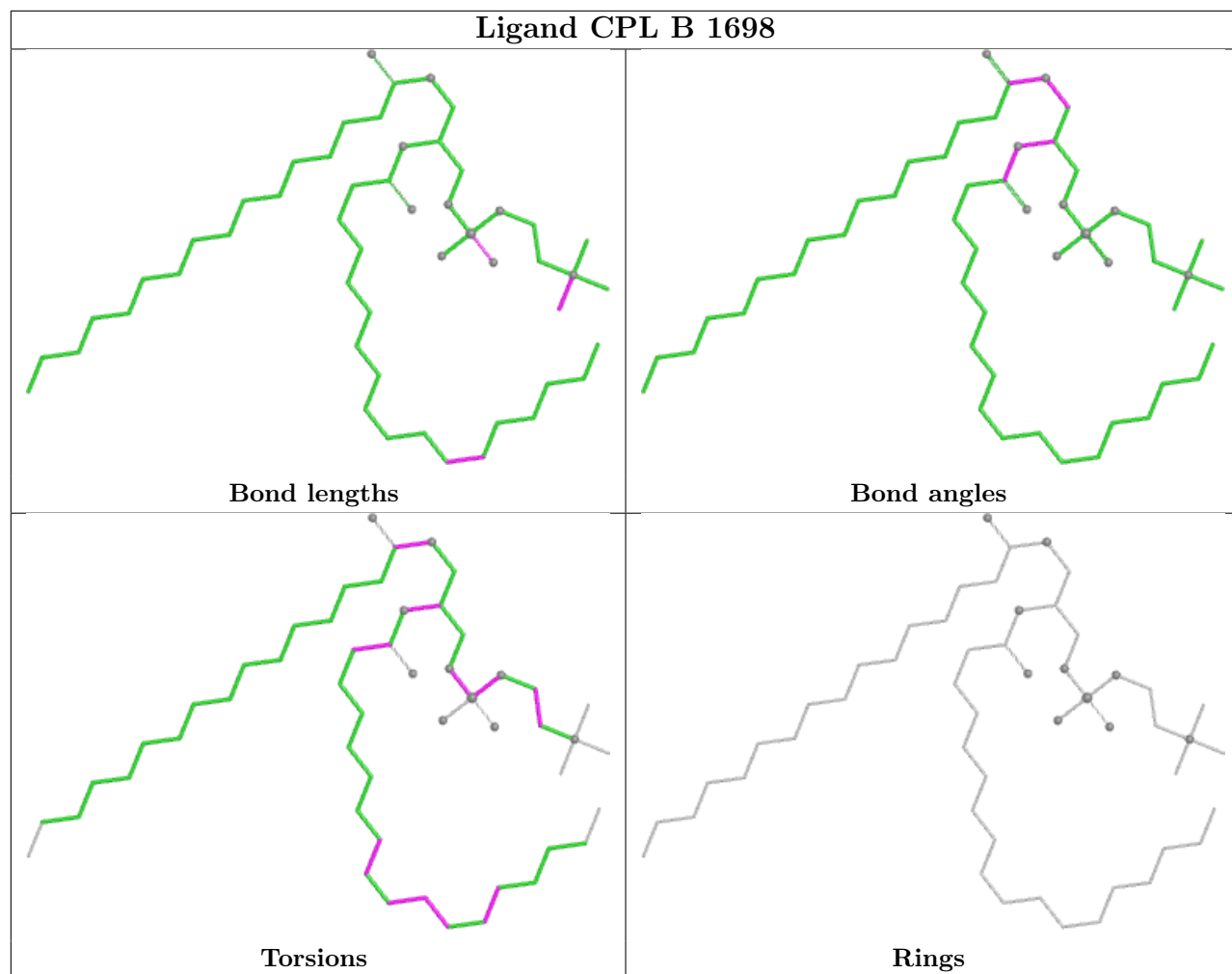


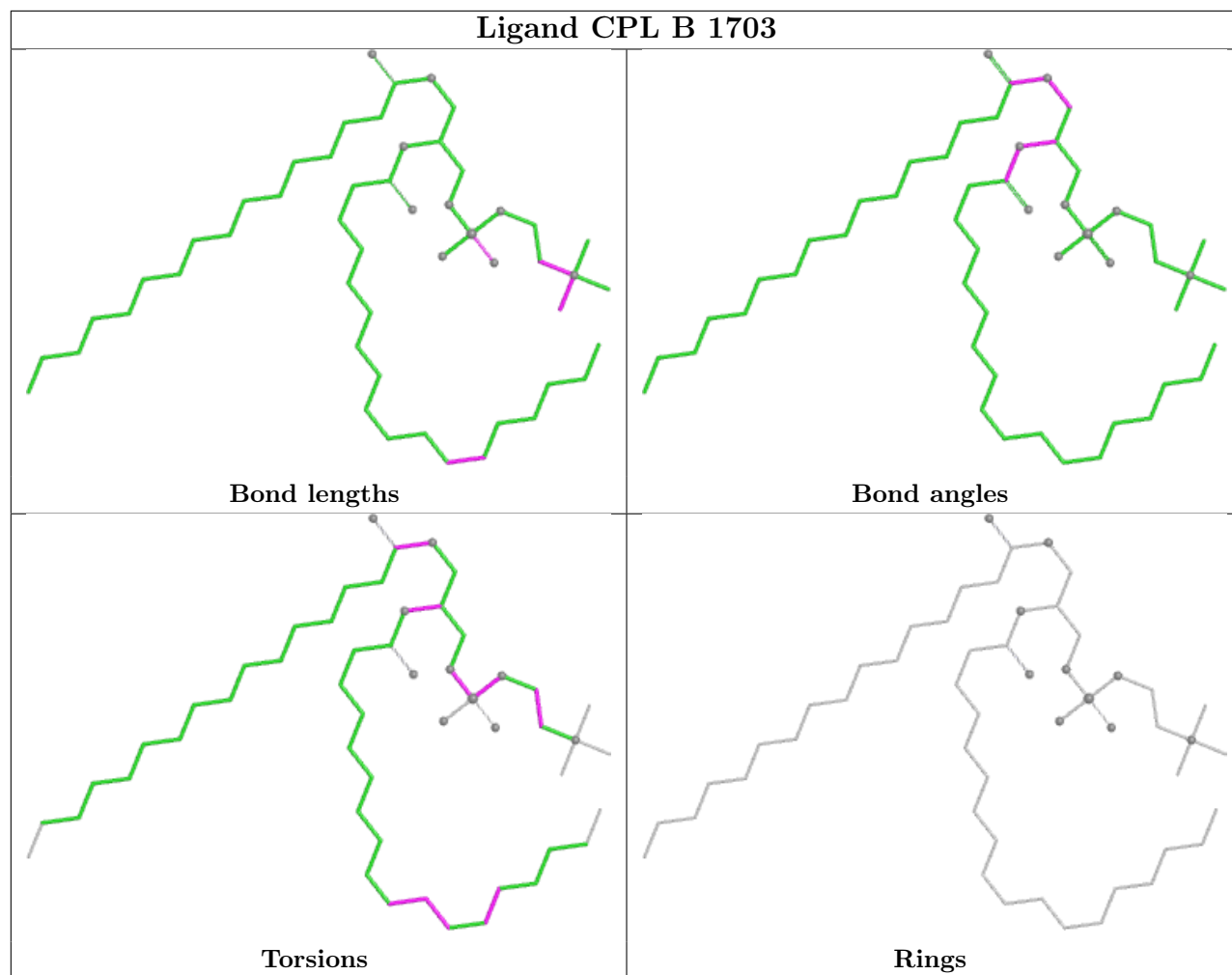


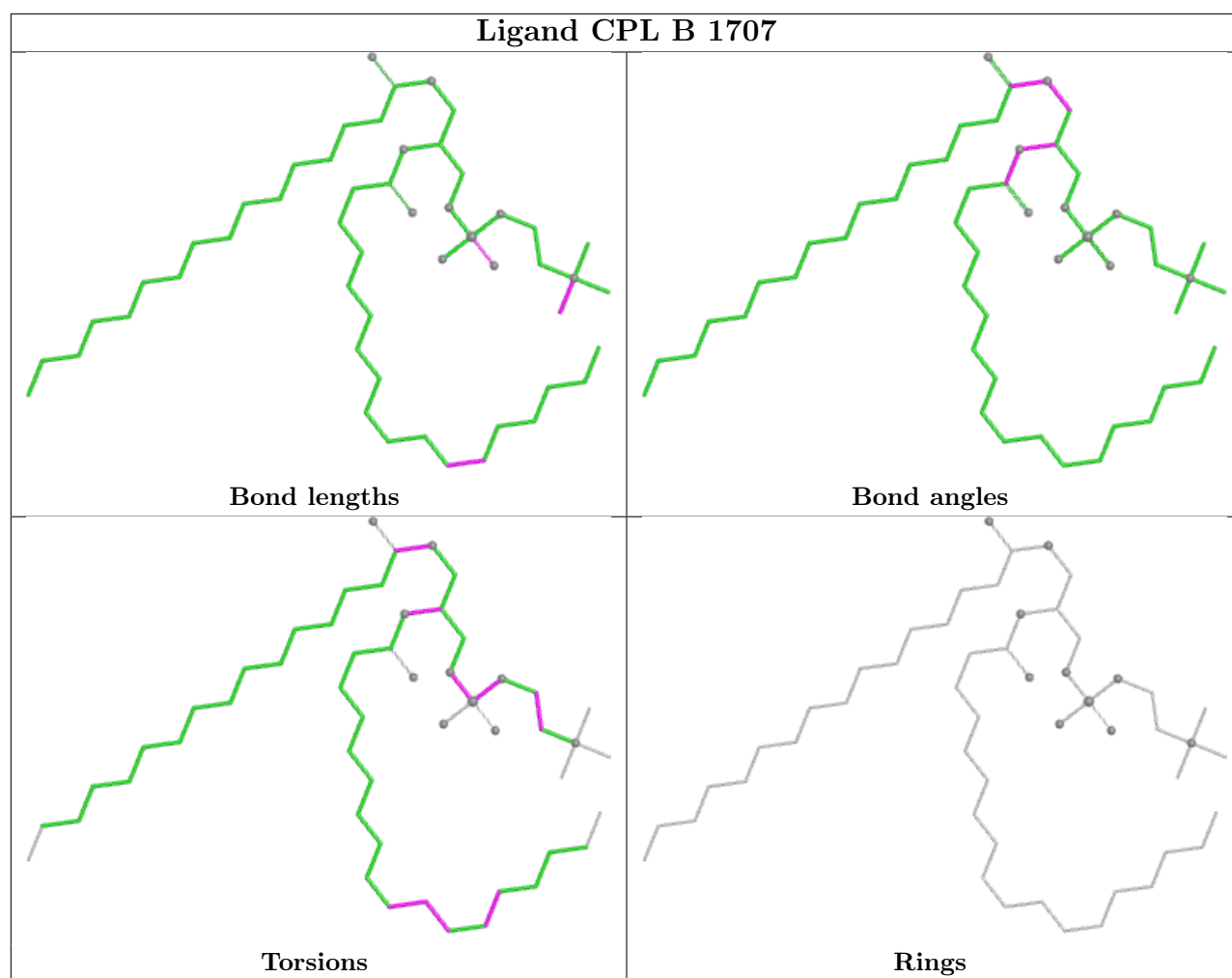


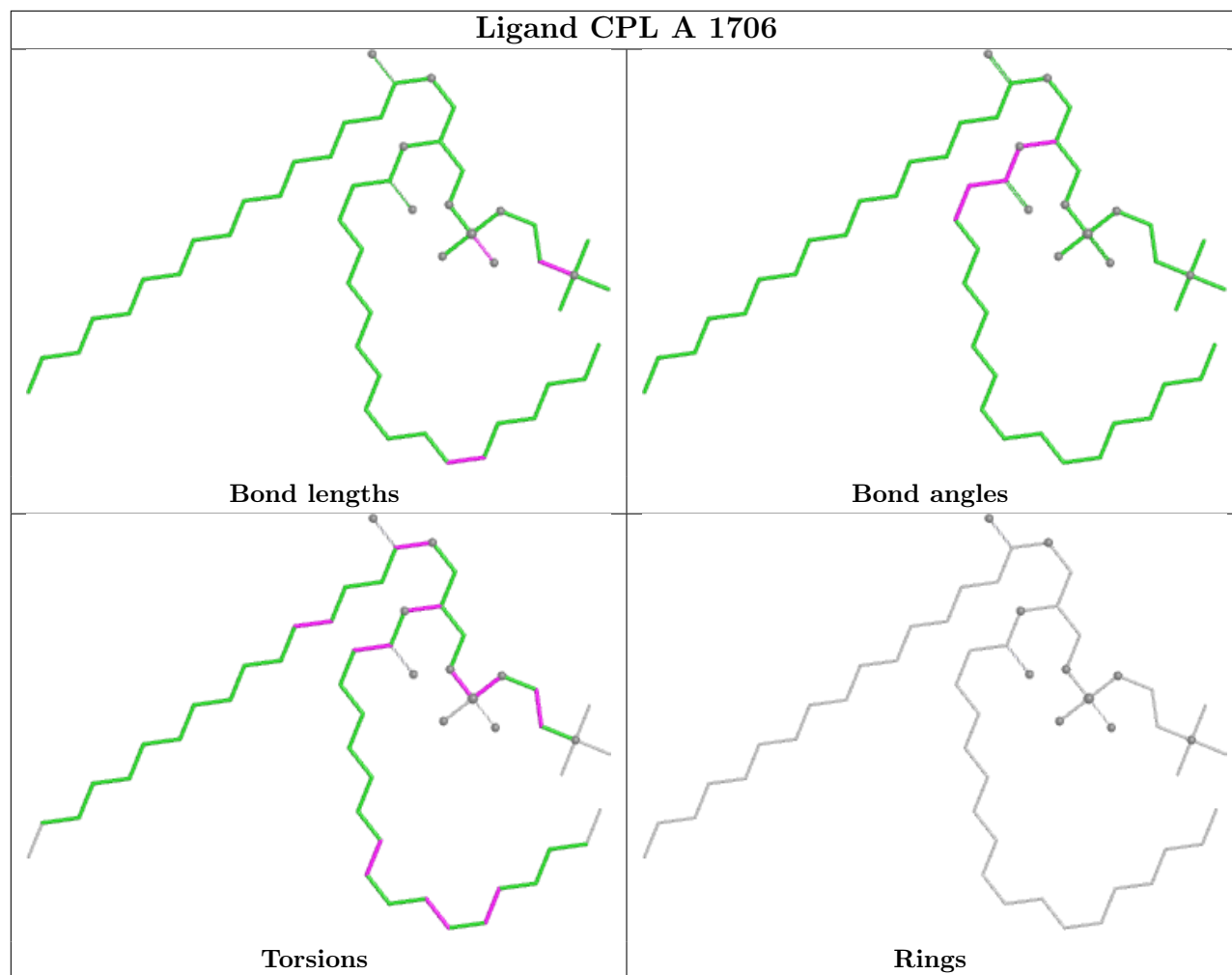


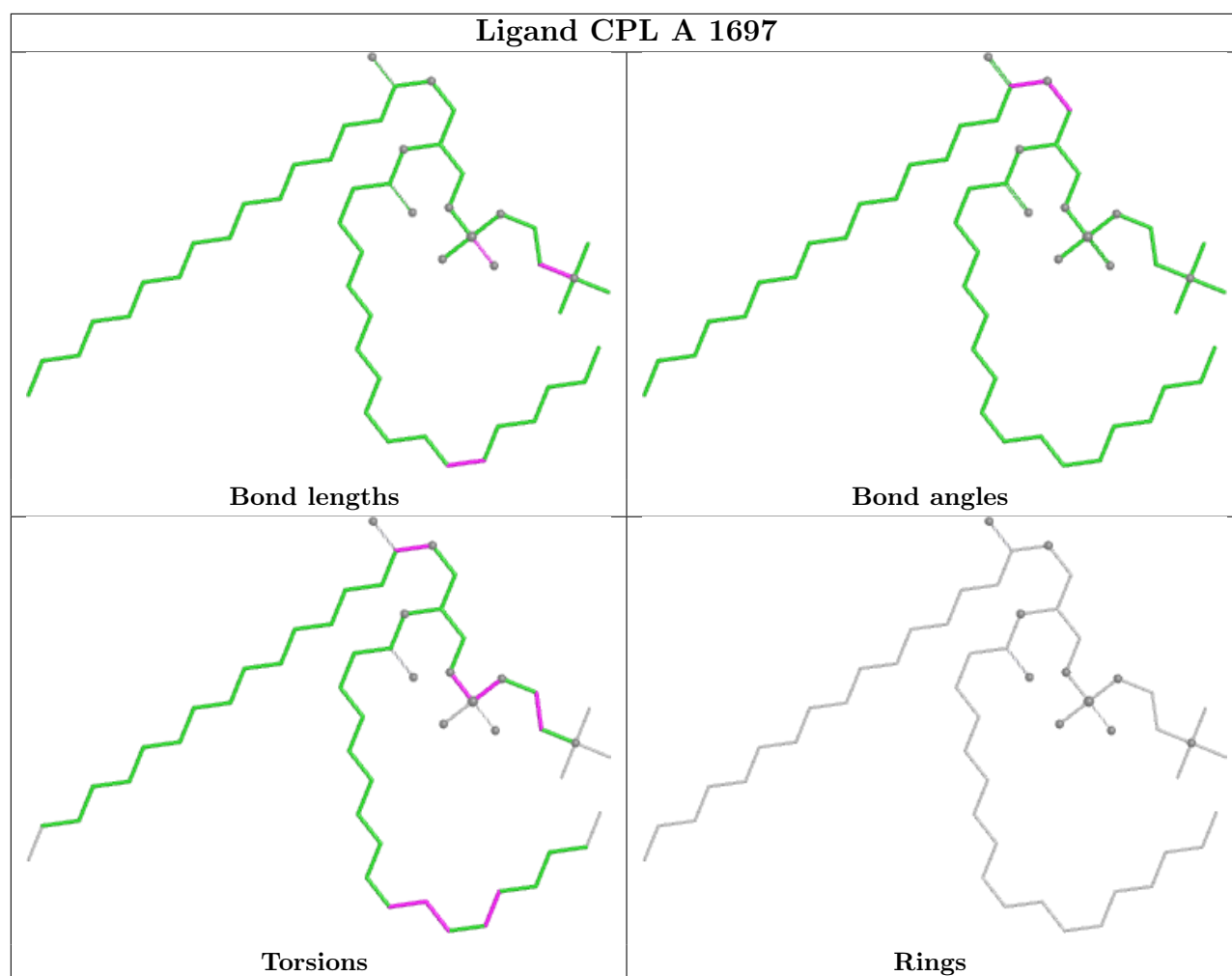


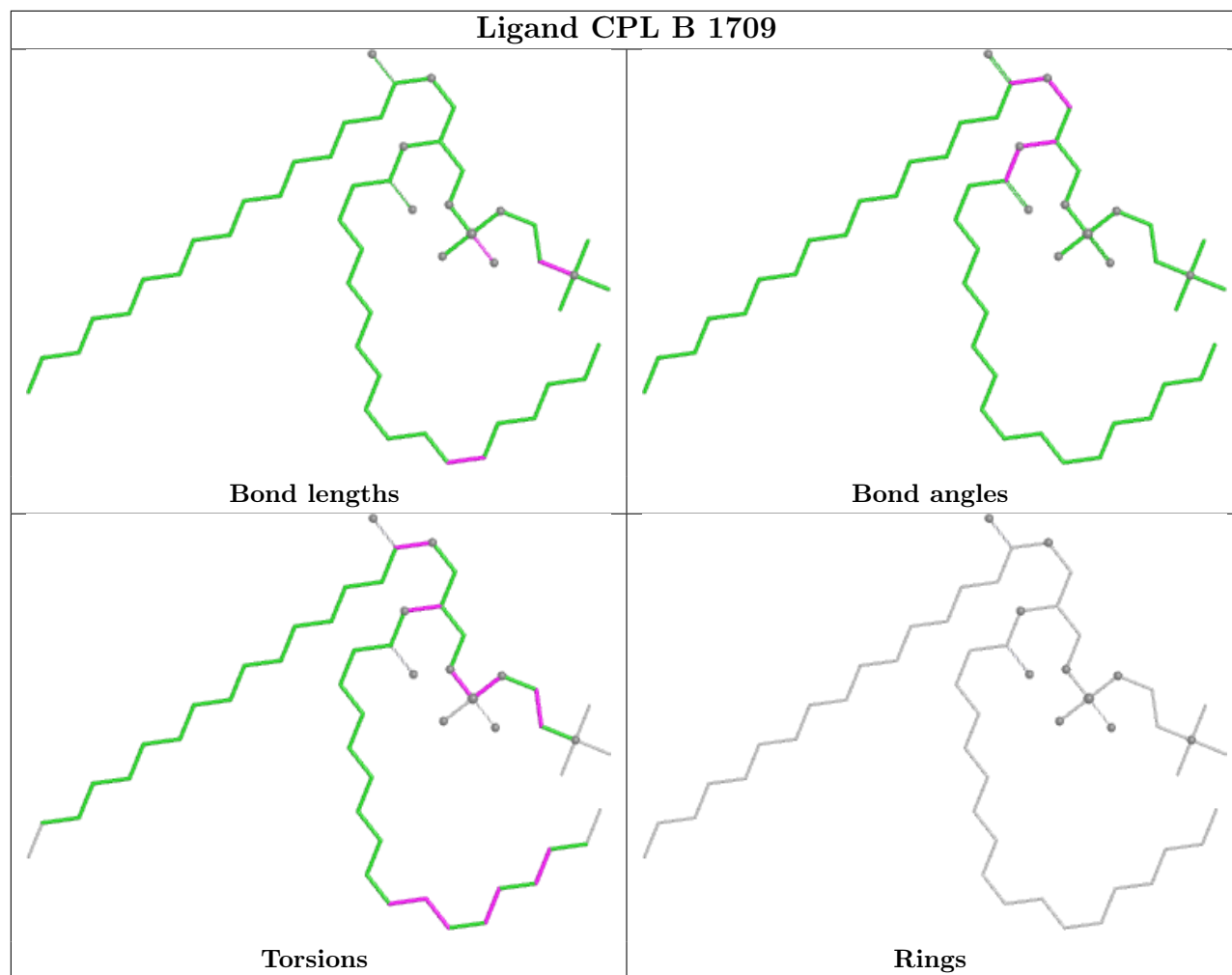


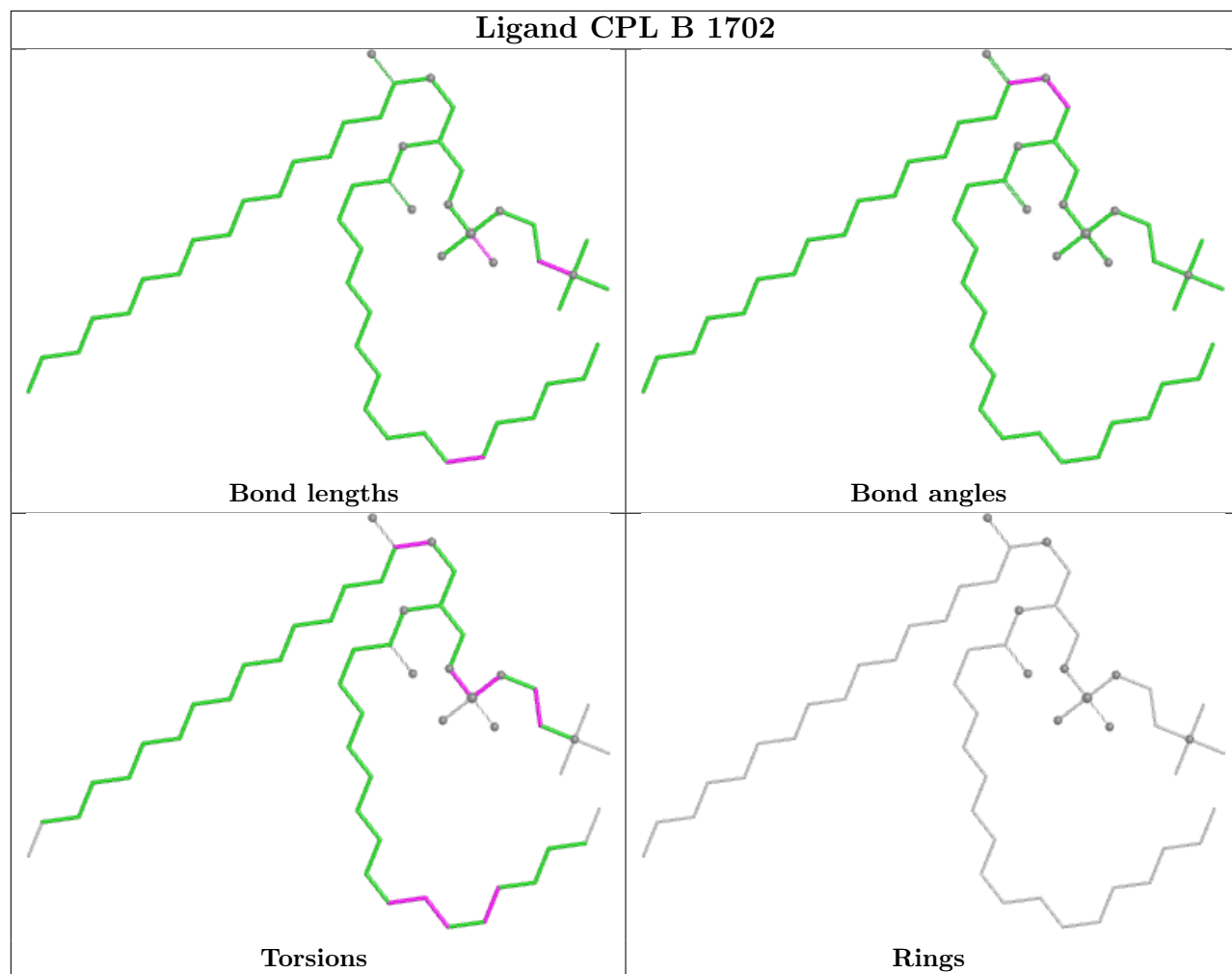


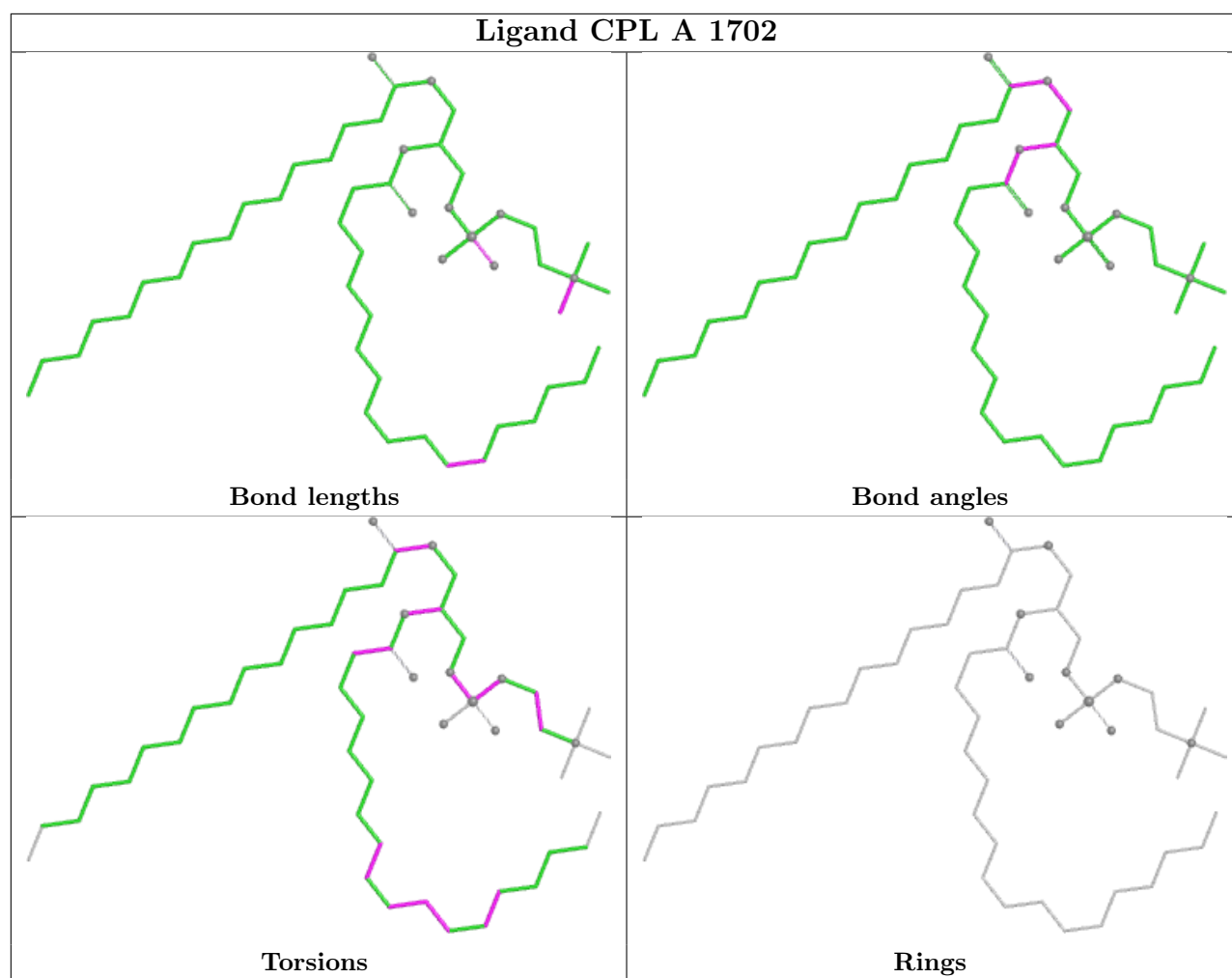


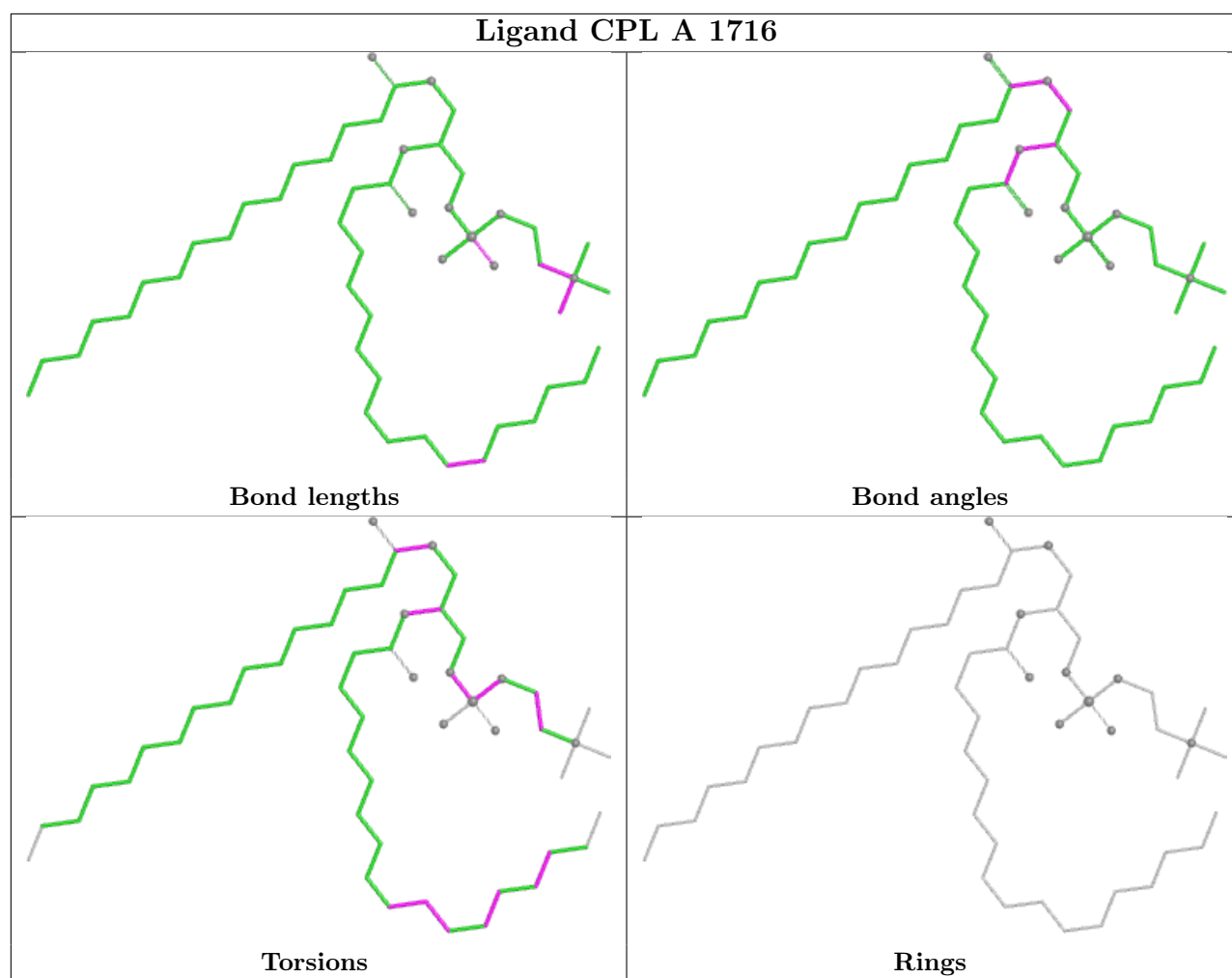


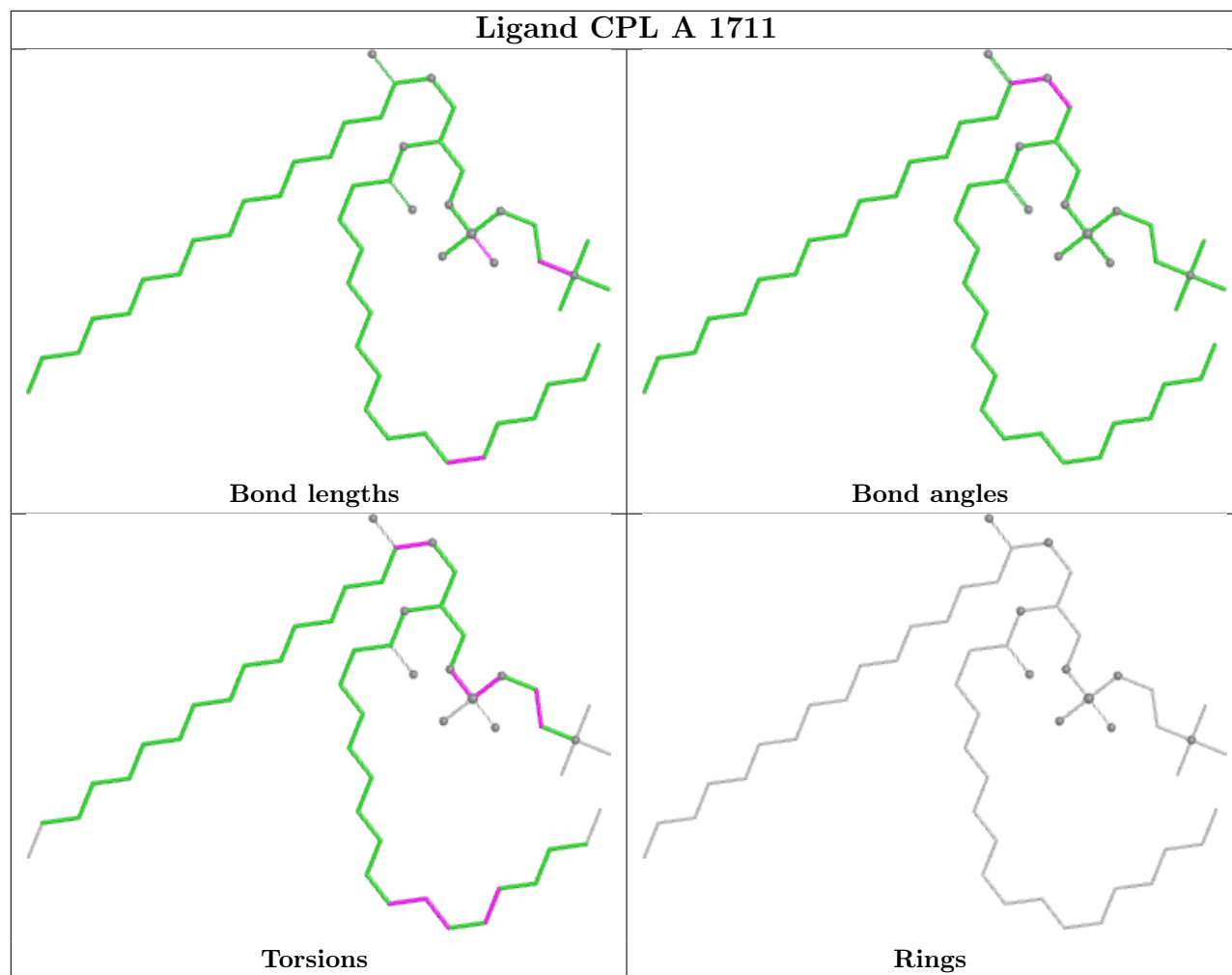


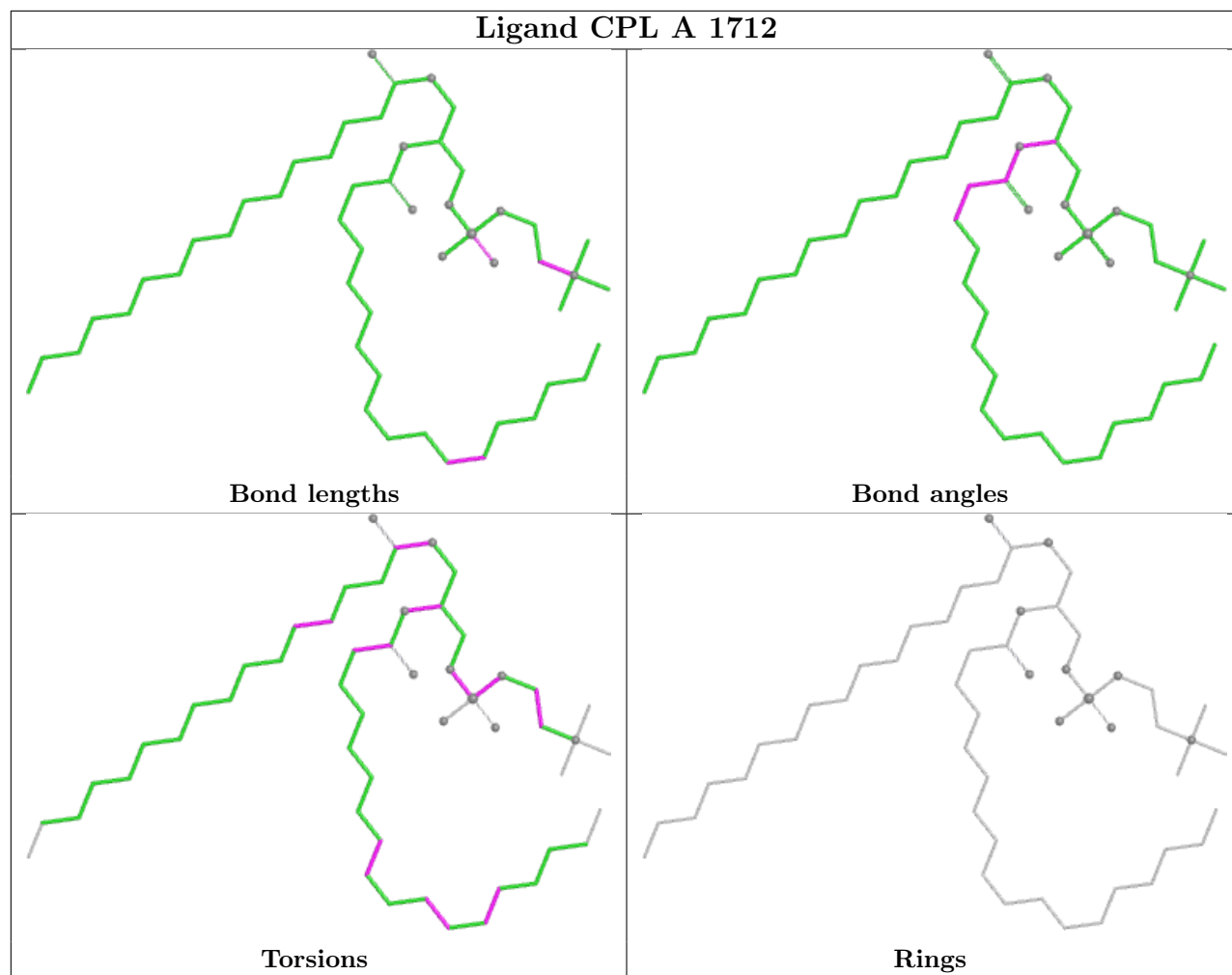


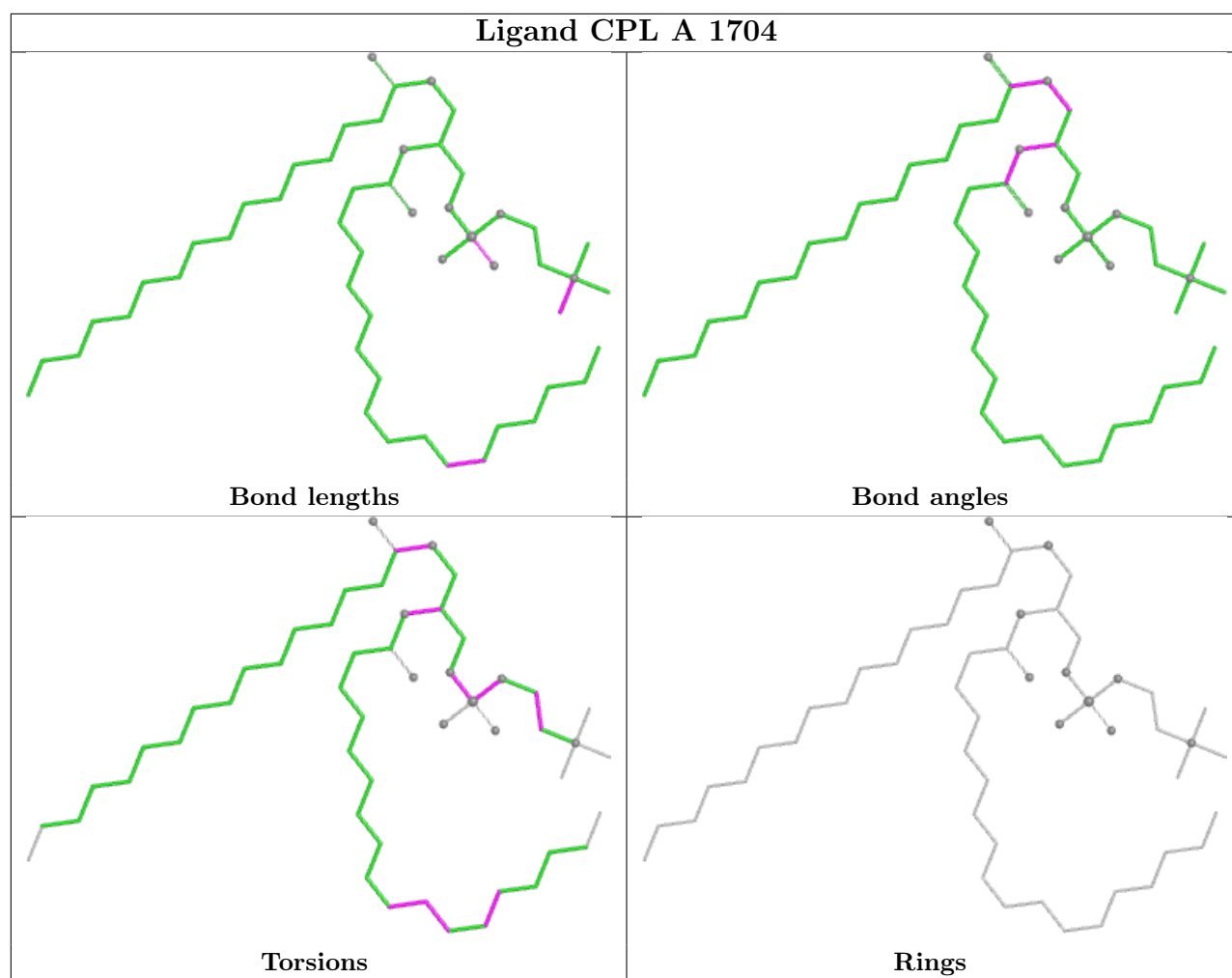


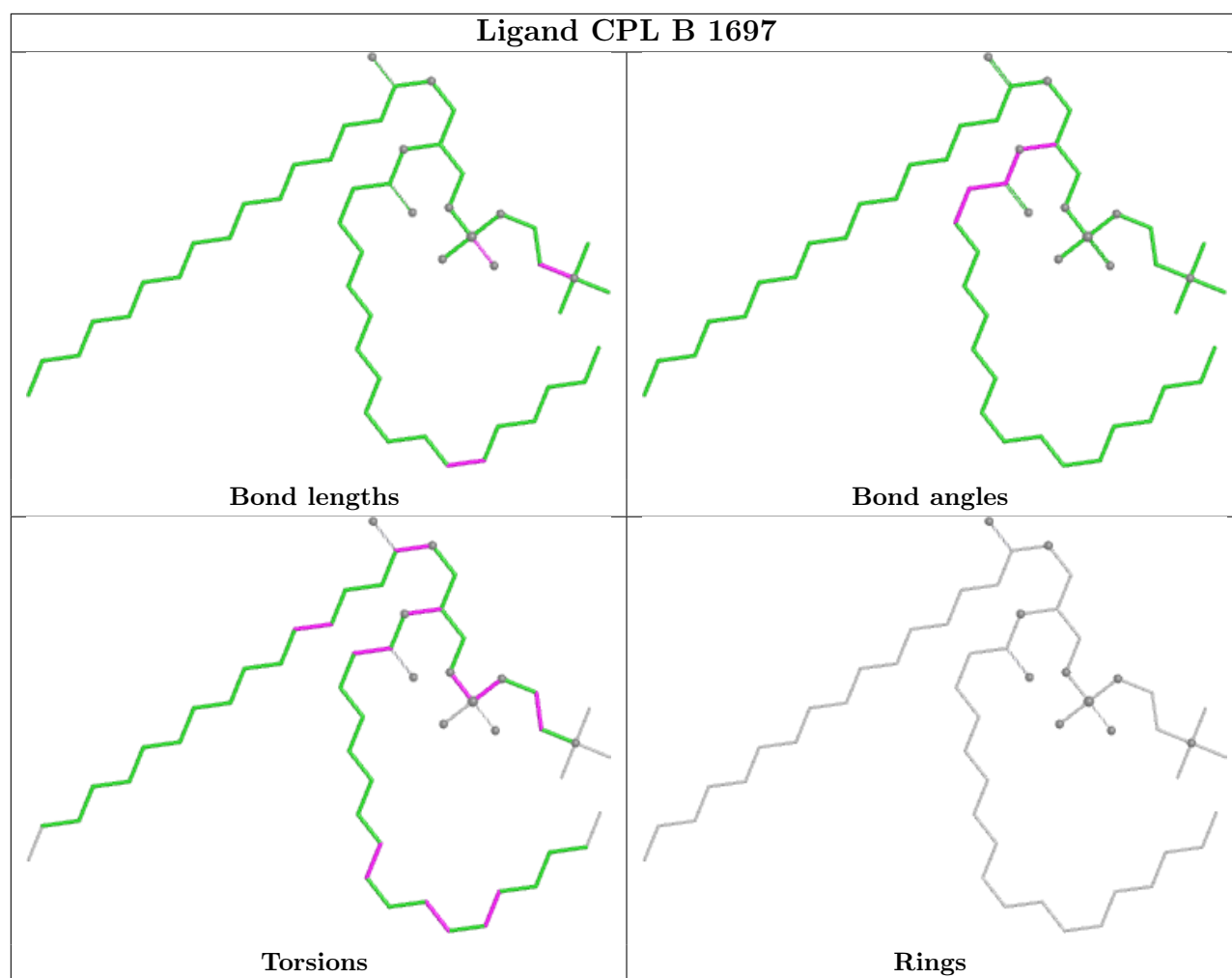


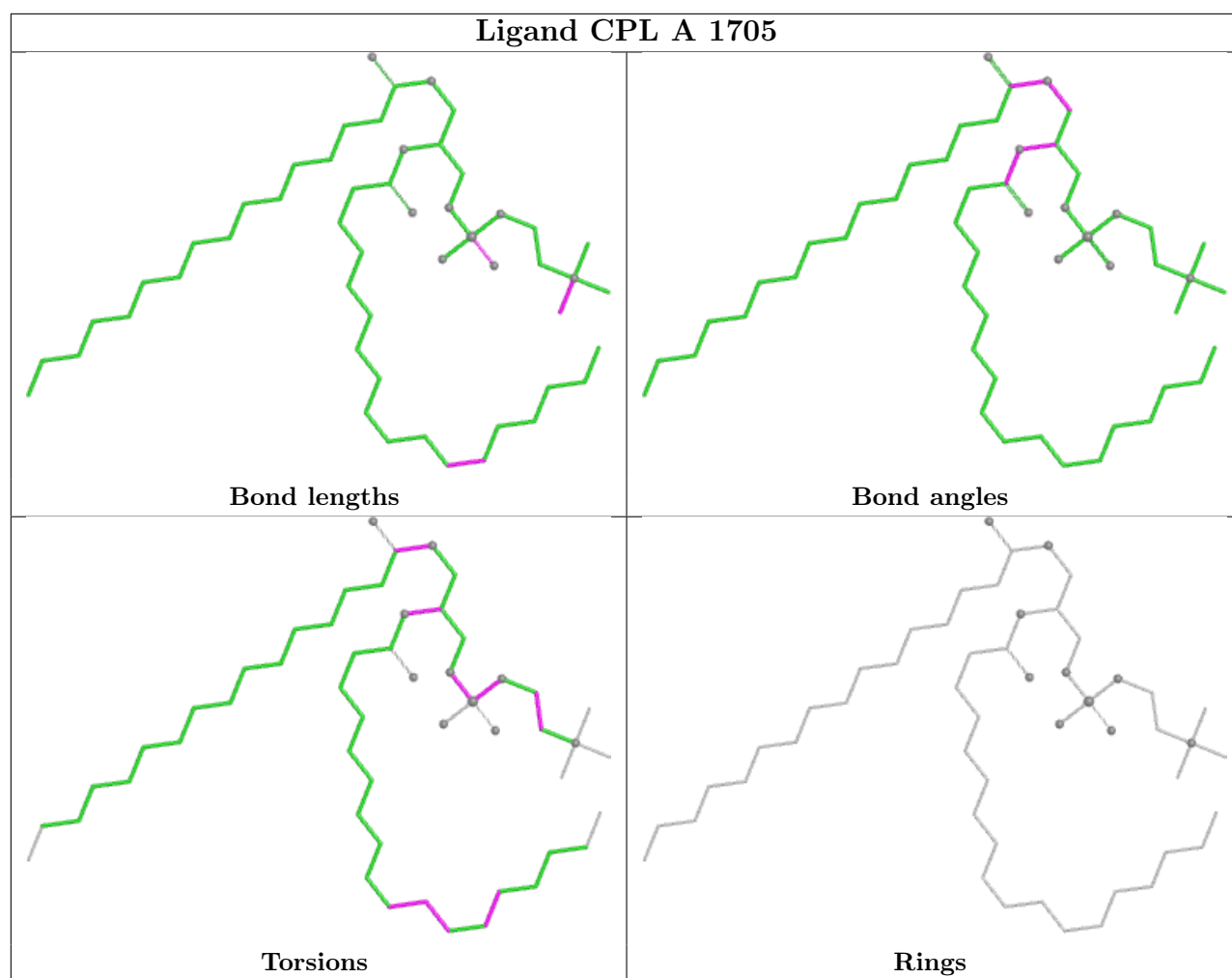


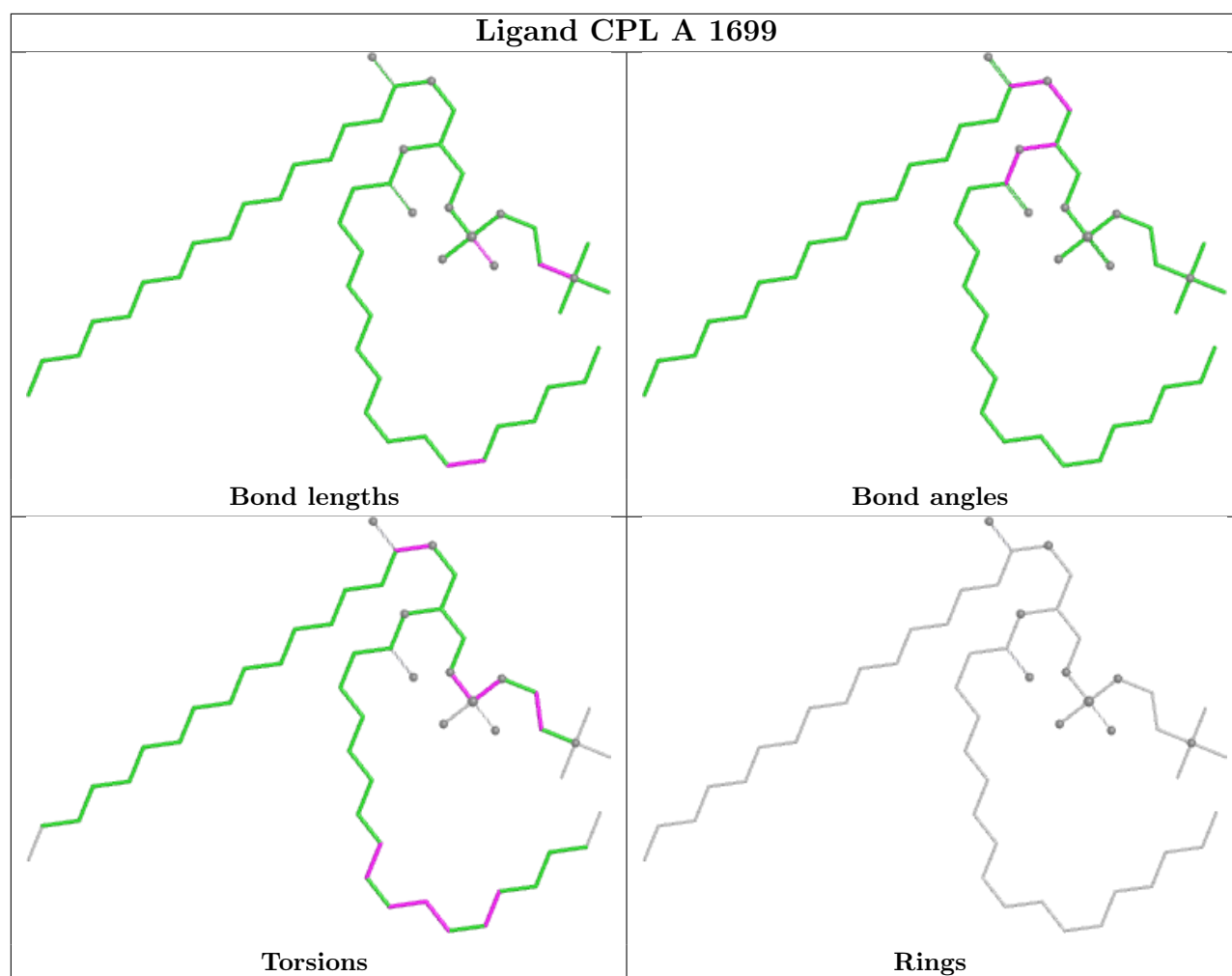


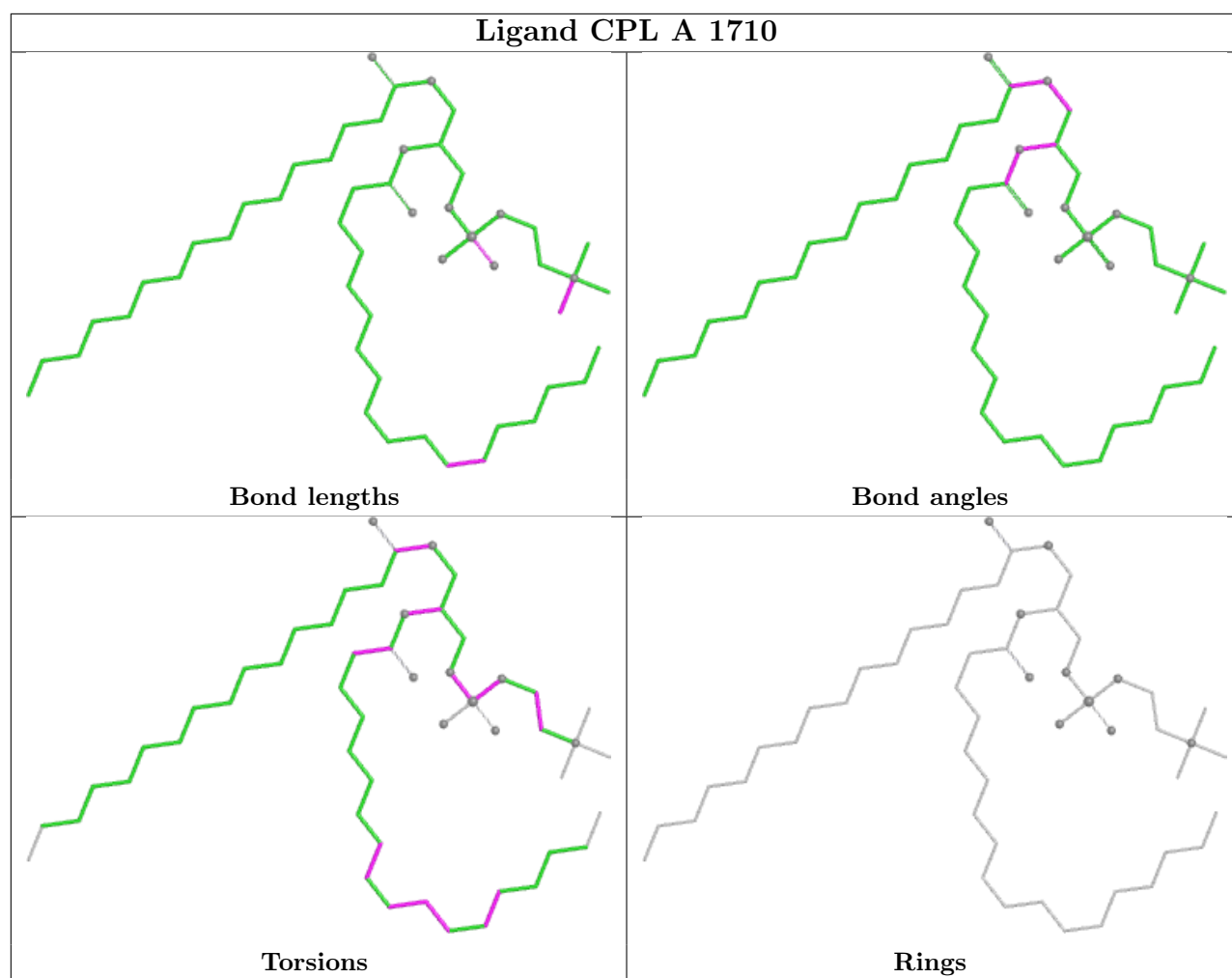


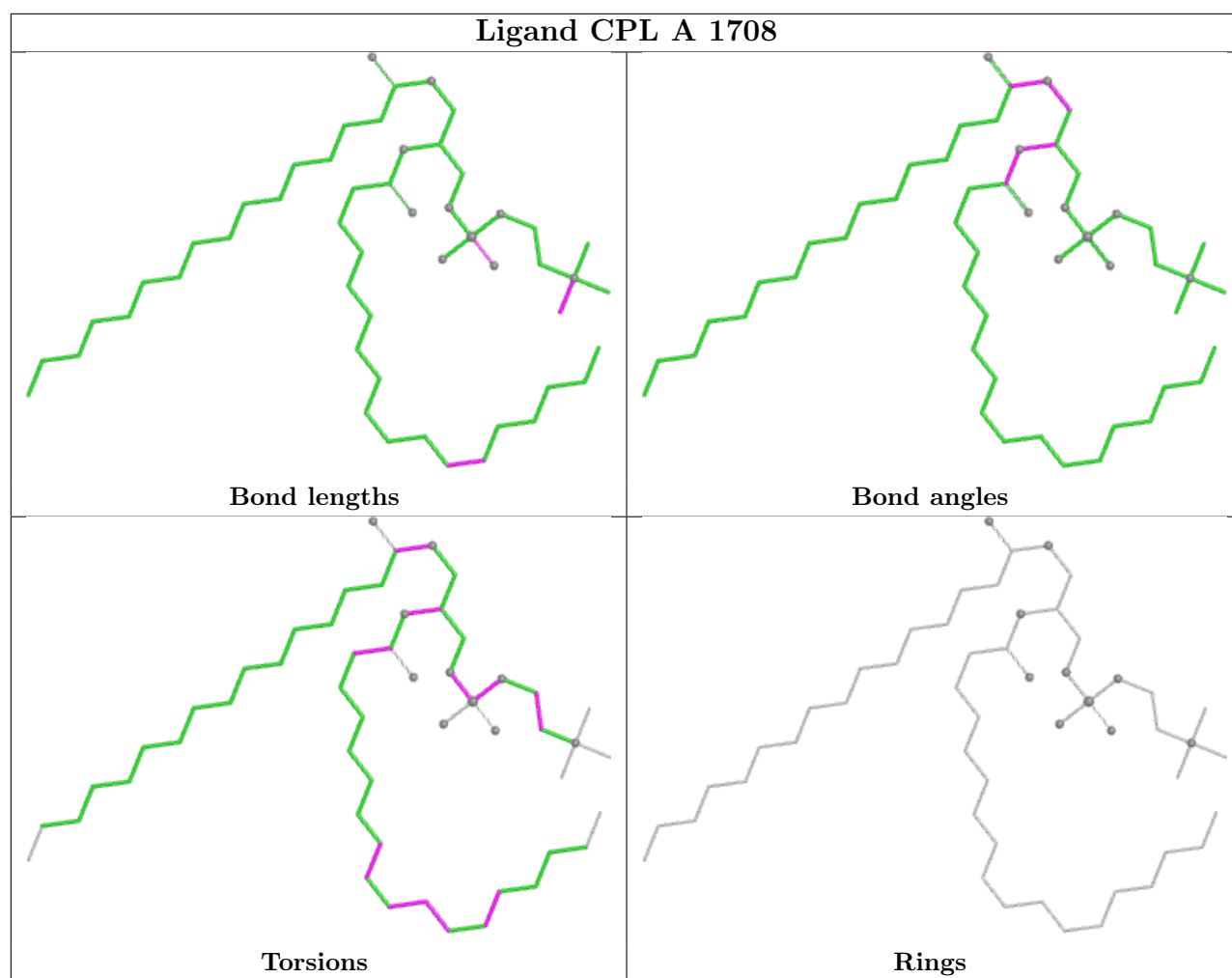


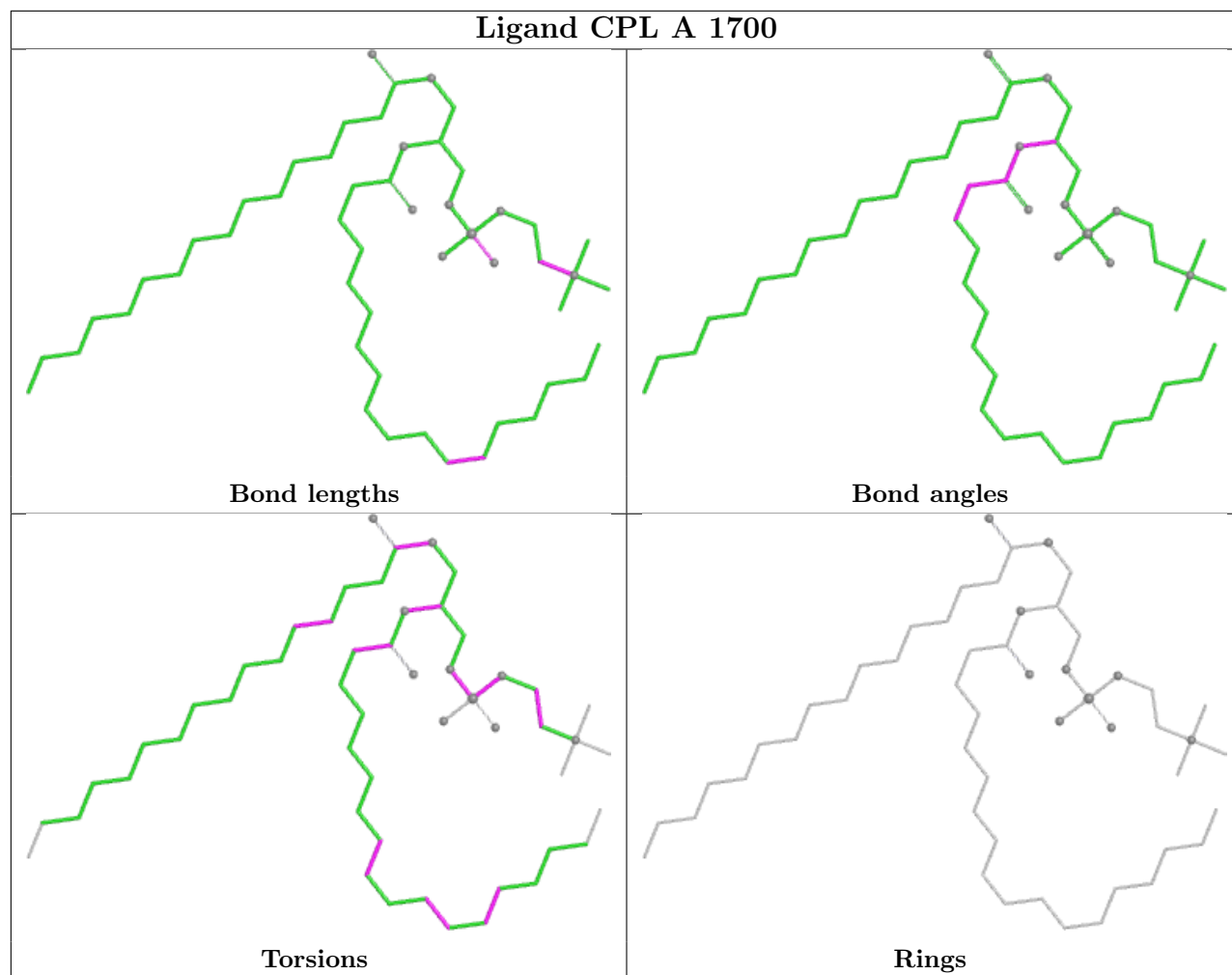


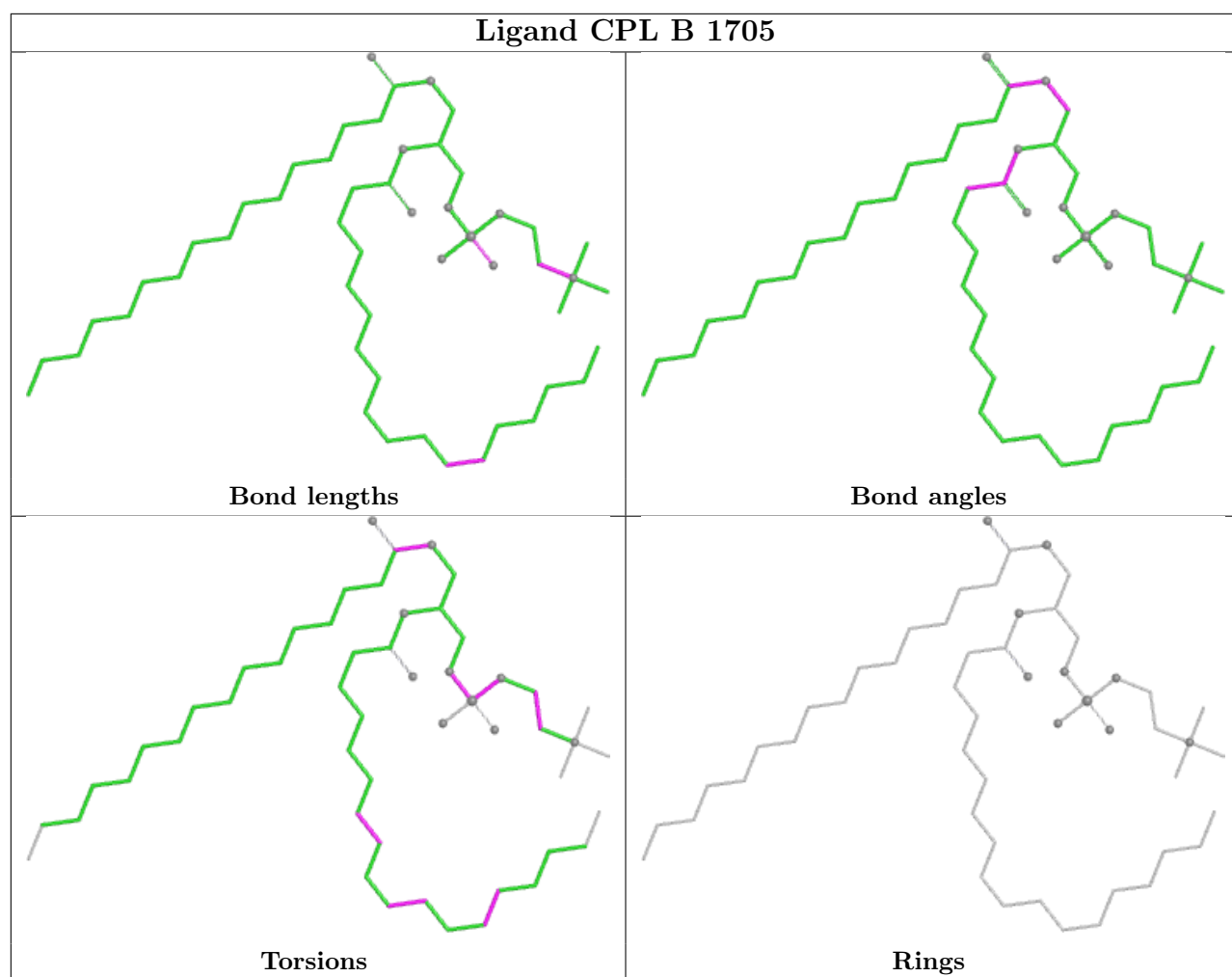


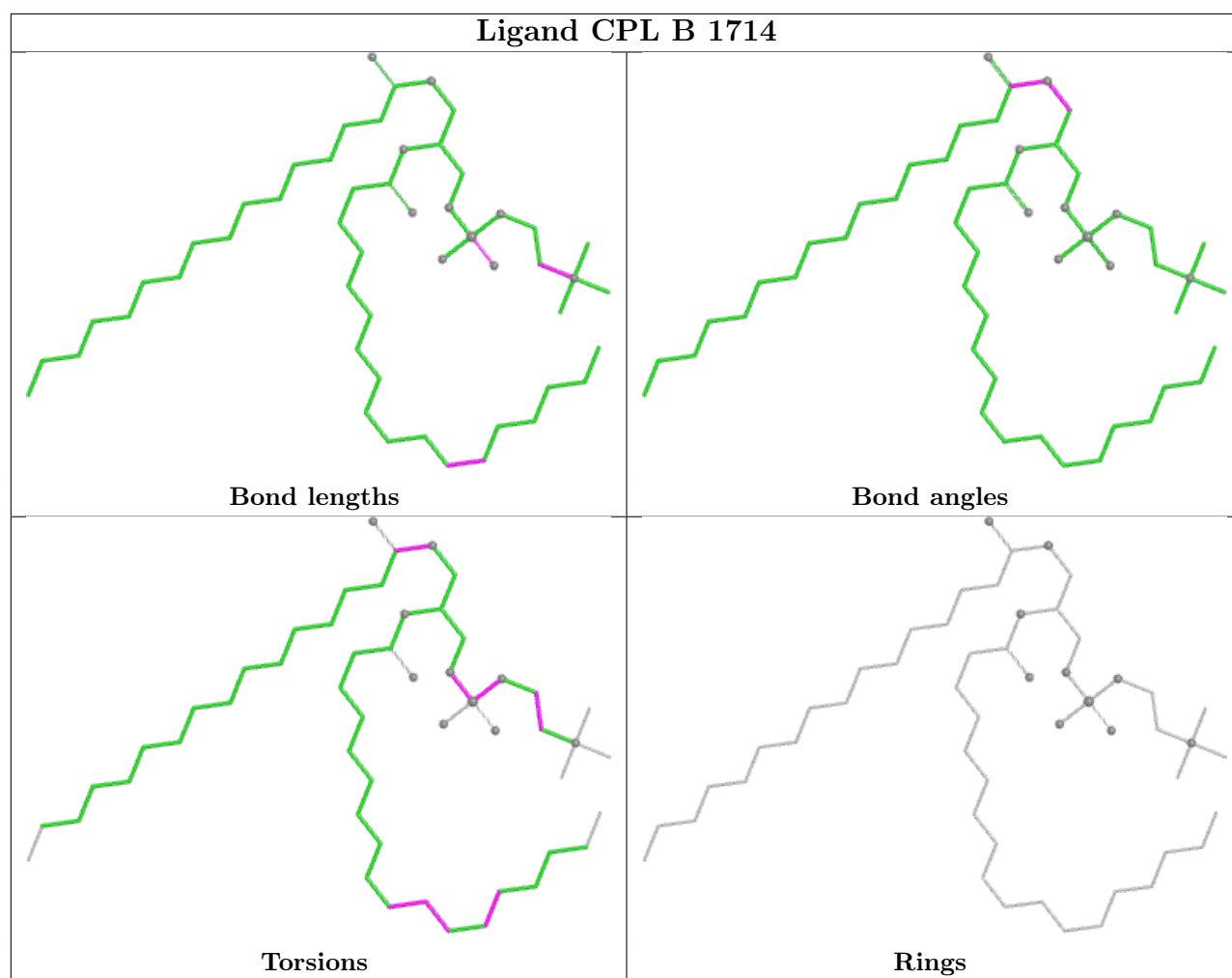


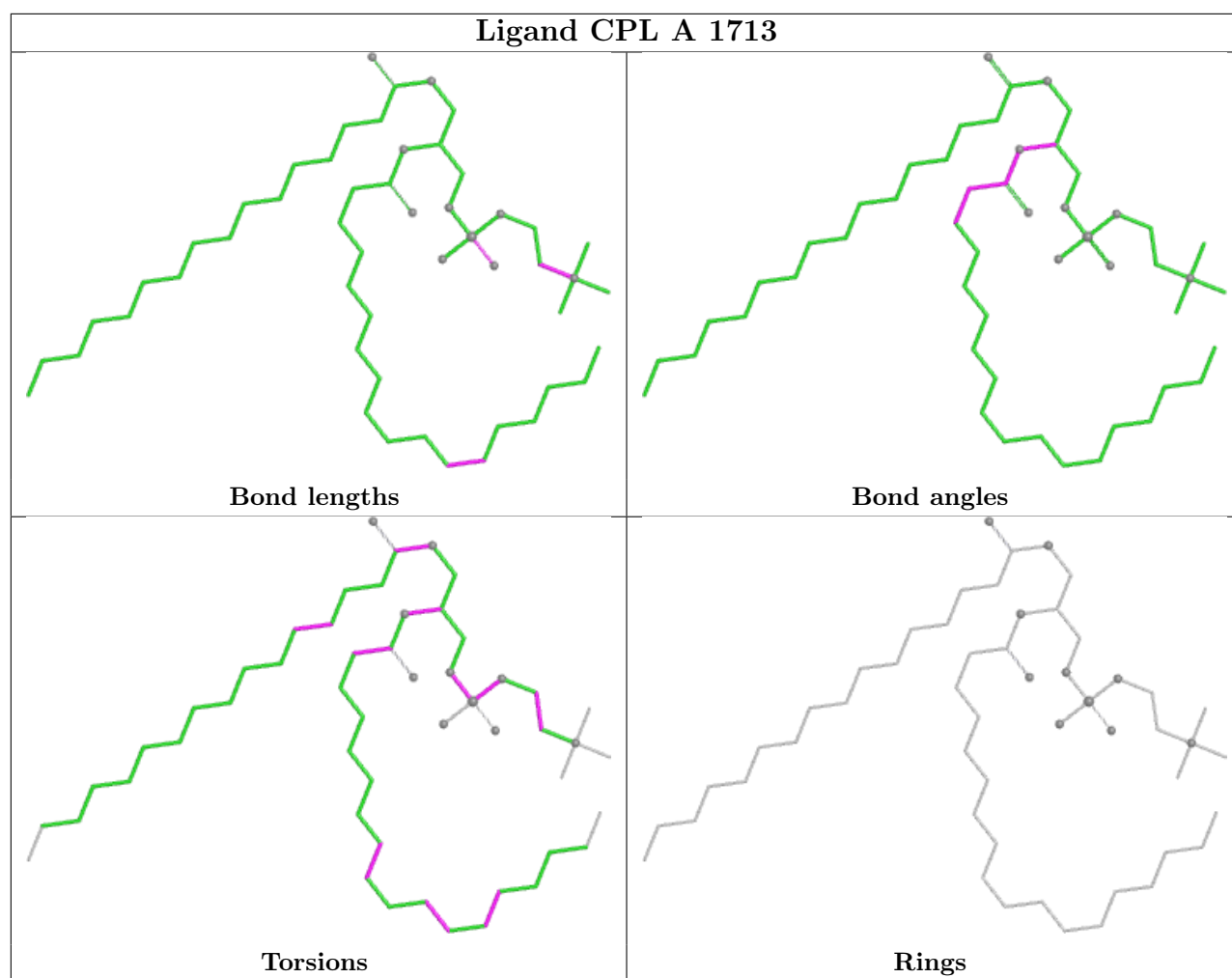


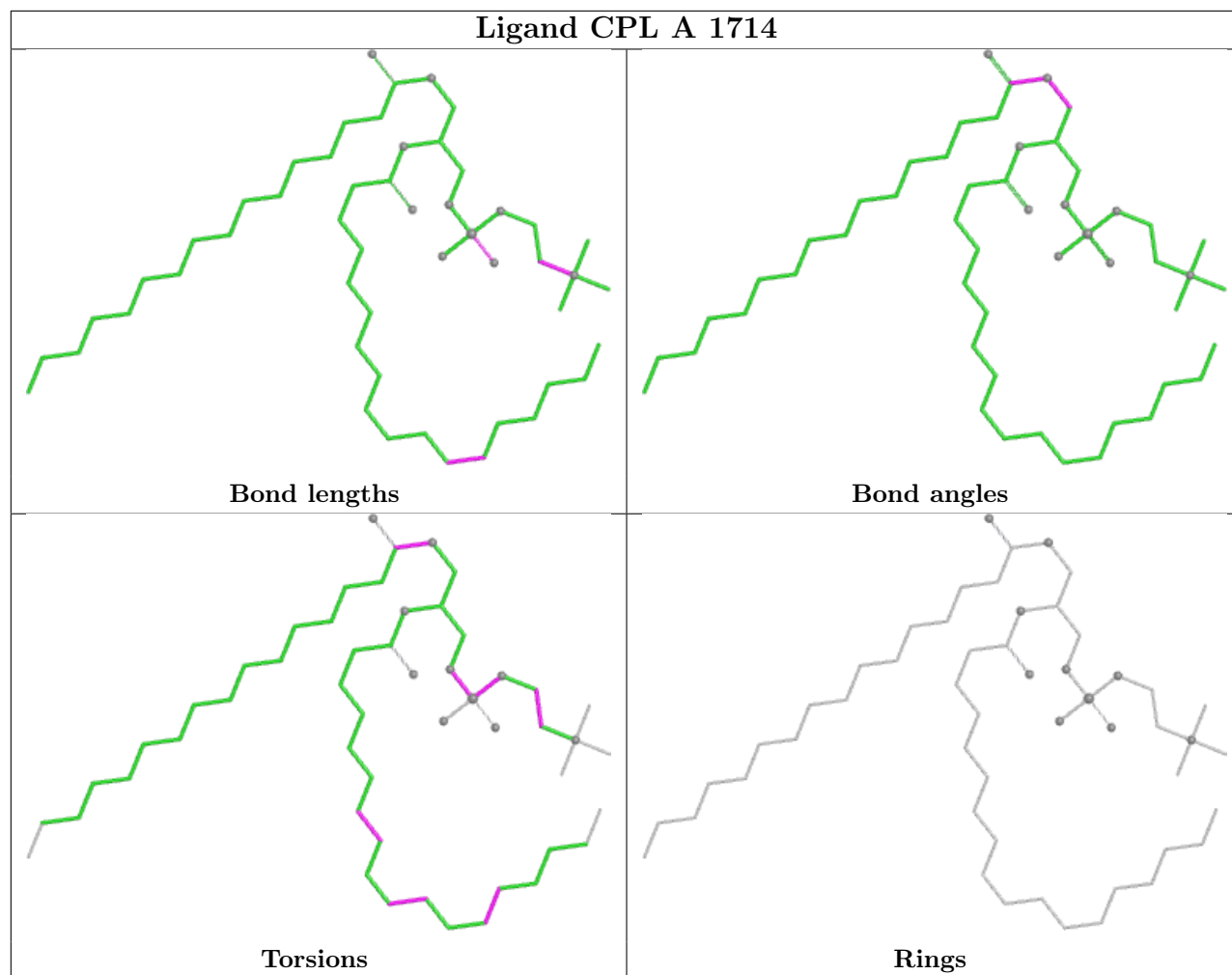


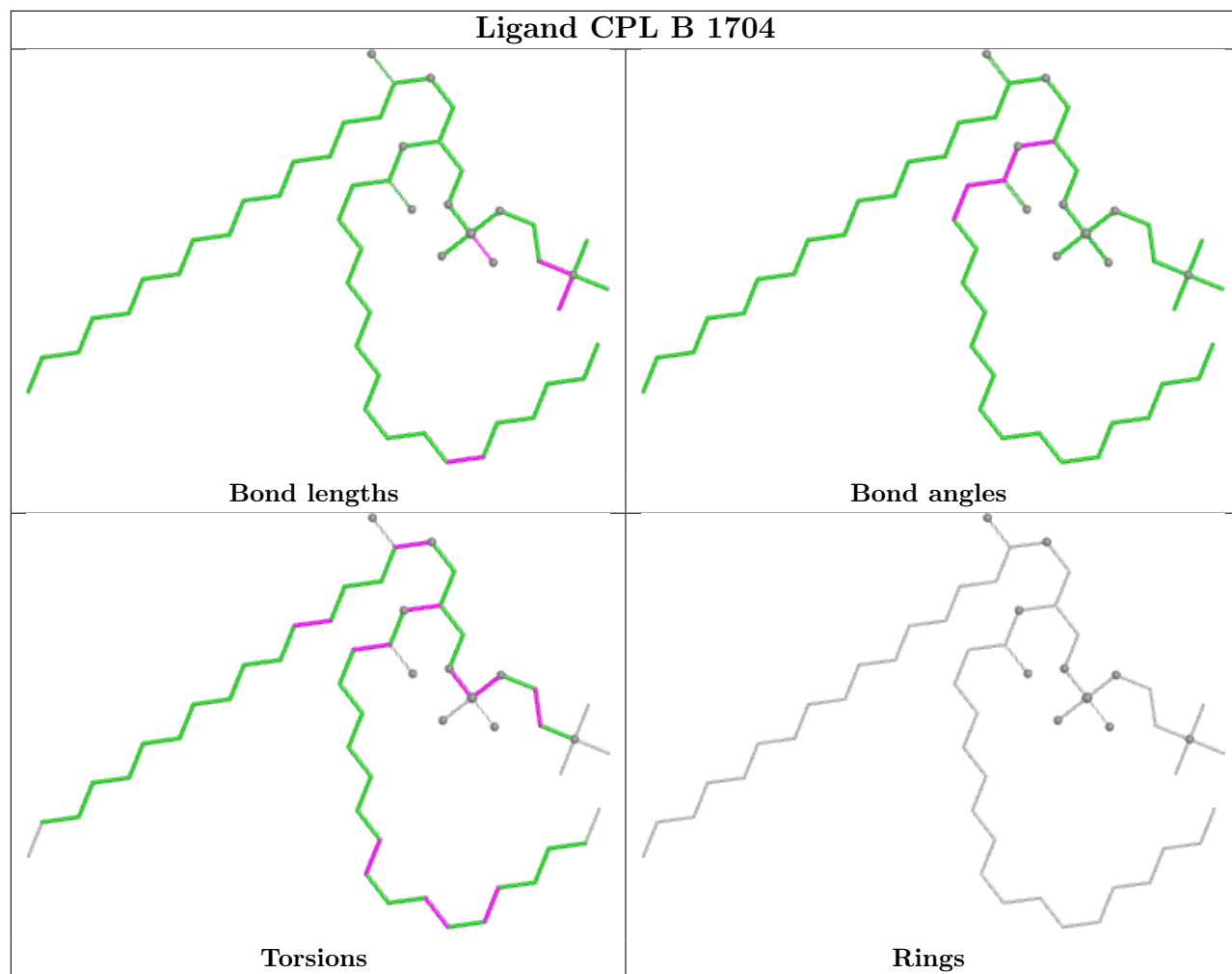


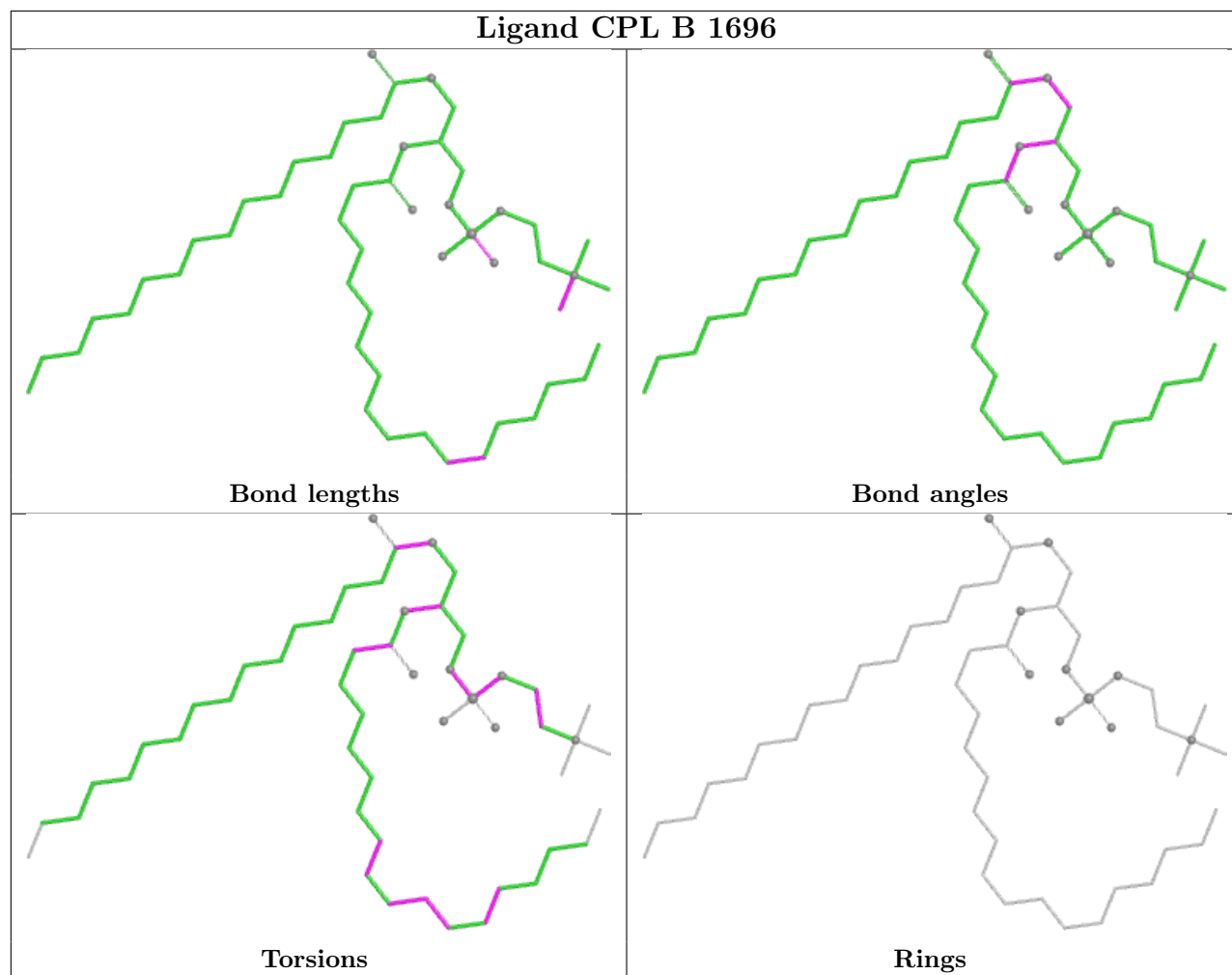


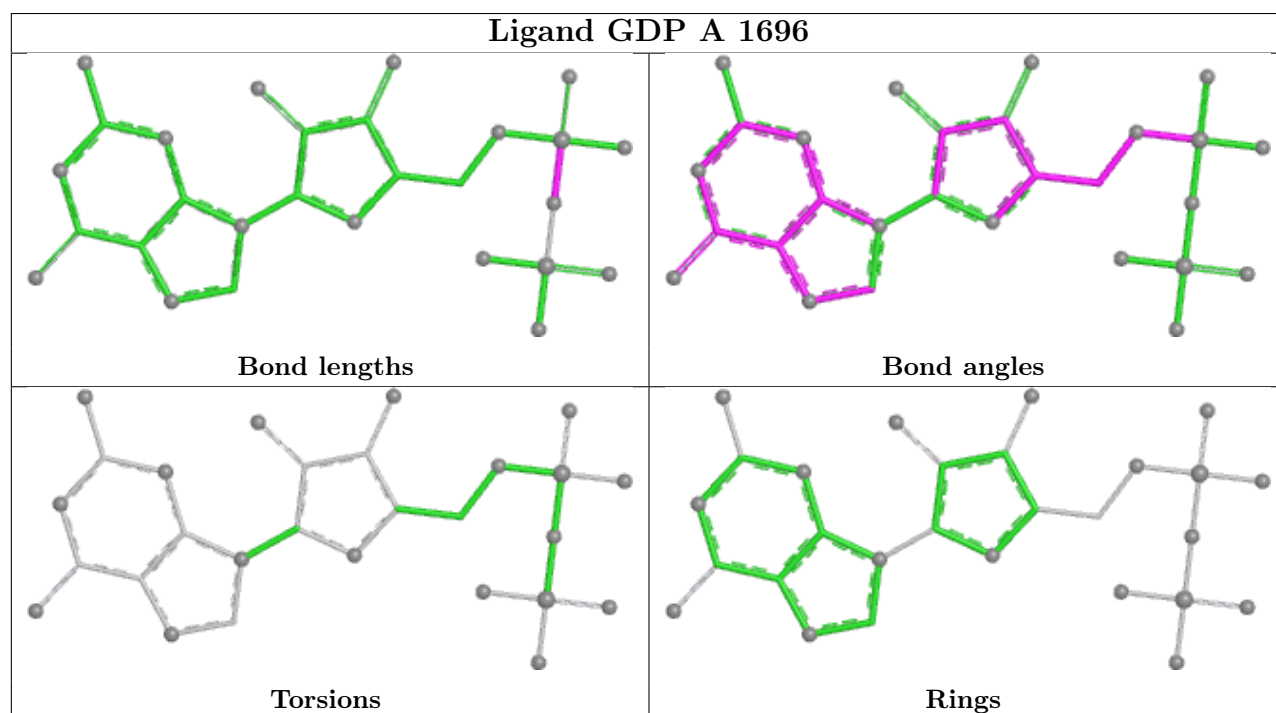
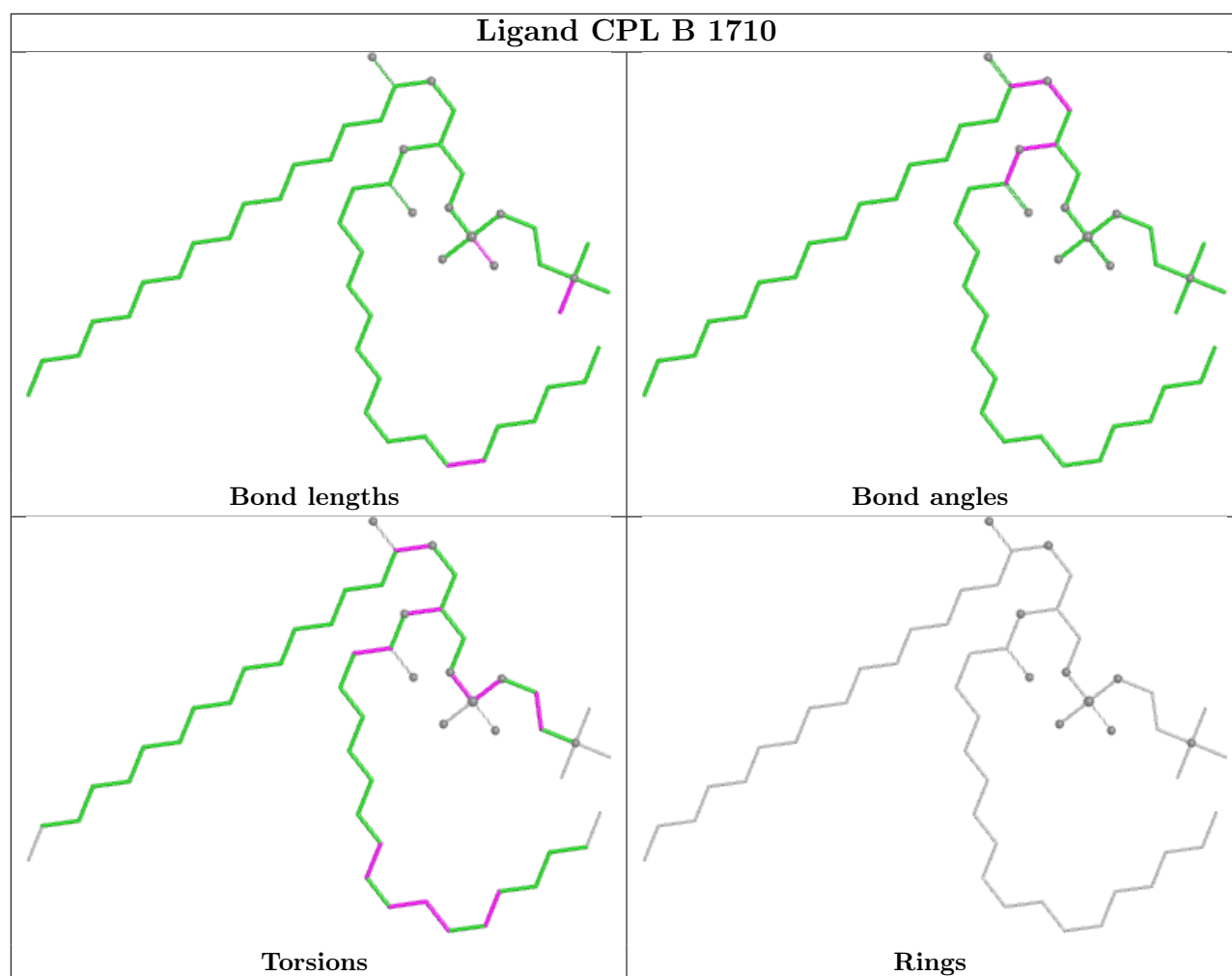


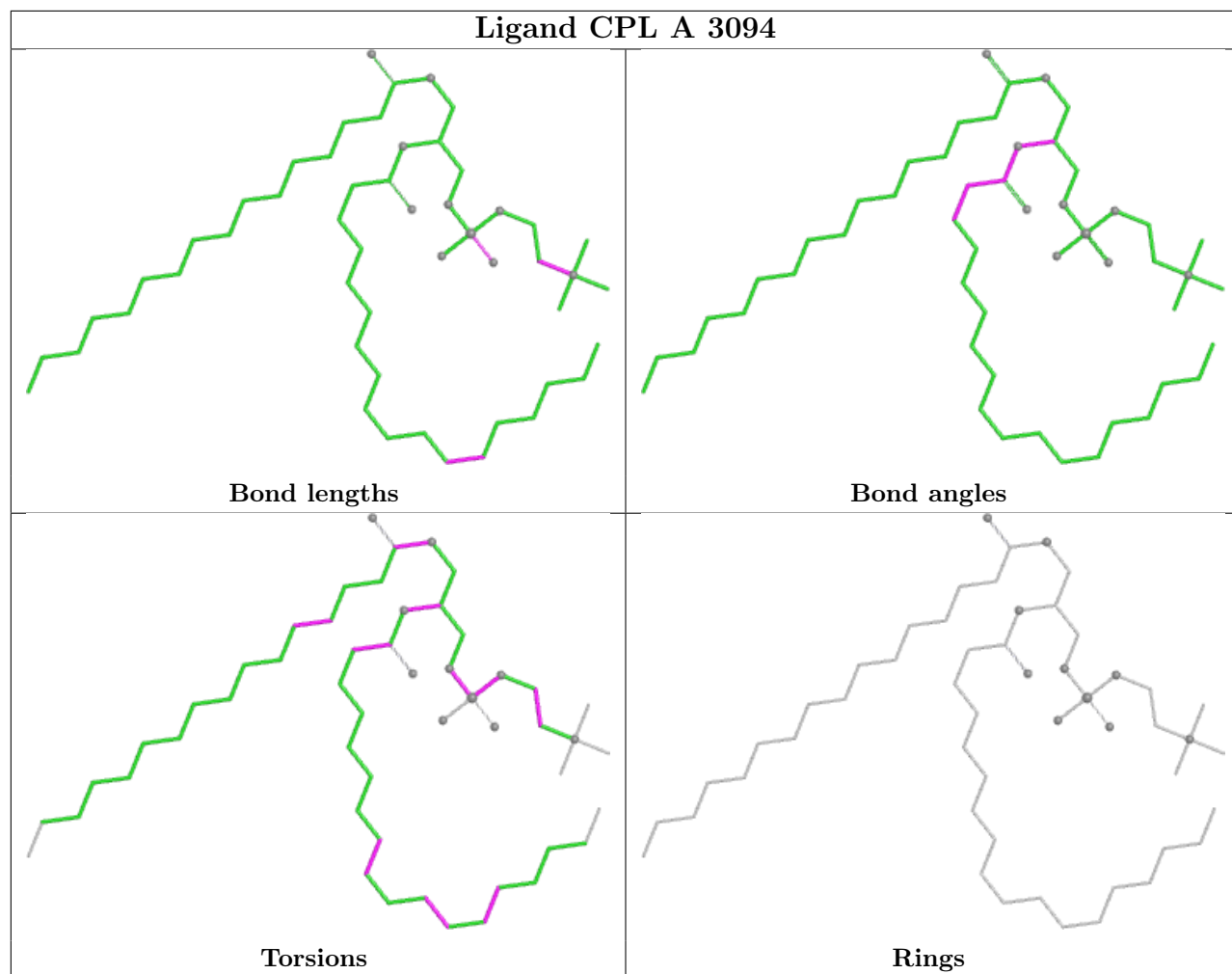


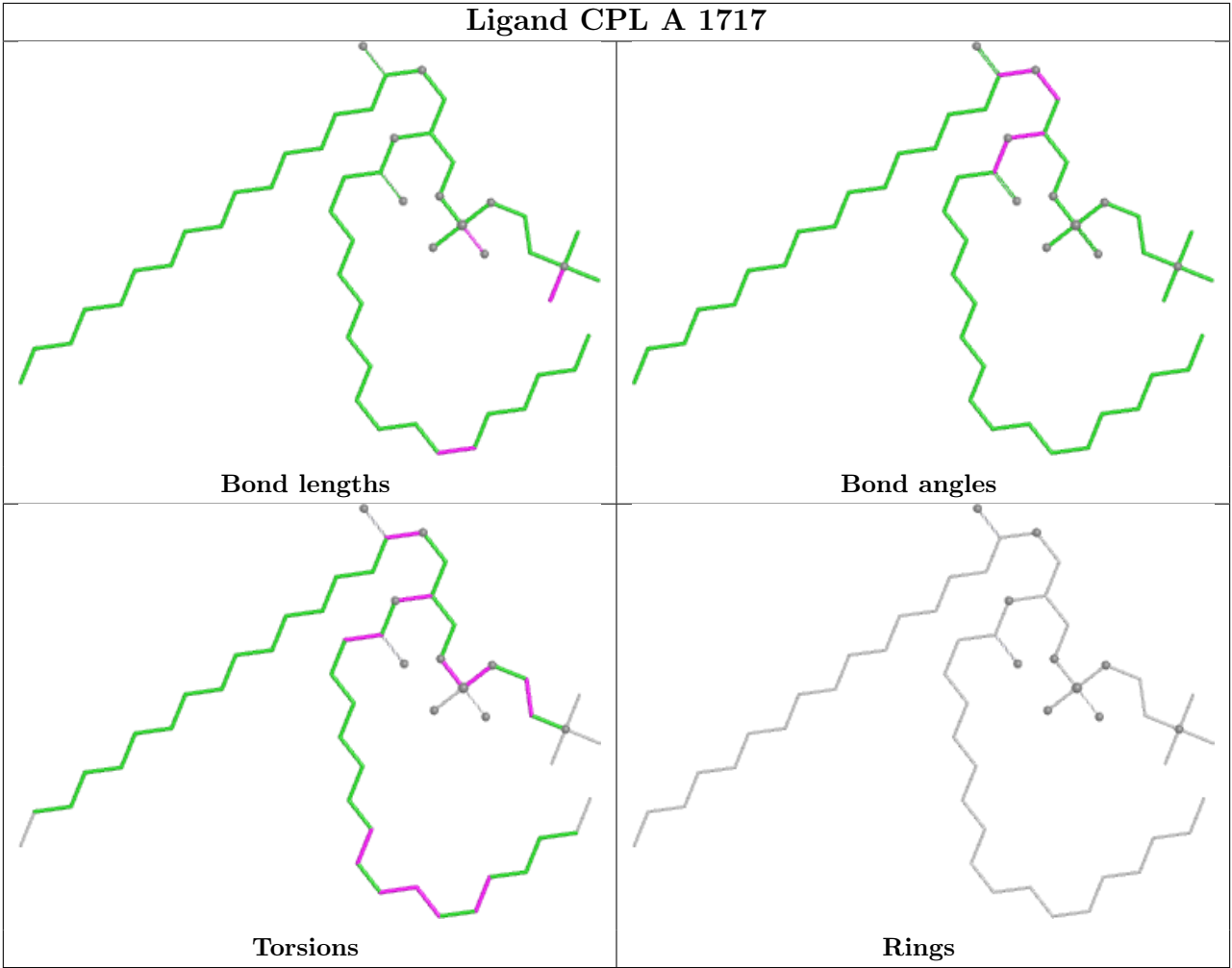












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	4
1	A	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	309:GLY	C	310:THR	N	31.27
1	A	309:GLY	C	310:THR	N	30.13

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	656:ARG	C	657:GLU	N	17.03
1	A	656:ARG	C	657:GLU	N	15.14
1	B	360:ASP	C	361:VAL	N	13.73
1	A	360:ASP	C	361:VAL	N	13.00
1	A	68:GLY	C	69:VAL	N	4.32
1	B	68:GLY	C	69:VAL	N	3.32

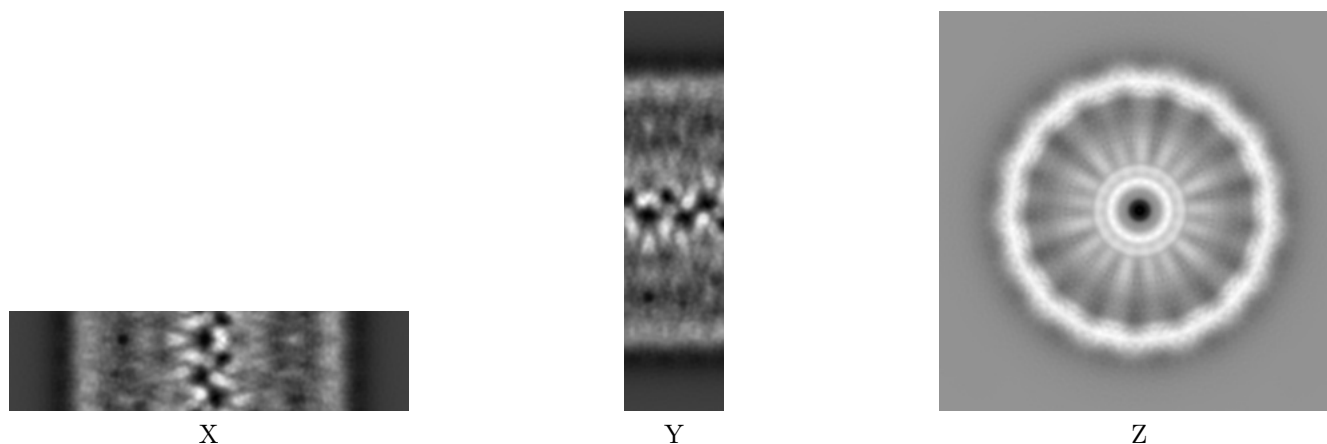
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1589. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



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

6.2 Central slices [i](#)

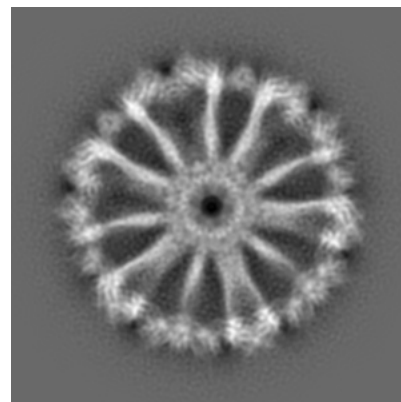
6.2.1 Primary map



X Index: 165



Y Index:
165



Z Index: 40

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

6.3 Largest variance slices [i](#)

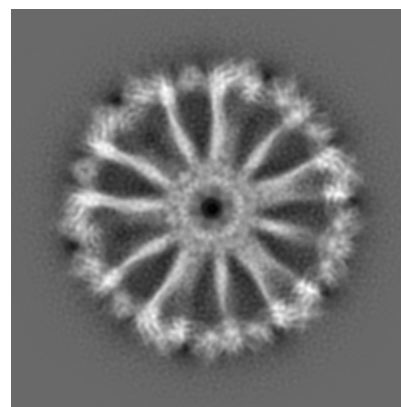
6.3.1 Primary map



X Index: 166



Y Index:
167

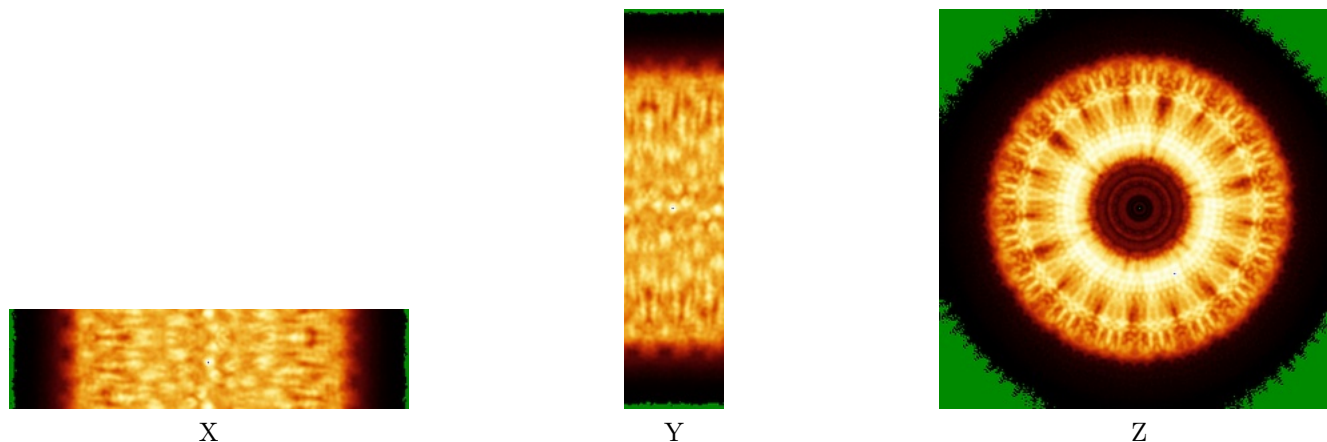


Z Index: 50

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



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](#)

This section was not generated.

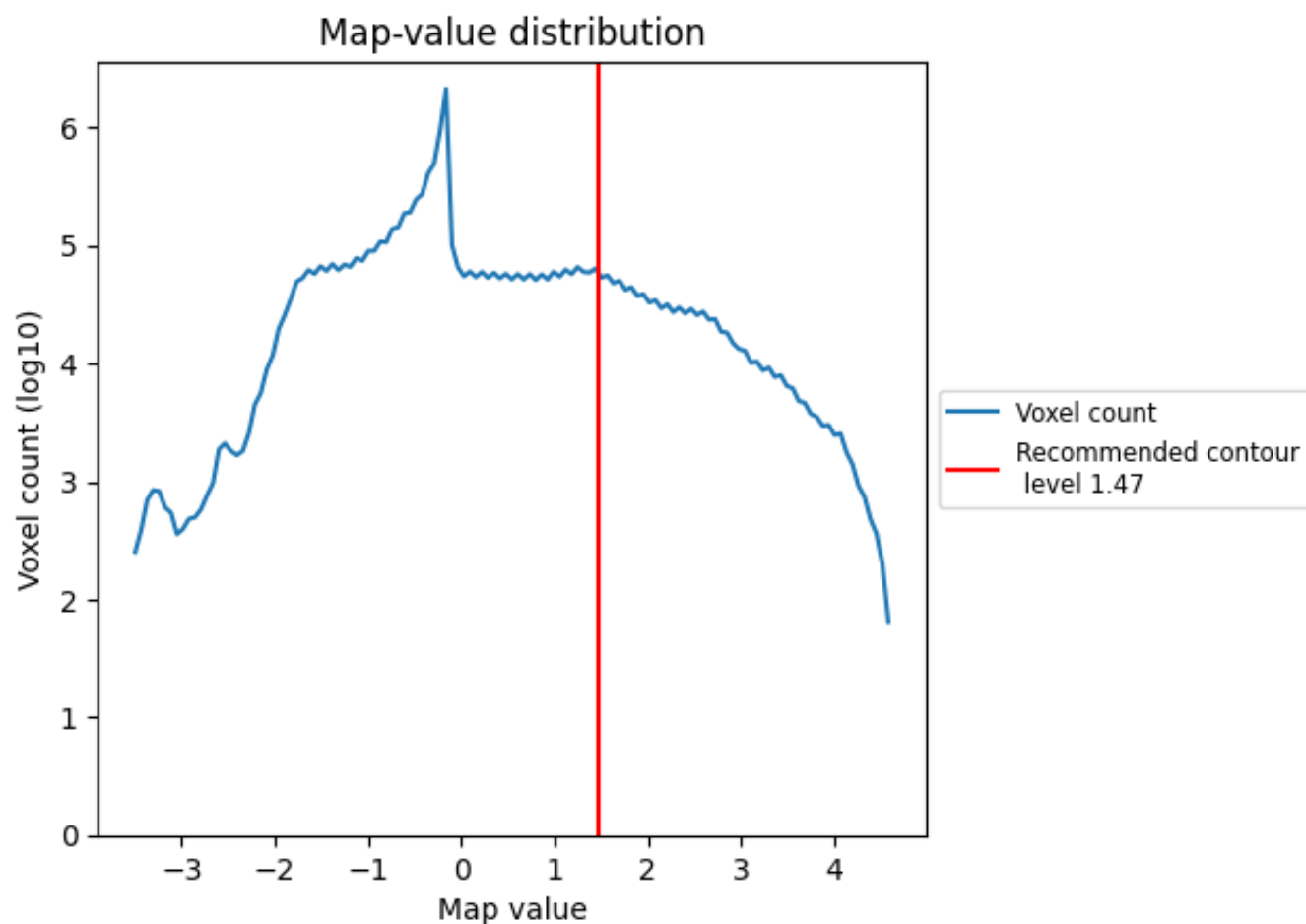
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

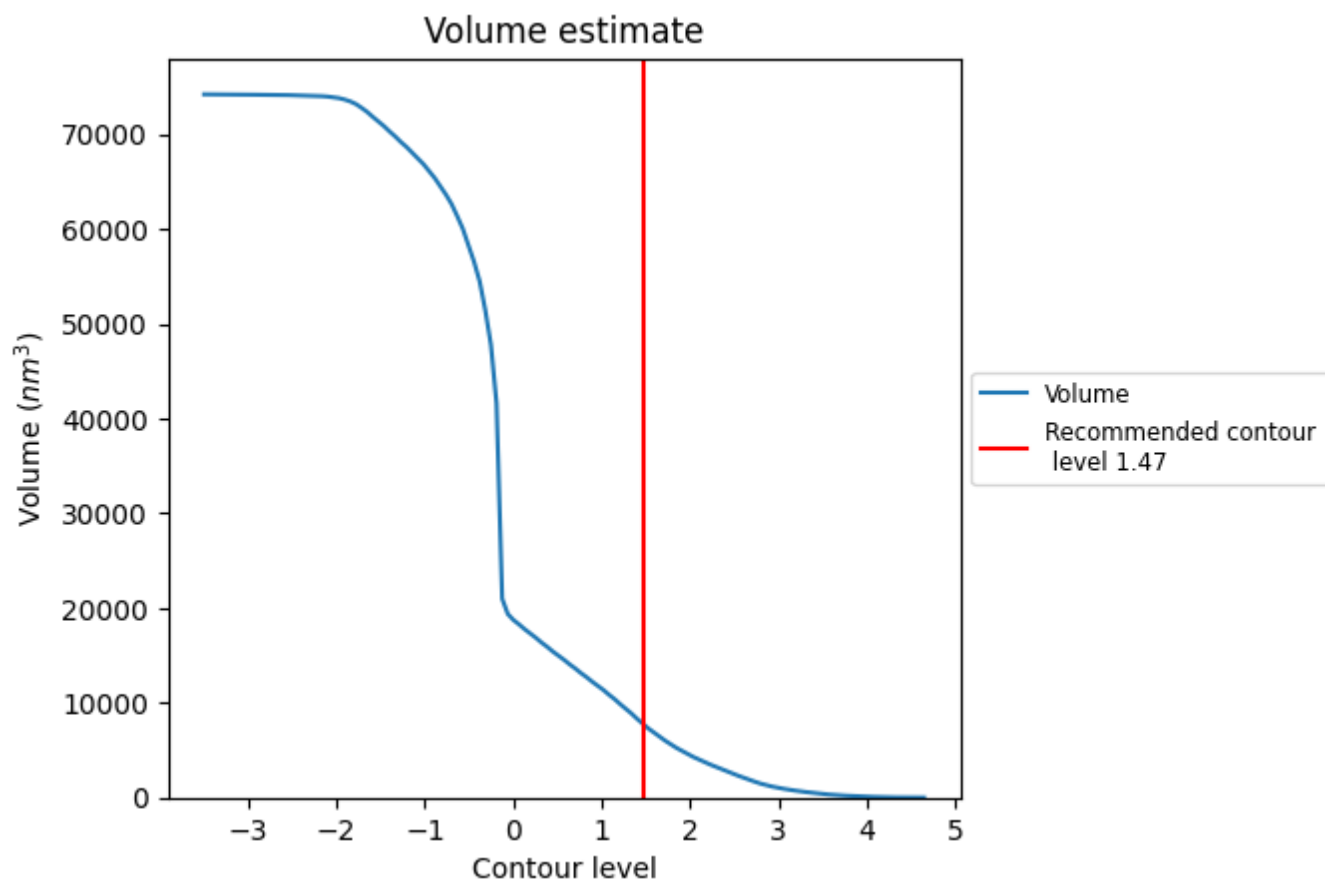
This section contains the results of statistical analysis of the map.

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 7767 nm³; this corresponds to an approximate mass of 7016 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 [i](#)

This section was not generated. The rotationally averaged power spectrum could not be displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

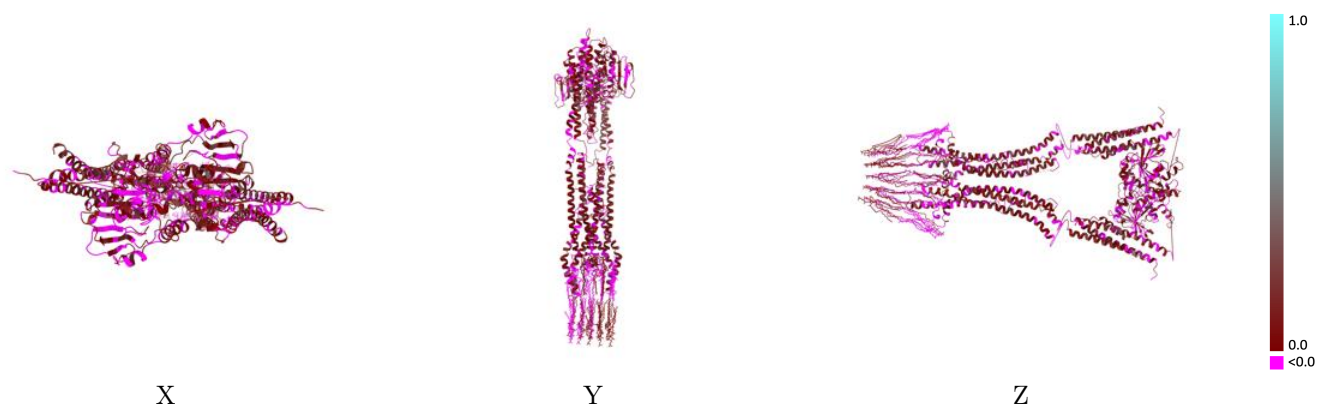
This section contains information regarding the fit between EMDB map EMD-1589 and PDB model 2W6D. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 1.47 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

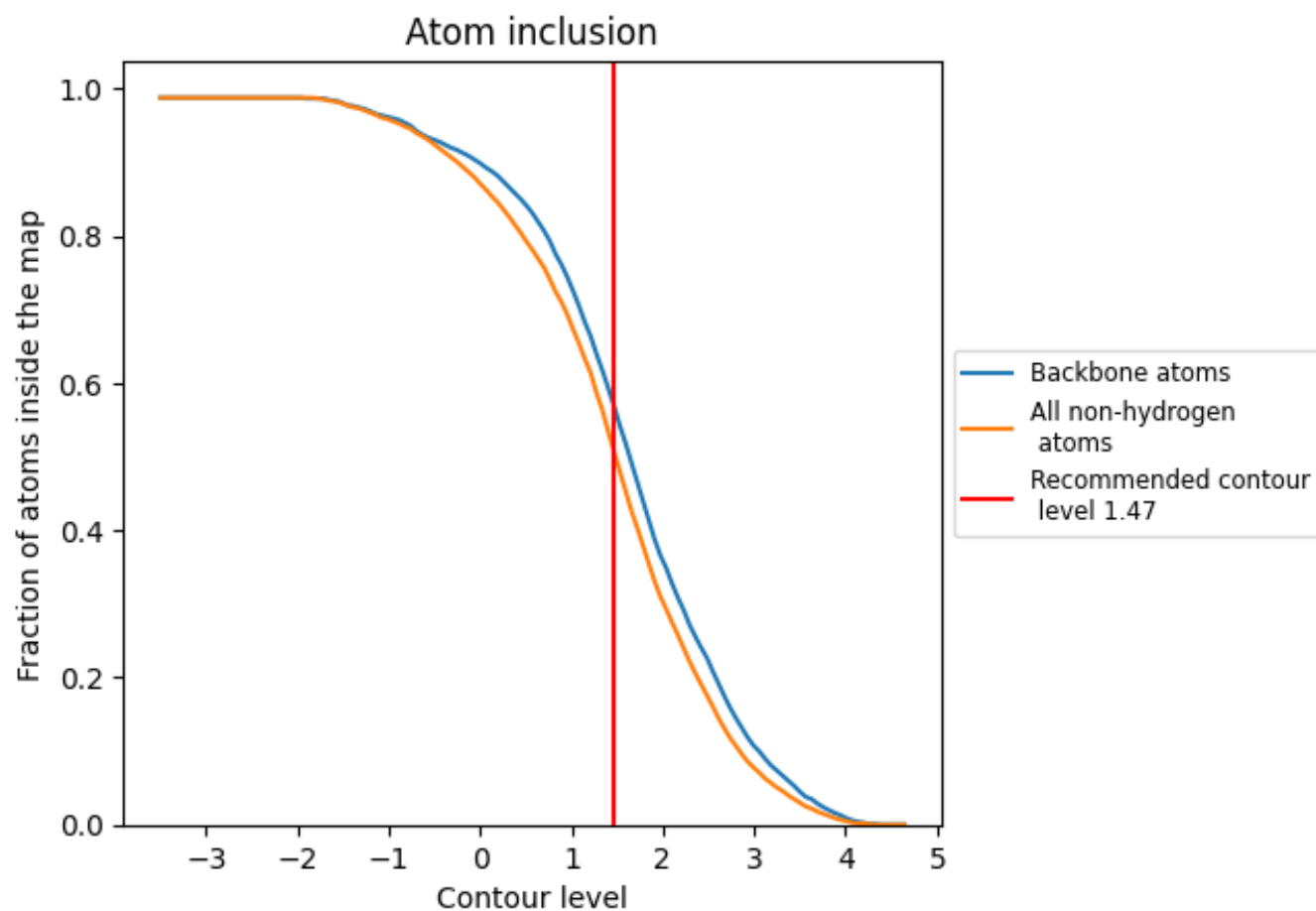


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 51% 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 (1.47) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5060	0.0410
A	0.5080	0.0390
B	0.5030	0.0430

