



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:17 PM UTC

PDB ID : 8RR0 / pdb_00008rr0
EMDB ID : EMD-19452
Title : CryoEM structure of Molybdenum bispyranopterin guanine dinucleotide formate dehydrogenases ForCE1 from *Bacillus subtilis*
Authors : Cherrier, M.V.; Arnoux, P.; Martin, L.; Nicolet, Y.; Schoehn, G.; Legrand, P.; Broc, M.; Seduk, F.; Brasseur, G.; Arias-Cartin, R.; Magalon, A.; Walburger, A.; Uzel, A.; Guigliarelli, B.; Grimaldi, S.; Pierrel, F.; Mate, M.
Deposited on : 2024-01-22
Resolution : 3.35 Å(reported)
Based on initial model : 8RQZ

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)

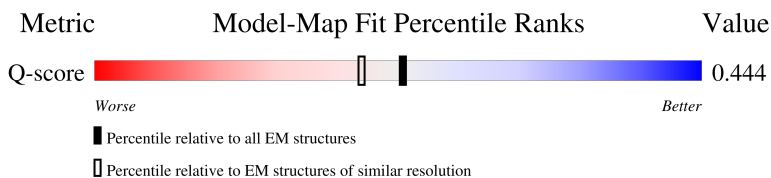
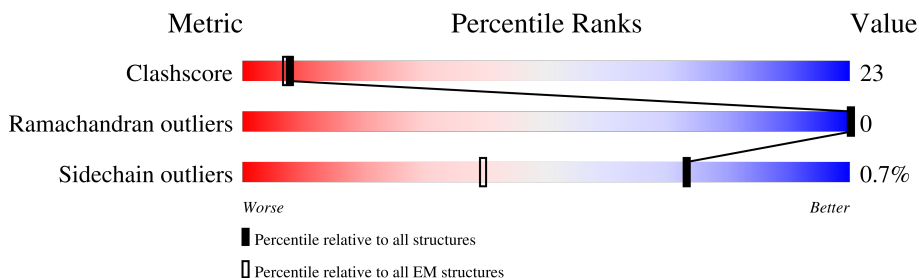
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.35 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	14390 (2.85 - 3.85)

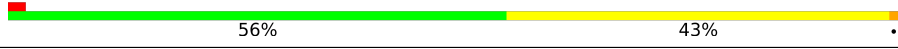
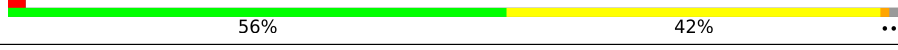
The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment 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	186	 52% 28% 20%
1	C	186	 52% 27% 20%
1	E	186	 53% 27% 20%

Continued on next page...

Validation Pipeline (wwPDB-VP) : 2.49

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	186	
2	B	985	
2	D	985	
2	F	985	
2	H	985	

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
9	SF4	B	1003	-	-	X	-
9	SF4	F	1003	-	-	X	-
9	SF4	H	1003	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 37080 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.

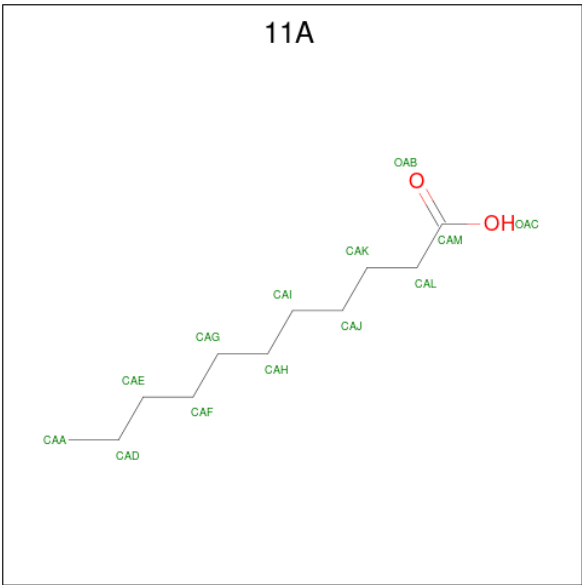
- Molecule 1 is a protein called Uncharacterized protein YjgD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	148	Total	C	N	O	S	0	0
			1166	742	201	219	4		
1	C	148	Total	C	N	O	S	0	0
			1166	742	201	219	4		
1	E	148	Total	C	N	O	S	0	0
			1166	742	201	219	4		
1	G	148	Total	C	N	O	S	0	0
			1166	742	201	219	4		

- Molecule 2 is a protein called Probable oxidoreductase YjgC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	975	Total	C	N	O	S	0	0
			7636	4794	1307	1487	48		
2	D	975	Total	C	N	O	S	0	0
			7636	4794	1307	1487	48		
2	F	975	Total	C	N	O	S	0	0
			7636	4794	1307	1487	48		
2	H	975	Total	C	N	O	S	0	0
			7636	4794	1307	1487	48		

- Molecule 3 is UNDECANOIC ACID (CCD ID: 11A) (formula: C₁₁H₂₂O₂).



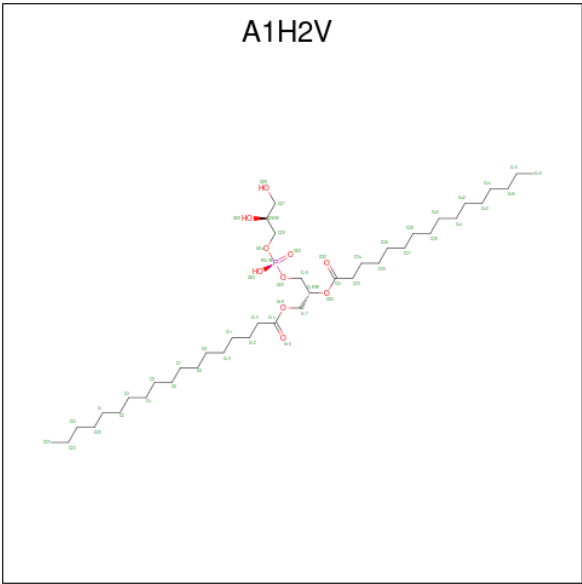
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			12	10	2	
3	A	1	Total	C	O	0
			13	11	2	
3	A	1	Total	C	O	0
			13	11	2	
3	A	1	Total	C	O	0
			13	11	2	
3	A	1	Total	C	O	0
			13	11	2	
3	A	1	Total	C	O	0
			13	11	2	
3	C	1	Total	C	O	0
			12	10	2	
3	C	1	Total	C	O	0
			13	11	2	
3	C	1	Total	C	O	0
			13	11	2	
3	C	1	Total	C	O	0
			13	11	2	
3	C	1	Total	C	O	0
			13	11	2	
3	E	1	Total	C	O	0
			12	10	2	
3	E	1	Total	C	O	0
			13	11	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
3	E	1	Total	C	O	0
			13	11	2	
3	E	1	Total	C	O	0
			13	11	2	
3	E	1	Total	C	O	0
			13	11	2	
3	E	1	Total	C	O	0
			13	11	2	
3	G	1	Total	C	O	0
			12	10	2	
3	G	1	Total	C	O	0
			13	11	2	
3	G	1	Total	C	O	0
			13	11	2	
3	G	1	Total	C	O	0
			13	11	2	
3	G	1	Total	C	O	0
			13	11	2	

- Molecule 4 is [(2 {R})-3-[[[(2 {R})-2,3-bis(oxidanyl)propoxy]-oxidanyl-phosphoryl]oxy-2-hexadecanoyloxy-propyl] octadecanoate (CCD ID: A1H2V) (formula: C₄₀H₇₉O₁₀P).



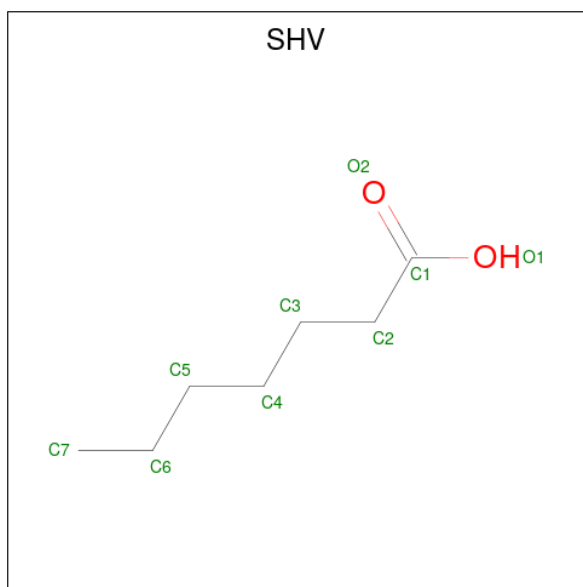
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			45	34	10	1	

Continued on next page...

Continued from previous page...

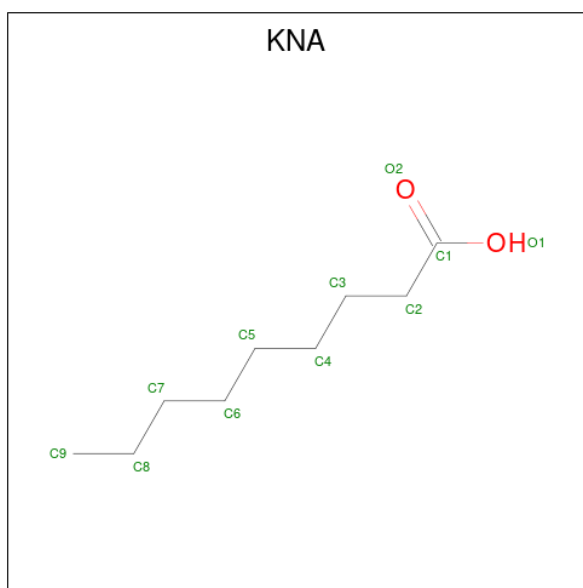
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			51	40	10	1	
4	A	1	Total	C	O	P	0
			51	40	10	1	
4	C	1	Total	C	O	P	0
			51	40	10	1	
4	C	1	Total	C	O	P	0
			45	34	10	1	
4	C	1	Total	C	O	P	0
			51	40	10	1	
4	E	1	Total	C	O	P	0
			51	40	10	1	
4	E	1	Total	C	O	P	0
			45	34	10	1	
4	E	1	Total	C	O	P	0
			51	40	10	1	
4	G	1	Total	C	O	P	0
			51	40	10	1	
4	G	1	Total	C	O	P	0
			45	34	10	1	
4	G	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 5 is HEPTANOIC ACID (CCD ID: SHV) (formula: $C_7H_{14}O_2$).



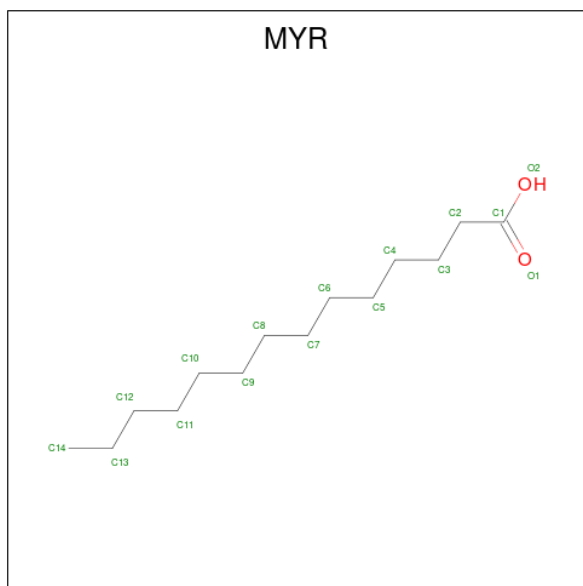
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			9	7	2	
5	A	1	Total	C	O	0
			9	7	2	
5	C	1	Total	C	O	0
			9	7	2	
5	C	1	Total	C	O	0
			9	7	2	
5	E	1	Total	C	O	0
			9	7	2	
5	E	1	Total	C	O	0
			9	7	2	
5	G	1	Total	C	O	0
			9	7	2	
5	G	1	Total	C	O	0
			9	7	2	

- Molecule 6 is nonanoic acid (CCD ID: KNA) (formula: $C_9H_{18}O_2$).



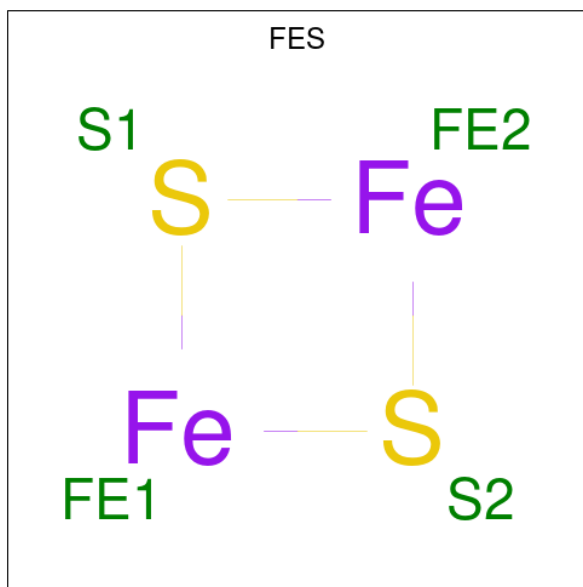
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			11	9	2	
6	C	1	Total	C	O	0
			11	9	2	
6	E	1	Total	C	O	0
			11	9	2	
6	G	1	Total	C	O	0
			11	9	2	

- Molecule 7 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



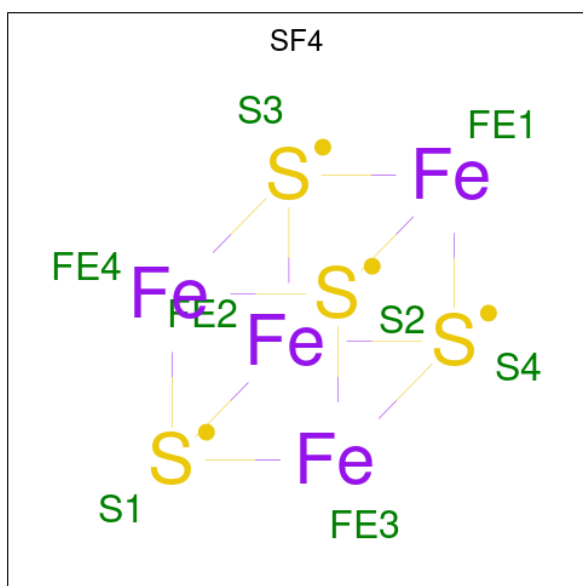
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			14	12	2	
7	C	1	Total	C	O	0
			14	12	2	
7	E	1	Total	C	O	0
			14	12	2	
7	G	1	Total	C	O	0
			14	12	2	

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



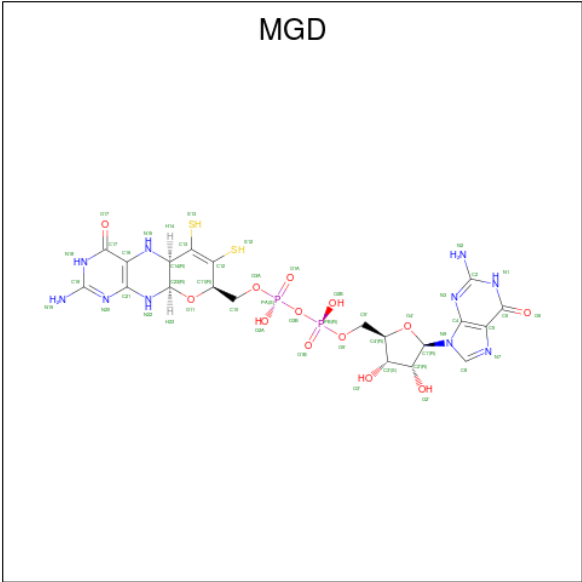
Mol	Chain	Residues	Atoms			AltConf
8	B	1	Total	Fe	S	0
			4	2	2	
8	D	1	Total	Fe	S	0
			4	2	2	
8	F	1	Total	Fe	S	0
			4	2	2	
8	H	1	Total	Fe	S	0
			4	2	2	

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
9	B	1	Total	Fe	S	0
			8	4	4	
9	B	1	Total	Fe	S	0
			8	4	4	
9	B	1	Total	Fe	S	0
			8	4	4	
9	B	1	Total	Fe	S	0
			8	4	4	
9	D	1	Total	Fe	S	0
			8	4	4	
9	D	1	Total	Fe	S	0
			8	4	4	
9	D	1	Total	Fe	S	0
			8	4	4	
9	D	1	Total	Fe	S	0
			8	4	4	
9	F	1	Total	Fe	S	0
			8	4	4	
9	F	1	Total	Fe	S	0
			8	4	4	
9	F	1	Total	Fe	S	0
			8	4	4	
9	F	1	Total	Fe	S	0
			8	4	4	
9	H	1	Total	Fe	S	0
			8	4	4	
9	H	1	Total	Fe	S	0
			8	4	4	
9	H	1	Total	Fe	S	0
			8	4	4	
9	H	1	Total	Fe	S	0
			8	4	4	

- Molecule 10 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
10	B	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	
10	B	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	
10	D	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	
10	D	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	
10	F	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	
10	F	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	
10	H	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	
10	H	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	

- Molecule 11 is MOLYBDENUM(IV) ION (CCD ID: 4MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

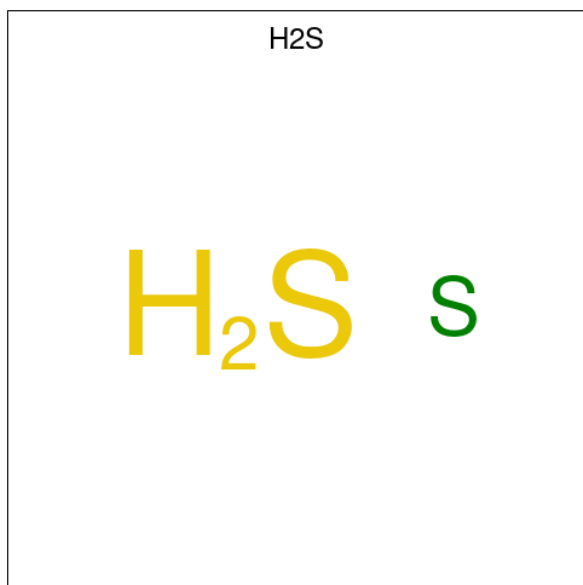
Mol	Chain	Residues	Atoms		AltConf
11	B	1	Total	Mo	0
			1	1	
11	D	1	Total	Mo	0
			1	1	
11	F	1	Total	Mo	0
			1	1	

Continued on next page...

Continued from previous page...

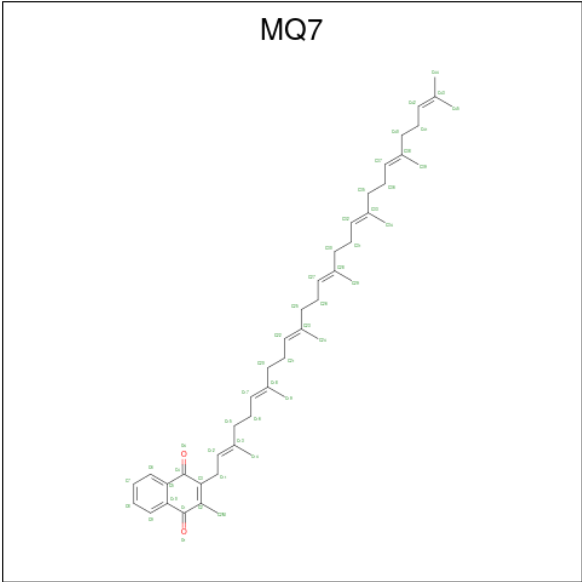
Mol	Chain	Residues	Atoms		AltConf
11	H	1	Total	Mo	0
			1	1	

- Molecule 12 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
12	B	1	Total	S	0
			1	1	
12	D	1	Total	S	0
			1	1	
12	F	1	Total	S	0
			1	1	
12	H	1	Total	S	0
			1	1	

- Molecule 13 is MENAQUINONE-7 (CCD ID: MQ7) (formula: C₄₆H₆₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
13	B	1	Total	C	O	0
			48	46	2	
13	D	1	Total	C	O	0
			48	46	2	
13	F	1	Total	C	O	0
			48	46	2	
13	H	1	Total	C	O	0
			48	46	2	

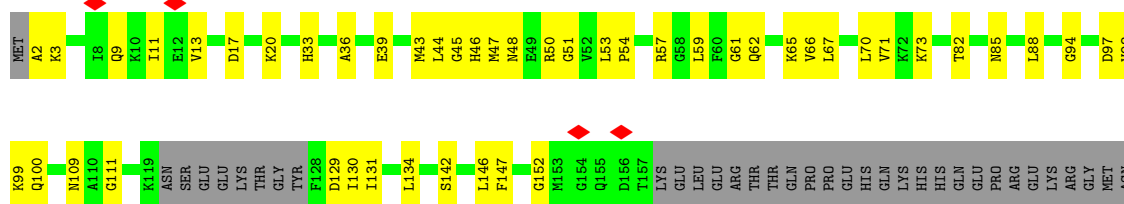
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		AltConf
14	B	21	Total	O	0
			21	21	
14	D	21	Total	O	0
			21	21	
14	F	21	Total	O	0
			21	21	
14	H	21	Total	O	0
			21	21	

LYS
ARG
ASP

• Molecule 1: Uncharacterized protein YjgD

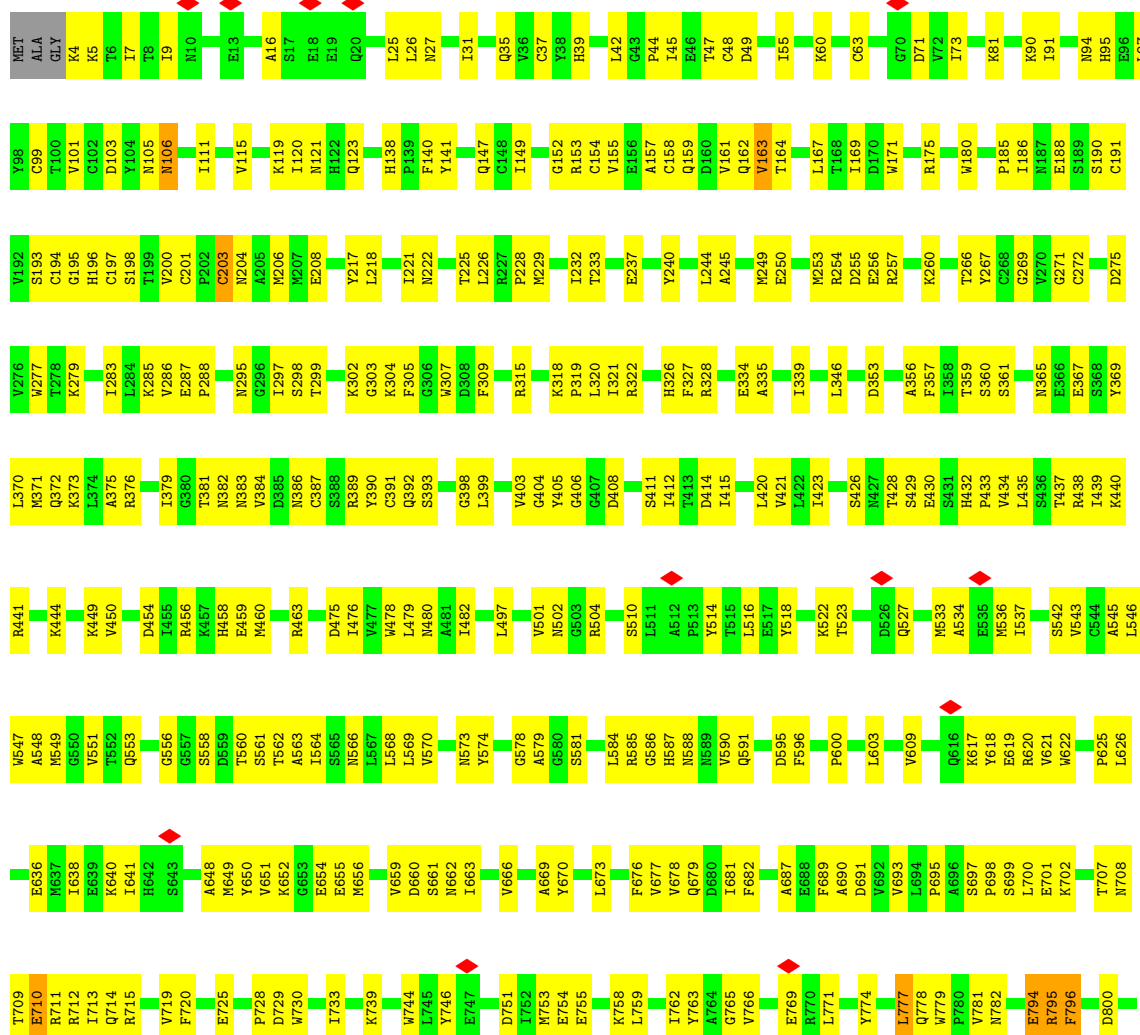
Chain G:  54% 26% 20%

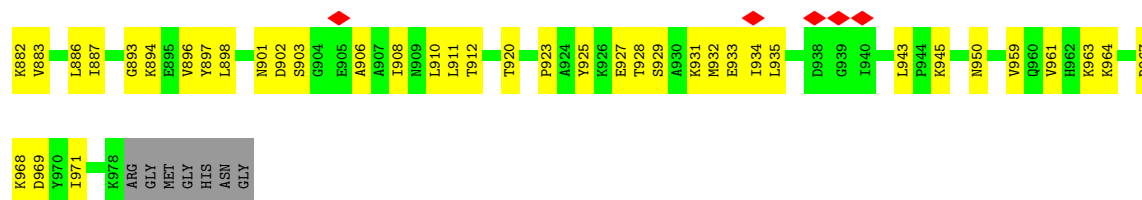


LYS
ARG
ASP

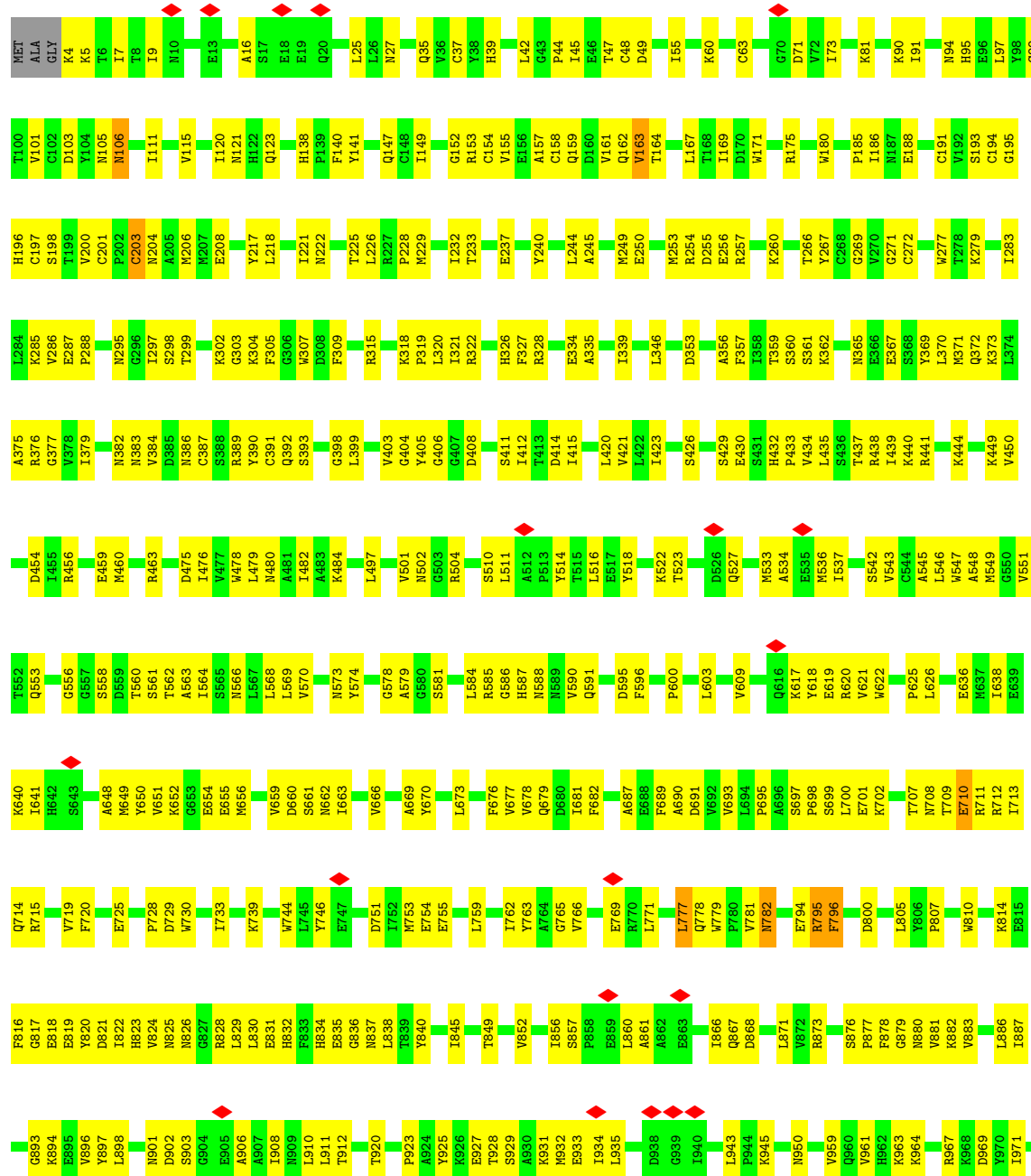
• Molecule 2: Probable oxidoreductase YjgC

Chain B:  56% 43% ..





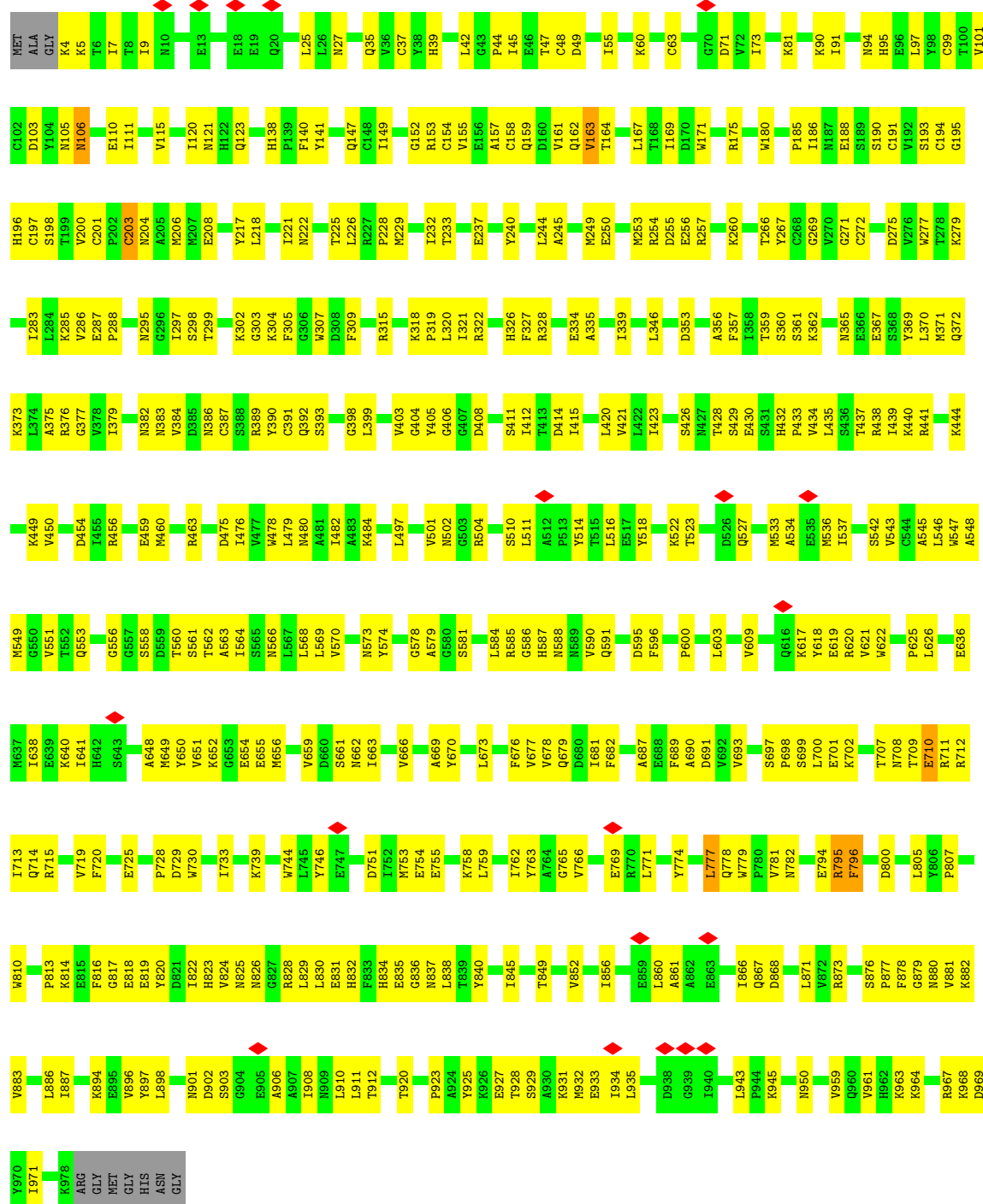
• Molecule 2: Probable oxidoreductase YjgC



K978
ARG
GLY
MET
GLY
HIS
ASN
GLY

• Molecule 2: Probable oxidoreductase YjgC

Chain H:  56% 42% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	112095	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	45000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.409	Depositor
Minimum map value	-0.669	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	352.0, 352.0, 352.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MQ7, A1H2V, SF4, 11A, SHV, MYR, MGD, FES, KNA, 4MO, H2S

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	0.11	0/1175	0.29	0/1574
1	C	0.11	0/1175	0.29	0/1574
1	E	0.11	0/1175	0.29	0/1574
1	G	0.11	0/1175	0.29	0/1574
2	B	0.28	0/7797	0.54	8/10558 (0.1%)
2	D	0.28	0/7797	0.54	8/10558 (0.1%)
2	F	0.28	0/7797	0.54	8/10558 (0.1%)
2	H	0.28	0/7797	0.54	8/10558 (0.1%)
All	All	0.26	0/35888	0.51	32/48528 (0.1%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	106	ASN	N-CA-C	-8.07	102.99	112.92
2	D	106	ASN	N-CA-C	-8.07	102.99	112.92
2	H	106	ASN	N-CA-C	-8.07	102.99	112.92
2	F	106	ASN	N-CA-C	-8.05	103.02	112.92
2	B	164	THR	N-CA-C	-6.53	104.01	112.23
2	D	164	THR	N-CA-C	-6.53	104.01	112.23
2	F	164	THR	N-CA-C	-6.53	104.01	112.23
2	H	164	THR	N-CA-C	-6.53	104.01	112.23
2	B	777	LEU	CA-C-N	-5.26	115.68	123.05
2	B	777	LEU	C-N-CA	-5.26	115.68	123.05
2	D	777	LEU	CA-C-N	-5.26	115.68	123.05
2	D	777	LEU	C-N-CA	-5.26	115.68	123.05
2	F	777	LEU	CA-C-N	-5.26	115.68	123.05
2	F	777	LEU	C-N-CA	-5.26	115.68	123.05
2	H	777	LEU	CA-C-N	-5.26	115.68	123.05
2	H	777	LEU	C-N-CA	-5.26	115.68	123.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	796	PHE	CA-C-N	5.23	124.89	119.56
2	B	796	PHE	C-N-CA	5.23	124.89	119.56
2	D	796	PHE	CA-C-N	5.23	124.89	119.56
2	D	796	PHE	C-N-CA	5.23	124.89	119.56
2	F	796	PHE	CA-C-N	5.23	124.89	119.56
2	F	796	PHE	C-N-CA	5.23	124.89	119.56
2	H	796	PHE	CA-C-N	5.23	124.89	119.56
2	H	796	PHE	C-N-CA	5.23	124.89	119.56
2	B	105	ASN	CB-CA-C	-5.23	103.59	112.00
2	D	105	ASN	CB-CA-C	-5.23	103.59	112.00
2	F	105	ASN	CB-CA-C	-5.23	103.59	112.00
2	H	105	ASN	CB-CA-C	-5.23	103.59	112.00
2	B	710	GLU	N-CA-C	-5.16	107.15	112.93
2	D	710	GLU	N-CA-C	-5.16	107.15	112.93
2	H	710	GLU	N-CA-C	-5.16	107.15	112.93
2	F	710	GLU	N-CA-C	-5.15	107.17	112.93

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	1166	0	1237	59	0
1	C	1166	0	1237	60	0
1	E	1166	0	1237	55	0
1	G	1166	0	1237	55	0
2	B	7636	0	7467	380	0
2	D	7636	0	7467	379	0
2	F	7636	0	7467	370	0
2	H	7636	0	7467	370	0
3	A	77	0	121	4	0
3	C	77	0	121	3	0
3	E	77	0	121	3	0
3	G	77	0	121	3	0
4	A	147	0	0	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	147	0	0	6	0
4	E	147	0	0	6	0
4	G	147	0	0	6	0
5	A	18	0	26	0	0
5	C	18	0	26	0	0
5	E	18	0	26	0	0
5	G	18	0	26	0	0
6	A	11	0	17	0	0
6	C	11	0	17	0	0
6	E	11	0	17	0	0
6	G	11	0	17	0	0
7	A	14	0	20	2	0
7	C	14	0	20	2	0
7	E	14	0	20	2	0
7	G	14	0	20	2	0
8	B	4	0	0	1	0
8	D	4	0	0	1	0
8	F	4	0	0	1	0
8	H	4	0	0	1	0
9	B	32	0	0	5	0
9	D	32	0	0	4	0
9	F	32	0	0	5	0
9	H	32	0	0	5	0
10	B	94	0	44	20	0
10	D	94	0	44	22	0
10	F	94	0	44	22	0
10	H	94	0	44	22	0
11	B	1	0	0	0	0
11	D	1	0	0	0	0
11	F	1	0	0	0	0
11	H	1	0	0	0	0
12	B	1	0	0	1	0
12	D	1	0	0	1	0
12	F	1	0	0	1	0
12	H	1	0	0	1	0
13	B	48	0	64	2	0
13	D	48	0	64	2	0
13	F	48	0	64	2	0
13	H	48	0	64	2	0
14	B	21	0	0	0	0
14	D	21	0	0	0	0
14	F	21	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	H	21	0	0	0	0
All	All	37080	0	35984	1647	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 23.

All (1647) 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)
2:B:387:CYS:SG	12:B:1009:H2S:S	2.30	1.30
2:H:387:CYS:SG	12:H:1009:H2S:S	2.30	1.30
2:D:387:CYS:SG	12:D:1009:H2S:S	2.30	1.29
2:F:387:CYS:SG	12:F:1009:H2S:S	2.30	1.27
2:B:387:CYS:SG	2:B:587:HIS:HD2	1.81	1.03
2:F:387:CYS:SG	2:F:587:HIS:HD2	1.81	1.03
2:H:387:CYS:SG	2:H:587:HIS:HD2	1.81	1.03
2:D:387:CYS:SG	2:D:587:HIS:HD2	1.81	1.02
2:F:766:VAL:HG13	2:F:781:VAL:HG11	1.44	0.99
2:H:766:VAL:HG13	2:H:781:VAL:HG11	1.44	0.99
2:D:766:VAL:HG13	2:D:781:VAL:HG11	1.44	0.96
2:B:766:VAL:HG13	2:B:781:VAL:HG11	1.44	0.96
2:B:361:SER:OG	2:B:387:CYS:SG	2.26	0.94
2:F:361:SER:OG	2:F:387:CYS:SG	2.26	0.94
2:D:361:SER:OG	2:D:387:CYS:SG	2.26	0.93
2:H:361:SER:OG	2:H:387:CYS:SG	2.26	0.93
2:F:387:CYS:SG	2:F:587:HIS:CD2	2.65	0.90
2:H:387:CYS:SG	2:H:587:HIS:CD2	2.65	0.89
2:B:387:CYS:SG	2:B:587:HIS:CD2	2.65	0.89
2:D:387:CYS:SG	2:D:587:HIS:CD2	2.65	0.88
1:C:43:MET:HE1	1:E:57:ARG:HB2	1.57	0.87
1:A:57:ARG:HB2	1:G:43:MET:HE1	1.57	0.87
1:E:43:MET:HE1	1:G:57:ARG:HB2	1.57	0.87
2:D:873:ARG:HH22	2:D:880:ASN:HD21	1.23	0.86
1:A:43:MET:HE1	1:C:57:ARG:HB2	1.57	0.86
4:A:203:A1H2V:O29	4:G:205:A1H2V:C25	2.24	0.86
4:E:205:A1H2V:C25	4:G:205:A1H2V:O29	2.24	0.86
4:C:205:A1H2V:C25	4:E:205:A1H2V:O29	2.24	0.85
2:B:873:ARG:HH22	2:B:880:ASN:HD21	1.23	0.85
4:A:203:A1H2V:C25	4:C:205:A1H2V:O29	2.24	0.85
2:H:826:ASN:HB3	2:H:908:ILE:HG12	1.59	0.85
2:F:826:ASN:HB3	2:F:908:ILE:HG12	1.59	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:856:ILE:HD13	2:F:866:ILE:HG21	1.59	0.84
2:H:856:ILE:HD13	2:H:866:ILE:HG21	1.59	0.84
2:F:873:ARG:HH22	2:F:880:ASN:HD21	1.23	0.84
2:H:663:ILE:HD11	2:H:910:LEU:HD12	1.60	0.83
2:B:826:ASN:HB3	2:B:908:ILE:HG12	1.59	0.83
2:B:856:ILE:HD13	2:B:866:ILE:HG21	1.59	0.83
2:D:663:ILE:HD11	2:D:910:LEU:HD12	1.60	0.83
2:D:826:ASN:HB3	2:D:908:ILE:HG12	1.59	0.83
2:B:663:ILE:HD11	2:B:910:LEU:HD12	1.60	0.82
2:D:856:ILE:HD13	2:D:866:ILE:HG21	1.59	0.82
2:F:663:ILE:HD11	2:F:910:LEU:HD12	1.60	0.82
2:H:873:ARG:HH22	2:H:880:ASN:HD21	1.23	0.82
2:B:266:THR:HG23	2:B:307:TRP:CH2	2.17	0.80
2:D:663:ILE:HA	2:D:666:VAL:HG22	1.65	0.79
2:F:266:THR:HG23	2:F:307:TRP:CH2	2.17	0.79
2:D:545:ALA:HB3	2:D:568:LEU:HD11	1.65	0.78
2:F:663:ILE:HA	2:F:666:VAL:HG22	1.65	0.78
2:D:266:THR:HG23	2:D:307:TRP:CH2	2.17	0.78
2:B:454:ASP:HB2	10:B:1007:MGD:H1'	1.66	0.78
2:H:266:THR:HG23	2:H:307:TRP:CH2	2.17	0.77
2:B:545:ALA:HB3	2:B:568:LEU:HD11	1.65	0.77
2:H:663:ILE:HA	2:H:666:VAL:HG22	1.65	0.77
2:B:482:ILE:HD12	2:B:534:ALA:HB2	1.67	0.77
2:B:663:ILE:HA	2:B:666:VAL:HG22	1.65	0.77
2:D:482:ILE:HD12	2:D:534:ALA:HB2	1.67	0.77
2:H:454:ASP:HB2	10:H:1007:MGD:H1'	1.66	0.77
2:D:454:ASP:HB2	10:D:1007:MGD:H1'	1.66	0.76
2:F:454:ASP:HB2	10:F:1007:MGD:H1'	1.66	0.76
2:H:545:ALA:HB3	2:H:568:LEU:HD11	1.65	0.76
2:F:545:ALA:HB3	2:F:568:LEU:HD11	1.65	0.76
2:F:482:ILE:HD12	2:F:534:ALA:HB2	1.67	0.76
2:B:435:LEU:HD13	2:B:584:LEU:HD21	1.67	0.75
2:H:482:ILE:HD12	2:H:534:ALA:HB2	1.67	0.75
2:D:435:LEU:HD13	2:D:584:LEU:HD21	1.67	0.75
2:F:435:LEU:HD13	2:F:584:LEU:HD21	1.67	0.75
2:H:299:THR:HG21	2:H:304:LYS:HB2	1.69	0.75
2:H:435:LEU:HD13	2:H:584:LEU:HD21	1.67	0.75
2:H:266:THR:HG23	2:H:307:TRP:HH2	1.52	0.75
2:B:266:THR:HG23	2:B:307:TRP:HH2	1.52	0.75
2:F:299:THR:HG21	2:F:304:LYS:HB2	1.69	0.74
2:H:713:ILE:HD13	2:H:766:VAL:HG11	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:713:ILE:HD13	2:B:766:VAL:HG11	1.70	0.74
2:D:266:THR:HG23	2:D:307:TRP:HH2	1.52	0.73
2:F:266:THR:HG23	2:F:307:TRP:HH2	1.52	0.73
2:D:638:ILE:HG13	2:D:666:VAL:HG12	1.71	0.73
2:D:299:THR:HG21	2:D:304:LYS:HB2	1.69	0.73
2:D:866:ILE:HD13	2:D:934:ILE:HD12	1.70	0.73
2:D:820:TYR:HB3	2:D:929:SER:HB2	1.71	0.73
2:F:866:ILE:HD13	2:F:934:ILE:HD12	1.70	0.73
2:B:299:THR:HG21	2:B:304:LYS:HB2	1.69	0.73
2:B:638:ILE:HG13	2:B:666:VAL:HG12	1.71	0.73
2:F:713:ILE:HD13	2:F:766:VAL:HG11	1.70	0.73
2:D:295:ASN:O	2:D:438:ARG:NH2	2.22	0.72
2:F:295:ASN:O	2:F:438:ARG:NH2	2.22	0.72
2:H:361:SER:CB	2:H:387:CYS:SG	2.77	0.72
2:B:361:SER:CB	2:B:387:CYS:SG	2.77	0.72
2:F:820:TYR:HB3	2:F:929:SER:HB2	1.71	0.72
2:H:638:ILE:HG13	2:H:666:VAL:HG12	1.71	0.72
2:B:713:ILE:HD11	2:B:779:TRP:HB3	1.72	0.72
2:B:866:ILE:HD13	2:B:934:ILE:HD12	1.70	0.72
2:D:713:ILE:HD13	2:D:766:VAL:HG11	1.70	0.72
2:H:866:ILE:HD13	2:H:934:ILE:HD12	1.70	0.72
2:F:55:ILE:HD11	2:F:60:LYS:HD2	1.72	0.72
2:B:820:TYR:HB3	2:B:929:SER:HB2	1.71	0.72
2:H:295:ASN:O	2:H:438:ARG:NH2	2.22	0.72
2:B:295:ASN:O	2:B:438:ARG:NH2	2.22	0.71
2:D:55:ILE:HD11	2:D:60:LYS:HD2	1.72	0.71
2:D:713:ILE:HD11	2:D:779:TRP:HB3	1.72	0.71
2:H:713:ILE:HD11	2:H:779:TRP:HB3	1.72	0.71
2:B:55:ILE:HD11	2:B:60:LYS:HD2	1.72	0.71
2:D:361:SER:CB	2:D:387:CYS:SG	2.77	0.71
2:F:361:SER:CB	2:F:387:CYS:SG	2.77	0.71
2:F:638:ILE:HG13	2:F:666:VAL:HG12	1.71	0.71
2:H:55:ILE:HD11	2:H:60:LYS:HD2	1.72	0.71
2:F:713:ILE:HD11	2:F:779:TRP:HB3	1.72	0.71
2:H:820:TYR:HB3	2:H:929:SER:HB2	1.71	0.70
2:D:195:GLY:HA3	2:D:304:LYS:HD3	1.74	0.70
2:B:195:GLY:HA3	2:B:304:LYS:HD3	1.74	0.70
2:F:195:GLY:HA3	2:F:304:LYS:HD3	1.74	0.70
2:B:95:HIS:CE1	2:B:203:CYS:HB3	2.27	0.70
2:H:111:ILE:HD11	2:H:149:ILE:HD13	1.74	0.70
2:D:95:HIS:CE1	2:D:203:CYS:HB3	2.27	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:195:GLY:HA3	2:H:304:LYS:HD3	1.74	0.69
2:B:497:LEU:HD21	2:B:570:VAL:HA	1.75	0.69
2:D:497:LEU:HD21	2:D:570:VAL:HA	1.75	0.69
2:F:423:ILE:HG23	2:F:426:SER:HB3	1.75	0.69
2:F:95:HIS:CE1	2:F:203:CYS:HB3	2.27	0.69
2:F:497:LEU:HD21	2:F:570:VAL:HA	1.75	0.69
2:F:861:ALA:HA	2:F:866:ILE:HG22	1.75	0.69
2:H:95:HIS:CE1	2:H:203:CYS:HB3	2.27	0.69
2:H:497:LEU:HD21	2:H:570:VAL:HA	1.75	0.69
2:H:838:LEU:HD21	10:H:1006:MGD:H8	1.75	0.69
2:B:111:ILE:HD11	2:B:149:ILE:HD13	1.74	0.69
2:B:678:VAL:HG11	2:B:687:ALA:HA	1.76	0.68
2:D:111:ILE:HD11	2:D:149:ILE:HD13	1.74	0.68
2:F:678:VAL:HG11	2:F:687:ALA:HA	1.76	0.68
2:D:861:ALA:HA	2:D:866:ILE:HG22	1.75	0.68
2:F:398:GLY:HA2	2:F:562:THR:HG22	1.75	0.68
2:F:155:VAL:HG21	2:F:169:ILE:HG13	1.76	0.68
2:F:838:LEU:HD21	10:F:1006:MGD:H8	1.75	0.68
2:H:678:VAL:HG11	2:H:687:ALA:HA	1.76	0.68
2:B:155:VAL:HG21	2:B:169:ILE:HG13	1.76	0.68
2:B:398:GLY:HA2	2:B:562:THR:HG22	1.75	0.68
2:H:861:ALA:HA	2:H:866:ILE:HG22	1.75	0.68
2:D:398:GLY:HA2	2:D:562:THR:HG22	1.75	0.68
2:F:111:ILE:HD11	2:F:149:ILE:HD13	1.74	0.68
2:D:201:CYS:HA	9:D:1003:SF4:S2	2.34	0.68
2:D:423:ILE:HG23	2:D:426:SER:HB3	1.75	0.68
2:D:655:GLU:OE2	2:D:837:ASN:ND2	2.27	0.68
2:F:655:GLU:OE2	2:F:837:ASN:ND2	2.27	0.68
2:H:655:GLU:OE2	2:H:837:ASN:ND2	2.27	0.67
2:D:678:VAL:HG11	2:D:687:ALA:HA	1.76	0.67
2:H:155:VAL:HG21	2:H:169:ILE:HG13	1.76	0.67
2:H:201:CYS:HA	9:H:1003:SF4:S2	2.34	0.67
2:B:250:GLU:OE1	2:B:254:ARG:NH1	2.27	0.67
2:B:838:LEU:HD21	10:B:1006:MGD:H8	1.75	0.67
2:D:838:LEU:HD21	10:D:1006:MGD:H8	1.75	0.67
2:H:398:GLY:HA2	2:H:562:THR:HG22	1.75	0.67
2:D:155:VAL:HG21	2:D:169:ILE:HG13	1.76	0.67
2:B:423:ILE:HG23	2:B:426:SER:HB3	1.75	0.67
2:B:201:CYS:HA	9:B:1003:SF4:S2	2.34	0.67
2:F:250:GLU:OE1	2:F:254:ARG:NH1	2.27	0.67
2:H:423:ILE:HG23	2:H:426:SER:HB3	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:ILE:HD12	2:B:149:ILE:HD12	1.77	0.67
2:B:861:ALA:HA	2:B:866:ILE:HG22	1.75	0.67
2:F:201:CYS:HA	9:F:1003:SF4:S2	2.34	0.67
2:D:250:GLU:OE1	2:D:254:ARG:NH1	2.27	0.66
2:H:250:GLU:OE1	2:H:254:ARG:NH1	2.27	0.66
2:B:655:GLU:OE2	2:B:837:ASN:ND2	2.27	0.66
2:D:91:ILE:HD12	2:D:149:ILE:HD12	1.77	0.66
2:B:879:GLY:HA3	2:B:910:LEU:HB3	1.77	0.66
2:D:656:MET:SD	2:D:670:TYR:OH	2.48	0.66
2:H:585:ARG:NH1	2:H:591:GLN:OE1	2.28	0.65
2:H:656:MET:SD	2:H:670:TYR:OH	2.48	0.65
2:F:585:ARG:NH1	2:F:591:GLN:OE1	2.28	0.65
4:A:203:A1H2V:O29	4:G:205:A1H2V:C26	2.45	0.65
2:B:194:CYS:SG	2:B:196:HIS:ND1	2.65	0.65
3:C:203:11A:HAL1	3:E:203:11A:HAL2	1.79	0.65
2:D:879:GLY:HA3	2:D:910:LEU:HB3	1.77	0.65
2:F:879:GLY:HA3	2:F:910:LEU:HB3	1.77	0.65
3:E:203:11A:HAL1	3:G:203:11A:HAL2	1.79	0.65
2:H:879:GLY:HA3	2:H:910:LEU:HB3	1.77	0.65
2:B:585:ARG:NH1	2:B:591:GLN:OE1	2.28	0.65
4:C:205:A1H2V:C26	4:E:205:A1H2V:O29	2.45	0.65
2:F:91:ILE:HD12	2:F:149:ILE:HD12	1.77	0.65
4:A:203:A1H2V:C13	4:C:205:A1H2V:O32	2.45	0.65
2:D:320:LEU:HD12	2:D:327:PHE:HB3	1.79	0.64
2:F:299:THR:CG2	2:F:304:LYS:HB2	2.27	0.64
4:C:205:A1H2V:C13	4:E:205:A1H2V:O32	2.45	0.64
2:D:299:THR:CG2	2:D:304:LYS:HB2	2.27	0.64
2:B:656:MET:SD	2:B:670:TYR:OH	2.48	0.64
2:F:194:CYS:SG	2:F:196:HIS:ND1	2.65	0.64
2:F:320:LEU:HD12	2:F:327:PHE:HB3	1.79	0.64
3:A:201:11A:HAL1	3:C:203:11A:HAL2	1.79	0.64
4:A:203:A1H2V:C26	4:C:205:A1H2V:O29	2.45	0.64
4:E:205:A1H2V:C26	4:G:205:A1H2V:O29	2.45	0.64
1:C:2:ALA:N	2:F:670:TYR:O	2.31	0.64
2:D:194:CYS:SG	2:D:196:HIS:ND1	2.65	0.64
2:D:408:ASP:O	2:D:711:ARG:HD3	1.98	0.64
2:D:708:ASN:ND2	2:D:712:ARG:HB3	2.12	0.64
2:H:299:THR:CG2	2:H:304:LYS:HB2	2.27	0.64
2:H:408:ASP:O	2:H:711:ARG:HD3	1.98	0.64
2:B:221:ILE:HB	2:B:226:LEU:HD13	1.80	0.64
2:B:299:THR:CG2	2:B:304:LYS:HB2	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:670:TYR:O	1:G:2:ALA:N	2.31	0.64
2:D:547:TRP:HB2	2:D:551:VAL:HG11	1.80	0.64
2:F:656:MET:SD	2:F:670:TYR:OH	2.48	0.64
3:A:201:11A:HAL2	3:G:203:11A:HAL1	1.79	0.63
2:B:408:ASP:O	2:B:711:ARG:HD3	1.98	0.63
2:D:221:ILE:HB	2:D:226:LEU:HD13	1.80	0.63
2:F:45:ILE:HD12	2:F:153:ARG:HG2	1.80	0.63
2:F:708:ASN:ND2	2:F:712:ARG:HB3	2.12	0.63
2:H:708:ASN:ND2	2:H:712:ARG:HB3	2.12	0.63
2:B:285:LYS:HD3	2:B:287:GLU:HB2	1.80	0.63
2:B:547:TRP:HB2	2:B:551:VAL:HG11	1.80	0.63
4:A:203:A1H2V:O32	4:G:205:A1H2V:C13	2.45	0.63
2:B:320:LEU:HD12	2:B:327:PHE:HB3	1.79	0.63
2:H:91:ILE:HD12	2:H:149:ILE:HD12	1.77	0.63
2:F:547:TRP:HB2	2:F:551:VAL:HG11	1.80	0.63
2:H:820:TYR:HB3	2:H:929:SER:CB	2.28	0.63
2:B:708:ASN:ND2	2:B:712:ARG:HB3	2.12	0.63
2:D:820:TYR:HB3	2:D:929:SER:CB	2.28	0.63
2:F:408:ASP:O	2:F:711:ARG:HD3	1.98	0.63
2:H:320:LEU:HD12	2:H:327:PHE:HB3	1.79	0.63
1:A:2:ALA:N	2:D:670:TYR:O	2.31	0.63
2:B:371:MET:HE3	2:B:652:LYS:HE3	1.81	0.63
2:B:828:ARG:NH2	10:B:1006:MGD:O17	2.32	0.63
2:B:545:ALA:HB2	2:B:568:LEU:HD21	1.80	0.63
2:D:285:LYS:HD3	2:D:287:GLU:HB2	1.80	0.63
2:D:585:ARG:NH1	2:D:591:GLN:OE1	2.28	0.63
2:B:820:TYR:HB3	2:B:929:SER:CB	2.28	0.63
1:E:2:ALA:N	2:H:670:TYR:O	2.31	0.63
4:E:205:A1H2V:C13	4:G:205:A1H2V:O32	2.45	0.63
2:D:318:LYS:HG3	2:D:319:PRO:HD2	1.81	0.62
2:H:45:ILE:HD12	2:H:153:ARG:HG2	1.80	0.62
2:D:545:ALA:HB2	2:D:568:LEU:HD21	1.80	0.62
2:F:371:MET:HE3	2:F:652:LYS:HE3	1.81	0.62
2:H:547:TRP:HB2	2:H:551:VAL:HG11	1.80	0.62
2:D:828:ARG:NH2	10:D:1006:MGD:O17	2.32	0.62
2:F:820:TYR:HB3	2:F:929:SER:CB	2.28	0.62
2:B:852:VAL:HB	2:B:902:ASP:HB2	1.81	0.62
2:D:45:ILE:HD12	2:D:153:ARG:HG2	1.80	0.62
2:F:828:ARG:NH2	10:F:1006:MGD:O17	2.32	0.62
2:H:828:ARG:NH2	10:H:1006:MGD:O17	2.32	0.62
2:B:318:LYS:HG3	2:B:319:PRO:HD2	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:339:ILE:HD12	2:B:677:VAL:HG21	1.82	0.62
2:H:221:ILE:HB	2:H:226:LEU:HD13	1.80	0.62
2:H:285:LYS:HD3	2:H:287:GLU:HB2	1.80	0.62
2:H:339:ILE:HD12	2:H:677:VAL:HG21	1.82	0.62
2:F:432:HIS:CE1	2:F:584:LEU:HB3	2.35	0.62
2:B:45:ILE:HD12	2:B:153:ARG:HG2	1.80	0.62
2:H:371:MET:HE3	2:H:652:LYS:HE3	1.81	0.62
2:H:432:HIS:CE1	2:H:584:LEU:HB3	2.35	0.62
2:D:157:ALA:HB1	2:D:196:HIS:HB3	1.82	0.62
2:F:221:ILE:HB	2:F:226:LEU:HD13	1.80	0.61
1:A:59:LEU:HA	2:H:253:MET:HE1	1.83	0.61
2:F:285:LYS:HD3	2:F:287:GLU:HB2	1.80	0.61
2:F:852:VAL:HB	2:F:902:ASP:HB2	1.81	0.61
2:H:852:VAL:HB	2:H:902:ASP:HB2	1.81	0.61
2:D:852:VAL:HB	2:D:902:ASP:HB2	1.81	0.61
2:F:545:ALA:HB2	2:F:568:LEU:HD21	1.80	0.61
2:H:361:SER:HB2	2:H:387:CYS:SG	2.41	0.61
2:B:432:HIS:CE1	2:B:584:LEU:HB3	2.35	0.61
2:F:339:ILE:HD12	2:F:677:VAL:HG21	1.82	0.61
2:H:194:CYS:SG	2:H:196:HIS:ND1	2.65	0.61
1:A:85:ASN:HD22	1:C:98:VAL:HG23	1.66	0.61
2:B:157:ALA:HB1	2:B:196:HIS:HB3	1.82	0.61
2:D:253:MET:HE1	1:E:59:LEU:HA	1.83	0.61
2:D:371:MET:HE3	2:D:652:LYS:HE3	1.81	0.61
2:D:391:CYS:SG	2:D:392:GLN:NE2	2.74	0.61
2:D:566:ASN:HA	2:D:569:LEU:HB2	1.83	0.61
2:B:391:CYS:SG	2:B:392:GLN:NE2	2.74	0.61
2:H:318:LYS:HG3	2:H:319:PRO:HD2	1.81	0.61
2:B:361:SER:HB2	2:B:387:CYS:SG	2.41	0.61
2:H:545:ALA:HB2	2:H:568:LEU:HD21	1.80	0.61
1:A:152:GLY:HA3	1:C:111:GLY:HA2	1.83	0.61
2:D:432:HIS:CE1	2:D:584:LEU:HB3	2.35	0.61
2:B:390:TYR:HB3	2:B:925:TYR:HE2	1.66	0.61
2:D:339:ILE:HD12	2:D:677:VAL:HG21	1.82	0.61
2:F:318:LYS:HG3	2:F:319:PRO:HD2	1.81	0.60
2:H:390:TYR:HB3	2:H:925:TYR:HE2	1.66	0.60
2:H:566:ASN:HA	2:H:569:LEU:HB2	1.83	0.60
2:B:9:ILE:HG21	2:B:25:LEU:HD21	1.84	0.60
2:F:566:ASN:HA	2:F:569:LEU:HB2	1.83	0.60
2:B:253:MET:HE1	1:C:59:LEU:HA	1.83	0.60
2:B:266:THR:O	2:B:588:ASN:ND2	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:883:VAL:HG12	2:D:906:ALA:HB1	1.84	0.60
2:F:883:VAL:HG12	2:F:906:ALA:HB1	1.84	0.60
2:H:298:SER:OG	2:H:438:ARG:NH1	2.32	0.60
2:F:157:ALA:HB1	2:F:196:HIS:HB3	1.82	0.60
2:H:391:CYS:SG	2:H:392:GLN:NE2	2.74	0.60
2:F:298:SER:OG	2:F:438:ARG:NH1	2.32	0.60
2:H:9:ILE:HG21	2:H:25:LEU:HD21	1.84	0.60
2:H:542:SER:HB2	2:H:579:ALA:HB2	1.84	0.60
2:H:883:VAL:HG12	2:H:906:ALA:HB1	1.84	0.60
2:H:931:LYS:HD3	2:H:933:GLU:OE2	2.02	0.60
2:F:253:MET:HE1	1:G:59:LEU:HA	1.82	0.60
1:A:111:GLY:HA2	1:G:152:GLY:HA3	1.83	0.60
2:B:566:ASN:HA	2:B:569:LEU:HB2	1.83	0.60
2:B:826:ASN:HD22	10:B:1006:MGD:H191	1.49	0.60
2:B:883:VAL:HG12	2:B:906:ALA:HB1	1.84	0.60
2:B:931:LYS:HD3	2:B:933:GLU:OE2	2.02	0.60
1:A:98:VAL:HG23	1:G:85:ASN:HD22	1.66	0.60
1:E:152:GLY:HA3	1:G:111:GLY:HA2	1.83	0.60
2:F:361:SER:HB2	2:F:387:CYS:SG	2.41	0.60
1:C:85:ASN:HD22	1:E:98:VAL:HG23	1.66	0.60
2:D:9:ILE:HG21	2:D:25:LEU:HD21	1.84	0.60
2:D:931:LYS:HD3	2:D:933:GLU:OE2	2.02	0.60
2:F:147:GLN:NE2	2:F:204:ASN:OD1	2.35	0.60
2:F:391:CYS:SG	2:F:392:GLN:NE2	2.74	0.60
2:H:157:ALA:HB1	2:H:196:HIS:HB3	1.82	0.60
2:B:147:GLN:NE2	2:B:204:ASN:OD1	2.35	0.59
2:D:361:SER:HB2	2:D:387:CYS:SG	2.41	0.59
2:D:542:SER:HB2	2:D:579:ALA:HB2	1.84	0.59
2:F:9:ILE:HG21	2:F:25:LEU:HD21	1.84	0.59
2:H:518:TYR:OH	2:H:522:LYS:NZ	2.35	0.59
1:C:152:GLY:HA3	1:E:111:GLY:HA2	1.83	0.59
2:H:147:GLN:NE2	2:H:204:ASN:OD1	2.35	0.59
2:D:266:THR:O	2:D:588:ASN:ND2	2.32	0.59
2:D:361:SER:HB2	2:D:587:HIS:CD2	2.37	0.59
2:H:266:THR:O	2:H:588:ASN:ND2	2.32	0.59
2:D:390:TYR:HB3	2:D:925:TYR:HE2	1.66	0.59
2:F:361:SER:HB2	2:F:587:HIS:CD2	2.37	0.59
2:H:180:TRP:CE2	2:H:186:ILE:HG12	2.38	0.59
2:D:147:GLN:NE2	2:D:204:ASN:OD1	2.35	0.59
2:F:180:TRP:CE2	2:F:186:ILE:HG12	2.38	0.59
2:F:542:SER:HB2	2:F:579:ALA:HB2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:433:PRO:O	2:H:437:THR:HG23	2.02	0.59
2:F:433:PRO:O	2:F:437:THR:HG23	2.02	0.59
2:F:931:LYS:HD3	2:F:933:GLU:OE2	2.02	0.59
2:H:826:ASN:HD22	10:H:1006:MGD:H191	1.49	0.59
2:B:361:SER:HB2	2:B:587:HIS:CD2	2.37	0.59
2:F:390:TYR:HB3	2:F:925:TYR:HE2	1.66	0.59
2:F:826:ASN:HD22	10:F:1006:MGD:H191	1.49	0.59
1:A:98:VAL:HB	1:G:88:LEU:HB3	1.85	0.59
2:B:180:TRP:CE2	2:B:186:ILE:HG12	2.38	0.59
2:D:298:SER:OG	2:D:438:ARG:NH1	2.32	0.59
1:E:88:LEU:HB3	1:G:98:VAL:HB	1.85	0.59
2:F:162:GLN:HA	2:F:437:THR:HB	1.85	0.59
2:F:826:ASN:ND2	10:F:1006:MGD:H191	2.01	0.59
2:H:162:GLN:HA	2:H:437:THR:HB	1.85	0.59
1:E:85:ASN:HD22	1:G:98:VAL:HG23	1.66	0.58
2:B:542:SER:HB2	2:B:579:ALA:HB2	1.84	0.58
2:D:180:TRP:CE2	2:D:186:ILE:HG12	2.38	0.58
2:F:266:THR:O	2:F:588:ASN:ND2	2.32	0.58
2:H:818:GLU:HG3	2:H:819:GLU:H	1.68	0.58
2:F:818:GLU:HG3	2:F:819:GLU:H	1.68	0.58
2:H:361:SER:HB2	2:H:587:HIS:CD2	2.37	0.58
2:D:433:PRO:O	2:D:437:THR:HG23	2.02	0.58
2:D:818:GLU:HG3	2:D:819:GLU:H	1.68	0.58
1:G:13:VAL:HG13	1:G:17:ASP:HB2	1.86	0.58
2:B:115:VAL:HG12	2:B:244:LEU:HD11	1.86	0.58
2:B:698:PRO:HG2	2:B:701:GLU:HG3	1.86	0.58
2:D:826:ASN:ND2	10:D:1006:MGD:H191	2.01	0.58
2:H:698:PRO:HG2	2:H:701:GLU:HG3	1.86	0.58
1:A:88:LEU:HB3	1:C:98:VAL:HB	1.85	0.58
2:B:162:GLN:HA	2:B:437:THR:HB	1.85	0.58
2:H:115:VAL:HG12	2:H:244:LEU:HD11	1.86	0.58
2:B:433:PRO:O	2:B:437:THR:HG23	2.02	0.58
2:D:115:VAL:HG12	2:D:244:LEU:HD11	1.86	0.58
2:D:162:GLN:HA	2:D:437:THR:HB	1.85	0.58
2:F:115:VAL:HG12	2:F:244:LEU:HD11	1.86	0.58
2:H:826:ASN:ND2	10:H:1006:MGD:H191	2.01	0.58
2:D:826:ASN:HD22	10:D:1006:MGD:H191	1.49	0.57
2:B:547:TRP:NE1	2:B:561:SER:OG	2.37	0.57
1:C:88:LEU:HB3	1:E:98:VAL:HB	1.85	0.57
1:E:13:VAL:HG13	1:E:17:ASP:HB2	1.86	0.57
2:F:373:LYS:NZ	2:F:746:TYR:OH	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:873:ARG:HH21	2:F:882:LYS:HE2	1.69	0.57
2:B:818:GLU:HG3	2:B:819:GLU:H	1.68	0.57
2:D:873:ARG:HH21	2:D:882:LYS:HE2	1.69	0.57
2:F:501:VAL:HG13	2:F:569:LEU:HD13	1.87	0.57
2:B:250:GLU:O	2:B:253:MET:HB2	2.04	0.57
2:D:820:TYR:CZ	2:D:877:PRO:HD3	2.40	0.57
2:F:518:TYR:OH	2:F:522:LYS:NZ	2.35	0.57
1:A:13:VAL:HG13	1:A:17:ASP:HB2	1.86	0.57
2:F:547:TRP:NE1	2:F:561:SER:OG	2.37	0.57
2:B:707:THR:HA	2:B:712:ARG:O	2.05	0.57
2:F:698:PRO:HG2	2:F:701:GLU:HG3	1.86	0.57
2:H:501:VAL:HG13	2:H:569:LEU:HD13	1.87	0.57
2:F:820:TYR:CZ	2:F:877:PRO:HD3	2.40	0.57
1:G:129:ASP:N	1:G:129:ASP:OD1	2.36	0.57
2:D:547:TRP:NE1	2:D:561:SER:OG	2.37	0.56
2:D:558:SER:O	2:D:562:THR:HG23	2.05	0.56
2:D:698:PRO:HG2	2:D:701:GLU:HG3	1.86	0.56
1:C:13:VAL:HG13	1:C:17:ASP:HB2	1.86	0.56
2:D:250:GLU:O	2:D:253:MET:HB2	2.04	0.56
2:D:382:ASN:HD21	2:D:609:VAL:HG11	1.71	0.56
2:F:382:ASN:HD21	2:F:609:VAL:HG11	1.71	0.56
2:H:547:TRP:NE1	2:H:561:SER:OG	2.37	0.56
1:A:129:ASP:OD1	1:A:129:ASP:N	2.36	0.56
2:B:558:SER:O	2:B:562:THR:HG23	2.05	0.56
2:B:826:ASN:ND2	10:B:1006:MGD:H191	2.01	0.56
2:D:373:LYS:NZ	2:D:746:TYR:OH	2.37	0.56
2:D:707:THR:HA	2:D:712:ARG:O	2.05	0.56
2:F:157:ALA:HA	2:F:161:VAL:HG12	1.88	0.56
2:F:250:GLU:O	2:F:253:MET:HB2	2.04	0.56
2:H:157:ALA:HA	2:H:161:VAL:HG12	1.88	0.56
2:H:873:ARG:HH21	2:H:882:LYS:HE2	1.69	0.56
2:B:621:VAL:HG21	2:B:759:LEU:HD21	1.88	0.56
2:F:367:GLU:OE2	2:F:730:TRP:N	2.39	0.56
2:H:373:LYS:NZ	2:H:746:TYR:OH	2.37	0.56
2:H:382:ASN:HD21	2:H:609:VAL:HG11	1.71	0.56
2:B:157:ALA:HA	2:B:161:VAL:HG12	1.88	0.56
2:B:367:GLU:OE2	2:B:730:TRP:N	2.39	0.56
2:F:673:LEU:HD11	2:F:676:PHE:HB2	1.88	0.56
2:H:707:THR:HA	2:H:712:ARG:O	2.05	0.56
2:B:298:SER:OG	2:B:438:ARG:NH1	2.32	0.56
2:D:157:ALA:HA	2:D:161:VAL:HG12	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:673:LEU:HD11	2:D:676:PHE:HB2	1.88	0.56
2:H:558:SER:O	2:H:562:THR:HG23	2.05	0.56
2:B:382:ASN:HD21	2:B:609:VAL:HG11	1.71	0.56
2:B:873:ARG:HH21	2:B:882:LYS:HE2	1.69	0.56
2:D:621:VAL:HG21	2:D:759:LEU:HD21	1.88	0.56
2:D:871:LEU:CD2	2:D:935:LEU:HD12	2.36	0.56
2:H:621:VAL:HG21	2:H:759:LEU:HD21	1.88	0.56
2:H:641:ILE:HD11	2:H:649:MET:HE1	1.88	0.56
2:H:673:LEU:HD11	2:H:676:PHE:HB2	1.88	0.56
1:A:36:ALA:HB2	1:C:45:GLY:HA2	1.88	0.56
2:B:373:LYS:NZ	2:B:746:TYR:OH	2.37	0.56
2:B:820:TYR:CZ	2:B:877:PRO:HD3	2.40	0.56
2:H:250:GLU:O	2:H:253:MET:HB2	2.04	0.56
1:A:45:GLY:HA2	1:G:36:ALA:HB2	1.88	0.56
2:B:141:TYR:OH	2:B:191:CYS:SG	2.64	0.56
2:B:501:VAL:HG13	2:B:569:LEU:HD13	1.87	0.56
2:B:673:LEU:HD11	2:B:676:PHE:HB2	1.88	0.56
1:E:36:ALA:HB2	1:G:45:GLY:HA2	1.88	0.56
2:F:707:THR:HA	2:F:712:ARG:O	2.05	0.56
2:H:141:TYR:OH	2:H:191:CYS:SG	2.64	0.56
2:B:255:ASP:HB3	1:C:62:GLN:HG2	1.88	0.56
2:F:871:LEU:CD2	2:F:935:LEU:HD12	2.36	0.56
2:H:837:ASN:ND2	10:H:1006:MGD:O3'	2.36	0.56
1:A:62:GLN:HG2	2:H:255:ASP:HB3	1.88	0.55
2:D:255:ASP:HB3	1:E:62:GLN:HG2	1.88	0.55
2:F:255:ASP:HB3	1:G:62:GLN:HG2	1.88	0.55
2:H:820:TYR:CZ	2:H:877:PRO:HD3	2.40	0.55
2:D:501:VAL:HG13	2:D:569:LEU:HD13	1.87	0.55
2:F:621:VAL:HG21	2:F:759:LEU:HD21	1.88	0.55
2:H:873:ARG:HB2	2:H:933:GLU:HB2	1.87	0.55
2:B:288:PRO:HB2	2:B:297:ILE:HA	1.88	0.55
2:B:641:ILE:HD11	2:B:649:MET:HE1	1.88	0.55
2:B:814:LYS:N	2:B:927:GLU:OE1	2.39	0.55
1:C:36:ALA:HB2	1:E:45:GLY:HA2	1.88	0.55
2:F:824:VAL:O	2:F:928:THR:OG1	2.23	0.55
2:D:288:PRO:HB2	2:D:297:ILE:HA	1.88	0.55
2:D:367:GLU:OE2	2:D:730:TRP:N	2.39	0.55
2:D:824:VAL:O	2:D:928:THR:OG1	2.23	0.55
1:A:43:MET:HE1	1:C:57:ARG:CB	2.35	0.55
2:B:873:ARG:HB2	2:B:933:GLU:HB2	1.87	0.55
2:D:873:ARG:HB2	2:D:933:GLU:HB2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:370:LEU:HB3	2:F:733:ILE:HG21	1.89	0.55
2:F:558:SER:O	2:F:562:THR:HG23	2.05	0.55
2:B:769:GLU:OE2	2:B:769:GLU:N	2.28	0.55
2:H:439:ILE:HG21	2:H:460:MET:HE1	1.89	0.55
2:D:586:GLY:HA3	10:D:1007:MGD:S12	2.47	0.55
2:H:288:PRO:HB2	2:H:297:ILE:HA	1.88	0.55
2:B:518:TYR:OH	2:B:522:LYS:NZ	2.35	0.55
2:D:587:HIS:NE2	10:D:1006:MGD:O1A	2.31	0.55
2:F:101:VAL:HG12	2:F:218:LEU:HB3	1.89	0.55
2:F:873:ARG:HB2	2:F:933:GLU:HB2	1.88	0.55
2:B:586:GLY:HA3	10:B:1007:MGD:S12	2.47	0.55
2:D:141:TYR:OH	2:D:191:CYS:SG	2.64	0.55
2:D:478:TRP:HB3	2:D:523:THR:HG21	1.90	0.54
2:D:856:ILE:HG13	2:D:896:VAL:HG11	1.89	0.54
2:F:641:ILE:HD11	2:F:649:MET:HE1	1.88	0.54
2:H:440:LYS:NZ	2:H:459:GLU:OE2	2.40	0.54
2:H:814:LYS:N	2:H:927:GLU:OE1	2.39	0.54
2:H:871:LEU:CD2	2:H:935:LEU:HD12	2.36	0.54
2:B:370:LEU:HB3	2:B:733:ILE:HG21	1.89	0.54
2:B:816:PHE:HE2	2:B:929:SER:H	1.55	0.54
2:B:871:LEU:CD2	2:B:935:LEU:HD12	2.36	0.54
2:F:586:GLY:HA3	10:F:1007:MGD:S12	2.47	0.54
2:H:367:GLU:OE2	2:H:730:TRP:N	2.39	0.54
2:H:423:ILE:HG12	2:H:546:LEU:HB2	1.89	0.54
2:F:37:CYS:HB3	2:F:48:CYS:HB3	1.89	0.54
2:F:141:TYR:OH	2:F:191:CYS:SG	2.64	0.54
2:H:370:LEU:HB3	2:H:733:ILE:HG21	1.89	0.54
2:D:37:CYS:HB3	2:D:48:CYS:HB3	1.89	0.54
2:D:502:ASN:ND2	2:D:800:ASP:OD2	2.41	0.54
2:F:430:GLU:OE1	2:F:456:ARG:NH2	2.41	0.54
2:F:439:ILE:HG21	2:F:460:MET:HE1	1.89	0.54
2:H:586:GLY:HA3	10:H:1007:MGD:S12	2.47	0.54
2:H:856:ILE:HG13	2:H:896:VAL:HG11	1.89	0.54
2:B:37:CYS:HB3	2:B:48:CYS:HB3	1.89	0.54
2:B:228:PRO:HB2	1:E:71:VAL:HB	1.89	0.54
2:B:856:ILE:HG13	2:B:896:VAL:HG11	1.89	0.54
2:B:475:ASP:HA	2:B:478:TRP:NE1	2.23	0.54
2:B:479:LEU:HD21	2:B:564:ILE:HA	1.90	0.54
2:D:423:ILE:HG12	2:D:546:LEU:HB2	1.89	0.54
2:D:475:ASP:HA	2:D:478:TRP:NE1	2.23	0.54
2:F:502:ASN:ND2	2:F:800:ASP:OD2	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:101:VAL:HG12	2:H:218:LEU:HB3	1.89	0.54
2:H:479:LEU:HD21	2:H:564:ILE:HA	1.90	0.54
2:B:439:ILE:HG21	2:B:460:MET:HE1	1.89	0.54
2:B:502:ASN:ND2	2:B:800:ASP:OD2	2.41	0.54
2:D:221:ILE:HG22	2:D:225:THR:HG23	1.89	0.54
2:D:430:GLU:OE1	2:D:456:ARG:NH2	2.41	0.54
2:F:816:PHE:HE2	2:F:929:SER:H	1.55	0.54
2:H:221:ILE:HG22	2:H:225:THR:HG23	1.89	0.54
2:H:824:VAL:O	2:H:928:THR:OG1	2.23	0.54
1:A:57:ARG:CB	1:G:43:MET:HE1	2.35	0.54
1:C:142:SER:O	1:C:146:LEU:HG	2.08	0.54
2:D:121:ASN:HA	2:D:240:TYR:HB2	1.90	0.54
2:D:641:ILE:HD11	2:D:649:MET:HE1	1.88	0.54
2:D:769:GLU:OE2	2:D:769:GLU:N	2.28	0.54
2:F:475:ASP:HA	2:F:478:TRP:NE1	2.23	0.54
2:F:479:LEU:HD21	2:F:564:ILE:HA	1.90	0.54
2:F:587:HIS:NE2	10:F:1006:MGD:O1A	2.31	0.54
2:H:502:ASN:ND2	2:H:800:ASP:OD2	2.41	0.54
2:B:516:LEU:HB3	2:B:527:GLN:HE22	1.73	0.54
2:B:837:ASN:ND2	10:B:1006:MGD:O3'	2.36	0.54
2:F:288:PRO:HB2	2:F:297:ILE:HA	1.88	0.54
2:F:837:ASN:ND2	10:F:1006:MGD:O3'	2.36	0.54
2:F:856:ILE:HG13	2:F:896:VAL:HG11	1.89	0.54
2:B:478:TRP:HB3	2:B:523:THR:HG21	1.90	0.53
2:F:221:ILE:HG22	2:F:225:THR:HG23	1.89	0.53
2:H:585:ARG:HG3	2:H:591:GLN:HB2	1.90	0.53
2:B:101:VAL:HG12	2:B:218:LEU:HB3	1.89	0.53
2:B:585:ARG:HG3	2:B:591:GLN:HB2	1.90	0.53
1:C:43:MET:HE1	1:E:57:ARG:CB	2.35	0.53
2:D:370:LEU:HB3	2:D:733:ILE:HG21	1.89	0.53
2:D:439:ILE:HG21	2:D:460:MET:HE1	1.89	0.53
2:D:479:LEU:HD21	2:D:564:ILE:HA	1.90	0.53
1:E:142:SER:O	1:E:146:LEU:HG	2.08	0.53
2:F:420:LEU:HD23	2:F:543:VAL:HG22	1.89	0.53
2:H:475:ASP:HA	2:H:478:TRP:NE1	2.23	0.53
2:B:155:VAL:HG22	2:B:167:LEU:HB3	1.91	0.53
2:B:391:CYS:HB2	10:B:1006:MGD:S13	2.48	0.53
2:B:430:GLU:HG2	2:B:830:LEU:HB2	1.90	0.53
1:C:71:VAL:HB	2:H:228:PRO:HB2	1.89	0.53
2:F:423:ILE:HG12	2:F:546:LEU:HB2	1.89	0.53
2:F:549:MET:N	2:F:549:MET:HE2	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:769:GLU:OE2	2:F:769:GLU:N	2.28	0.53
2:B:121:ASN:HA	2:B:240:TYR:HB2	1.90	0.53
2:B:549:MET:HE2	2:B:549:MET:N	2.24	0.53
2:B:824:VAL:O	2:B:928:THR:OG1	2.23	0.53
2:D:837:ASN:ND2	10:D:1006:MGD:O3'	2.36	0.53
1:E:97:ASP:OD2	1:E:100:GLN:NE2	2.42	0.53
2:F:233:THR:HB	13:F:1010:MQ7:H2M1	1.90	0.53
2:F:430:GLU:HG2	2:F:830:LEU:HB2	1.90	0.53
1:G:97:ASP:OD2	1:G:100:GLN:NE2	2.42	0.53
2:H:37:CYS:HB3	2:H:48:CYS:HB3	1.89	0.53
2:H:816:PHE:HE2	2:H:929:SER:H	1.55	0.53
2:D:101:VAL:HG12	2:D:218:LEU:HB3	1.89	0.53
2:D:391:CYS:HB2	10:D:1006:MGD:S13	2.48	0.53
2:D:549:MET:N	2:D:549:MET:HE2	2.24	0.53
2:F:516:LEU:HB3	2:F:527:GLN:HE22	1.73	0.53
2:H:430:GLU:OE1	2:H:456:ARG:NH2	2.41	0.53
2:H:516:LEU:HB3	2:H:527:GLN:HE22	1.73	0.53
2:H:549:MET:N	2:H:549:MET:HE2	2.24	0.53
2:H:945:LYS:HA	2:H:950:ASN:HD22	1.74	0.53
2:B:221:ILE:HG22	2:B:225:THR:HG23	1.89	0.53
2:B:430:GLU:OE1	2:B:456:ARG:NH2	2.41	0.53
2:D:228:PRO:HB2	1:G:71:VAL:HB	1.89	0.53
2:D:420:LEU:HD23	2:D:543:VAL:HG22	1.89	0.53
2:F:945:LYS:HA	2:F:950:ASN:HD22	1.74	0.53
2:D:518:TYR:OH	2:D:522:LYS:NZ	2.35	0.53
2:F:121:ASN:HA	2:F:240:TYR:HB2	1.90	0.53
2:B:423:ILE:HG12	2:B:546:LEU:HB2	1.89	0.53
2:D:516:LEU:HB3	2:D:527:GLN:HE22	1.73	0.53
2:D:945:LYS:HA	2:D:950:ASN:HD22	1.74	0.53
2:F:138:HIS:NE2	2:F:193:SER:OG	2.41	0.53
2:F:712:ARG:HG2	2:F:714:GLN:HG2	1.91	0.53
2:H:478:TRP:HB3	2:H:523:THR:HG21	1.90	0.53
2:H:659:VAL:O	10:H:1006:MGD:N22	2.35	0.53
1:A:71:VAL:HB	2:F:228:PRO:HB2	1.89	0.53
2:B:945:LYS:HA	2:B:950:ASN:HD22	1.74	0.53
2:D:430:GLU:HG2	2:D:830:LEU:HB2	1.90	0.53
2:H:430:GLU:HG2	2:H:830:LEU:HB2	1.90	0.53
2:B:208:GLU:OE2	2:B:304:LYS:NZ	2.42	0.53
2:D:155:VAL:HG22	2:D:167:LEU:HB3	1.91	0.53
2:F:391:CYS:HB2	10:F:1006:MGD:S13	2.48	0.53
2:B:217:TYR:CE2	2:B:253:MET:HB3	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:420:LEU:HD23	2:B:543:VAL:HG22	1.89	0.52
2:D:208:GLU:OE2	2:D:304:LYS:NZ	2.42	0.52
2:D:328:ARG:NH1	2:D:334:GLU:OE2	2.42	0.52
2:D:814:LYS:N	2:D:927:GLU:OE1	2.39	0.52
2:H:155:VAL:HG22	2:H:167:LEU:HB3	1.91	0.52
2:D:233:THR:HB	13:D:1010:MQ7:H2M1	1.90	0.52
2:D:585:ARG:HG3	2:D:591:GLN:HB2	1.90	0.52
2:F:328:ARG:NH1	2:F:334:GLU:OE2	2.42	0.52
2:H:233:THR:HB	13:H:1010:MQ7:H2M1	1.90	0.52
2:H:391:CYS:HB2	10:H:1006:MGD:S13	2.48	0.52
1:A:142:SER:O	1:A:146:LEU:HG	2.08	0.52
2:D:217:TYR:CE2	2:D:253:MET:HB3	2.44	0.52
2:F:357:PHE:HE2	2:F:375:ALA:HA	1.74	0.52
2:H:328:ARG:NH1	2:H:334:GLU:OE2	2.42	0.52
2:H:420:LEU:HD23	2:H:543:VAL:HG22	1.89	0.52
2:B:659:VAL:O	10:B:1006:MGD:N22	2.35	0.52
2:H:121:ASN:HA	2:H:240:TYR:HB2	1.90	0.52
1:A:97:ASP:OD2	1:A:100:GLN:NE2	2.42	0.52
2:B:233:THR:HB	13:B:1010:MQ7:H2M1	1.90	0.52
2:B:357:PHE:HE2	2:B:375:ALA:HA	1.74	0.52
1:C:97:ASP:OD2	1:C:100:GLN:NE2	2.42	0.52
2:F:155:VAL:HG22	2:F:167:LEU:HB3	1.91	0.52
1:G:142:SER:O	1:G:146:LEU:HG	2.08	0.52
2:H:712:ARG:HG2	2:H:714:GLN:HG2	1.91	0.52
2:B:440:LYS:NZ	2:B:459:GLU:OE2	2.40	0.52
2:B:650:TYR:OH	2:B:679:GLN:NE2	2.43	0.52
2:F:478:TRP:HB3	2:F:523:THR:HG21	1.90	0.52
2:F:585:ARG:HG3	2:F:591:GLN:HB2	1.90	0.52
2:F:814:LYS:N	2:F:927:GLU:OE1	2.39	0.52
2:B:328:ARG:NH1	2:B:334:GLU:OE2	2.42	0.52
1:C:129:ASP:OD1	1:C:129:ASP:N	2.36	0.52
2:F:217:TYR:CE2	2:F:253:MET:HB3	2.44	0.52
2:D:712:ARG:HG2	2:D:714:GLN:HG2	1.91	0.52
2:B:27:ASN:OD1	2:B:35:GLN:NE2	2.43	0.52
2:B:411:SER:HA	2:B:710:GLU:HB2	1.92	0.52
2:B:825:ASN:HD21	10:B:1007:MGD:H2'	1.75	0.52
2:D:357:PHE:HE2	2:D:375:ALA:HA	1.74	0.52
2:F:27:ASN:OD1	2:F:35:GLN:NE2	2.43	0.52
2:H:217:TYR:CE2	2:H:253:MET:HB3	2.44	0.52
1:A:11:ILE:HG23	1:A:13:VAL:HG23	1.92	0.52
2:B:712:ARG:HG2	2:B:714:GLN:HG2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:652:LYS:HB2	2:F:679:GLN:HB3	1.92	0.52
2:F:659:VAL:O	10:F:1006:MGD:N22	2.35	0.52
2:H:357:PHE:HE2	2:H:375:ALA:HA	1.74	0.52
2:D:650:TYR:OH	2:D:679:GLN:NE2	2.43	0.51
2:F:208:GLU:OE2	2:F:304:LYS:NZ	2.42	0.51
2:H:650:TYR:OH	2:H:679:GLN:NE2	2.43	0.51
2:H:652:LYS:HB2	2:H:679:GLN:HB3	1.92	0.51
2:H:825:ASN:HD21	10:H:1007:MGD:H2'	1.75	0.51
1:A:131:ILE:HA	1:A:134:LEU:HD23	1.92	0.51
1:E:43:MET:HE1	1:G:57:ARG:CB	2.35	0.51
1:G:46:HIS:NE2	2:H:256:GLU:OE2	2.44	0.51
2:H:656:MET:HA	2:H:659:VAL:HG22	1.93	0.51
2:H:769:GLU:OE2	2:H:769:GLU:N	2.28	0.51
2:D:659:VAL:O	10:D:1006:MGD:N22	2.35	0.51
1:E:11:ILE:HG23	1:E:13:VAL:HG23	1.93	0.51
2:F:825:ASN:HD21	10:F:1007:MGD:H2'	1.75	0.51
2:B:816:PHE:HD2	2:B:929:SER:HB2	1.76	0.51
2:B:867:GLN:N	2:B:867:GLN:OE1	2.44	0.51
1:C:11:ILE:HG23	1:C:13:VAL:HG23	1.92	0.51
2:D:816:PHE:HE2	2:D:929:SER:H	1.55	0.51
2:H:365:ASN:HB3	2:H:596:PHE:CE2	2.45	0.51
2:B:196:HIS:NE2	2:B:298:SER:HA	2.26	0.51
2:B:221:ILE:HD12	2:B:229:MET:HE1	1.93	0.51
2:B:656:MET:HA	2:B:659:VAL:HG22	1.93	0.51
2:D:825:ASN:HD21	10:D:1007:MGD:H2'	1.75	0.51
2:D:898:LEU:HD23	2:D:908:ILE:HD13	1.92	0.51
2:F:449:LYS:HB2	2:F:536:MET:HE2	1.92	0.51
2:F:650:TYR:OH	2:F:679:GLN:NE2	2.43	0.51
2:H:196:HIS:NE2	2:H:298:SER:HA	2.26	0.51
2:H:816:PHE:HD2	2:H:929:SER:HB2	1.76	0.51
1:A:46:HIS:NE2	2:B:256:GLU:OE2	2.44	0.51
2:B:426:SER:OG	2:B:428:THR:OG1	2.21	0.51
2:D:652:LYS:HB2	2:D:679:GLN:HB3	1.92	0.51
2:D:867:GLN:N	2:D:867:GLN:OE1	2.44	0.51
2:B:652:LYS:HB2	2:B:679:GLN:HB3	1.92	0.51
1:C:131:ILE:HA	1:C:134:LEU:HD23	1.92	0.51
2:D:196:HIS:NE2	2:D:298:SER:HA	2.26	0.51
2:D:221:ILE:HD12	2:D:229:MET:HE1	1.93	0.51
2:D:411:SER:HA	2:D:710:GLU:HB2	1.92	0.51
2:D:816:PHE:HD2	2:D:929:SER:HB2	1.76	0.51
2:F:365:ASN:HB3	2:F:596:PHE:CE2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:365:ASN:HB3	2:B:596:PHE:CE2	2.45	0.51
2:F:816:PHE:HD2	2:F:929:SER:HB2	1.76	0.51
2:H:449:LYS:HB2	2:H:536:MET:HE2	1.92	0.51
2:D:829:LEU:O	10:D:1007:MGD:N19	2.44	0.51
2:F:361:SER:HB2	2:F:587:HIS:HD2	1.76	0.51
2:F:399:LEU:O	2:F:404:GLY:N	2.29	0.51
1:G:11:ILE:HG23	1:G:13:VAL:HG23	1.92	0.51
2:H:361:SER:HB2	2:H:587:HIS:HD2	1.76	0.51
2:H:411:SER:N	2:H:414:ASP:OD2	2.38	0.51
2:F:898:LEU:HD23	2:F:908:ILE:HD13	1.92	0.51
2:H:898:LEU:HD23	2:H:908:ILE:HD13	1.92	0.51
2:B:618:TYR:HA	2:B:621:VAL:HG12	1.93	0.50
2:D:27:ASN:OD1	2:D:35:GLN:NE2	2.43	0.50
2:F:196:HIS:NE2	2:F:298:SER:HA	2.26	0.50
2:F:867:GLN:N	2:F:867:GLN:OE1	2.44	0.50
2:H:27:ASN:OD1	2:H:35:GLN:NE2	2.43	0.50
2:B:898:LEU:HD23	2:B:908:ILE:HD13	1.92	0.50
1:C:46:HIS:NE2	2:D:256:GLU:OE2	2.44	0.50
1:E:131:ILE:HA	1:E:134:LEU:HD23	1.92	0.50
2:F:411:SER:HA	2:F:710:GLU:HB2	1.92	0.50
2:H:411:SER:HA	2:H:710:GLU:HB2	1.92	0.50
2:H:587:HIS:NE2	10:H:1006:MGD:O1A	2.31	0.50
2:B:322:ARG:NH2	1:G:3:LYS:O	2.43	0.50
2:D:967:ARG:NH2	2:D:969:ASP:OD2	2.45	0.50
2:F:497:LEU:HD12	2:F:504:ARG:HB2	1.93	0.50
2:H:618:TYR:HA	2:H:621:VAL:HG12	1.93	0.50
2:H:867:GLN:OE1	2:H:867:GLN:N	2.44	0.50
2:B:449:LYS:HB2	2:B:536:MET:HE2	1.92	0.50
2:B:587:HIS:NE2	10:B:1006:MGD:O1A	2.31	0.50
2:F:271:GLY:O	2:F:714:GLN:NE2	2.38	0.50
2:F:829:LEU:O	10:F:1007:MGD:N19	2.44	0.50
2:H:162:GLN:HB2	2:H:196:HIS:CE1	2.47	0.50
2:H:221:ILE:HD12	2:H:229:MET:HE1	1.93	0.50
2:H:240:TYR:O	2:H:244:LEU:HB2	2.12	0.50
2:B:829:LEU:O	10:B:1007:MGD:N19	2.44	0.50
2:D:365:ASN:HB3	2:D:596:PHE:CE2	2.45	0.50
2:F:656:MET:HA	2:F:659:VAL:HG22	1.93	0.50
2:F:831:GLU:OE2	2:F:849:THR:OG1	2.30	0.50
1:G:131:ILE:HA	1:G:134:LEU:HD23	1.92	0.50
2:H:662:ASN:H	2:H:912:THR:HG23	1.77	0.50
2:H:831:GLU:OE2	2:H:849:THR:OG1	2.30	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:ASN:OD1	2:D:175:ARG:NH2	2.45	0.50
2:D:190:SER:O	2:D:190:SER:OG	2.29	0.50
2:D:286:VAL:O	2:D:304:LYS:NZ	2.44	0.50
2:D:449:LYS:HB2	2:D:536:MET:HE2	1.92	0.50
1:E:46:HIS:NE2	2:F:256:GLU:OE2	2.44	0.50
2:F:221:ILE:HD12	2:F:229:MET:HE1	1.93	0.50
2:B:233:THR:O	2:B:237:GLU:HG3	2.12	0.50
2:B:715:ARG:HB3	2:B:771:LEU:HB3	1.94	0.50
2:B:831:GLU:OE2	2:B:849:THR:OG1	2.30	0.50
2:B:860:LEU:HD13	2:B:894:LYS:HA	1.94	0.50
2:D:619:GLU:HG2	2:D:625:PRO:HA	1.94	0.50
2:D:656:MET:HA	2:D:659:VAL:HG22	1.93	0.50
2:F:662:ASN:H	2:F:912:THR:HG23	1.77	0.50
2:F:860:LEU:HD13	2:F:894:LYS:HA	1.94	0.50
1:A:47:MET:HE3	1:A:53:LEU:HG	1.94	0.50
2:B:55:ILE:HG13	2:B:55:ILE:O	2.11	0.50
2:B:399:LEU:O	2:B:404:GLY:N	2.29	0.50
2:D:831:GLU:OE2	2:D:849:THR:OG1	2.30	0.50
2:F:162:GLN:HB2	2:F:196:HIS:CE1	2.47	0.50
1:A:50:ARG:NH2	1:C:61:GLY:O	2.30	0.50
2:B:162:GLN:HB2	2:B:196:HIS:CE1	2.47	0.50
2:D:55:ILE:O	2:D:55:ILE:HG13	2.11	0.50
2:D:715:ARG:HB3	2:D:771:LEU:HB3	1.94	0.50
1:E:3:LYS:O	2:H:322:ARG:NH2	2.43	0.50
2:F:618:TYR:HA	2:F:621:VAL:HG12	1.93	0.50
2:H:233:THR:O	2:H:237:GLU:HG3	2.12	0.50
2:H:497:LEU:HD12	2:H:504:ARG:HB2	1.93	0.50
2:D:240:TYR:O	2:D:244:LEU:HB2	2.12	0.49
2:D:497:LEU:HD12	2:D:504:ARG:HB2	1.93	0.49
2:D:547:TRP:HB2	2:D:551:VAL:CG1	2.42	0.49
1:E:47:MET:HE3	1:E:53:LEU:HG	1.94	0.49
2:F:765:GLY:H	2:F:781:VAL:HG13	1.77	0.49
2:B:240:TYR:O	2:B:244:LEU:HB2	2.12	0.49
2:D:159:GLN:O	2:D:444:LYS:NZ	2.45	0.49
2:H:829:LEU:O	10:H:1007:MGD:N19	2.44	0.49
2:B:373:LYS:NZ	2:B:755:GLU:OE2	2.42	0.49
2:B:497:LEU:HD12	2:B:504:ARG:HB2	1.93	0.49
2:D:162:GLN:HB2	2:D:196:HIS:CE1	2.47	0.49
2:D:320:LEU:HB2	2:D:693:VAL:HB	1.94	0.49
2:D:765:GLY:H	2:D:781:VAL:HG13	1.77	0.49
2:F:320:LEU:HB2	2:F:693:VAL:HB	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:55:ILE:O	2:H:55:ILE:HG13	2.11	0.49
1:A:9:GLN:HG3	2:D:326:HIS:CD2	2.47	0.49
2:B:326:HIS:CD2	1:G:9:GLN:HG3	2.47	0.49
2:B:353:ASP:OD1	2:B:353:ASP:N	2.45	0.49
2:B:420:LEU:HD21	2:B:537:ILE:HG12	1.94	0.49
2:B:619:GLU:HG2	2:B:625:PRO:HA	1.94	0.49
2:D:233:THR:O	2:D:237:GLU:HG3	2.12	0.49
2:D:618:TYR:HA	2:D:621:VAL:HG12	1.93	0.49
2:D:860:LEU:HD13	2:D:894:LYS:HA	1.94	0.49
2:F:420:LEU:HD21	2:F:537:ILE:HG12	1.94	0.49
1:G:47:MET:HE3	1:G:53:LEU:HG	1.94	0.49
1:C:47:MET:HE3	1:C:53:LEU:HG	1.94	0.49
2:F:715:ARG:HB3	2:F:771:LEU:HB3	1.94	0.49
2:H:286:VAL:O	2:H:304:LYS:NZ	2.44	0.49
2:D:638:ILE:HG23	2:D:669:ALA:HB2	1.95	0.49
2:F:233:THR:O	2:F:237:GLU:HG3	2.12	0.49
2:F:547:TRP:HB2	2:F:551:VAL:CG1	2.42	0.49
2:H:320:LEU:HB2	2:H:693:VAL:HB	1.94	0.49
2:H:619:GLU:HG2	2:H:625:PRO:HA	1.94	0.49
2:B:94:ASN:OD1	2:B:175:ARG:NH2	2.45	0.49
2:F:55:ILE:O	2:F:55:ILE:HG13	2.11	0.49
2:H:638:ILE:HG23	2:H:669:ALA:HB2	1.95	0.49
2:H:860:LEU:HD13	2:H:894:LYS:HA	1.94	0.49
2:B:159:GLN:O	2:B:444:LYS:NZ	2.45	0.49
2:B:361:SER:HB2	2:B:587:HIS:HD2	1.76	0.49
2:D:440:LYS:NZ	2:D:459:GLU:OE2	2.40	0.49
1:E:50:ARG:NH2	1:G:61:GLY:O	2.30	0.49
2:F:857:SER:OG	2:F:893:GLY:O	2.28	0.49
1:C:9:GLN:HG3	2:F:326:HIS:CD2	2.47	0.49
2:D:360:SER:H	2:D:652:LYS:NZ	2.11	0.49
2:F:353:ASP:N	2:F:353:ASP:OD1	2.45	0.49
2:H:94:ASN:OD1	2:H:175:ARG:NH2	2.45	0.49
2:H:715:ARG:HB3	2:H:771:LEU:HB3	1.94	0.49
2:B:7:ILE:HD11	2:B:71:ASP:HB2	1.95	0.48
2:B:320:LEU:HB2	2:B:693:VAL:HB	1.94	0.48
2:B:547:TRP:HB2	2:B:551:VAL:CG1	2.42	0.48
2:B:765:GLY:H	2:B:781:VAL:HG13	1.77	0.48
2:H:7:ILE:HD11	2:H:71:ASP:HB2	1.95	0.48
2:H:159:GLN:O	2:H:444:LYS:NZ	2.45	0.48
2:H:208:GLU:OE2	2:H:304:LYS:NZ	2.42	0.48
2:H:353:ASP:OD1	2:H:353:ASP:N	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:SER:H	2:B:652:LYS:NZ	2.11	0.48
2:B:662:ASN:H	2:B:912:THR:HG23	1.77	0.48
2:D:353:ASP:N	2:D:353:ASP:OD1	2.45	0.48
2:D:662:ASN:H	2:D:912:THR:HG23	1.77	0.48
2:F:360:SER:H	2:F:652:LYS:NZ	2.11	0.48
2:F:619:GLU:HG2	2:F:625:PRO:HA	1.94	0.48
2:H:420:LEU:HD21	2:H:537:ILE:HG12	1.94	0.48
2:F:7:ILE:HD11	2:F:71:ASP:HB2	1.95	0.48
2:F:240:TYR:O	2:F:244:LEU:HB2	2.12	0.48
2:F:421:VAL:HG11	2:F:439:ILE:HD13	1.95	0.48
2:F:440:LYS:NZ	2:F:459:GLU:OE2	2.40	0.48
2:H:190:SER:O	2:H:190:SER:OG	2.29	0.48
2:H:765:GLY:H	2:H:781:VAL:HG13	1.77	0.48
1:A:61:GLY:O	1:G:50:ARG:NH2	2.30	0.48
2:D:138:HIS:NE2	2:D:193:SER:OG	2.41	0.48
2:H:421:VAL:HG11	2:H:439:ILE:HD13	1.95	0.48
2:H:967:ARG:NH2	2:H:969:ASP:OD2	2.45	0.48
1:A:57:ARG:NH1	2:H:256:GLU:OE2	2.47	0.48
2:B:138:HIS:NE2	2:B:193:SER:OG	2.41	0.48
2:D:420:LEU:HD21	2:D:537:ILE:HG12	1.94	0.48
2:D:587:HIS:HB2	2:D:590:VAL:HB	1.96	0.48
2:D:762:ILE:HG13	2:D:763:TYR:HD1	1.78	0.48
2:F:140:PHE:HB3	2:F:305:PHE:CD1	2.49	0.48
2:H:482:ILE:HG13	2:H:533:MET:HE2	1.95	0.48
2:B:587:HIS:HB2	2:B:590:VAL:HB	1.96	0.48
2:B:638:ILE:HG23	2:B:669:ALA:HB2	1.95	0.48
2:D:7:ILE:HD11	2:D:71:ASP:HB2	1.95	0.48
2:D:563:ALA:HA	2:D:566:ASN:HD21	1.79	0.48
1:E:9:GLN:HG3	2:H:326:HIS:CD2	2.47	0.48
2:F:94:ASN:OD1	2:F:175:ARG:NH2	2.45	0.48
2:F:762:ILE:HG13	2:F:763:TYR:HD1	1.78	0.48
2:H:360:SER:H	2:H:652:LYS:NZ	2.11	0.48
2:B:171:TRP:CD1	2:B:963:LYS:HB2	2.49	0.48
2:B:563:ALA:HA	2:B:566:ASN:HD21	1.79	0.48
2:B:595:ASP:OD2	2:B:763:TYR:OH	2.30	0.48
1:C:62:GLN:O	1:C:66:VAL:HG23	2.14	0.48
2:F:961:VAL:O	2:F:964:LYS:N	2.47	0.48
2:H:140:PHE:HB3	2:H:305:PHE:CD1	2.49	0.48
2:H:171:TRP:CD1	2:H:963:LYS:HB2	2.49	0.48
2:H:547:TRP:HB2	2:H:551:VAL:CG1	2.42	0.48
2:H:762:ILE:HG13	2:H:763:TYR:HD1	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:PHE:HB3	2:B:305:PHE:CD1	2.49	0.48
2:B:271:GLY:O	2:B:714:GLN:NE2	2.38	0.48
2:B:676:PHE:HB3	2:B:690:ALA:HA	1.96	0.48
2:B:762:ILE:HG13	2:B:763:TYR:HD1	1.78	0.48
2:D:256:GLU:OE2	1:E:57:ARG:NH1	2.47	0.48
2:D:636:GLU:O	2:D:640:LYS:HG2	2.14	0.48
1:E:129:ASP:OD1	1:E:129:ASP:N	2.36	0.48
2:F:256:GLU:OE2	1:G:57:ARG:NH1	2.47	0.48
2:F:868:ASP:HB3	2:F:887:ILE:HG22	1.95	0.48
2:H:222:ASN:HB2	2:H:225:THR:HG22	1.96	0.48
2:H:961:VAL:O	2:H:964:LYS:N	2.47	0.48
2:B:359:THR:HB	2:B:371:MET:HG2	1.96	0.47
2:B:482:ILE:HG13	2:B:533:MET:HE2	1.95	0.47
2:B:636:GLU:O	2:B:640:LYS:HG2	2.14	0.47
2:D:90:LYS:NZ	2:D:971:ILE:O	2.47	0.47
2:D:222:ASN:HB2	2:D:225:THR:HG22	1.96	0.47
2:H:868:ASP:HB3	2:H:887:ILE:HG22	1.95	0.47
2:B:562:THR:O	2:B:566:ASN:ND2	2.48	0.47
2:D:140:PHE:HB3	2:D:305:PHE:CD1	2.49	0.47
2:D:257:ARG:CZ	2:D:279:LYS:HD2	2.44	0.47
2:D:421:VAL:HG11	2:D:439:ILE:HD13	1.95	0.47
2:F:171:TRP:CD1	2:F:963:LYS:HB2	2.49	0.47
2:H:359:THR:HB	2:H:371:MET:HG2	1.96	0.47
2:B:39:HIS:HB3	2:B:42:LEU:HB2	1.95	0.47
2:B:335:ALA:O	2:B:339:ILE:HG22	2.14	0.47
2:D:482:ILE:HG13	2:D:533:MET:HE2	1.95	0.47
2:F:482:ILE:HG13	2:F:533:MET:HE2	1.95	0.47
2:H:39:HIS:HB3	2:H:42:LEU:HB2	1.95	0.47
2:H:90:LYS:NZ	2:H:971:ILE:O	2.47	0.47
1:A:3:LYS:O	2:D:322:ARG:NH2	2.43	0.47
1:A:62:GLN:O	1:A:66:VAL:HG23	2.14	0.47
1:A:67:LEU:O	1:A:71:VAL:HG22	2.15	0.47
2:D:171:TRP:CD1	2:D:963:LYS:HB2	2.49	0.47
2:D:356:ALA:HA	2:D:383:ASN:HB2	1.97	0.47
2:F:39:HIS:HB3	2:F:42:LEU:HB2	1.95	0.47
2:F:563:ALA:HA	2:F:566:ASN:HD21	1.79	0.47
2:F:700:LEU:HD22	2:F:719:VAL:HG21	1.97	0.47
2:H:587:HIS:HB2	2:H:590:VAL:HB	1.96	0.47
2:H:636:GLU:O	2:H:640:LYS:HG2	2.14	0.47
2:B:90:LYS:NZ	2:B:971:ILE:O	2.47	0.47
2:B:961:VAL:O	2:B:964:LYS:N	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:676:PHE:HB3	2:D:690:ALA:HA	1.96	0.47
1:E:9:GLN:HB2	2:H:328:ARG:HA	1.96	0.47
2:F:286:VAL:O	2:F:304:LYS:NZ	2.44	0.47
2:F:356:ALA:HA	2:F:383:ASN:HB2	1.97	0.47
2:F:636:GLU:O	2:F:640:LYS:HG2	2.14	0.47
1:G:62:GLN:O	1:G:66:VAL:HG23	2.14	0.47
2:H:356:ALA:HA	2:H:383:ASN:HB2	1.97	0.47
1:A:36:ALA:HB1	1:C:44:LEU:HB3	1.96	0.47
2:B:55:ILE:HG12	2:B:60:LYS:HB2	1.97	0.47
2:B:257:ARG:CZ	2:B:279:LYS:HD2	2.44	0.47
2:B:283:ILE:HD13	2:B:307:TRP:HB3	1.97	0.47
2:B:421:VAL:HG11	2:B:439:ILE:HD13	1.95	0.47
2:B:700:LEU:HD22	2:B:719:VAL:HG21	1.97	0.47
2:D:55:ILE:HG12	2:D:60:LYS:HB2	1.97	0.47
2:D:361:SER:HB2	2:D:587:HIS:HD2	1.76	0.47
2:D:619:GLU:HG3	2:D:626:LEU:HD23	1.97	0.47
2:D:700:LEU:HD22	2:D:719:VAL:HG21	1.97	0.47
2:D:834:HIS:N	10:D:1007:MGD:O17	2.48	0.47
1:E:20:LYS:HD3	1:E:20:LYS:HA	1.62	0.47
1:E:62:GLN:O	1:E:66:VAL:HG23	2.14	0.47
2:F:359:THR:HB	2:F:371:MET:HG2	1.95	0.47
2:F:587:HIS:HB2	2:F:590:VAL:HB	1.96	0.47
2:F:638:ILE:HG23	2:F:669:ALA:HB2	1.95	0.47
2:H:257:ARG:CZ	2:H:279:LYS:HD2	2.44	0.47
2:H:700:LEU:HD22	2:H:719:VAL:HG21	1.97	0.47
2:B:222:ASN:HB2	2:B:225:THR:HG22	1.96	0.47
2:B:256:GLU:OE2	1:C:57:ARG:NH1	2.47	0.47
2:B:356:ALA:HA	2:B:383:ASN:HB2	1.97	0.47
1:C:9:GLN:HB2	2:F:328:ARG:HA	1.96	0.47
1:C:67:LEU:O	1:C:71:VAL:HG22	2.15	0.47
2:D:39:HIS:HB3	2:D:42:LEU:HB2	1.95	0.47
2:D:335:ALA:O	2:D:339:ILE:HG22	2.14	0.47
2:D:399:LEU:O	2:D:404:GLY:N	2.29	0.47
1:E:67:LEU:O	1:E:71:VAL:HG22	2.15	0.47
2:F:222:ASN:HB2	2:F:225:THR:HG22	1.96	0.47
2:F:257:ARG:CZ	2:F:279:LYS:HD2	2.44	0.47
2:F:432:HIS:ND1	2:F:584:LEU:HD13	2.30	0.47
2:F:676:PHE:HB3	2:F:690:ALA:HA	1.96	0.47
1:G:67:LEU:O	1:G:71:VAL:HG22	2.15	0.47
2:B:824:VAL:HG23	2:B:896:VAL:HG23	1.97	0.47
2:D:562:THR:O	2:D:566:ASN:ND2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:568:LEU:HB2	2:D:574:TYR:CE2	2.50	0.47
2:D:873:ARG:NH1	2:D:880:ASN:OD1	2.48	0.47
1:E:36:ALA:HB1	1:G:44:LEU:HB3	1.96	0.47
2:F:55:ILE:HG12	2:F:60:LYS:HB2	1.97	0.47
2:F:619:GLU:HG3	2:F:626:LEU:HD23	1.97	0.47
2:B:547:TRP:CZ3	2:B:581:SER:HB2	2.50	0.47
2:D:547:TRP:CZ3	2:D:581:SER:HB2	2.50	0.47
2:D:832:HIS:CD2	2:D:849:THR:HB	2.50	0.47
2:H:563:ALA:HA	2:H:566:ASN:HD21	1.79	0.47
2:B:711:ARG:O	2:B:778:GLN:HA	2.15	0.47
2:B:868:ASP:HB3	2:B:887:ILE:HG22	1.95	0.47
1:C:3:LYS:O	2:F:322:ARG:NH2	2.43	0.47
2:D:868:ASP:HB3	2:D:887:ILE:HG22	1.95	0.47
2:F:711:ARG:CZ	2:F:711:ARG:HB2	2.45	0.47
2:F:832:HIS:CD2	2:F:849:THR:HB	2.50	0.47
2:H:283:ILE:HD13	2:H:307:TRP:HB3	1.97	0.47
2:H:335:ALA:O	2:H:339:ILE:HG22	2.14	0.47
2:H:432:HIS:ND1	2:H:584:LEU:HD13	2.30	0.47
2:H:676:PHE:O	2:H:691:ASP:N	2.48	0.47
2:B:328:ARG:HA	1:G:9:GLN:HB2	1.96	0.46
2:B:832:HIS:CD2	2:B:849:THR:HB	2.50	0.46
2:B:873:ARG:NH1	2:B:880:ASN:OD1	2.48	0.46
2:D:359:THR:HB	2:D:371:MET:HG2	1.96	0.46
2:D:765:GLY:HA3	2:D:781:VAL:HG22	1.97	0.46
2:F:90:LYS:NZ	2:F:971:ILE:O	2.47	0.46
2:F:335:ALA:O	2:F:339:ILE:HG22	2.14	0.46
2:F:390:TYR:HB3	2:F:925:TYR:CE2	2.48	0.46
2:F:411:SER:N	2:F:414:ASP:OD2	2.38	0.46
2:H:765:GLY:HA3	2:H:781:VAL:HG22	1.97	0.46
2:B:260:LYS:HG2	2:B:277:TRP:CD1	2.51	0.46
2:B:432:HIS:ND1	2:B:584:LEU:HD13	2.30	0.46
2:D:81:LYS:HD3	2:D:81:LYS:HA	1.74	0.46
2:D:432:HIS:ND1	2:D:584:LEU:HD13	2.30	0.46
2:F:123:GLN:NE2	2:F:240:TYR:OH	2.49	0.46
2:F:765:GLY:HA3	2:F:781:VAL:HG22	1.97	0.46
2:F:871:LEU:HD22	2:F:935:LEU:HD12	1.98	0.46
2:H:711:ARG:CZ	2:H:711:ARG:HB2	2.45	0.46
2:H:824:VAL:HG23	2:H:896:VAL:HG23	1.97	0.46
1:A:44:LEU:HB3	1:G:36:ALA:HB1	1.96	0.46
2:B:190:SER:O	2:B:190:SER:OG	2.29	0.46
2:B:568:LEU:HB2	2:B:574:TYR:CE2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:123:GLN:NE2	2:D:240:TYR:OH	2.49	0.46
2:D:603:LEU:HG	2:D:609:VAL:HG12	1.98	0.46
2:D:711:ARG:O	2:D:778:GLN:HA	2.15	0.46
2:D:871:LEU:HD22	2:D:935:LEU:HD12	1.98	0.46
2:D:961:VAL:O	2:D:964:LYS:N	2.47	0.46
2:F:547:TRP:CZ3	2:F:581:SER:HB2	2.50	0.46
2:F:568:LEU:HB2	2:F:574:TYR:CE2	2.50	0.46
2:F:655:GLU:O	2:F:655:GLU:HG2	2.16	0.46
2:H:302:LYS:HE3	2:H:302:LYS:HB2	1.75	0.46
2:H:619:GLU:HG3	2:H:626:LEU:HD23	1.97	0.46
2:H:655:GLU:HG2	2:H:655:GLU:O	2.16	0.46
2:H:661:SER:HB3	2:H:923:PRO:HB3	1.97	0.46
1:A:9:GLN:HB2	2:D:328:ARG:HA	1.96	0.46
2:B:765:GLY:HA3	2:B:781:VAL:HG22	1.97	0.46
1:C:36:ALA:HB1	1:E:44:LEU:HB3	1.96	0.46
2:D:249:MET:HE1	1:E:70:LEU:HB2	1.98	0.46
2:D:260:LYS:HG2	2:D:277:TRP:CD1	2.51	0.46
2:F:283:ILE:HD13	2:F:307:TRP:HB3	1.97	0.46
2:F:562:THR:O	2:F:566:ASN:ND2	2.48	0.46
2:F:661:SER:HB3	2:F:923:PRO:HB3	1.97	0.46
2:F:873:ARG:NH1	2:F:880:ASN:OD1	2.48	0.46
2:H:504:ARG:HA	2:H:805:LEU:HD12	1.98	0.46
2:H:568:LEU:HB2	2:H:574:TYR:CE2	2.50	0.46
2:B:249:MET:HE1	1:C:70:LEU:HB2	1.98	0.46
2:B:390:TYR:HB3	2:B:925:TYR:CE2	2.48	0.46
2:B:967:ARG:NH2	2:B:969:ASP:OD2	2.45	0.46
2:D:543:VAL:HB	2:D:573:ASN:CG	2.41	0.46
2:F:158:CYS:HB3	2:F:167:LEU:HB2	1.98	0.46
2:F:357:PHE:O	2:F:384:VAL:HA	2.15	0.46
2:F:504:ARG:HA	2:F:805:LEU:HD12	1.98	0.46
2:F:603:LEU:HG	2:F:609:VAL:HG12	1.98	0.46
2:F:967:ARG:NH2	2:F:969:ASP:OD2	2.45	0.46
2:H:158:CYS:HB3	2:H:167:LEU:HB2	1.98	0.46
1:A:97:ASP:HA	1:G:85:ASN:HD21	1.81	0.46
2:B:655:GLU:O	2:B:655:GLU:HG2	2.16	0.46
2:F:249:MET:HE1	1:G:70:LEU:HB2	1.98	0.46
2:F:267:TYR:CD2	2:F:302:LYS:HB3	2.51	0.46
2:F:373:LYS:NZ	2:F:755:GLU:OE2	2.42	0.46
2:H:141:TYR:HA	2:H:208:GLU:HA	1.97	0.46
2:H:357:PHE:O	2:H:384:VAL:HA	2.15	0.46
2:H:547:TRP:CZ3	2:H:581:SER:HB2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:562:THR:O	2:H:566:ASN:ND2	2.48	0.46
2:H:873:ARG:NH1	2:H:880:ASN:OD1	2.48	0.46
2:B:267:TYR:CD2	2:B:302:LYS:HB3	2.51	0.46
2:B:676:PHE:O	2:B:691:ASP:N	2.48	0.46
2:D:283:ILE:HD13	2:D:307:TRP:HB3	1.97	0.46
2:D:361:SER:HB3	2:D:590:VAL:HA	1.97	0.46
2:D:426:SER:HA	2:D:548:ALA:HB3	1.98	0.46
2:D:699:SER:HA	2:D:702:LYS:HG2	1.98	0.46
2:F:249:MET:CE	1:G:70:LEU:HB2	2.46	0.46
2:F:699:SER:HA	2:F:702:LYS:HG2	1.98	0.46
2:F:711:ARG:O	2:F:778:GLN:HA	2.15	0.46
1:G:99:LYS:HD2	1:G:99:LYS:HA	1.76	0.46
2:H:123:GLN:NE2	2:H:240:TYR:OH	2.49	0.46
1:C:85:ASN:HD21	1:E:97:ASP:HA	1.81	0.46
2:D:302:LYS:HB2	2:D:302:LYS:HE3	1.75	0.46
2:D:357:PHE:O	2:D:384:VAL:HA	2.15	0.46
2:D:504:ARG:HA	2:D:805:LEU:HD12	1.98	0.46
2:F:271:GLY:HA3	2:F:708:ASN:HB3	1.98	0.46
2:H:55:ILE:HG12	2:H:60:LYS:HB2	1.97	0.46
2:H:399:LEU:O	2:H:404:GLY:N	2.29	0.46
2:B:123:GLN:NE2	2:B:240:TYR:OH	2.49	0.46
2:B:271:GLY:HA3	2:B:708:ASN:HB3	1.98	0.46
2:D:141:TYR:HA	2:D:208:GLU:HA	1.97	0.46
2:D:676:PHE:O	2:D:691:ASP:N	2.48	0.46
2:F:260:LYS:HG2	2:F:277:TRP:CD1	2.51	0.46
2:F:369:TYR:HB2	2:F:596:PHE:CD2	2.51	0.46
2:H:361:SER:HB3	2:H:590:VAL:HA	1.97	0.46
2:H:372:GLN:HE22	2:H:622:TRP:HZ2	1.64	0.46
2:H:676:PHE:HB3	2:H:690:ALA:HA	1.96	0.46
2:B:619:GLU:HG3	2:B:626:LEU:HD23	1.97	0.46
2:B:711:ARG:HB2	2:B:711:ARG:CZ	2.45	0.46
2:D:617:LYS:HB3	2:D:617:LYS:HE2	1.82	0.46
2:H:138:HIS:NE2	2:H:193:SER:OG	2.41	0.46
2:H:271:GLY:HA3	2:H:708:ASN:HB3	1.98	0.46
1:A:70:LEU:HB2	2:H:249:MET:CE	2.46	0.45
2:B:372:GLN:HE22	2:B:622:TRP:HZ2	1.64	0.45
2:B:426:SER:HA	2:B:548:ALA:HB3	1.98	0.45
2:B:661:SER:HB3	2:B:923:PRO:HB3	1.97	0.45
2:D:661:SER:HB3	2:D:923:PRO:HB3	1.97	0.45
2:F:111:ILE:HD11	2:F:149:ILE:CD1	2.46	0.45
2:F:676:PHE:O	2:F:691:ASP:N	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:824:VAL:HG23	2:F:896:VAL:HG23	1.97	0.45
2:F:834:HIS:N	10:F:1007:MGD:O17	2.48	0.45
2:H:543:VAL:HB	2:H:573:ASN:CG	2.41	0.45
2:H:711:ARG:O	2:H:778:GLN:HA	2.15	0.45
2:B:543:VAL:HB	2:B:573:ASN:CG	2.41	0.45
2:D:271:GLY:HA3	2:D:708:ASN:HB3	1.98	0.45
2:F:171:TRP:CD2	2:F:964:LYS:HB2	2.52	0.45
2:F:372:GLN:HE22	2:F:622:TRP:HZ2	1.64	0.45
2:F:818:GLU:HG3	2:F:819:GLU:N	2.32	0.45
2:H:260:LYS:HG2	2:H:277:TRP:CD1	2.51	0.45
2:H:271:GLY:O	2:H:714:GLN:NE2	2.38	0.45
2:H:871:LEU:HD22	2:H:935:LEU:HD12	1.98	0.45
1:A:70:LEU:HB2	2:H:249:MET:HE1	1.98	0.45
1:A:97:ASP:H	1:C:109:ASN:CG	2.24	0.45
1:A:99:LYS:HD2	1:A:99:LYS:HA	1.76	0.45
2:B:361:SER:HB3	2:B:590:VAL:HA	1.97	0.45
2:B:818:GLU:HG3	2:B:819:GLU:N	2.32	0.45
2:D:158:CYS:HB3	2:D:167:LEU:HB2	1.98	0.45
2:D:171:TRP:CD2	2:D:964:LYS:HB2	2.52	0.45
2:D:249:MET:CE	1:E:70:LEU:HB2	2.46	0.45
2:D:711:ARG:HB2	2:D:711:ARG:CZ	2.45	0.45
2:F:421:VAL:HB	2:F:450:VAL:HG12	1.99	0.45
2:H:185:PRO:HB2	2:H:188:GLU:OE1	2.17	0.45
2:H:357:PHE:CZ	2:H:379:ILE:HG13	2.52	0.45
2:H:369:TYR:HB2	2:H:596:PHE:CD2	2.51	0.45
2:B:115:VAL:HG13	2:B:120:ILE:HG22	1.99	0.45
2:B:158:CYS:HB3	2:B:167:LEU:HB2	1.98	0.45
2:B:357:PHE:O	2:B:384:VAL:HA	2.15	0.45
2:B:585:ARG:HB2	2:B:709:THR:HA	1.99	0.45
2:D:421:VAL:HB	2:D:450:VAL:HG12	1.99	0.45
2:D:824:VAL:HG23	2:D:896:VAL:HG23	1.97	0.45
2:D:876:SER:C	2:D:878:PHE:H	2.25	0.45
1:E:85:ASN:HD21	1:G:97:ASP:HA	1.81	0.45
2:F:357:PHE:CZ	2:F:379:ILE:HG13	2.52	0.45
2:F:543:VAL:HB	2:F:573:ASN:CG	2.41	0.45
2:H:267:TYR:CD2	2:H:302:LYS:HB3	2.51	0.45
2:B:141:TYR:HA	2:B:208:GLU:HA	1.97	0.45
2:B:421:VAL:HB	2:B:450:VAL:HG12	1.99	0.45
2:B:871:LEU:HD22	2:B:935:LEU:HD12	1.98	0.45
2:D:267:TYR:CD2	2:D:302:LYS:HB3	2.51	0.45
2:D:390:TYR:HB3	2:D:925:TYR:CE2	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:426:SER:OG	2:D:428:THR:OG1	2.21	0.45
2:F:141:TYR:HA	2:F:208:GLU:HA	1.98	0.45
2:F:362:LYS:HE2	2:F:362:LYS:HB3	1.76	0.45
2:F:393:SER:HB3	2:F:920:THR:HB	1.98	0.45
2:H:161:VAL:HA	2:H:441:ARG:HD2	1.99	0.45
2:H:390:TYR:HB3	2:H:925:TYR:CE2	2.48	0.45
2:B:249:MET:CE	1:C:70:LEU:HB2	2.46	0.45
2:B:275:ASP:OD1	2:B:774:TYR:OH	2.23	0.45
2:B:286:VAL:O	2:B:304:LYS:NZ	2.44	0.45
2:B:357:PHE:CZ	2:B:379:ILE:HG13	2.52	0.45
2:B:504:ARG:HA	2:B:805:LEU:HD12	1.98	0.45
2:D:161:VAL:HA	2:D:441:ARG:HD2	1.99	0.45
2:D:655:GLU:O	2:D:655:GLU:HG2	2.16	0.45
2:H:115:VAL:HG13	2:H:120:ILE:HG22	1.99	0.45
2:H:585:ARG:HB2	2:H:709:THR:HA	1.99	0.45
1:A:48:ASN:HA	1:A:54:PRO:HD3	1.99	0.45
2:B:161:VAL:HA	2:B:441:ARG:HD2	1.99	0.45
2:B:171:TRP:CD2	2:B:964:LYS:HB2	2.52	0.45
2:B:391:CYS:CB	10:B:1006:MGD:S13	3.05	0.45
2:D:357:PHE:CZ	2:D:379:ILE:HG13	2.52	0.45
2:D:369:TYR:HB2	2:D:596:PHE:CD2	2.51	0.45
2:D:393:SER:HB3	2:D:920:THR:HB	1.98	0.45
2:D:818:GLU:HG3	2:D:819:GLU:N	2.32	0.45
2:F:161:VAL:HA	2:F:441:ARG:HD2	1.99	0.45
2:F:361:SER:HB3	2:F:590:VAL:HA	1.97	0.45
2:H:163:VAL:HG11	2:H:440:LYS:HB3	1.99	0.45
2:H:391:CYS:CB	10:H:1006:MGD:S13	3.05	0.45
2:H:426:SER:HA	2:H:548:ALA:HB3	1.98	0.45
2:H:832:HIS:CD2	2:H:849:THR:HB	2.50	0.45
2:D:346:LEU:HD22	2:D:648:ALA:HB2	1.99	0.45
2:D:372:GLN:HE22	2:D:622:TRP:HZ2	1.64	0.45
2:F:141:TYR:OH	9:F:1004:SF4:S1	2.75	0.45
2:F:222:ASN:O	2:F:226:LEU:N	2.50	0.45
2:F:426:SER:HA	2:F:548:ALA:HB3	1.98	0.45
1:A:109:ASN:CG	1:G:97:ASP:H	2.24	0.45
2:B:699:SER:HA	2:B:702:LYS:HG2	1.98	0.45
1:C:48:ASN:HA	1:C:54:PRO:HD3	1.99	0.45
2:D:391:CYS:CB	10:D:1006:MGD:S13	3.05	0.45
2:F:585:ARG:HB2	2:F:709:THR:HA	1.99	0.45
1:G:48:ASN:HA	1:G:54:PRO:HD3	1.99	0.45
2:H:152:GLY:HA3	2:H:959:VAL:HG11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:171:TRP:CD2	2:H:964:LYS:HB2	2.52	0.45
2:H:699:SER:HA	2:H:702:LYS:HG2	1.98	0.45
2:H:739:LYS:HA	2:H:739:LYS:HD3	1.76	0.45
2:B:369:TYR:HB2	2:B:596:PHE:CD2	2.51	0.45
2:B:603:LEU:HG	2:B:609:VAL:HG12	1.98	0.45
2:D:152:GLY:HA3	2:D:959:VAL:HG11	1.99	0.45
2:D:454:ASP:OD2	10:D:1007:MGD:O2'	2.35	0.45
2:D:566:ASN:HB2	2:D:805:LEU:HD22	1.99	0.45
2:D:585:ARG:HB2	2:D:709:THR:HA	1.99	0.45
2:F:640:LYS:HA	2:F:640:LYS:HD3	1.79	0.45
2:F:651:VAL:HG13	2:F:678:VAL:HG23	1.99	0.45
2:H:346:LEU:HD22	2:H:648:ALA:HB2	1.99	0.45
2:H:603:LEU:HG	2:H:609:VAL:HG12	1.98	0.45
2:B:309:PHE:HB2	2:B:682:PHE:CZ	2.52	0.44
2:B:566:ASN:HB2	2:B:805:LEU:HD22	1.99	0.44
1:C:62:GLN:HG3	1:C:65:LYS:HD2	1.99	0.44
2:D:185:PRO:HB2	2:D:188:GLU:OE1	2.17	0.44
2:D:825:ASN:N	2:D:896:VAL:O	2.38	0.44
2:F:185:PRO:HB2	2:F:188:GLU:OE1	2.17	0.44
2:F:876:SER:C	2:F:878:PHE:H	2.25	0.44
1:C:97:ASP:H	1:E:109:ASN:CG	2.24	0.44
2:D:271:GLY:O	2:D:714:GLN:NE2	2.38	0.44
2:D:283:ILE:HG13	2:D:720:PHE:HZ	1.83	0.44
1:E:48:ASN:HA	1:E:54:PRO:HD3	1.99	0.44
1:E:62:GLN:HG3	1:E:65:LYS:HD2	1.99	0.44
2:F:163:VAL:HG11	2:F:440:LYS:HB3	1.99	0.44
2:F:372:GLN:HB2	2:F:376:ARG:NH1	2.32	0.44
2:H:309:PHE:HB2	2:H:682:PHE:CZ	2.52	0.44
2:H:393:SER:HB3	2:H:920:THR:HB	1.98	0.44
2:H:421:VAL:HB	2:H:450:VAL:HG12	1.99	0.44
2:H:818:GLU:HG3	2:H:819:GLU:N	2.32	0.44
1:A:20:LYS:HA	1:A:20:LYS:HD3	1.62	0.44
1:A:85:ASN:HD21	1:C:97:ASP:HA	1.81	0.44
2:B:429:SER:O	2:B:830:LEU:HD12	2.18	0.44
2:B:454:ASP:OD2	10:B:1007:MGD:O2'	2.35	0.44
2:B:739:LYS:HA	2:B:739:LYS:HD3	1.76	0.44
2:D:617:LYS:HA	2:D:620:ARG:NH1	2.33	0.44
2:D:753:MET:HA	2:D:753:MET:HE2	2.00	0.44
2:F:391:CYS:CB	10:F:1006:MGD:S13	3.05	0.44
2:F:595:ASP:OD2	2:F:763:TYR:OH	2.30	0.44
2:F:753:MET:HE2	2:F:753:MET:HA	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:138:HIS:CE1	2:H:140:PHE:HB2	2.53	0.44
2:H:141:TYR:OH	9:H:1004:SF4:S1	2.75	0.44
2:H:362:LYS:HE2	2:H:362:LYS:HB3	1.76	0.44
2:H:373:LYS:NZ	2:H:755:GLU:OE2	2.42	0.44
2:H:651:VAL:HG13	2:H:678:VAL:HG23	2.00	0.44
2:B:185:PRO:HB2	2:B:188:GLU:OE1	2.17	0.44
2:D:9:ILE:O	2:D:9:ILE:HG13	2.17	0.44
2:D:372:GLN:HB2	2:D:376:ARG:NH1	2.32	0.44
2:D:475:ASP:OD1	10:D:1007:MGD:N2	2.43	0.44
2:F:152:GLY:HA3	2:F:959:VAL:HG11	1.99	0.44
2:F:283:ILE:HG13	2:F:720:PHE:HZ	1.83	0.44
2:F:302:LYS:HE3	2:F:302:LYS:HB2	1.75	0.44
2:F:617:LYS:HA	2:F:620:ARG:NH1	2.33	0.44
1:G:62:GLN:HG3	1:G:65:LYS:HD2	1.99	0.44
2:H:9:ILE:O	2:H:9:ILE:HG13	2.17	0.44
2:H:217:TYR:CD2	2:H:253:MET:HB3	2.52	0.44
2:H:372:GLN:HB2	2:H:376:ARG:NH1	2.32	0.44
2:H:753:MET:HE2	2:H:753:MET:HA	2.00	0.44
2:H:876:SER:C	2:H:878:PHE:H	2.25	0.44
2:B:97:LEU:HD12	9:B:1002:SF4:S2	2.58	0.44
2:B:222:ASN:O	2:B:226:LEU:N	2.50	0.44
1:C:20:LYS:HD3	1:C:20:LYS:HA	1.62	0.44
2:D:217:TYR:CD2	2:D:253:MET:HB3	2.52	0.44
2:D:429:SER:O	2:D:830:LEU:HD12	2.18	0.44
2:D:651:VAL:HG13	2:D:678:VAL:HG23	2.00	0.44
7:E:201:MYR:H92	7:G:201:MYR:H51	2.00	0.44
2:F:217:TYR:CD2	2:F:253:MET:HB3	2.52	0.44
2:F:403:VAL:HG23	2:F:405:TYR:H	1.83	0.44
2:H:198:SER:HA	2:H:206:MET:O	2.18	0.44
2:H:556:GLY:O	2:H:560:THR:HG22	2.17	0.44
2:H:828:ARG:N	2:H:897:TYR:OH	2.51	0.44
7:A:212:MYR:H51	7:G:201:MYR:H92	2.00	0.44
2:B:217:TYR:CD2	2:B:253:MET:HB3	2.52	0.44
2:B:753:MET:HA	2:B:753:MET:HE2	2.00	0.44
2:B:828:ARG:N	2:B:897:TYR:OH	2.51	0.44
2:B:835:GLU:HB2	2:B:903:SER:HB3	2.00	0.44
7:C:201:MYR:H92	7:E:201:MYR:H51	2.00	0.44
2:D:309:PHE:HB2	2:D:682:PHE:CZ	2.52	0.44
2:D:835:GLU:HB2	2:D:903:SER:HB3	2.00	0.44
2:F:309:PHE:HB2	2:F:682:PHE:CZ	2.52	0.44
2:F:568:LEU:HD12	2:F:581:SER:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:111:ILE:HD11	2:H:149:ILE:CD1	2.46	0.44
2:H:403:VAL:HG23	2:H:405:TYR:H	1.83	0.44
2:H:835:GLU:HB2	2:H:903:SER:HB3	2.00	0.44
2:B:99:CYS:HB2	13:B:1010:MQ7:H6	2.00	0.44
2:B:138:HIS:CE1	2:B:140:PHE:HB2	2.53	0.44
2:B:617:LYS:HA	2:B:620:ARG:NH1	2.33	0.44
2:B:651:VAL:HG13	2:B:678:VAL:HG23	2.00	0.44
2:D:115:VAL:HG13	2:D:120:ILE:HG22	1.99	0.44
2:D:403:VAL:HG23	2:D:405:TYR:H	1.83	0.44
2:D:414:ASP:HB3	2:D:578:GLY:HA2	2.00	0.44
2:D:556:GLY:O	2:D:560:THR:HG22	2.17	0.44
2:F:198:SER:HA	2:F:206:MET:O	2.18	0.44
2:F:414:ASP:HB3	2:F:578:GLY:HA2	2.00	0.44
2:F:556:GLY:O	2:F:560:THR:HG22	2.17	0.44
2:H:222:ASN:O	2:H:226:LEU:N	2.50	0.44
2:H:298:SER:HB3	2:H:434:VAL:HG22	2.00	0.44
2:H:429:SER:O	2:H:830:LEU:HD12	2.18	0.44
2:H:834:HIS:N	10:H:1007:MGD:O17	2.48	0.44
2:H:836:GLY:HA3	2:H:840:TYR:HD2	1.83	0.44
1:A:62:GLN:HG3	1:A:65:LYS:HD2	1.99	0.44
2:B:152:GLY:HA3	2:B:959:VAL:HG11	1.99	0.44
2:B:198:SER:HA	2:B:206:MET:O	2.18	0.44
2:B:556:GLY:O	2:B:560:THR:HG22	2.17	0.44
2:D:163:VAL:HG11	2:D:440:LYS:HB3	1.99	0.44
2:D:828:ARG:N	2:D:897:TYR:OH	2.51	0.44
1:E:10:LYS:HE2	1:E:10:LYS:HB2	1.86	0.44
2:F:269:GLY:N	2:F:586:GLY:O	2.51	0.44
2:F:835:GLU:HB2	2:F:903:SER:HB3	2.00	0.44
2:H:566:ASN:HB2	2:H:805:LEU:HD22	1.99	0.44
2:H:617:LYS:HA	2:H:620:ARG:NH1	2.33	0.44
2:H:828:ARG:HD3	10:H:1007:MGD:C16	2.48	0.44
2:D:568:LEU:HD12	2:D:581:SER:HB3	2.00	0.44
2:F:97:LEU:HD12	9:F:1002:SF4:S2	2.58	0.44
2:F:115:VAL:HG13	2:F:120:ILE:HG22	1.99	0.44
2:H:269:GLY:N	2:H:586:GLY:O	2.51	0.44
2:B:141:TYR:OH	9:B:1004:SF4:S1	2.75	0.43
2:B:163:VAL:HG11	2:B:440:LYS:HB3	1.99	0.43
2:B:393:SER:HB3	2:B:920:THR:HB	1.98	0.43
2:D:222:ASN:O	2:D:226:LEU:N	2.50	0.43
2:D:729:ASP:O	2:D:733:ILE:HG12	2.18	0.43
2:D:751:ASP:O	2:D:754:GLU:HG3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:729:ASP:O	2:F:733:ILE:HG12	2.18	0.43
2:H:81:LYS:HA	2:H:81:LYS:HD3	1.74	0.43
2:H:99:CYS:HB2	13:H:1010:MQ7:H6	2.00	0.43
2:H:595:ASP:OD2	2:H:763:TYR:OH	2.30	0.43
7:A:212:MYR:H92	7:C:201:MYR:H51	2.00	0.43
2:B:302:LYS:HB2	2:B:302:LYS:HE3	1.75	0.43
2:B:346:LEU:HD22	2:B:648:ALA:HB2	1.99	0.43
1:C:50:ARG:NH2	1:E:61:GLY:O	2.30	0.43
2:D:198:SER:HA	2:D:206:MET:O	2.18	0.43
1:G:20:LYS:HA	1:G:20:LYS:HD3	1.62	0.43
2:B:372:GLN:HB2	2:B:376:ARG:NH1	2.32	0.43
2:B:414:ASP:HB3	2:B:578:GLY:HA2	2.00	0.43
2:B:823:HIS:HE1	2:B:927:GLU:HA	1.84	0.43
2:B:876:SER:C	2:B:878:PHE:H	2.25	0.43
2:D:196:HIS:O	2:D:200:VAL:HG22	2.18	0.43
2:F:90:LYS:HE3	2:F:90:LYS:HB2	1.84	0.43
2:F:138:HIS:CE1	2:F:140:PHE:HB2	2.53	0.43
2:F:828:ARG:N	2:F:897:TYR:OH	2.51	0.43
2:H:729:ASP:O	2:H:733:ILE:HG12	2.18	0.43
2:B:119:LYS:HE3	2:B:119:LYS:HB2	1.94	0.43
2:B:269:GLY:N	2:B:586:GLY:O	2.51	0.43
2:B:751:ASP:O	2:B:754:GLU:HG3	2.19	0.43
2:B:834:HIS:N	10:B:1007:MGD:O17	2.48	0.43
2:D:49:ASP:N	8:D:1001:FES:S2	2.90	0.43
2:D:141:TYR:OH	9:D:1004:SF4:S1	2.75	0.43
2:F:836:GLY:HA3	2:F:840:TYR:HD2	1.83	0.43
2:H:97:LEU:HD12	9:H:1002:SF4:S2	2.58	0.43
2:H:283:ILE:HG13	2:H:720:PHE:HZ	1.83	0.43
2:B:196:HIS:O	2:B:200:VAL:HG22	2.18	0.43
2:B:814:LYS:HA	2:B:814:LYS:HD3	1.76	0.43
2:B:828:ARG:HD3	10:B:1007:MGD:C16	2.48	0.43
2:D:97:LEU:HD12	9:D:1002:SF4:S2	2.58	0.43
2:D:269:GLY:N	2:D:586:GLY:O	2.51	0.43
2:D:367:GLU:CG	2:D:729:ASP:HB2	2.49	0.43
1:E:39:GLU:HB3	1:G:53:LEU:HD13	2.01	0.43
2:F:298:SER:HB3	2:F:434:VAL:HG22	2.00	0.43
2:F:566:ASN:HB2	2:F:805:LEU:HD22	1.99	0.43
2:F:751:ASP:O	2:F:754:GLU:HG3	2.19	0.43
2:F:880:ASN:H	2:F:910:LEU:HD23	1.84	0.43
2:H:751:ASP:O	2:H:754:GLU:HG3	2.19	0.43
2:H:814:LYS:HA	2:H:814:LYS:HD3	1.76	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:817:GLY:O	2:H:818:GLU:HG2	2.19	0.43
2:B:836:GLY:HA3	2:B:840:TYR:HD2	1.83	0.43
2:D:823:HIS:HE1	2:D:927:GLU:HA	1.84	0.43
2:F:367:GLU:CG	2:F:729:ASP:HB2	2.49	0.43
2:F:454:ASP:OD2	10:F:1007:MGD:O2'	2.35	0.43
2:F:828:ARG:HD3	10:F:1007:MGD:C16	2.48	0.43
2:H:367:GLU:CG	2:H:729:ASP:HB2	2.49	0.43
1:A:53:LEU:HD13	1:G:39:GLU:HB3	2.01	0.43
1:A:67:LEU:HD12	1:A:67:LEU:HA	1.86	0.43
2:B:367:GLU:CG	2:B:729:ASP:HB2	2.49	0.43
2:D:298:SER:HB3	2:D:434:VAL:HG22	2.00	0.43
2:D:318:LYS:HD2	2:D:725:GLU:CD	2.44	0.43
2:F:429:SER:O	2:F:830:LEU:HD12	2.18	0.43
2:H:408:ASP:O	2:H:711:ARG:NH1	2.50	0.43
2:H:476:ILE:HB	2:H:560:THR:HB	2.01	0.43
2:B:49:ASP:N	8:B:1001:FES:S2	2.90	0.43
2:B:283:ILE:HG13	2:B:720:PHE:HZ	1.83	0.43
2:B:298:SER:HB3	2:B:434:VAL:HG22	2.00	0.43
2:B:821:ASP:OD1	2:B:821:ASP:N	2.52	0.43
2:B:826:ASN:ND2	2:B:925:TYR:O	2.51	0.43
2:D:408:ASP:O	2:D:711:ARG:NH1	2.50	0.43
2:F:159:GLN:O	2:F:444:LYS:NZ	2.45	0.43
2:F:303:GLY:HA3	9:F:1005:SF4:S2	2.59	0.43
2:F:670:TYR:HD2	2:F:689:PHE:HB2	1.84	0.43
2:F:886:LEU:HD21	2:F:943:LEU:HD22	2.01	0.43
2:H:568:LEU:HD12	2:H:581:SER:HB3	2.00	0.43
2:D:303:GLY:HA3	9:D:1005:SF4:S2	2.59	0.43
2:D:670:TYR:HD2	2:D:689:PHE:HB2	1.84	0.43
2:D:880:ASN:H	2:D:910:LEU:HD23	1.84	0.43
2:F:9:ILE:O	2:F:9:ILE:HG13	2.17	0.43
2:F:147:GLN:HE21	2:F:204:ASN:CG	2.27	0.43
2:F:269:GLY:O	2:F:708:ASN:HB2	2.19	0.43
2:F:346:LEU:HD22	2:F:648:ALA:HB2	1.99	0.43
2:F:459:GLU:HG3	2:F:463:ARG:HH21	1.84	0.43
2:F:823:HIS:HE1	2:F:927:GLU:HA	1.84	0.43
2:H:163:VAL:HG21	2:H:440:LYS:C	2.44	0.43
2:H:196:HIS:O	2:H:200:VAL:HG22	2.18	0.43
2:H:318:LYS:HD2	2:H:725:GLU:CD	2.44	0.43
2:H:834:HIS:O	2:H:901:ASN:HA	2.19	0.43
2:D:272:CYS:SG	2:D:295:ASN:HB3	2.59	0.43
2:D:412:ILE:HG23	2:D:435:LEU:HG	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:476:ILE:HB	2:D:560:THR:HB	2.01	0.43
2:F:4:LYS:HG3	2:F:5:LYS:HG2	2.01	0.43
2:F:163:VAL:HG21	2:F:440:LYS:C	2.44	0.43
2:H:272:CYS:SG	2:H:295:ASN:HB3	2.59	0.43
2:H:303:GLY:HA3	9:H:1005:SF4:S2	2.59	0.43
2:H:569:LEU:HD23	2:H:569:LEU:HA	1.85	0.43
2:B:403:VAL:HG23	2:B:405:TYR:H	1.83	0.42
2:B:476:ILE:HB	2:B:560:THR:HB	2.01	0.42
2:B:514:TYR:OH	2:B:810:TRP:N	2.52	0.42
2:B:729:ASP:O	2:B:733:ILE:HG12	2.18	0.42
2:D:138:HIS:CE1	2:D:140:PHE:HB2	2.53	0.42
2:D:459:GLU:HG3	2:D:463:ARG:HH21	1.84	0.42
2:D:595:ASP:OD2	2:D:763:TYR:OH	2.30	0.42
1:E:97:ASP:H	1:G:109:ASN:CG	2.24	0.42
2:F:81:LYS:HD3	2:F:81:LYS:HA	1.74	0.42
2:F:272:CYS:SG	2:F:295:ASN:HB3	2.59	0.42
2:F:514:TYR:OH	2:F:810:TRP:N	2.52	0.42
2:F:516:LEU:HD13	2:F:516:LEU:HA	1.93	0.42
2:F:617:LYS:HB3	2:F:617:LYS:HE2	1.82	0.42
2:H:414:ASP:HB3	2:H:578:GLY:HA2	2.00	0.42
1:A:10:LYS:HE2	1:A:10:LYS:HB2	1.86	0.42
2:B:303:GLY:HA3	9:B:1005:SF4:S2	2.59	0.42
2:B:318:LYS:HD2	2:B:725:GLU:CD	2.44	0.42
2:B:834:HIS:O	2:B:901:ASN:HA	2.19	0.42
1:C:53:LEU:HD23	1:C:53:LEU:HA	1.77	0.42
1:C:99:LYS:HA	1:C:99:LYS:HD2	1.76	0.42
2:D:415:ILE:HD12	2:D:546:LEU:HD11	2.01	0.42
2:D:649:MET:HE2	2:D:649:MET:HB2	1.81	0.42
2:F:196:HIS:O	2:F:200:VAL:HG22	2.18	0.42
2:F:318:LYS:HD2	2:F:725:GLU:CD	2.44	0.42
2:F:408:ASP:O	2:F:711:ARG:NH1	2.50	0.42
2:H:42:LEU:HD21	2:H:200:VAL:HG11	2.01	0.42
2:H:260:LYS:HG2	2:H:277:TRP:CG	2.55	0.42
2:H:670:TYR:HD2	2:H:689:PHE:HB2	1.84	0.42
2:B:549:MET:HG2	10:B:1007:MGD:H101	2.01	0.42
2:B:568:LEU:HD12	2:B:581:SER:HB3	2.00	0.42
2:D:163:VAL:HG21	2:D:440:LYS:C	2.44	0.42
2:D:514:TYR:OH	2:D:810:TRP:N	2.52	0.42
2:D:817:GLY:O	2:D:818:GLU:HG2	2.19	0.42
2:D:968:LYS:HE3	2:D:968:LYS:HB2	1.83	0.42
2:F:39:HIS:HB3	2:F:42:LEU:HD23	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:HIS:HB3	2:H:42:LEU:HD23	2.01	0.42
2:H:49:ASP:N	8:H:1001:FES:S2	2.90	0.42
2:H:415:ILE:HD12	2:H:546:LEU:HD11	2.01	0.42
2:H:881:VAL:HG22	2:H:911:LEU:HD21	2.02	0.42
2:B:272:CYS:SG	2:B:295:ASN:HB3	2.59	0.42
2:D:147:GLN:HE21	2:D:204:ASN:CG	2.27	0.42
2:D:356:ALA:O	2:D:649:MET:HA	2.20	0.42
2:D:828:ARG:HD3	10:D:1007:MGD:C16	2.48	0.42
2:F:822:ILE:HD13	2:F:932:MET:HE3	2.02	0.42
2:F:834:HIS:O	2:F:901:ASN:HA	2.19	0.42
2:H:514:TYR:OH	2:H:810:TRP:N	2.52	0.42
2:B:163:VAL:HG21	2:B:440:LYS:C	2.44	0.42
2:B:260:LYS:HG2	2:B:277:TRP:CG	2.55	0.42
2:B:516:LEU:HD13	2:B:516:LEU:HA	1.93	0.42
2:B:817:GLY:O	2:B:818:GLU:HG2	2.19	0.42
1:C:39:GLU:HB3	1:E:53:LEU:HD13	2.01	0.42
2:D:99:CYS:HB2	13:D:1010:MQ7:H6	2.00	0.42
2:D:584:LEU:HD23	2:D:584:LEU:HA	1.82	0.42
2:D:886:LEU:HD21	2:D:943:LEU:HD22	2.01	0.42
2:F:832:HIS:NE2	2:F:849:THR:O	2.53	0.42
3:G:213:11A:HAI2	3:G:213:11A:HAL2	1.81	0.42
2:H:828:ARG:HD3	10:H:1007:MGD:N15	2.35	0.42
2:H:832:HIS:NE2	2:H:849:THR:O	2.53	0.42
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.77	0.42
1:A:147:PHE:CE2	1:C:130:ILE:HG23	2.55	0.42
2:B:9:ILE:O	2:B:9:ILE:HG13	2.17	0.42
2:D:269:GLY:O	2:D:708:ASN:HB2	2.19	0.42
2:D:697:SER:HB3	2:D:728:PRO:HA	2.02	0.42
2:D:826:ASN:ND2	2:D:925:TYR:O	2.51	0.42
2:F:42:LEU:HD21	2:F:200:VAL:HG11	2.01	0.42
2:F:99:CYS:HB2	13:F:1010:MQ7:H6	2.00	0.42
2:F:415:ILE:HD12	2:F:546:LEU:HD11	2.01	0.42
2:H:140:PHE:HZ	2:H:845:ILE:HG13	1.85	0.42
2:H:766:VAL:HG12	2:H:777:LEU:HD12	2.02	0.42
2:B:4:LYS:HG3	2:B:5:LYS:HG2	2.01	0.42
2:B:42:LEU:HD21	2:B:200:VAL:HG11	2.01	0.42
2:B:670:TYR:HD2	2:B:689:PHE:HB2	1.84	0.42
2:B:828:ARG:HD3	10:B:1007:MGD:N15	2.35	0.42
2:D:90:LYS:HE3	2:D:90:LYS:HB2	1.84	0.42
2:D:154:CYS:HB2	2:D:197:CYS:HB2	2.02	0.42
2:D:834:HIS:O	2:D:901:ASN:HA	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:213:11A:HAL2	3:E:213:11A:HAI2	1.81	0.42
2:F:140:PHE:HZ	2:F:845:ILE:HG13	1.85	0.42
2:F:828:ARG:HG2	10:F:1007:MGD:O1B	2.20	0.42
2:H:659:VAL:HB	10:H:1006:MGD:O11	2.20	0.42
2:H:823:HIS:HE1	2:H:927:GLU:HA	1.84	0.42
2:B:356:ALA:O	2:B:649:MET:HA	2.20	0.42
2:B:415:ILE:HD12	2:B:546:LEU:HD11	2.01	0.42
3:C:213:11A:HAL2	3:C:213:11A:HAI2	1.81	0.42
2:D:260:LYS:HG2	2:D:277:TRP:CG	2.55	0.42
2:D:828:ARG:HG2	10:D:1007:MGD:O1B	2.20	0.42
2:D:836:GLY:HA3	2:D:840:TYR:HD2	1.83	0.42
2:F:315:ARG:HD2	2:F:681:ILE:HB	2.01	0.42
2:F:817:GLY:O	2:F:818:GLU:HG2	2.19	0.42
2:H:4:LYS:HG3	2:H:5:LYS:HG2	2.01	0.42
2:H:147:GLN:HE21	2:H:204:ASN:CG	2.27	0.42
2:H:822:ILE:HD13	2:H:932:MET:HE3	2.02	0.42
2:H:880:ASN:H	2:H:910:LEU:HD23	1.84	0.42
2:H:886:LEU:HD21	2:H:943:LEU:HD22	2.01	0.42
2:B:111:ILE:HD11	2:B:149:ILE:CD1	2.46	0.42
2:B:154:CYS:HB2	2:B:197:CYS:HB2	2.02	0.42
2:B:245:ALA:HB2	1:C:73:LYS:HG2	2.02	0.42
2:D:245:ALA:HB2	1:E:73:LYS:HG2	2.02	0.42
2:D:549:MET:O	2:D:553:GLN:HB2	2.20	0.42
2:D:817:GLY:C	2:D:818:GLU:HG2	2.45	0.42
2:D:828:ARG:HD3	10:D:1007:MGD:N15	2.35	0.42
2:F:245:ALA:HB2	1:G:73:LYS:HG2	2.02	0.42
2:F:476:ILE:HB	2:F:560:THR:HB	2.01	0.42
2:F:814:LYS:HA	2:F:814:LYS:HD3	1.76	0.42
1:A:73:LYS:HG2	2:H:245:ALA:HB2	2.02	0.42
2:B:140:PHE:HZ	2:B:845:ILE:HG13	1.85	0.42
2:B:549:MET:HB3	2:B:553:GLN:CD	2.45	0.42
2:B:617:LYS:HB3	2:B:617:LYS:HE2	1.82	0.42
2:D:42:LEU:HD21	2:D:200:VAL:HG11	2.01	0.42
2:D:321:ILE:HD11	2:D:335:ALA:HA	2.02	0.42
2:D:710:GLU:CD	2:D:712:ARG:HE	2.27	0.42
2:D:766:VAL:HG12	2:D:777:LEU:HD12	2.02	0.42
2:D:881:VAL:HG22	2:D:911:LEU:HD21	2.02	0.42
2:F:260:LYS:HG2	2:F:277:TRP:CG	2.55	0.42
2:F:549:MET:HG2	10:F:1007:MGD:H101	2.01	0.42
2:F:659:VAL:HB	10:F:1006:MGD:O11	2.20	0.42
2:F:828:ARG:HD3	10:F:1007:MGD:N15	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:881:VAL:HG22	2:F:911:LEU:HD21	2.02	0.42
1:G:53:LEU:HA	1:G:53:LEU:HD23	1.77	0.42
2:H:412:ILE:HG23	2:H:435:LEU:HG	2.01	0.42
2:H:549:MET:HG2	10:H:1007:MGD:H101	2.01	0.42
2:H:617:LYS:HB3	2:H:617:LYS:HE2	1.82	0.42
1:A:39:GLU:HB3	1:C:53:LEU:HD13	2.01	0.41
2:B:39:HIS:HB3	2:B:42:LEU:HD23	2.01	0.41
2:B:81:LYS:HA	2:B:81:LYS:HD3	1.74	0.41
2:B:147:GLN:HE21	2:B:204:ASN:CG	2.27	0.41
2:B:758:LYS:HB3	2:B:758:LYS:HE2	1.85	0.41
2:B:817:GLY:C	2:B:818:GLU:HG2	2.45	0.41
1:C:147:PHE:CE2	1:E:130:ILE:HG23	2.55	0.41
2:D:42:LEU:HD13	2:D:42:LEU:HA	1.91	0.41
2:D:315:ARG:HD2	2:D:681:ILE:HB	2.01	0.41
2:D:484:LYS:HG3	2:D:511:LEU:HB3	2.03	0.41
2:F:549:MET:O	2:F:553:GLN:HB2	2.20	0.41
2:F:710:GLU:CD	2:F:712:ARG:HE	2.27	0.41
2:H:315:ARG:HD2	2:H:681:ILE:HB	2.01	0.41
2:H:516:LEU:HD13	2:H:516:LEU:HA	1.93	0.41
3:A:209:11A:HAI1	3:A:209:11A:HAL2	1.92	0.41
2:B:408:ASP:O	2:B:711:ARG:NH1	2.50	0.41
2:B:659:VAL:HB	10:B:1006:MGD:O11	2.20	0.41
1:C:73:LYS:HA	1:C:73:LYS:HD2	1.91	0.41
2:D:638:ILE:HD11	2:D:656:MET:HE1	2.02	0.41
2:D:659:VAL:HB	10:D:1006:MGD:O11	2.20	0.41
2:F:389:ARG:NH2	2:F:600:PRO:HD2	2.35	0.41
2:F:697:SER:HB3	2:F:728:PRO:HA	2.02	0.41
2:H:454:ASP:OD2	10:H:1007:MGD:O2'	2.35	0.41
3:A:211:11A:HAL2	3:A:211:11A:HAI2	1.81	0.41
2:B:315:ARG:HD2	2:B:681:ILE:HB	2.01	0.41
2:B:321:ILE:HD11	2:B:335:ALA:HA	2.02	0.41
2:B:389:ARG:NH2	2:B:600:PRO:HD2	2.35	0.41
2:B:399:LEU:HD12	2:B:406:GLY:HA2	2.02	0.41
2:B:510:SER:HB3	2:B:807:PRO:HB3	2.02	0.41
2:B:543:VAL:O	2:B:579:ALA:HB1	2.21	0.41
2:B:697:SER:HB3	2:B:728:PRO:HA	2.02	0.41
2:B:836:GLY:O	2:B:840:TYR:HB2	2.21	0.41
2:D:389:ARG:NH2	2:D:600:PRO:HD2	2.35	0.41
1:E:82:THR:HA	1:G:94:GLY:HA3	2.02	0.41
2:F:569:LEU:HD23	2:F:569:LEU:HA	1.85	0.41
2:F:766:VAL:HG12	2:F:777:LEU:HD12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:795:ARG:HD2	2:F:796:PHE:O	2.20	0.41
2:H:269:GLY:O	2:H:708:ASN:HB2	2.19	0.41
2:H:389:ARG:NH2	2:H:600:PRO:HD2	2.35	0.41
2:H:549:MET:HB3	2:H:553:GLN:CD	2.45	0.41
2:H:795:ARG:HD2	2:H:796:PHE:O	2.20	0.41
1:A:130:ILE:HG23	1:G:147:PHE:CE2	2.55	0.41
2:B:475:ASP:OD1	10:B:1007:MGD:N2	2.43	0.41
2:B:968:LYS:HB2	2:B:968:LYS:HE3	1.83	0.41
1:C:67:LEU:HD12	1:C:67:LEU:HA	1.86	0.41
2:D:640:LYS:HA	2:D:640:LYS:HD3	1.79	0.41
2:D:739:LYS:HA	2:D:739:LYS:HD3	1.76	0.41
2:D:795:ARG:HD2	2:D:796:PHE:O	2.20	0.41
2:F:549:MET:HB3	2:F:553:GLN:CD	2.45	0.41
2:F:654:GLU:HG2	2:F:656:MET:HB3	2.02	0.41
2:F:821:ASP:OD1	2:F:821:ASP:N	2.52	0.41
2:H:106:ASN:OD1	2:H:254:ARG:HD2	2.21	0.41
2:H:321:ILE:HD11	2:H:335:ALA:HA	2.02	0.41
2:H:828:ARG:HG2	10:H:1007:MGD:O1B	2.20	0.41
2:B:857:SER:OG	2:B:893:GLY:O	2.28	0.41
2:B:886:LEU:HD21	2:B:943:LEU:HD22	2.01	0.41
1:C:50:ARG:HD3	1:C:50:ARG:HA	1.75	0.41
2:D:39:HIS:HB3	2:D:42:LEU:HD23	2.01	0.41
2:D:480:ASN:HD22	2:D:514:TYR:HE2	1.69	0.41
2:D:617:LYS:HA	2:D:620:ARG:HH11	1.86	0.41
1:E:147:PHE:CE2	1:G:130:ILE:HG23	2.55	0.41
2:F:154:CYS:HB2	2:F:197:CYS:HB2	2.02	0.41
2:F:356:ALA:O	2:F:649:MET:HA	2.20	0.41
2:F:480:ASN:HD22	2:F:514:TYR:HE2	1.68	0.41
2:F:484:LYS:HG3	2:F:511:LEU:HB3	2.02	0.41
2:F:739:LYS:HA	2:F:739:LYS:HD3	1.76	0.41
2:H:399:LEU:HD12	2:H:406:GLY:HA2	2.02	0.41
2:H:459:GLU:HG3	2:H:463:ARG:HH21	1.84	0.41
2:H:543:VAL:O	2:H:579:ALA:HB1	2.21	0.41
2:H:968:LYS:HE3	2:H:968:LYS:HB2	1.83	0.41
2:B:459:GLU:HG3	2:B:463:ARG:HH21	1.84	0.41
2:B:549:MET:O	2:B:553:GLN:HB2	2.20	0.41
2:D:281:ARG:HA	2:D:281:ARG:HD2	1.89	0.41
2:D:549:MET:HG2	10:D:1007:MGD:H101	2.01	0.41
2:D:710:GLU:OE2	2:D:712:ARG:NE	2.46	0.41
2:D:822:ILE:HD13	2:D:932:MET:HE3	2.02	0.41
2:D:836:GLY:O	2:D:840:TYR:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:LYS:HD2	1:E:99:LYS:HA	1.76	0.41
2:F:5:LYS:HB2	2:F:16:ALA:HB3	2.02	0.41
2:F:412:ILE:HG23	2:F:435:LEU:HG	2.01	0.41
2:H:758:LYS:HB3	2:H:758:LYS:HE2	1.85	0.41
2:B:106:ASN:OD1	2:B:254:ARG:HD2	2.21	0.41
2:B:269:GLY:O	2:B:708:ASN:HB2	2.19	0.41
2:B:373:LYS:HE2	2:B:744:TRP:NE1	2.36	0.41
2:B:411:SER:N	2:B:414:ASP:OD2	2.38	0.41
2:B:617:LYS:HA	2:B:620:ARG:HH11	1.86	0.41
2:B:795:ARG:HD2	2:B:796:PHE:O	2.20	0.41
2:D:4:LYS:HG3	2:D:5:LYS:HG2	2.01	0.41
2:D:106:ASN:OD1	2:D:254:ARG:HD2	2.21	0.41
2:D:843:LYS:HD3	2:D:843:LYS:HA	1.79	0.41
2:D:932:MET:HA	2:D:932:MET:HE2	2.03	0.41
2:F:49:ASP:N	8:F:1001:FES:S2	2.90	0.41
2:F:825:ASN:HD21	10:F:1007:MGD:H8	1.86	0.41
2:H:154:CYS:HB2	2:H:197:CYS:HB2	2.02	0.41
2:H:426:SER:OG	2:H:428:THR:OG1	2.21	0.41
2:H:836:GLY:O	2:H:840:TYR:HB2	2.21	0.41
1:A:23:LEU:HD13	1:A:23:LEU:HA	1.96	0.41
2:B:5:LYS:HB2	2:B:16:ALA:HB3	2.02	0.41
2:B:9:ILE:HA	2:B:73:ILE:HB	2.03	0.41
2:B:386:ASN:OD1	2:B:386:ASN:N	2.54	0.41
2:B:569:LEU:HD23	2:B:569:LEU:HA	1.85	0.41
2:B:822:ILE:HD13	2:B:932:MET:HE3	2.02	0.41
2:B:832:HIS:NE2	2:B:849:THR:O	2.53	0.41
2:D:140:PHE:HZ	2:D:845:ILE:HG13	1.85	0.41
2:D:386:ASN:OD1	2:D:386:ASN:N	2.54	0.41
2:D:399:LEU:HD12	2:D:406:GLY:HA2	2.02	0.41
2:D:832:HIS:NE2	2:D:849:THR:O	2.53	0.41
2:F:399:LEU:HD12	2:F:406:GLY:HA2	2.02	0.41
2:F:543:VAL:O	2:F:579:ALA:HB1	2.21	0.41
2:F:638:ILE:HD11	2:F:656:MET:HE1	2.02	0.41
2:H:9:ILE:HA	2:H:73:ILE:HB	2.03	0.41
2:H:362:LYS:HZ1	10:H:1006:MGD:H8	1.85	0.41
2:H:373:LYS:HE2	2:H:744:TRP:NE1	2.36	0.41
2:H:710:GLU:OE2	2:H:712:ARG:NE	2.46	0.41
1:A:82:THR:HA	1:C:94:GLY:HA3	2.02	0.41
2:B:26:LEU:HD22	2:B:31:ILE:HG21	2.03	0.41
2:B:149:ILE:HG12	9:B:1003:SF4:S4	2.61	0.41
2:B:375:ALA:O	2:B:381:THR:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:ILE:HG23	2:B:435:LEU:HG	2.01	0.41
2:B:654:GLU:HG2	2:B:656:MET:HB3	2.02	0.41
2:B:766:VAL:HG12	2:B:777:LEU:HD12	2.02	0.41
2:B:866:ILE:HD12	2:B:866:ILE:HA	1.89	0.41
1:C:10:LYS:HE2	1:C:10:LYS:HB2	1.86	0.41
1:C:156:ASP:OD1	1:C:156:ASP:N	2.54	0.41
2:D:319:PRO:HA	2:D:695:PRO:HD3	2.02	0.41
2:D:373:LYS:HE2	2:D:744:TRP:NE1	2.36	0.41
2:D:549:MET:HB3	2:D:553:GLN:CD	2.45	0.41
2:F:9:ILE:HA	2:F:73:ILE:HB	2.03	0.41
2:F:106:ASN:OD1	2:F:254:ARG:HD2	2.21	0.41
2:F:321:ILE:HD11	2:F:335:ALA:HA	2.02	0.41
2:F:660:ASP:OD1	2:F:661:SER:N	2.54	0.41
2:F:866:ILE:HD12	2:F:866:ILE:HA	1.89	0.41
1:G:50:ARG:HA	1:G:50:ARG:HD3	1.75	0.41
2:H:149:ILE:HG12	9:H:1003:SF4:S4	2.61	0.41
2:H:549:MET:O	2:H:553:GLN:HB2	2.20	0.41
2:H:617:LYS:HA	2:H:620:ARG:HH11	1.86	0.41
2:B:649:MET:HE2	2:B:649:MET:HB2	1.81	0.41
1:C:33:HIS:CE1	1:E:42:HIS:HA	2.57	0.41
1:C:74:ALA:O	2:H:232:ILE:HD11	2.21	0.41
2:D:44:PRO:HB3	2:D:63:CYS:O	2.21	0.41
2:D:456:ARG:HH21	2:D:458:HIS:HB3	1.86	0.41
2:D:654:GLU:HG2	2:D:656:MET:HB3	2.02	0.41
2:D:660:ASP:OD1	2:D:661:SER:N	2.54	0.41
2:F:149:ILE:HG12	9:F:1003:SF4:S4	2.61	0.41
2:F:836:GLY:O	2:F:840:TYR:HB2	2.21	0.41
2:H:480:ASN:HD22	2:H:514:TYR:HE2	1.69	0.41
2:H:510:SER:HB3	2:H:807:PRO:HB3	2.02	0.41
2:H:638:ILE:HD11	2:H:656:MET:HE1	2.02	0.41
2:H:654:GLU:HG2	2:H:656:MET:HB3	2.02	0.41
1:A:94:GLY:HA3	1:G:82:THR:HA	2.02	0.40
2:B:456:ARG:HH21	2:B:458:HIS:HB3	1.86	0.40
2:B:584:LEU:HD23	2:B:584:LEU:HA	1.82	0.40
1:C:82:THR:HA	1:E:94:GLY:HA3	2.02	0.40
2:D:9:ILE:HA	2:D:73:ILE:HB	2.03	0.40
2:D:309:PHE:CE2	2:D:838:LEU:HD23	2.56	0.40
2:D:373:LYS:O	2:D:377:GLY:N	2.54	0.40
2:D:415:ILE:HD11	2:D:582:TYR:CG	2.56	0.40
2:D:563:ALA:HA	2:D:566:ASN:ND2	2.36	0.40
2:D:825:ASN:HD21	10:D:1007:MGD:H8	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:GLY:C	1:E:54:PRO:HD2	2.46	0.40
2:H:697:SER:HB3	2:H:728:PRO:HA	2.02	0.40
2:H:817:GLY:C	2:H:818:GLU:HG2	2.45	0.40
1:A:51:GLY:C	1:A:54:PRO:HD2	2.46	0.40
1:A:74:ALA:O	2:F:232:ILE:HD11	2.21	0.40
2:B:42:LEU:HD13	2:B:42:LEU:HA	1.91	0.40
2:B:44:PRO:HB3	2:B:63:CYS:O	2.21	0.40
2:B:90:LYS:HB2	2:B:90:LYS:HE3	1.84	0.40
2:B:309:PHE:CE2	2:B:838:LEU:HD23	2.56	0.40
2:B:480:ASN:HD22	2:B:514:TYR:HE2	1.69	0.40
2:B:880:ASN:H	2:B:910:LEU:HD23	1.84	0.40
2:B:881:VAL:HG22	2:B:911:LEU:HD21	2.02	0.40
2:B:932:MET:HE2	2:B:932:MET:HA	2.03	0.40
2:D:5:LYS:HB2	2:D:16:ALA:HB3	2.02	0.40
2:D:411:SER:N	2:D:414:ASP:OD2	2.38	0.40
2:D:857:SER:OG	2:D:893:GLY:O	2.28	0.40
2:F:617:LYS:HA	2:F:620:ARG:HH11	1.86	0.40
2:F:782:ASN:OD1	2:F:782:ASN:N	2.54	0.40
2:F:826:ASN:ND2	2:F:925:TYR:O	2.51	0.40
2:H:484:LYS:HG3	2:H:511:LEU:HB3	2.03	0.40
2:H:649:MET:HE2	2:H:649:MET:HB2	1.81	0.40
1:A:42:HIS:HA	1:G:33:HIS:CE1	2.57	0.40
2:B:232:ILE:HD11	1:E:74:ALA:O	2.21	0.40
2:B:794:GLU:OE1	2:B:795:ARG:HG2	2.22	0.40
2:F:362:LYS:HZ1	10:F:1006:MGD:H8	1.86	0.40
2:F:373:LYS:O	2:F:377:GLY:N	2.54	0.40
2:H:44:PRO:HB3	2:H:63:CYS:O	2.21	0.40
2:H:356:ALA:O	2:H:649:MET:HA	2.20	0.40
2:H:386:ASN:OD1	2:H:386:ASN:N	2.54	0.40
1:A:33:HIS:CE1	1:C:42:HIS:HA	2.57	0.40
2:B:157:ALA:HB2	2:B:200:VAL:HG21	2.03	0.40
2:B:319:PRO:HA	2:B:695:PRO:HD3	2.02	0.40
2:B:547:TRP:CE3	2:B:564:ILE:HG21	2.57	0.40
2:D:543:VAL:O	2:D:579:ALA:HB1	2.21	0.40
2:D:569:LEU:HD23	2:D:569:LEU:HA	1.85	0.40
2:F:319:PRO:HA	2:F:695:PRO:HD3	2.02	0.40
2:F:386:ASN:N	2:F:386:ASN:OD1	2.54	0.40
1:G:51:GLY:C	1:G:54:PRO:HD2	2.46	0.40
2:H:110:GLU:O	2:H:111:ILE:C	2.64	0.40
2:H:309:PHE:CE2	2:H:838:LEU:HD23	2.56	0.40
2:H:547:TRP:CE3	2:H:564:ILE:HG21	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:ILE:CD1	2:B:153:ARG:HA	2.52	0.40
2:B:638:ILE:HD11	2:B:656:MET:HE1	2.02	0.40
2:B:660:ASP:OD1	2:B:661:SER:N	2.54	0.40
2:D:119:LYS:HE3	2:D:119:LYS:HB2	1.94	0.40
2:D:375:ALA:O	2:D:381:THR:N	2.54	0.40
2:D:547:TRP:CE3	2:D:564:ILE:HG21	2.57	0.40
2:D:821:ASP:OD1	2:D:821:ASP:N	2.52	0.40
2:D:866:ILE:HD11	2:D:870:THR:OG1	2.22	0.40
2:F:44:PRO:HB3	2:F:63:CYS:O	2.21	0.40
2:F:309:PHE:CE2	2:F:838:LEU:HD23	2.56	0.40
2:F:373:LYS:HE2	2:F:744:TRP:NE1	2.36	0.40
2:F:510:SER:HB3	2:F:807:PRO:HB3	2.02	0.40
2:H:275:ASP:OD1	2:H:774:TYR:OH	2.23	0.40
2:H:373:LYS:O	2:H:377:GLY:N	2.54	0.40
2:H:810:TRP:CZ2	2:H:813:PRO:HD2	2.57	0.40
2:H:825:ASN:HD21	10:H:1007:MGD:H8	1.86	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	144/186 (77%)	141 (98%)	3 (2%)	0	100	100
1	C	144/186 (77%)	141 (98%)	3 (2%)	0	100	100
1	E	144/186 (77%)	141 (98%)	3 (2%)	0	100	100
1	G	144/186 (77%)	141 (98%)	3 (2%)	0	100	100
2	B	973/985 (99%)	940 (97%)	33 (3%)	0	100	100
2	D	973/985 (99%)	940 (97%)	33 (3%)	0	100	100
2	F	973/985 (99%)	940 (97%)	33 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	973/985 (99%)	940 (97%)	33 (3%)	0	100	100
All	All	4468/4684 (95%)	4324 (97%)	144 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	129/165 (78%)	129 (100%)	0	100	100
1	C	129/165 (78%)	129 (100%)	0	100	100
1	E	129/165 (78%)	129 (100%)	0	100	100
1	G	129/165 (78%)	129 (100%)	0	100	100
2	B	840/845 (99%)	833 (99%)	7 (1%)	73	76
2	D	840/845 (99%)	833 (99%)	7 (1%)	73	76
2	F	840/845 (99%)	833 (99%)	7 (1%)	73	76
2	H	840/845 (99%)	833 (99%)	7 (1%)	73	76
All	All	3876/4040 (96%)	3848 (99%)	28 (1%)	73	77

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

Mol	Chain	Res	Type
2	B	47	THR
2	B	103	ASP
2	B	163	VAL
2	B	203	CYS
2	B	782	ASN
2	B	794	GLU
2	B	795	ARG
2	D	47	THR
2	D	103	ASP
2	D	163	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	203	CYS
2	D	782	ASN
2	D	794	GLU
2	D	795	ARG
2	F	47	THR
2	F	103	ASP
2	F	163	VAL
2	F	203	CYS
2	F	782	ASN
2	F	794	GLU
2	F	795	ARG
2	H	47	THR
2	H	103	ASP
2	H	163	VAL
2	H	203	CYS
2	H	782	ASN
2	H	794	GLU
2	H	795	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	155	GLN
2	B	123	GLN
2	B	129	HIS
2	B	182	ASN
2	B	417	GLN
2	B	502	ASN
2	B	527	GLN
2	B	573	ASN
2	B	587	HIS
2	B	613	GLN
2	B	635	HIS
2	B	642	HIS
2	B	679	GLN
2	B	775	ASN
2	B	909	ASN
2	B	937	HIS
2	B	950	ASN
1	C	85	ASN
1	C	155	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	123	GLN
2	D	129	HIS
2	D	182	ASN
2	D	417	GLN
2	D	502	ASN
2	D	527	GLN
2	D	573	ASN
2	D	587	HIS
2	D	613	GLN
2	D	635	HIS
2	D	642	HIS
2	D	679	GLN
2	D	775	ASN
2	D	909	ASN
2	D	937	HIS
2	D	950	ASN
1	E	85	ASN
1	E	155	GLN
2	F	123	GLN
2	F	129	HIS
2	F	182	ASN
2	F	417	GLN
2	F	502	ASN
2	F	527	GLN
2	F	573	ASN
2	F	587	HIS
2	F	613	GLN
2	F	635	HIS
2	F	642	HIS
2	F	679	GLN
2	F	775	ASN
2	F	909	ASN
2	F	937	HIS
2	F	950	ASN
1	G	85	ASN
1	G	155	GLN
2	H	123	GLN
2	H	182	ASN
2	H	417	GLN
2	H	502	ASN
2	H	527	GLN
2	H	573	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	587	HIS
2	H	613	GLN
2	H	635	HIS
2	H	642	HIS
2	H	679	GLN
2	H	825	ASN
2	H	909	ASN
2	H	937	HIS
2	H	950	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 92 ligands modelled in this entry, 4 are monoatomic and 4 are modelled with single atom - leaving 84 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	MYR	C	201	-	13,13,15	0.64	0	13,13,15	1.14	0
6	KNA	E	210	-	10,10,10	0.82	0	10,10,10	0.71	0
5	SHV	C	207	-	8,8,8	0.89	0	8,8,8	0.78	0
3	11A	A	207	-	12,12,12	0.68	0	12,12,12	1.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	11A	C	208	-	12,12,12	0.67	0	12,12,12	1.17	0
9	SF4	D	1005	2	0,12,12	-	-	-	-	-
10	MGD	H	1006	11	47,52,52	1.98	14 (29%)	58,81,81	1.26	8 (13%)
4	A1H2V	C	205	-	50,50,50	0.29	0	53,56,56	0.40	0
8	FES	F	1001	2	0,4,4	-	-	-	-	-
3	11A	G	208	-	12,12,12	0.67	0	12,12,12	1.17	0
3	11A	G	212	-	12,12,12	0.69	0	12,12,12	1.18	0
10	MGD	B	1006	11	47,52,52	1.98	14 (29%)	58,81,81	1.26	8 (13%)
5	SHV	A	205	-	8,8,8	0.89	0	8,8,8	0.78	0
4	A1H2V	G	204	-	44,44,50	0.32	0	47,50,56	0.35	0
3	11A	A	211	-	12,12,12	0.68	0	12,12,12	1.16	0
3	11A	E	213	-	12,12,12	0.68	0	12,12,12	1.16	0
9	SF4	D	1002	2	0,12,12	-	-	-	-	-
3	11A	A	210	-	12,12,12	0.69	0	12,12,12	1.18	0
5	SHV	G	206	-	8,8,8	0.89	0	8,8,8	0.73	0
7	MYR	G	201	-	13,13,15	0.64	0	13,13,15	1.14	0
4	A1H2V	E	202	-	50,50,50	0.29	0	53,56,56	0.27	0
4	A1H2V	E	204	-	44,44,50	0.31	0	47,50,56	0.35	0
9	SF4	H	1005	2	0,12,12	-	-	-	-	-
9	SF4	D	1004	2	0,12,12	-	-	-	-	-
13	MQ7	D	1010	-	49,49,49	0.23	0	61,63,63	0.40	1 (1%)
3	11A	G	211	-	12,12,12	0.68	0	12,12,12	1.17	0
3	11A	E	211	-	12,12,12	0.68	0	12,12,12	1.17	0
9	SF4	F	1003	2	0,12,12	-	-	-	-	-
10	MGD	F	1007	2,11	47,52,52	1.88	13 (27%)	58,81,81	1.35	7 (12%)
8	FES	H	1001	2	0,4,4	-	-	-	-	-
3	11A	C	212	-	12,12,12	0.69	0	12,12,12	1.18	0
4	A1H2V	E	205	-	50,50,50	0.29	0	53,56,56	0.40	0
5	SHV	E	207	-	8,8,8	0.89	0	8,8,8	0.78	0
9	SF4	F	1002	2	0,12,12	-	-	-	-	-
9	SF4	H	1004	2	0,12,12	-	-	-	-	-
9	SF4	D	1003	2	0,12,12	-	-	-	-	-
5	SHV	C	206	-	8,8,8	0.89	0	8,8,8	0.73	0
10	MGD	B	1007	2,11	47,52,52	1.87	13 (27%)	58,81,81	1.35	7 (12%)
8	FES	B	1001	2	0,4,4	-	-	-	-	-
5	SHV	A	204	-	8,8,8	0.89	0	8,8,8	0.73	0
9	SF4	B	1002	2	0,12,12	-	-	-	-	-
3	11A	G	209	-	12,12,12	0.68	0	12,12,12	1.17	0
3	11A	A	201	-	11,11,12	0.70	0	11,11,12	1.18	0
9	SF4	H	1003	2	0,12,12	-	-	-	-	-
13	MQ7	F	1010	-	49,49,49	0.23	0	61,63,63	0.40	1 (1%)
3	11A	G	203	-	11,11,12	0.70	0	11,11,12	1.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	11A	C	203	-	11,11,12	0.70	0	11,11,12	1.18	0
3	11A	G	213	-	12,12,12	0.68	0	12,12,12	1.16	0
6	KNA	A	208	-	10,10,10	0.81	0	10,10,10	0.70	0
3	11A	C	213	-	12,12,12	0.68	0	12,12,12	1.16	0
13	MQ7	B	1010	-	49,49,49	0.23	0	61,63,63	0.40	1 (1%)
9	SF4	B	1004	2	0,12,12	-	-	-	-	-
10	MGD	F	1006	11	47,52,52	1.97	14 (29%)	58,81,81	1.26	8 (13%)
6	KNA	G	210	-	10,10,10	0.81	0	10,10,10	0.70	0
7	MYR	E	201	-	13,13,15	0.64	0	13,13,15	1.14	0
8	FES	D	1001	2	0,4,4	-	-	-	-	-
3	11A	A	209	-	12,12,12	0.68	0	12,12,12	1.17	0
5	SHV	G	207	-	8,8,8	0.89	0	8,8,8	0.78	0
9	SF4	F	1004	2	0,12,12	-	-	-	-	-
6	KNA	C	210	-	10,10,10	0.81	0	10,10,10	0.70	0
3	11A	C	211	-	12,12,12	0.68	0	12,12,12	1.17	0
4	A1H2V	A	202	-	44,44,50	0.32	0	47,50,56	0.35	0
3	11A	E	212	-	12,12,12	0.69	0	12,12,12	1.18	0
4	A1H2V	G	205	-	50,50,50	0.29	0	53,56,56	0.40	0
9	SF4	B	1003	2	0,12,12	-	-	-	-	-
13	MQ7	H	1010	-	49,49,49	0.23	0	61,63,63	0.40	1 (1%)
3	11A	E	209	-	12,12,12	0.68	0	12,12,12	1.17	0
3	11A	A	206	-	12,12,12	0.67	0	12,12,12	1.17	0
5	SHV	E	206	-	8,8,8	0.89	0	8,8,8	0.73	0
3	11A	C	209	-	12,12,12	0.68	0	12,12,12	1.17	0
10	MGD	H	1007	2,11	47,52,52	1.87	13 (27%)	58,81,81	1.35	7 (12%)
4	A1H2V	C	204	-	44,44,50	0.32	0	47,50,56	0.35	0
9	SF4	F	1005	2	0,12,12	-	-	-	-	-
9	SF4	B	1005	2	0,12,12	-	-	-	-	-
10	MGD	D	1007	2,11	47,52,52	1.87	13 (27%)	58,81,81	1.35	7 (12%)
4	A1H2V	G	202	-	50,50,50	0.29	0	53,56,56	0.27	0
3	11A	E	208	-	12,12,12	0.68	0	12,12,12	1.17	0
4	A1H2V	C	202	-	50,50,50	0.29	0	53,56,56	0.27	0
3	11A	E	203	-	11,11,12	0.70	0	11,11,12	1.18	0
7	MYR	A	212	-	13,13,15	0.64	0	13,13,15	1.14	0
10	MGD	D	1006	11	47,52,52	1.98	14 (29%)	58,81,81	1.26	8 (13%)
4	A1H2V	A	203	-	50,50,50	0.29	0	53,56,56	0.40	0
4	A1H2V	A	213	-	50,50,50	0.29	0	53,56,56	0.27	0
9	SF4	H	1002	2	0,12,12	-	-	-	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MYR	C	201	-	-	5/11/11/13	-
6	KNA	E	210	-	-	3/8/8/8	-
5	SHV	C	207	-	-	2/6/6/6	-
3	11A	A	207	-	-	2/10/10/10	-
3	11A	C	208	-	-	1/10/10/10	-
10	MGD	H	1006	11	-	3/22/66/66	0/6/6/6
9	SF4	D	1005	2	-	-	0/6/5/5
4	A1H2V	C	205	-	-	22/55/55/55	-
8	FES	F	1001	2	-	-	0/1/1/1
3	11A	G	208	-	-	1/10/10/10	-
3	11A	G	212	-	-	6/10/10/10	-
10	MGD	B	1006	11	-	3/22/66/66	0/6/6/6
5	SHV	A	205	-	-	2/6/6/6	-
4	A1H2V	G	204	-	-	10/49/49/55	-
3	11A	A	211	-	-	3/10/10/10	-
3	11A	E	213	-	-	3/10/10/10	-
9	SF4	D	1002	2	-	-	0/6/5/5
3	11A	A	210	-	-	6/10/10/10	-
5	SHV	G	206	-	-	3/6/6/6	-
7	MYR	G	201	-	-	5/11/11/13	-
4	A1H2V	E	202	-	-	4/55/55/55	-
4	A1H2V	E	204	-	-	10/49/49/55	-
9	SF4	H	1005	2	-	-	0/6/5/5
9	SF4	D	1004	2	-	-	0/6/5/5
13	MQ7	D	1010	-	-	7/41/61/61	0/2/2/2
3	11A	G	211	-	-	2/10/10/10	-
3	11A	E	211	-	-	2/10/10/10	-
9	SF4	F	1003	2	-	-	0/6/5/5
10	MGD	F	1007	2,11	-	7/22/66/66	0/6/6/6
8	FES	H	1001	2	-	-	0/1/1/1
3	11A	C	212	-	-	6/10/10/10	-
4	A1H2V	E	205	-	-	22/55/55/55	-
5	SHV	E	207	-	-	2/6/6/6	-
9	SF4	F	1002	2	-	-	0/6/5/5
9	SF4	H	1004	2	-	-	0/6/5/5
10	MGD	B	1007	2,11	-	7/22/66/66	0/6/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SHV	C	206	-	-	3/6/6/6	-
9	SF4	D	1003	2	-	-	0/6/5/5
8	FES	B	1001	2	-	-	0/1/1/1
5	SHV	A	204	-	-	3/6/6/6	-
9	SF4	B	1002	2	-	-	0/6/5/5
3	11A	G	209	-	-	2/10/10/10	-
3	11A	A	201	-	-	1/9/9/10	-
9	SF4	H	1003	2	-	-	0/6/5/5
13	MQ7	F	1010	-	-	7/41/61/61	0/2/2/2
3	11A	G	203	-	-	1/9/9/10	-
3	11A	C	203	-	-	1/9/9/10	-
3	11A	G	213	-	-	3/10/10/10	-
6	KNA	A	208	-	-	3/8/8/8	-
3	11A	C	213	-	-	3/10/10/10	-
13	MQ7	B	1010	-	-	7/41/61/61	0/2/2/2
9	SF4	B	1004	2	-	-	0/6/5/5
10	MGD	F	1006	11	-	3/22/66/66	0/6/6/6
6	KNA	G	210	-	-	3/8/8/8	-
7	MYR	E	201	-	-	5/11/11/13	-
8	FES	D	1001	2	-	-	0/1/1/1
3	11A	A	209	-	-	2/10/10/10	-
5	SHV	G	207	-	-	2/6/6/6	-
9	SF4	F	1004	2	-	-	0/6/5/5
6	KNA	C	210	-	-	3/8/8/8	-
3	11A	C	211	-	-	2/10/10/10	-
4	A1H2V	A	202	-	-	10/49/49/55	-
3	11A	E	212	-	-	6/10/10/10	-
4	A1H2V	G	205	-	-	22/55/55/55	-
9	SF4	B	1003	2	-	-	0/6/5/5
13	MQ7	H	1010	-	-	7/41/61/61	0/2/2/2
3	11A	E	209	-	-	2/10/10/10	-
3	11A	A	206	-	-	1/10/10/10	-
5	SHV	E	206	-	-	3/6/6/6	-
3	11A	C	209	-	-	2/10/10/10	-
10	MGD	H	1007	2,11	-	7/22/66/66	0/6/6/6
4	A1H2V	C	204	-	-	10/49/49/55	-
9	SF4	F	1005	2	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SF4	B	1005	2	-	-	0/6/5/5
10	MGD	D	1007	2,11	-	7/22/66/66	0/6/6/6
4	A1H2V	G	202	-	-	4/55/55/55	-
3	11A	E	208	-	-	1/10/10/10	-
4	A1H2V	C	202	-	-	4/55/55/55	-
3	11A	E	203	-	-	1/9/9/10	-
7	MYR	A	212	-	-	5/11/11/13	-
10	MGD	D	1006	11	-	3/22/66/66	0/6/6/6
4	A1H2V	A	203	-	-	22/55/55/55	-
4	A1H2V	A	213	-	-	4/55/55/55	-
9	SF4	H	1002	2	-	-	0/6/5/5

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	1006	MGD	C23-C14	5.43	1.58	1.53
10	D	1006	MGD	C23-C14	5.43	1.58	1.53
10	F	1006	MGD	C23-C14	5.43	1.58	1.53
10	H	1006	MGD	C23-C14	5.43	1.58	1.53
10	B	1007	MGD	C21-N22	5.26	1.41	1.35
10	D	1007	MGD	C21-N22	5.26	1.41	1.35
10	F	1007	MGD	C21-N22	5.26	1.41	1.35
10	H	1007	MGD	C21-N22	5.26	1.41	1.35
10	B	1006	MGD	C21-N22	4.91	1.40	1.35
10	D	1006	MGD	C21-N22	4.91	1.40	1.35
10	H	1006	MGD	C21-N22	4.91	1.40	1.35
10	F	1006	MGD	C21-N22	4.85	1.40	1.35
10	B	1007	MGD	PB-O5'	4.06	1.75	1.59
10	D	1007	MGD	PB-O5'	4.06	1.75	1.59
10	H	1007	MGD	PB-O5'	4.06	1.75	1.59
10	B	1006	MGD	PB-O5'	4.05	1.75	1.59
10	D	1006	MGD	PB-O5'	4.05	1.75	1.59
10	F	1006	MGD	PB-O5'	4.05	1.75	1.59
10	H	1006	MGD	PB-O5'	4.05	1.75	1.59
10	F	1007	MGD	C23-C14	4.04	1.56	1.53
10	F	1007	MGD	PB-O5'	4.04	1.75	1.59
10	B	1007	MGD	C23-C14	3.96	1.56	1.53
10	D	1007	MGD	C23-C14	3.96	1.56	1.53
10	H	1007	MGD	C23-C14	3.96	1.56	1.53
10	B	1006	MGD	C10-C11	3.39	1.56	1.51
10	D	1006	MGD	C10-C11	3.39	1.56	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	H	1006	MGD	C10-C11	3.39	1.56	1.51
10	F	1006	MGD	C19-N19	3.39	1.42	1.34
10	F	1006	MGD	C10-C11	3.39	1.56	1.51
10	B	1006	MGD	C19-N19	3.38	1.42	1.34
10	D	1006	MGD	C19-N19	3.38	1.42	1.34
10	H	1006	MGD	C19-N19	3.38	1.42	1.34
10	B	1007	MGD	C19-N19	3.38	1.42	1.34
10	D	1007	MGD	C19-N19	3.38	1.42	1.34
10	H	1007	MGD	C19-N19	3.38	1.42	1.34
10	F	1007	MGD	C19-N19	3.36	1.42	1.34
10	F	1007	MGD	C2-N2	3.24	1.41	1.34
10	B	1007	MGD	C2-N2	3.21	1.41	1.34
10	D	1007	MGD	C2-N2	3.21	1.41	1.34
10	H	1007	MGD	C2-N2	3.21	1.41	1.34
10	B	1006	MGD	C2-N2	3.20	1.41	1.34
10	D	1006	MGD	C2-N2	3.20	1.41	1.34
10	F	1006	MGD	C2-N2	3.20	1.41	1.34
10	H	1006	MGD	C2-N2	3.20	1.41	1.34
10	F	1007	MGD	C6-N1	3.08	1.44	1.38
10	B	1007	MGD	C6-N1	3.05	1.44	1.38
10	D	1007	MGD	C6-N1	3.05	1.44	1.38
10	H	1007	MGD	C6-N1	3.05	1.44	1.38
10	F	1006	MGD	C6-N1	3.04	1.44	1.38
10	B	1006	MGD	C6-N1	3.03	1.44	1.38
10	D	1006	MGD	C6-N1	3.03	1.44	1.38
10	H	1006	MGD	C6-N1	3.03	1.44	1.38
10	B	1006	MGD	PA-O3A	2.98	1.71	1.59
10	D	1006	MGD	PA-O3A	2.98	1.71	1.59
10	F	1006	MGD	PA-O3A	2.98	1.71	1.59
10	H	1006	MGD	PA-O3A	2.98	1.71	1.59
10	B	1007	MGD	PA-O3A	2.83	1.70	1.59
10	D	1007	MGD	PA-O3A	2.83	1.70	1.59
10	F	1007	MGD	PA-O3A	2.83	1.70	1.59
10	H	1007	MGD	PA-O3A	2.83	1.70	1.59
10	F	1007	MGD	O11-C23	-2.48	1.40	1.43
10	B	1006	MGD	O11-C23	-2.46	1.40	1.43
10	D	1006	MGD	O11-C23	-2.46	1.40	1.43
10	H	1006	MGD	O11-C23	-2.46	1.40	1.43
10	F	1006	MGD	O11-C23	-2.46	1.40	1.43
10	B	1007	MGD	O11-C23	-2.42	1.40	1.43
10	D	1007	MGD	O11-C23	-2.42	1.40	1.43
10	H	1007	MGD	O11-C23	-2.42	1.40	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	1007	MGD	C21-N20	2.40	1.39	1.36
10	B	1007	MGD	C10-C11	2.39	1.55	1.51
10	D	1007	MGD	C10-C11	2.39	1.55	1.51
10	F	1007	MGD	C10-C11	2.39	1.55	1.51
10	H	1007	MGD	C10-C11	2.39	1.55	1.51
10	B	1007	MGD	C21-N20	2.38	1.39	1.36
10	D	1007	MGD	C21-N20	2.38	1.39	1.36
10	H	1007	MGD	C21-N20	2.38	1.39	1.36
10	B	1006	MGD	C21-N20	2.28	1.39	1.36
10	D	1006	MGD	C21-N20	2.28	1.39	1.36
10	F	1006	MGD	C21-N20	2.28	1.39	1.36
10	H	1006	MGD	C21-N20	2.28	1.39	1.36
10	B	1007	MGD	O3A-C10	-2.25	1.36	1.44
10	D	1007	MGD	O3A-C10	-2.25	1.36	1.44
10	F	1007	MGD	O3A-C10	-2.25	1.36	1.44
10	H	1007	MGD	O3A-C10	-2.25	1.36	1.44
10	B	1006	MGD	O3A-C10	-2.24	1.36	1.44
10	D	1006	MGD	O3A-C10	-2.24	1.36	1.44
10	F	1006	MGD	O3A-C10	-2.24	1.36	1.44
10	H	1006	MGD	O3A-C10	-2.24	1.36	1.44
10	B	1006	MGD	O5'-C5'	-2.10	1.36	1.44
10	D	1006	MGD	O5'-C5'	-2.10	1.36	1.44
10	F	1006	MGD	O5'-C5'	-2.10	1.36	1.44
10	H	1006	MGD	O5'-C5'	-2.10	1.36	1.44
10	B	1007	MGD	O5'-C5'	-2.09	1.36	1.44
10	D	1007	MGD	O5'-C5'	-2.09	1.36	1.44
10	F	1007	MGD	O5'-C5'	-2.09	1.36	1.44
10	H	1007	MGD	O5'-C5'	-2.09	1.36	1.44
10	B	1007	MGD	C4-N3	2.09	1.39	1.34
10	D	1007	MGD	C4-N3	2.09	1.39	1.34
10	H	1007	MGD	C4-N3	2.09	1.39	1.34
10	F	1007	MGD	C4-N3	2.06	1.39	1.34
10	B	1006	MGD	C17-N18	2.04	1.42	1.38
10	D	1006	MGD	C17-N18	2.04	1.42	1.38
10	F	1006	MGD	C17-N18	2.04	1.42	1.38
10	H	1006	MGD	C17-N18	2.04	1.42	1.38
10	F	1006	MGD	C4-N3	2.04	1.38	1.34
10	B	1006	MGD	C4-N3	2.03	1.38	1.34
10	D	1006	MGD	C4-N3	2.03	1.38	1.34
10	H	1006	MGD	C4-N3	2.03	1.38	1.34

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	1007	MGD	O11-C23-N22	-4.45	104.57	108.61
10	B	1007	MGD	O11-C23-N22	-4.44	104.58	108.61
10	D	1007	MGD	O11-C23-N22	-4.44	104.58	108.61
10	H	1007	MGD	O11-C23-N22	-4.44	104.58	108.61
10	B	1007	MGD	O11-C23-C14	-3.70	106.49	108.96
10	D	1007	MGD	O11-C23-C14	-3.70	106.49	108.96
10	H	1007	MGD	O11-C23-C14	-3.70	106.49	108.96
10	F	1007	MGD	O11-C23-C14	-3.68	106.51	108.96
10	B	1007	MGD	C19-N18-C17	-3.18	119.34	125.11
10	D	1007	MGD	C19-N18-C17	-3.18	119.34	125.11
10	H	1007	MGD	C19-N18-C17	-3.18	119.34	125.11
10	B	1006	MGD	C19-N18-C17	-3.17	119.36	125.11
10	D	1006	MGD	C19-N18-C17	-3.17	119.36	125.11
10	F	1006	MGD	C19-N18-C17	-3.17	119.36	125.11
10	H	1006	MGD	C19-N18-C17	-3.17	119.36	125.11
10	F	1007	MGD	C19-N18-C17	-3.15	119.40	125.11
13	B	1010	MQ7	C11-C3-C4	-2.61	115.83	118.58
13	D	1010	MQ7	C11-C3-C4	-2.61	115.83	118.58
13	F	1010	MQ7	C11-C3-C4	-2.61	115.83	118.58
13	H	1010	MQ7	C11-C3-C4	-2.61	115.83	118.58
10	B	1007	MGD	O2B-PB-O1B	2.54	124.27	112.44
10	D	1007	MGD	O2B-PB-O1B	2.54	124.27	112.44
10	H	1007	MGD	O2B-PB-O1B	2.54	124.27	112.44
10	F	1007	MGD	O2B-PB-O1B	2.54	124.25	112.44
10	B	1006	MGD	C23-C14-N15	2.52	110.34	107.87
10	D	1006	MGD	C23-C14-N15	2.52	110.34	107.87
10	F	1006	MGD	C23-C14-N15	2.52	110.34	107.87
10	H	1006	MGD	C23-C14-N15	2.52	110.34	107.87
10	B	1006	MGD	O2B-PB-O1B	2.51	124.13	112.44
10	D	1006	MGD	O2B-PB-O1B	2.51	124.13	112.44
10	F	1006	MGD	O2B-PB-O1B	2.51	124.13	112.44
10	H	1006	MGD	O2B-PB-O1B	2.51	124.13	112.44
10	F	1007	MGD	O6-C6-N1	-2.29	115.80	120.11
10	B	1007	MGD	O6-C6-N1	-2.28	115.82	120.11
10	D	1007	MGD	O6-C6-N1	-2.28	115.82	120.11
10	H	1007	MGD	O6-C6-N1	-2.28	115.82	120.11
10	F	1007	MGD	O2A-PA-O1A	2.23	122.84	112.44
10	B	1007	MGD	O2A-PA-O1A	2.23	122.82	112.44
10	D	1007	MGD	O2A-PA-O1A	2.23	122.82	112.44
10	H	1007	MGD	O2A-PA-O1A	2.23	122.82	112.44
10	F	1006	MGD	O11-C23-N22	-2.22	106.59	108.61
10	B	1006	MGD	O11-C23-N22	-2.21	106.60	108.61
10	D	1006	MGD	O11-C23-N22	-2.21	106.60	108.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	H	1006	MGD	O11-C23-N22	-2.21	106.60	108.61
10	B	1006	MGD	O2A-PA-O1A	2.18	122.61	112.44
10	D	1006	MGD	O2A-PA-O1A	2.18	122.61	112.44
10	F	1006	MGD	O2A-PA-O1A	2.18	122.61	112.44
10	H	1006	MGD	O2A-PA-O1A	2.18	122.61	112.44
10	F	1006	MGD	O6-C6-N1	-2.18	116.01	120.11
10	B	1006	MGD	O6-C6-N1	-2.17	116.03	120.11
10	D	1006	MGD	O6-C6-N1	-2.17	116.03	120.11
10	H	1006	MGD	O6-C6-N1	-2.17	116.03	120.11
10	B	1006	MGD	O5'-PB-O1B	-2.17	100.35	108.94
10	D	1006	MGD	O5'-PB-O1B	-2.17	100.35	108.94
10	F	1006	MGD	O5'-PB-O1B	-2.17	100.35	108.94
10	H	1006	MGD	O5'-PB-O1B	-2.17	100.35	108.94
10	B	1007	MGD	O5'-PB-O1B	-2.16	100.37	108.94
10	D	1007	MGD	O5'-PB-O1B	-2.16	100.37	108.94
10	H	1007	MGD	O5'-PB-O1B	-2.16	100.37	108.94
10	F	1007	MGD	O5'-PB-O1B	-2.16	100.38	108.94
10	B	1006	MGD	O11-C23-C14	-2.07	107.59	108.96
10	D	1006	MGD	O11-C23-C14	-2.07	107.59	108.96
10	H	1006	MGD	O11-C23-C14	-2.07	107.59	108.96
10	F	1006	MGD	O11-C23-C14	-2.04	107.60	108.96

There are no chirality outliers.

All (324) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	202	A1H2V	C13-C14-O16-C17
4	A	202	A1H2V	O15-C14-O16-C17
4	A	202	A1H2V	C19-O20-P21-O24
4	A	203	A1H2V	C19-O20-P21-O24
4	A	203	A1H2V	C25-O24-P21-O20
4	C	204	A1H2V	C13-C14-O16-C17
4	C	204	A1H2V	O15-C14-O16-C17
4	C	204	A1H2V	C19-O20-P21-O24
4	C	205	A1H2V	C19-O20-P21-O24
4	C	205	A1H2V	C25-O24-P21-O20
4	E	204	A1H2V	C13-C14-O16-C17
4	E	204	A1H2V	O15-C14-O16-C17
4	E	204	A1H2V	C19-O20-P21-O24
4	E	205	A1H2V	C19-O20-P21-O24
4	E	205	A1H2V	C25-O24-P21-O20
4	G	204	A1H2V	C13-C14-O16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	G	204	A1H2V	O15-C14-O16-C17
4	G	204	A1H2V	C19-O20-P21-O24
4	G	205	A1H2V	C19-O20-P21-O24
4	G	205	A1H2V	C25-O24-P21-O20
10	B	1006	MGD	O3A-C10-C11-O11
10	B	1006	MGD	O3A-C10-C11-C12
10	B	1007	MGD	C10-O3A-PA-O3B
10	B	1007	MGD	C10-O3A-PA-O1A
10	B	1007	MGD	C10-O3A-PA-O2A
10	B	1007	MGD	O3A-C10-C11-O11
10	D	1006	MGD	O3A-C10-C11-O11
10	D	1006	MGD	O3A-C10-C11-C12
10	D	1007	MGD	C10-O3A-PA-O3B
10	D	1007	MGD	C10-O3A-PA-O1A
10	D	1007	MGD	C10-O3A-PA-O2A
10	D	1007	MGD	O3A-C10-C11-O11
10	F	1006	MGD	O3A-C10-C11-O11
10	F	1006	MGD	O3A-C10-C11-C12
10	F	1007	MGD	C10-O3A-PA-O3B
10	F	1007	MGD	C10-O3A-PA-O1A
10	F	1007	MGD	C10-O3A-PA-O2A
10	F	1007	MGD	O3A-C10-C11-O11
10	H	1006	MGD	O3A-C10-C11-O11
10	H	1006	MGD	O3A-C10-C11-C12
10	H	1007	MGD	C10-O3A-PA-O3B
10	H	1007	MGD	C10-O3A-PA-O1A
10	H	1007	MGD	C10-O3A-PA-O2A
10	H	1007	MGD	O3A-C10-C11-O11
13	B	1010	MQ7	C23-C25-C26-C27
13	D	1010	MQ7	C23-C25-C26-C27
13	F	1010	MQ7	C23-C25-C26-C27
13	H	1010	MQ7	C23-C25-C26-C27
13	B	1010	MQ7	C13-C15-C16-C17
13	D	1010	MQ7	C13-C15-C16-C17
13	F	1010	MQ7	C13-C15-C16-C17
13	H	1010	MQ7	C13-C15-C16-C17
4	A	203	A1H2V	C20-C1-C2-C3
4	C	205	A1H2V	C20-C1-C2-C3
4	E	205	A1H2V	C20-C1-C2-C3
4	G	205	A1H2V	C20-C1-C2-C3
3	A	211	11A	CAD-CAE-CAF-CAG
3	C	213	11A	CAD-CAE-CAF-CAG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	E	213	11A	CAD-CAE-CAF-CAG
3	G	213	11A	CAD-CAE-CAF-CAG
4	A	203	A1H2V	C6-C7-C8-C9
4	C	205	A1H2V	C6-C7-C8-C9
4	G	205	A1H2V	C6-C7-C8-C9
4	E	205	A1H2V	C6-C7-C8-C9
3	A	211	11A	CAH-CAI-CAJ-CAK
3	C	213	11A	CAH-CAI-CAJ-CAK
3	E	213	11A	CAH-CAI-CAJ-CAK
3	G	213	11A	CAH-CAI-CAJ-CAK
4	A	203	A1H2V	C38-C39-C40-C41
4	C	205	A1H2V	C38-C39-C40-C41
4	G	205	A1H2V	C38-C39-C40-C41
4	E	205	A1H2V	C38-C39-C40-C41
7	A	212	MYR	C1-C2-C3-C4
7	C	201	MYR	C1-C2-C3-C4
7	E	201	MYR	C1-C2-C3-C4
7	G	201	MYR	C1-C2-C3-C4
4	A	203	A1H2V	C1-C20-C21-C22
4	C	205	A1H2V	C1-C20-C21-C22
4	E	205	A1H2V	C1-C20-C21-C22
4	G	205	A1H2V	C1-C20-C21-C22
4	A	213	A1H2V	C3-C4-C5-C6
4	C	202	A1H2V	C3-C4-C5-C6
4	E	202	A1H2V	C3-C4-C5-C6
4	G	202	A1H2V	C3-C4-C5-C6
3	A	210	11A	CAH-CAI-CAJ-CAK
3	C	212	11A	CAH-CAI-CAJ-CAK
3	E	212	11A	CAH-CAI-CAJ-CAK
3	G	212	11A	CAH-CAI-CAJ-CAK
3	A	210	11A	CAJ-CAK-CAL-CAM
3	C	212	11A	CAJ-CAK-CAL-CAM
3	E	212	11A	CAJ-CAK-CAL-CAM
3	G	212	11A	CAJ-CAK-CAL-CAM
3	A	210	11A	CAG-CAH-CAI-CAJ
3	C	212	11A	CAG-CAH-CAI-CAJ
3	E	212	11A	CAG-CAH-CAI-CAJ
3	G	212	11A	CAG-CAH-CAI-CAJ
6	A	208	KNA	C4-C5-C6-C7
6	C	210	KNA	C4-C5-C6-C7
6	E	210	KNA	C4-C5-C6-C7
6	G	210	KNA	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	E	205	A1H2V	C40-C41-C42-C43
4	A	203	A1H2V	C40-C41-C42-C43
4	C	205	A1H2V	C40-C41-C42-C43
4	G	205	A1H2V	C40-C41-C42-C43
3	A	207	11A	CAJ-CAK-CAL-CAM
3	C	209	11A	CAJ-CAK-CAL-CAM
3	E	209	11A	CAJ-CAK-CAL-CAM
3	G	209	11A	CAJ-CAK-CAL-CAM
7	A	212	MYR	C6-C7-C8-C9
7	C	201	MYR	C6-C7-C8-C9
7	E	201	MYR	C6-C7-C8-C9
7	G	201	MYR	C6-C7-C8-C9
4	A	203	A1H2V	C2-C1-C20-C21
4	C	205	A1H2V	C2-C1-C20-C21
4	E	205	A1H2V	C2-C1-C20-C21
4	G	205	A1H2V	C2-C1-C20-C21
10	B	1007	MGD	PA-O3B-PB-O5'
10	D	1007	MGD	PA-O3B-PB-O5'
10	F	1007	MGD	PA-O3B-PB-O5'
10	H	1007	MGD	PA-O3B-PB-O5'
4	A	203	A1H2V	C37-C38-C39-C40
4	C	205	A1H2V	C37-C38-C39-C40
4	E	205	A1H2V	C37-C38-C39-C40
4	G	205	A1H2V	C37-C38-C39-C40
4	A	203	A1H2V	C17-C18-C19-O20
4	C	205	A1H2V	C17-C18-C19-O20
4	E	205	A1H2V	C17-C18-C19-O20
4	G	205	A1H2V	C17-C18-C19-O20
4	A	202	A1H2V	O16-C17-C18-O30
4	C	204	A1H2V	O16-C17-C18-O30
4	E	204	A1H2V	O16-C17-C18-O30
4	G	204	A1H2V	O16-C17-C18-O30
7	A	212	MYR	C11-C10-C9-C8
7	C	201	MYR	C11-C10-C9-C8
7	E	201	MYR	C11-C10-C9-C8
7	G	201	MYR	C11-C10-C9-C8
4	A	203	A1H2V	O30-C18-C19-O20
4	C	205	A1H2V	O30-C18-C19-O20
4	E	205	A1H2V	O30-C18-C19-O20
4	G	205	A1H2V	O30-C18-C19-O20
7	A	212	MYR	C2-C3-C4-C5
7	C	201	MYR	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	E	201	MYR	C2-C3-C4-C5
7	G	201	MYR	C2-C3-C4-C5
4	A	202	A1H2V	C19-O20-P21-O22
4	A	203	A1H2V	C19-O20-P21-O22
4	A	203	A1H2V	C25-O24-P21-O22
4	C	204	A1H2V	C19-O20-P21-O22
4	C	205	A1H2V	C19-O20-P21-O22
4	C	205	A1H2V	C25-O24-P21-O22
4	E	204	A1H2V	C19-O20-P21-O22
4	E	205	A1H2V	C19-O20-P21-O22
4	E	205	A1H2V	C25-O24-P21-O22
4	G	204	A1H2V	C19-O20-P21-O22
4	G	205	A1H2V	C19-O20-P21-O22
4	G	205	A1H2V	C25-O24-P21-O22
4	A	203	A1H2V	C33-C34-C35-C36
4	C	205	A1H2V	C33-C34-C35-C36
4	E	205	A1H2V	C33-C34-C35-C36
4	G	205	A1H2V	C33-C34-C35-C36
4	A	202	A1H2V	C18-C19-O20-P21
4	A	203	A1H2V	C18-C19-O20-P21
4	C	204	A1H2V	C18-C19-O20-P21
4	C	205	A1H2V	C18-C19-O20-P21
4	E	204	A1H2V	C18-C19-O20-P21
4	E	205	A1H2V	C18-C19-O20-P21
4	G	204	A1H2V	C18-C19-O20-P21
4	G	205	A1H2V	C18-C19-O20-P21
3	E	213	11A	CAF-CAG-CAH-CAI
3	A	211	11A	CAF-CAG-CAH-CAI
3	C	213	11A	CAF-CAG-CAH-CAI
3	G	213	11A	CAF-CAG-CAH-CAI
4	A	203	A1H2V	C19-C18-O30-C31
4	C	205	A1H2V	C19-C18-O30-C31
4	E	205	A1H2V	C19-C18-O30-C31
4	G	205	A1H2V	C19-C18-O30-C31
4	A	202	A1H2V	C34-C35-C36-C37
4	C	204	A1H2V	C34-C35-C36-C37
4	G	204	A1H2V	C34-C35-C36-C37
4	E	204	A1H2V	C34-C35-C36-C37
5	A	204	SHV	C2-C3-C4-C5
5	C	206	SHV	C2-C3-C4-C5
5	E	206	SHV	C2-C3-C4-C5
5	G	206	SHV	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	203	A1H2V	C34-C35-C36-C37
4	C	205	A1H2V	C34-C35-C36-C37
4	E	205	A1H2V	C34-C35-C36-C37
4	G	205	A1H2V	C34-C35-C36-C37
4	A	203	A1H2V	C10-C11-C12-C13
4	C	205	A1H2V	C10-C11-C12-C13
4	E	205	A1H2V	C10-C11-C12-C13
4	G	205	A1H2V	C10-C11-C12-C13
4	A	202	A1H2V	C19-C18-O30-C31
4	C	204	A1H2V	C19-C18-O30-C31
4	E	204	A1H2V	C19-C18-O30-C31
4	G	204	A1H2V	C19-C18-O30-C31
4	A	203	A1H2V	C35-C36-C37-C38
4	C	205	A1H2V	C35-C36-C37-C38
4	E	205	A1H2V	C35-C36-C37-C38
4	G	205	A1H2V	C35-C36-C37-C38
4	A	203	A1H2V	C26-C25-O24-P21
4	C	205	A1H2V	C26-C25-O24-P21
4	E	205	A1H2V	C26-C25-O24-P21
4	G	205	A1H2V	C26-C25-O24-P21
3	A	209	11A	CAK-CAL-CAM-OAC
3	C	211	11A	CAK-CAL-CAM-OAC
3	E	211	11A	CAK-CAL-CAM-OAC
3	G	211	11A	CAK-CAL-CAM-OAC
5	A	205	SHV	O2-C1-C2-C3
5	C	207	SHV	O2-C1-C2-C3
5	E	207	SHV	O2-C1-C2-C3
5	G	207	SHV	O2-C1-C2-C3
3	A	209	11A	CAK-CAL-CAM-OAB
3	C	211	11A	CAK-CAL-CAM-OAB
3	E	211	11A	CAK-CAL-CAM-OAB
3	G	211	11A	CAK-CAL-CAM-OAB
3	A	210	11A	CAD-CAE-CAF-CAG
3	C	212	11A	CAD-CAE-CAF-CAG
3	G	212	11A	CAD-CAE-CAF-CAG
5	A	205	SHV	O1-C1-C2-C3
5	C	207	SHV	O1-C1-C2-C3
5	E	207	SHV	O1-C1-C2-C3
5	G	207	SHV	O1-C1-C2-C3
3	E	212	11A	CAD-CAE-CAF-CAG
13	B	1010	MQ7	C24-C23-C25-C26
13	D	1010	MQ7	C24-C23-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	F	1010	MQ7	C24-C23-C25-C26
13	H	1010	MQ7	C24-C23-C25-C26
4	E	204	A1H2V	C5-C6-C7-C8
4	A	202	A1H2V	C5-C6-C7-C8
4	C	204	A1H2V	C5-C6-C7-C8
4	G	204	A1H2V	C5-C6-C7-C8
13	B	1010	MQ7	C39-C38-C40-C41
13	D	1010	MQ7	C39-C38-C40-C41
13	F	1010	MQ7	C39-C38-C40-C41
13	H	1010	MQ7	C39-C38-C40-C41
3	A	210	11A	CAK-CAL-CAM-OAB
3	C	212	11A	CAK-CAL-CAM-OAB
3	E	212	11A	CAK-CAL-CAM-OAB
3	G	212	11A	CAK-CAL-CAM-OAB
13	B	1010	MQ7	C22-C23-C25-C26
13	D	1010	MQ7	C22-C23-C25-C26
13	F	1010	MQ7	C22-C23-C25-C26
13	H	1010	MQ7	C22-C23-C25-C26
6	A	208	KNA	O2-C1-C2-C3
6	C	210	KNA	O2-C1-C2-C3
6	E	210	KNA	O2-C1-C2-C3
6	G	210	KNA	O2-C1-C2-C3
4	A	213	A1H2V	C2-C3-C4-C5
4	C	202	A1H2V	C2-C3-C4-C5
4	E	202	A1H2V	C2-C3-C4-C5
4	G	202	A1H2V	C2-C3-C4-C5
4	A	203	A1H2V	C2-C3-C4-C5
4	C	205	A1H2V	C2-C3-C4-C5
4	G	205	A1H2V	C2-C3-C4-C5
10	B	1006	MGD	C11-C10-O3A-PA
10	D	1006	MGD	C11-C10-O3A-PA
10	F	1006	MGD	C11-C10-O3A-PA
10	H	1006	MGD	C11-C10-O3A-PA
4	E	205	A1H2V	C2-C3-C4-C5
10	B	1007	MGD	PB-O3B-PA-O1A
10	D	1007	MGD	PB-O3B-PA-O1A
10	F	1007	MGD	PB-O3B-PA-O1A
10	H	1007	MGD	PB-O3B-PA-O1A
4	A	203	A1H2V	C42-C43-C44-C45
4	C	205	A1H2V	C42-C43-C44-C45
4	G	205	A1H2V	C42-C43-C44-C45
4	E	205	A1H2V	C42-C43-C44-C45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	210	11A	CAK-CAL-CAM-OAC
3	C	212	11A	CAK-CAL-CAM-OAC
3	E	212	11A	CAK-CAL-CAM-OAC
3	G	212	11A	CAK-CAL-CAM-OAC
4	A	202	A1H2V	O30-C18-C19-O20
4	C	204	A1H2V	O30-C18-C19-O20
4	E	204	A1H2V	O30-C18-C19-O20
4	G	204	A1H2V	O30-C18-C19-O20
4	G	202	A1H2V	O30-C31-C33-C34
13	B	1010	MQ7	C29-C28-C30-C31
13	D	1010	MQ7	C29-C28-C30-C31
13	F	1010	MQ7	C29-C28-C30-C31
13	H	1010	MQ7	C29-C28-C30-C31
13	B	1010	MQ7	C40-C41-C42-C43
13	D	1010	MQ7	C40-C41-C42-C43
13	F	1010	MQ7	C40-C41-C42-C43
13	H	1010	MQ7	C40-C41-C42-C43
5	A	204	SHV	O2-C1-C2-C3
5	C	206	SHV	O2-C1-C2-C3
5	E	206	SHV	O2-C1-C2-C3
5	G	206	SHV	O2-C1-C2-C3
4	A	213	A1H2V	O30-C31-C33-C34
4	C	202	A1H2V	O30-C31-C33-C34
4	E	202	A1H2V	O30-C31-C33-C34
5	A	204	SHV	O1-C1-C2-C3
5	C	206	SHV	O1-C1-C2-C3
5	E	206	SHV	O1-C1-C2-C3
5	G	206	SHV	O1-C1-C2-C3
6	A	208	KNA	O1-C1-C2-C3
6	C	210	KNA	O1-C1-C2-C3
6	E	210	KNA	O1-C1-C2-C3
6	G	210	KNA	O1-C1-C2-C3
10	B	1007	MGD	O3A-C10-C11-C12
10	D	1007	MGD	O3A-C10-C11-C12
10	F	1007	MGD	O3A-C10-C11-C12
10	H	1007	MGD	O3A-C10-C11-C12
3	A	206	11A	CAK-CAL-CAM-OAC
3	C	208	11A	CAK-CAL-CAM-OAC
3	E	208	11A	CAK-CAL-CAM-OAC
3	G	208	11A	CAK-CAL-CAM-OAC
7	A	212	MYR	C3-C4-C5-C6
7	C	201	MYR	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	E	201	MYR	C3-C4-C5-C6
7	G	201	MYR	C3-C4-C5-C6
4	A	213	A1H2V	O32-C31-C33-C34
4	C	202	A1H2V	O32-C31-C33-C34
4	E	202	A1H2V	O32-C31-C33-C34
4	G	202	A1H2V	O32-C31-C33-C34
3	A	201	11A	CAK-CAL-CAM-OAC
3	A	207	11A	CAK-CAL-CAM-OAC
3	C	203	11A	CAK-CAL-CAM-OAC
3	C	209	11A	CAK-CAL-CAM-OAC
3	E	203	11A	CAK-CAL-CAM-OAC
3	E	209	11A	CAK-CAL-CAM-OAC
3	G	203	11A	CAK-CAL-CAM-OAC
3	G	209	11A	CAK-CAL-CAM-OAC

There are no ring outliers.

49 monomers are involved in 142 short contacts:

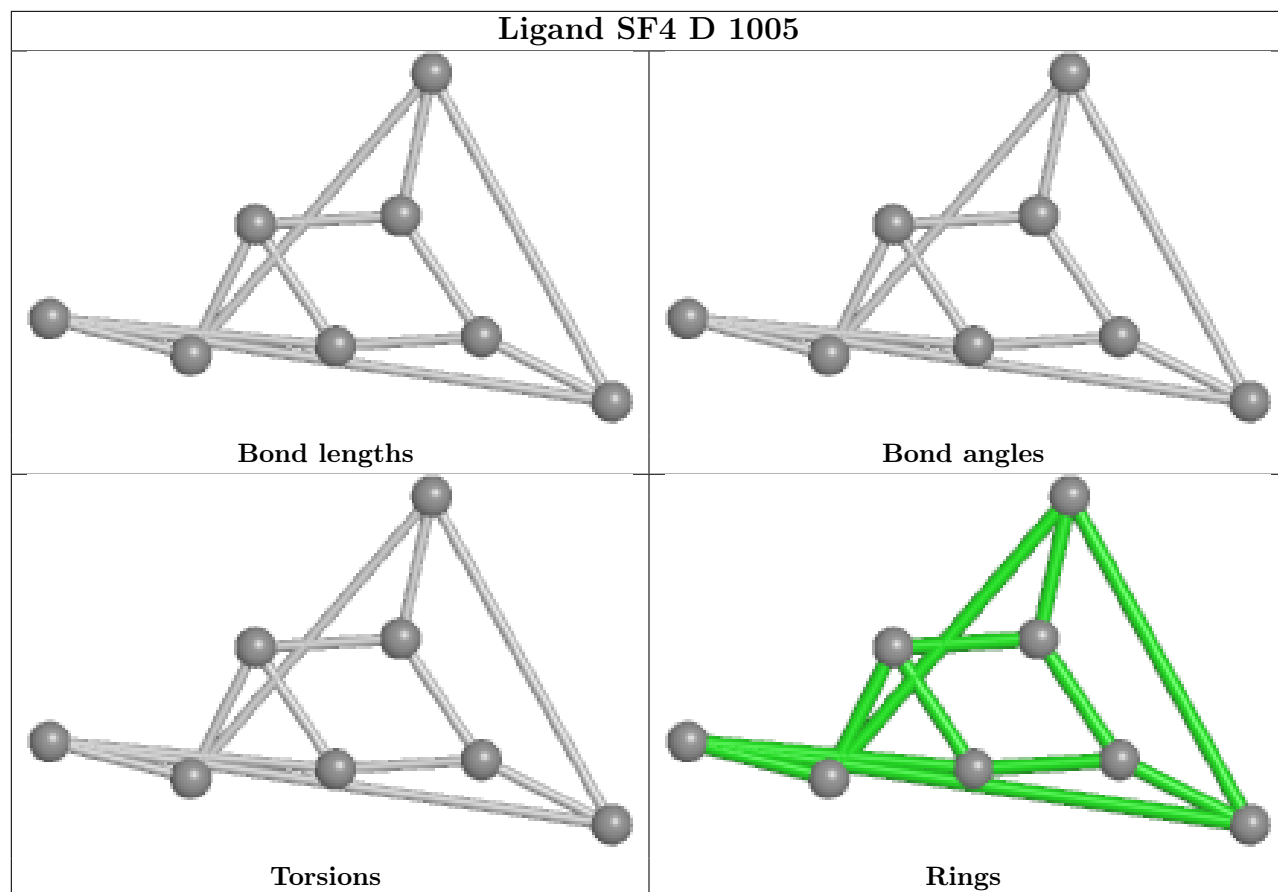
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	201	MYR	2	0
9	D	1005	SF4	1	0
10	H	1006	MGD	11	0
4	C	205	A1H2V	6	0
8	F	1001	FES	1	0
10	B	1006	MGD	10	0
3	A	211	11A	1	0
3	E	213	11A	1	0
9	D	1002	SF4	1	0
7	G	201	MYR	2	0
9	H	1005	SF4	1	0
9	D	1004	SF4	1	0
13	D	1010	MQ7	2	0
9	F	1003	SF4	2	0
10	F	1007	MGD	11	0
8	H	1001	FES	1	0
4	E	205	A1H2V	6	0
9	F	1002	SF4	1	0
9	H	1004	SF4	1	0
9	D	1003	SF4	1	0
10	B	1007	MGD	10	0
8	B	1001	FES	1	0
9	B	1002	SF4	1	0

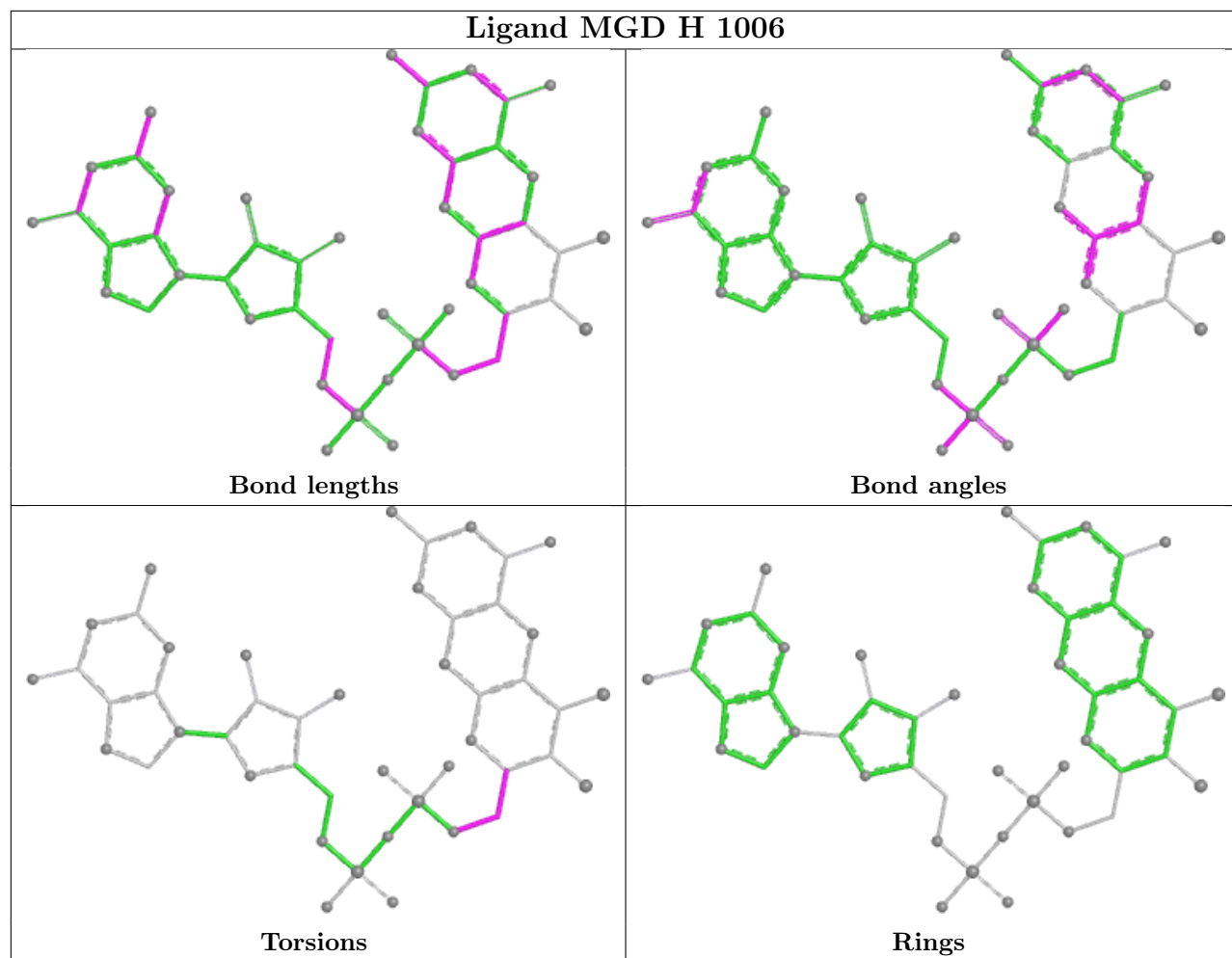
Continued on next page...

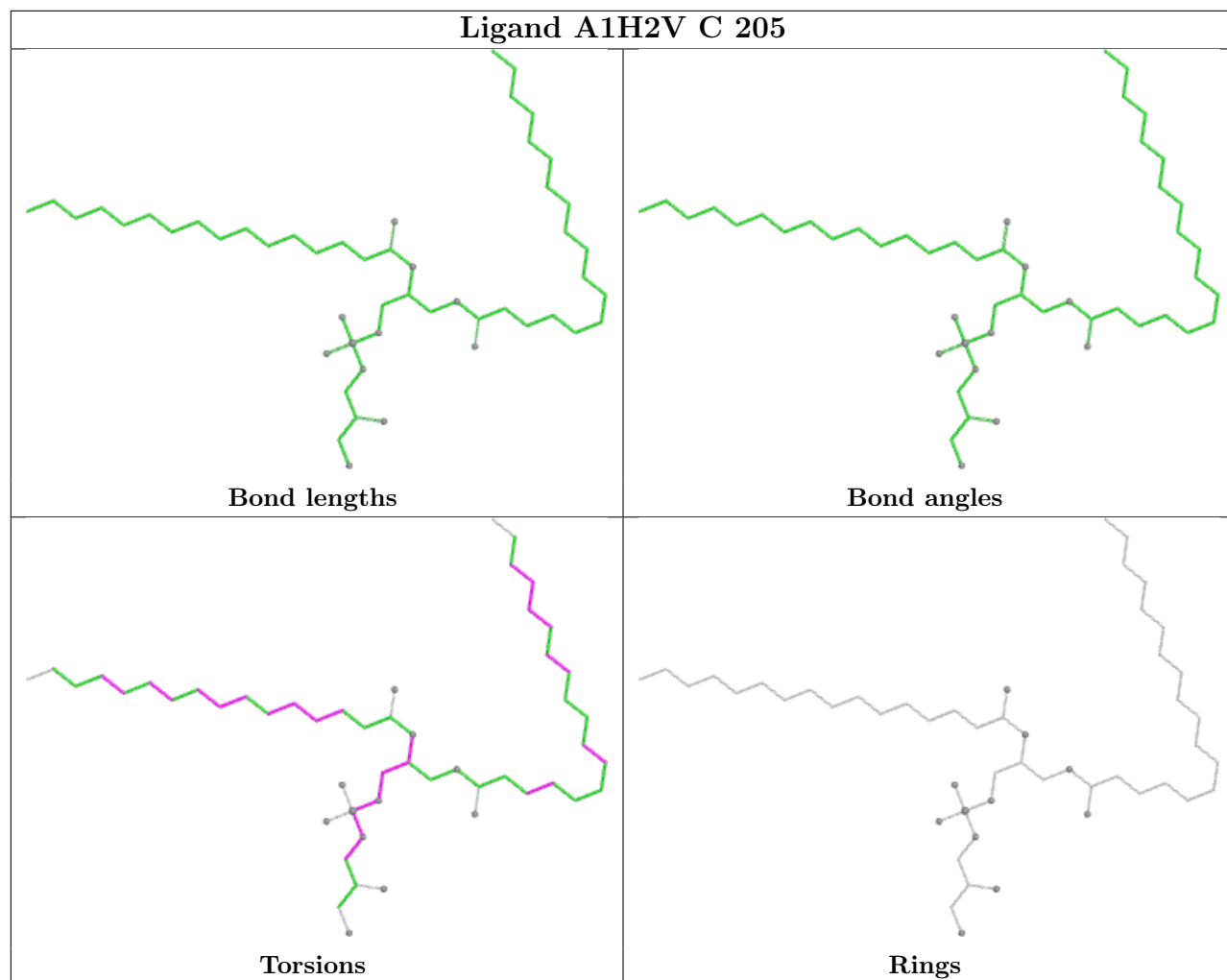
Continued from previous page...

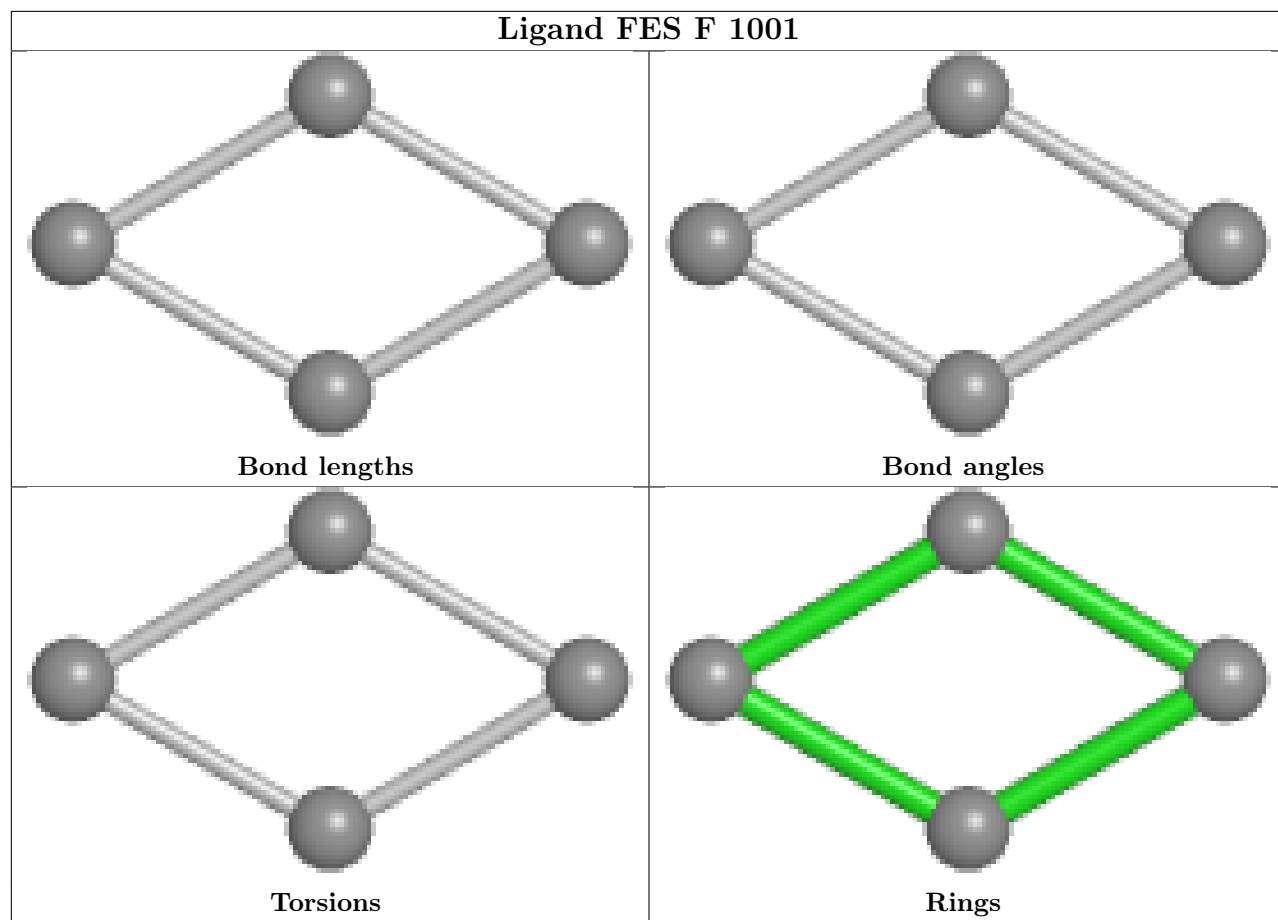
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	11A	2	0
9	H	1003	SF4	2	0
13	F	1010	MQ7	2	0
3	G	203	11A	2	0
3	C	203	11A	2	0
3	G	213	11A	1	0
3	C	213	11A	1	0
13	B	1010	MQ7	2	0
9	B	1004	SF4	1	0
10	F	1006	MGD	11	0
7	E	201	MYR	2	0
8	D	1001	FES	1	0
3	A	209	11A	1	0
9	F	1004	SF4	1	0
4	G	205	A1H2V	6	0
9	B	1003	SF4	2	0
13	H	1010	MQ7	2	0
10	H	1007	MGD	11	0
9	F	1005	SF4	1	0
9	B	1005	SF4	1	0
10	D	1007	MGD	12	0
3	E	203	11A	2	0
7	A	212	MYR	2	0
10	D	1006	MGD	10	0
4	A	203	A1H2V	6	0
9	H	1002	SF4	1	0

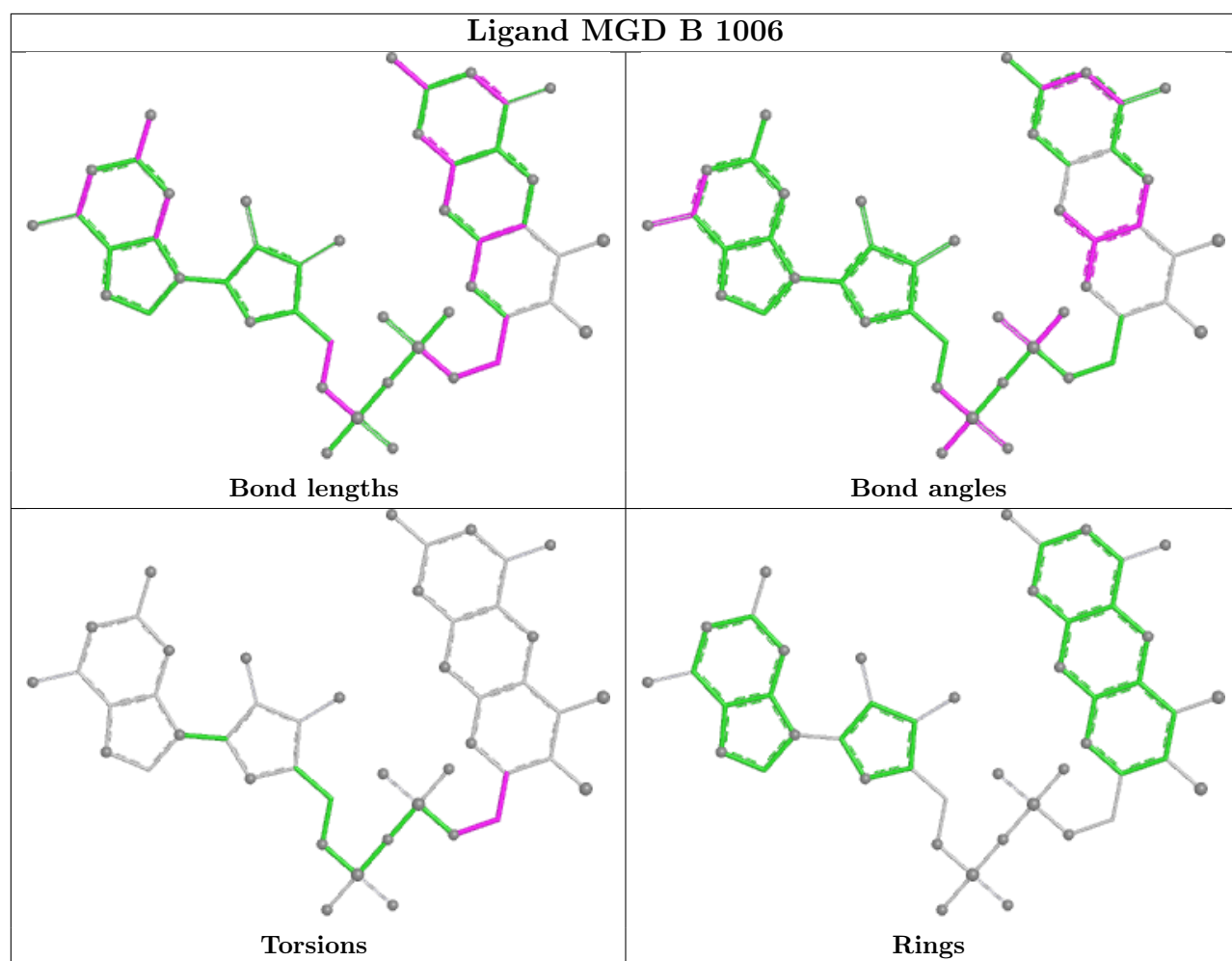
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

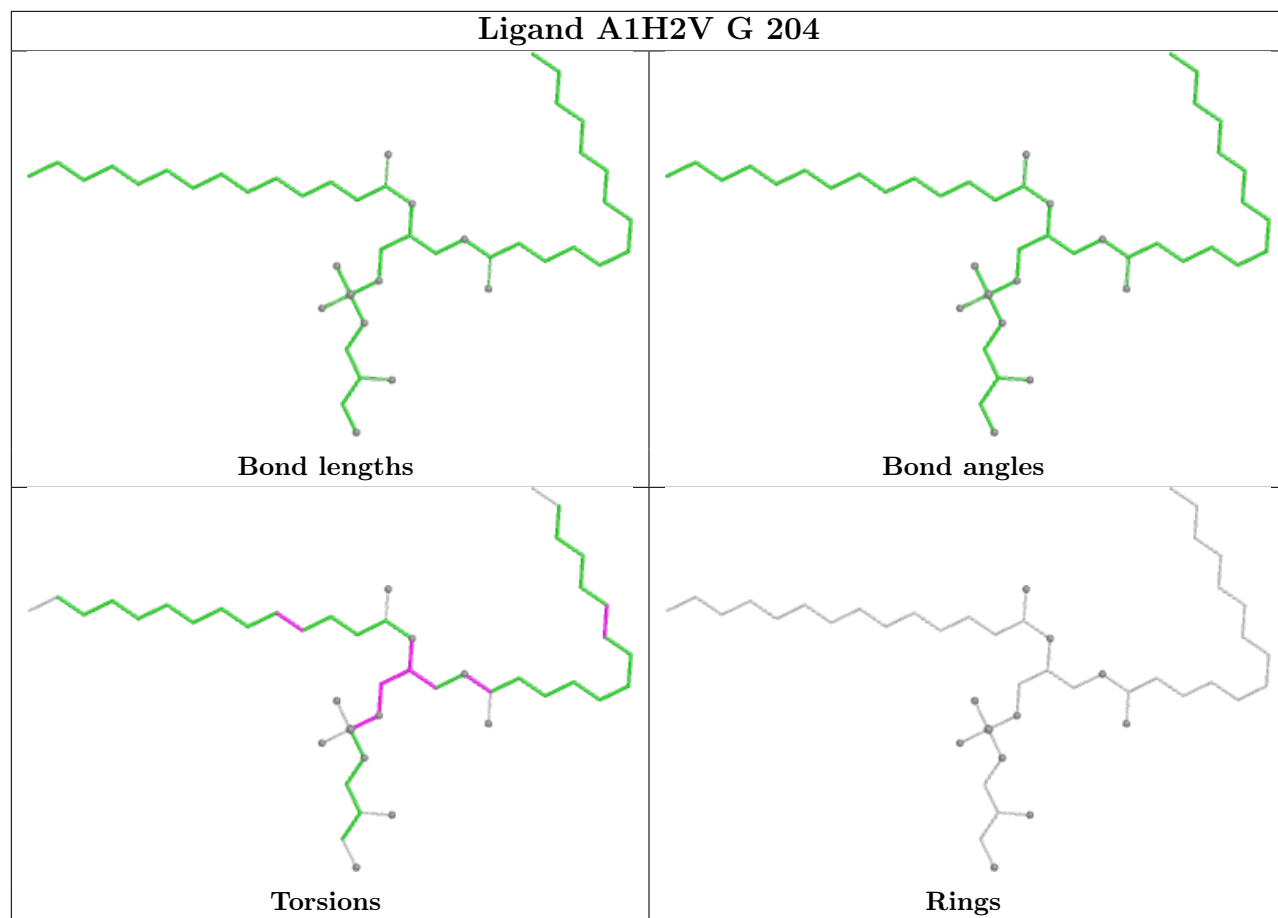


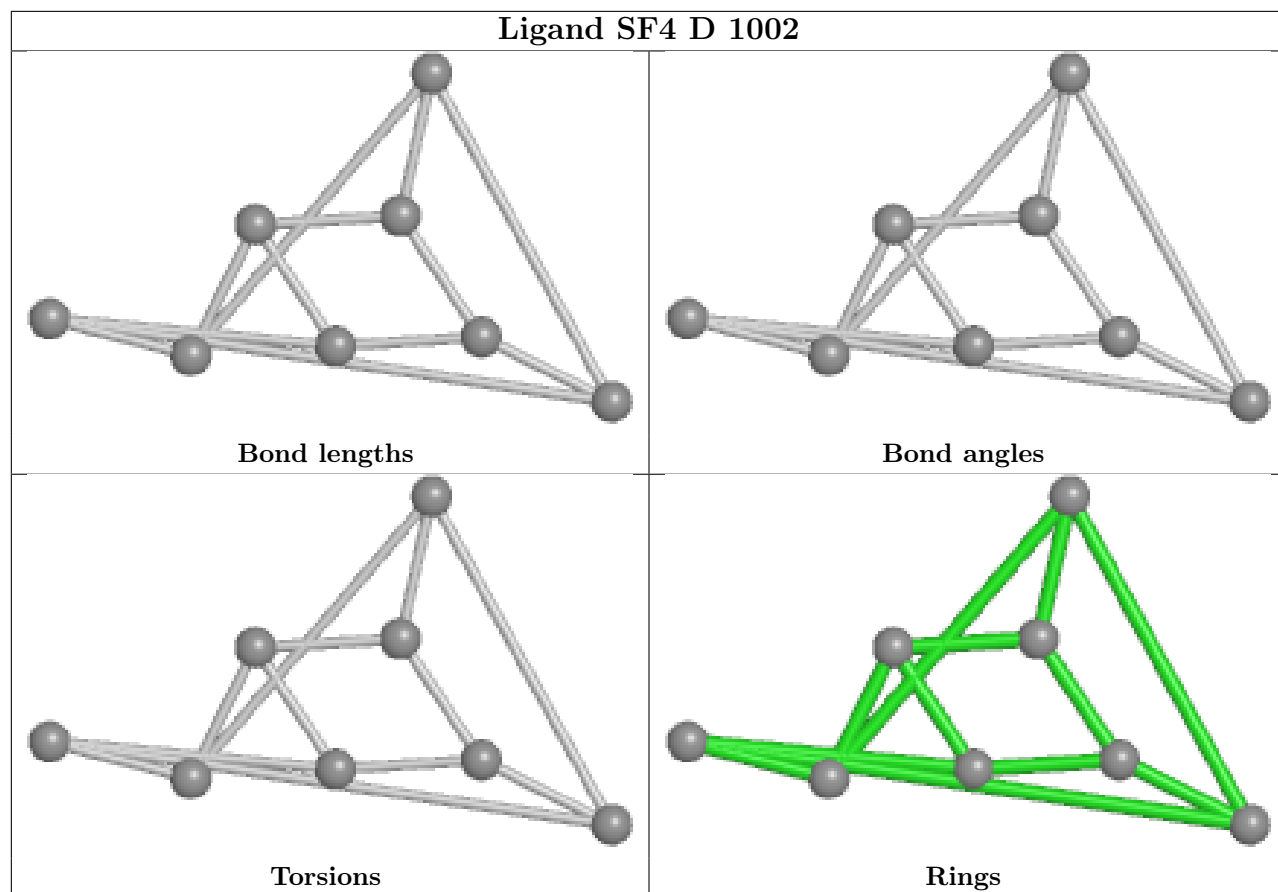


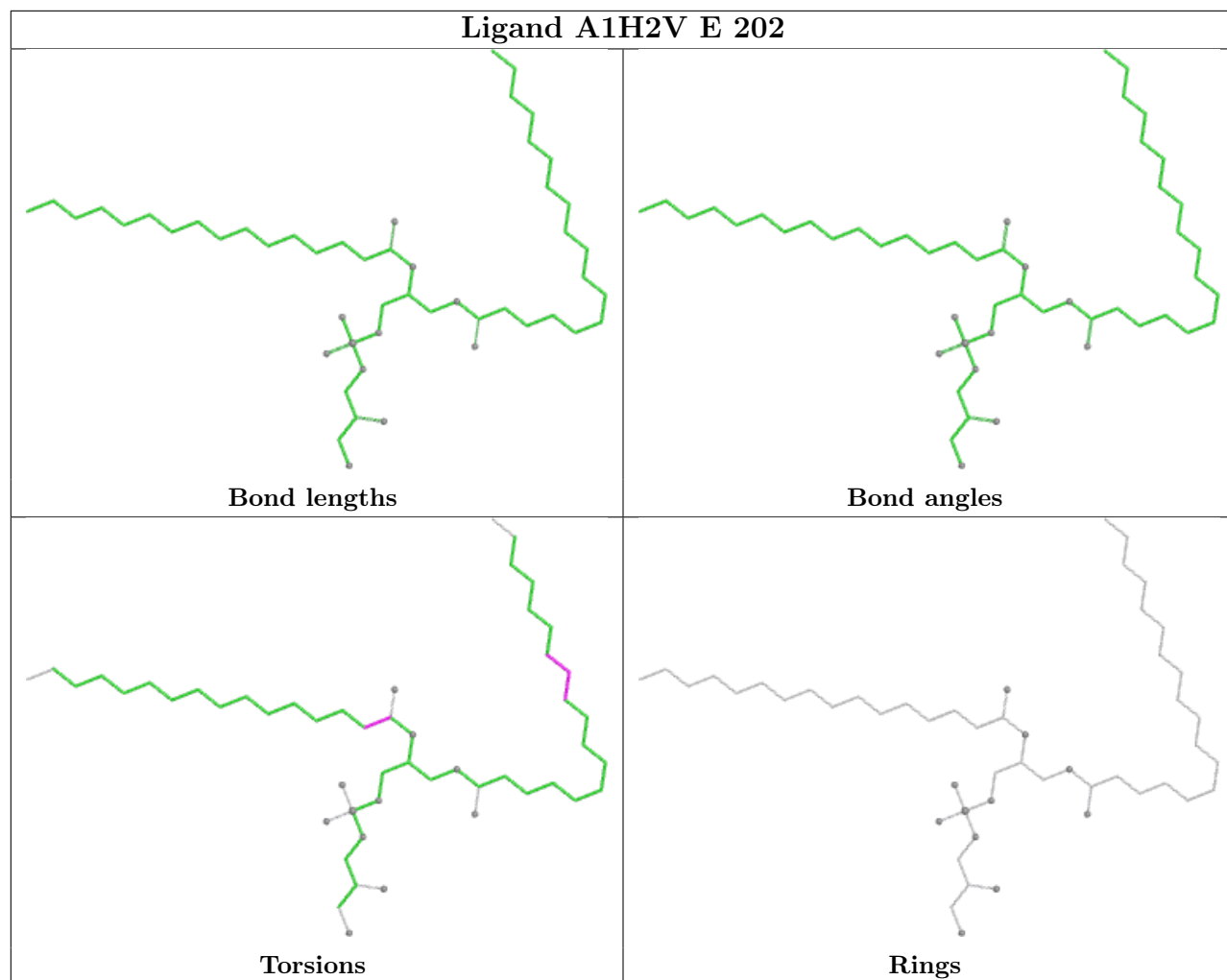


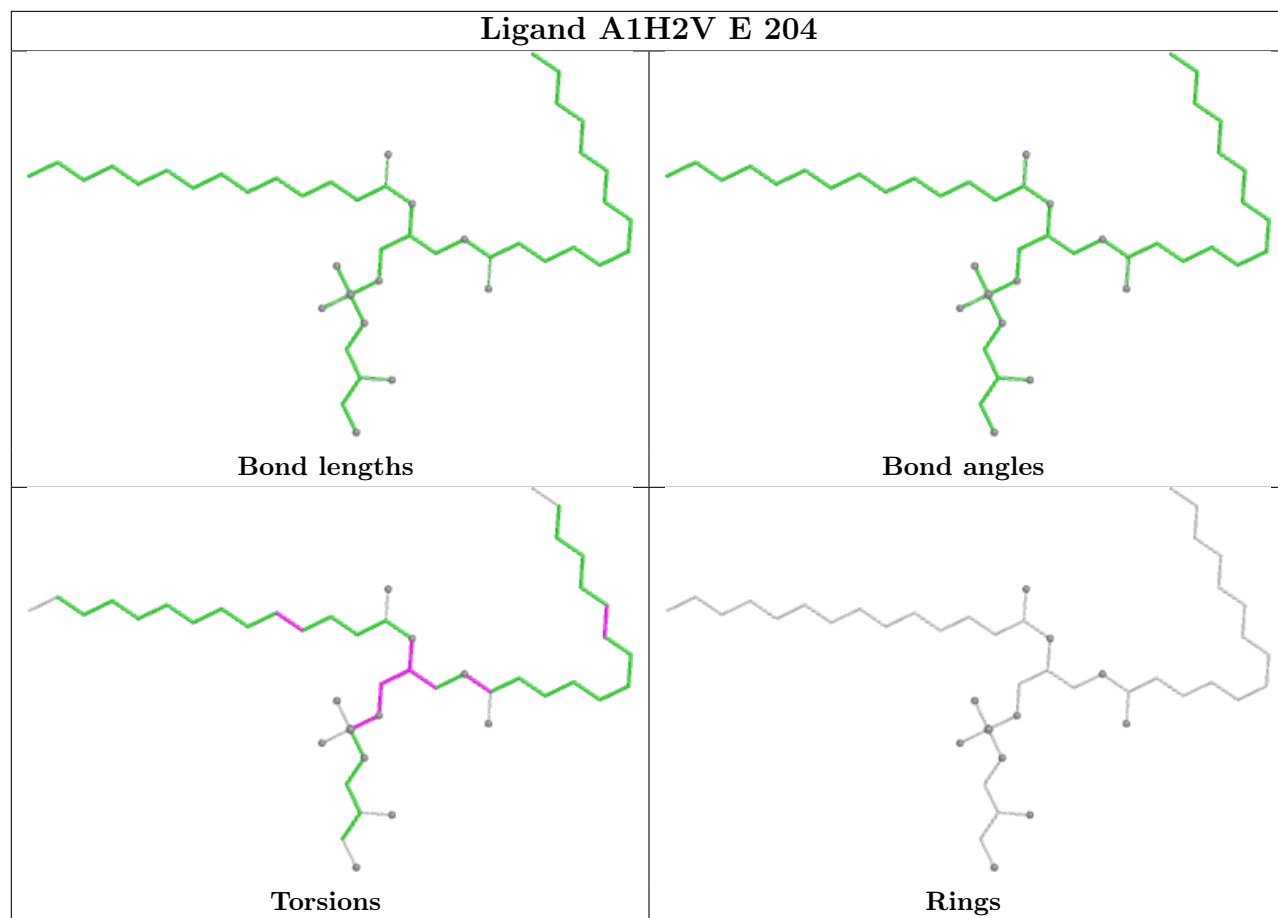


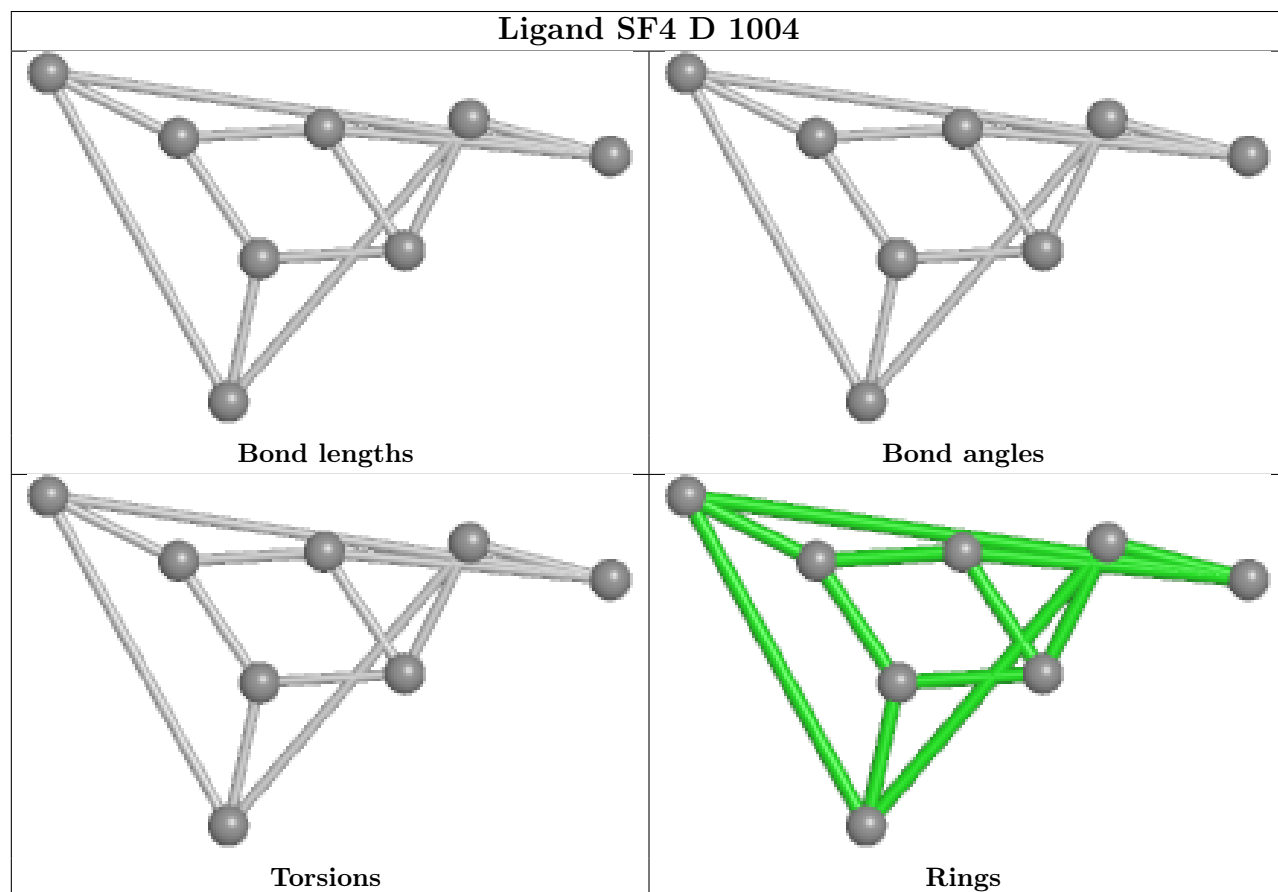
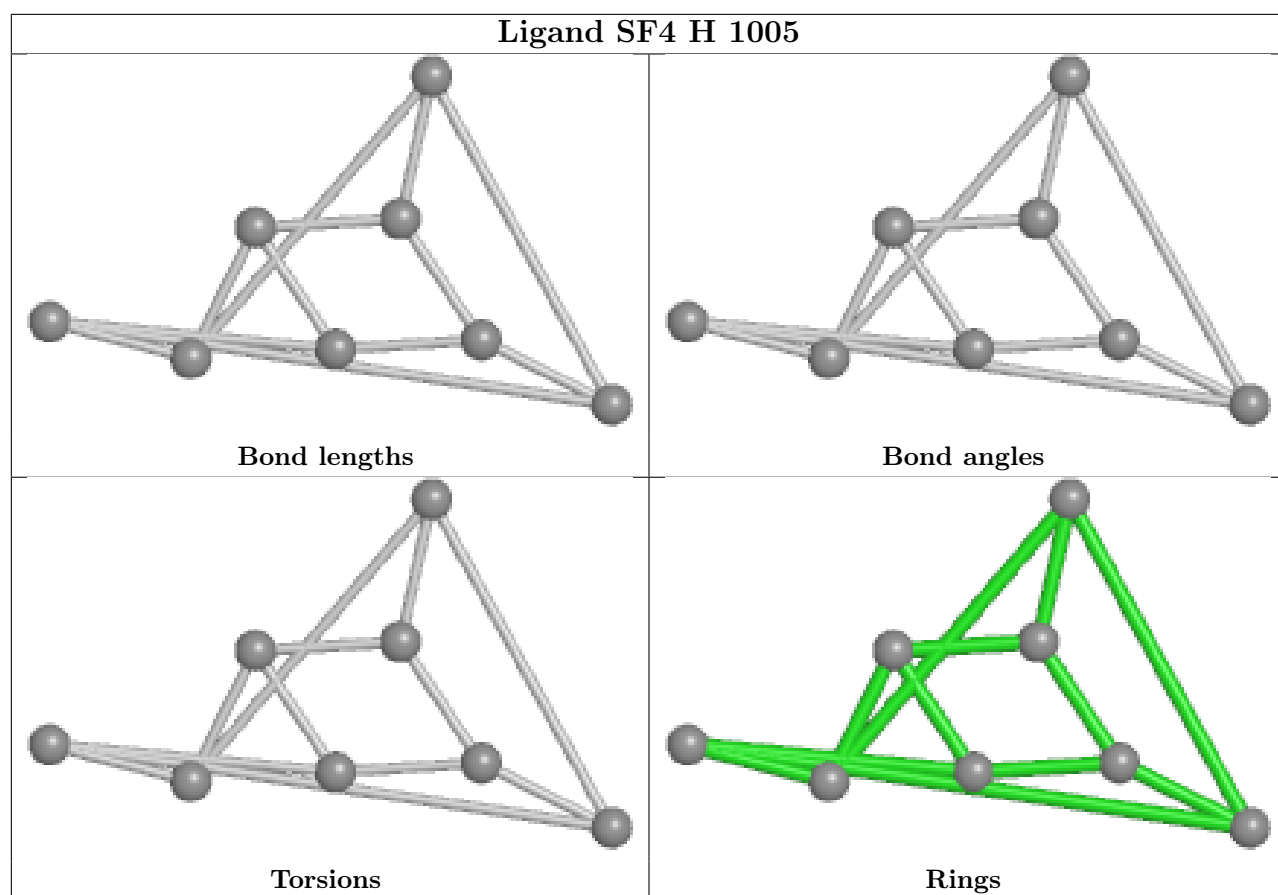


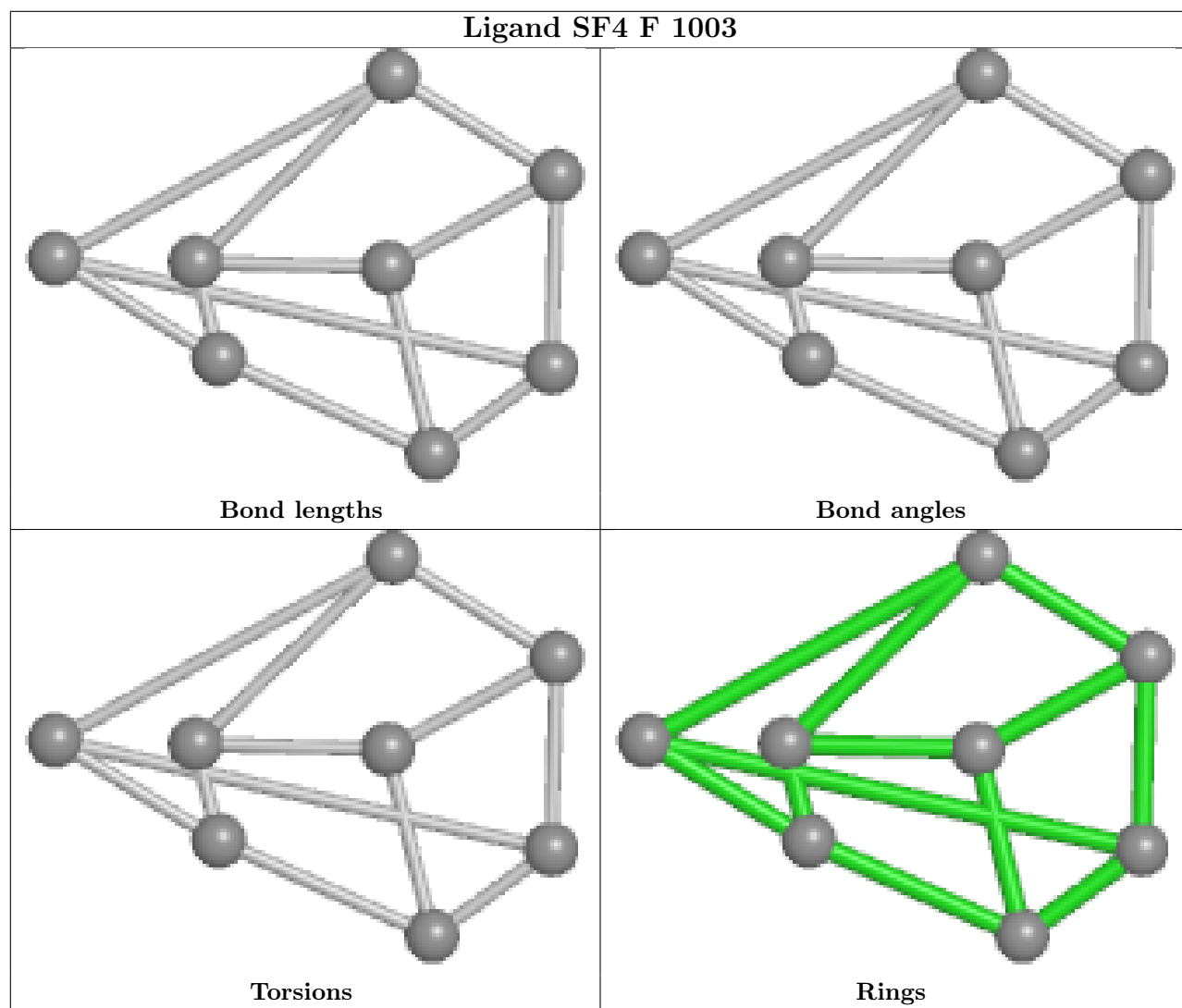
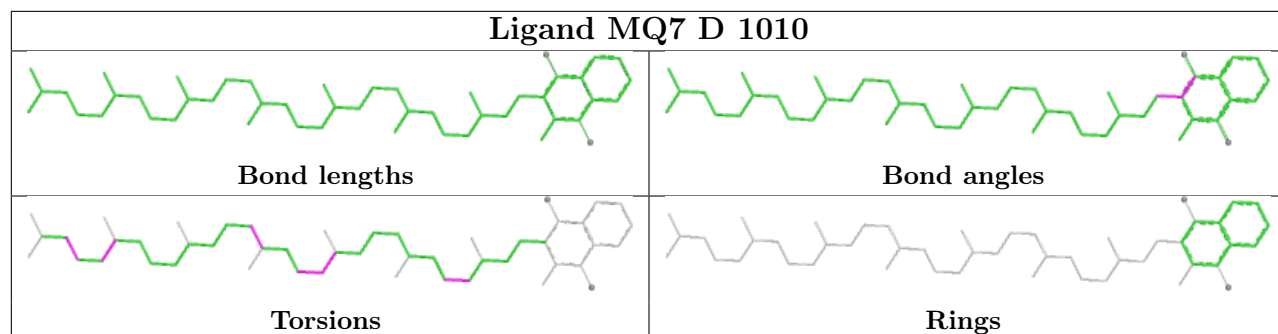


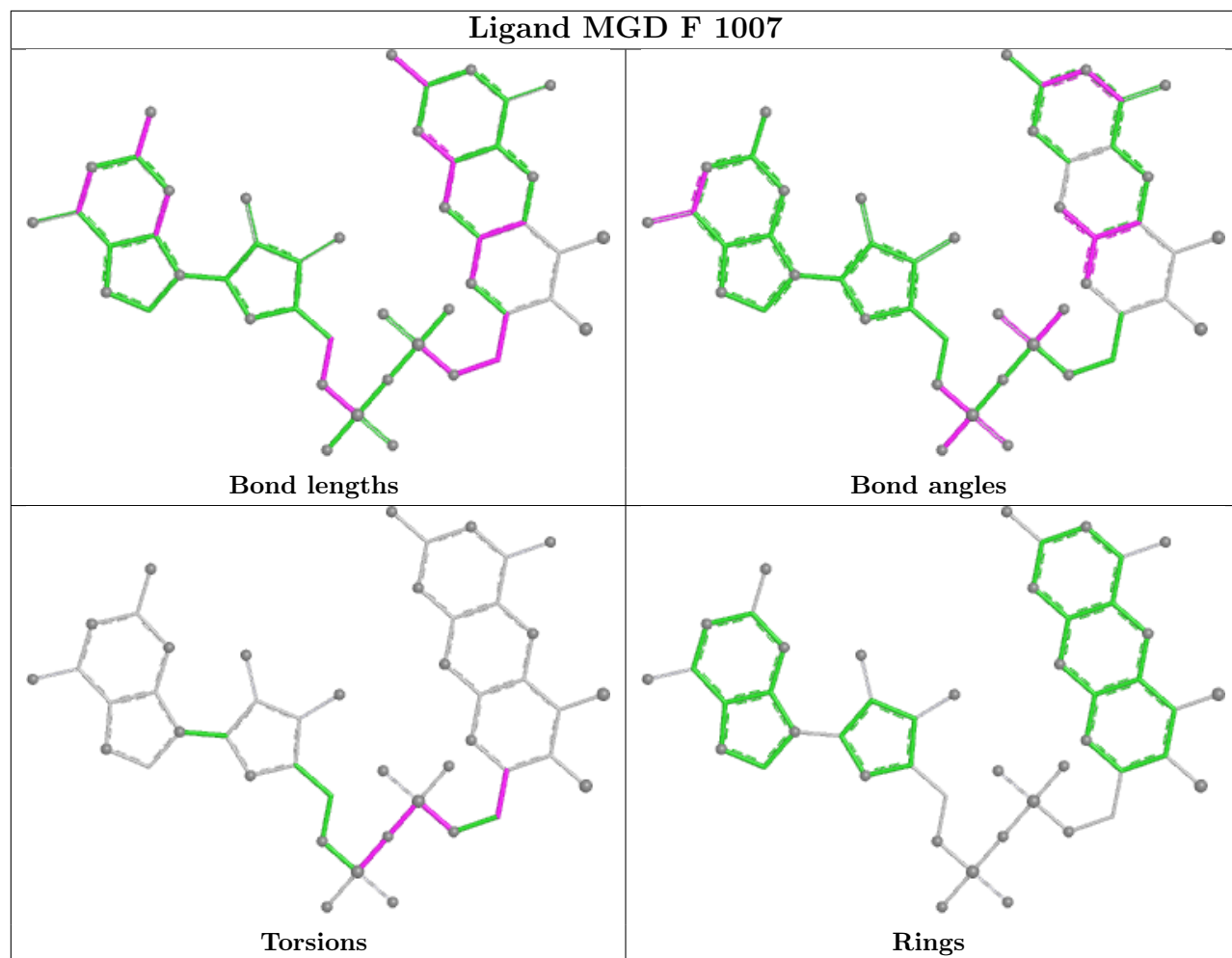


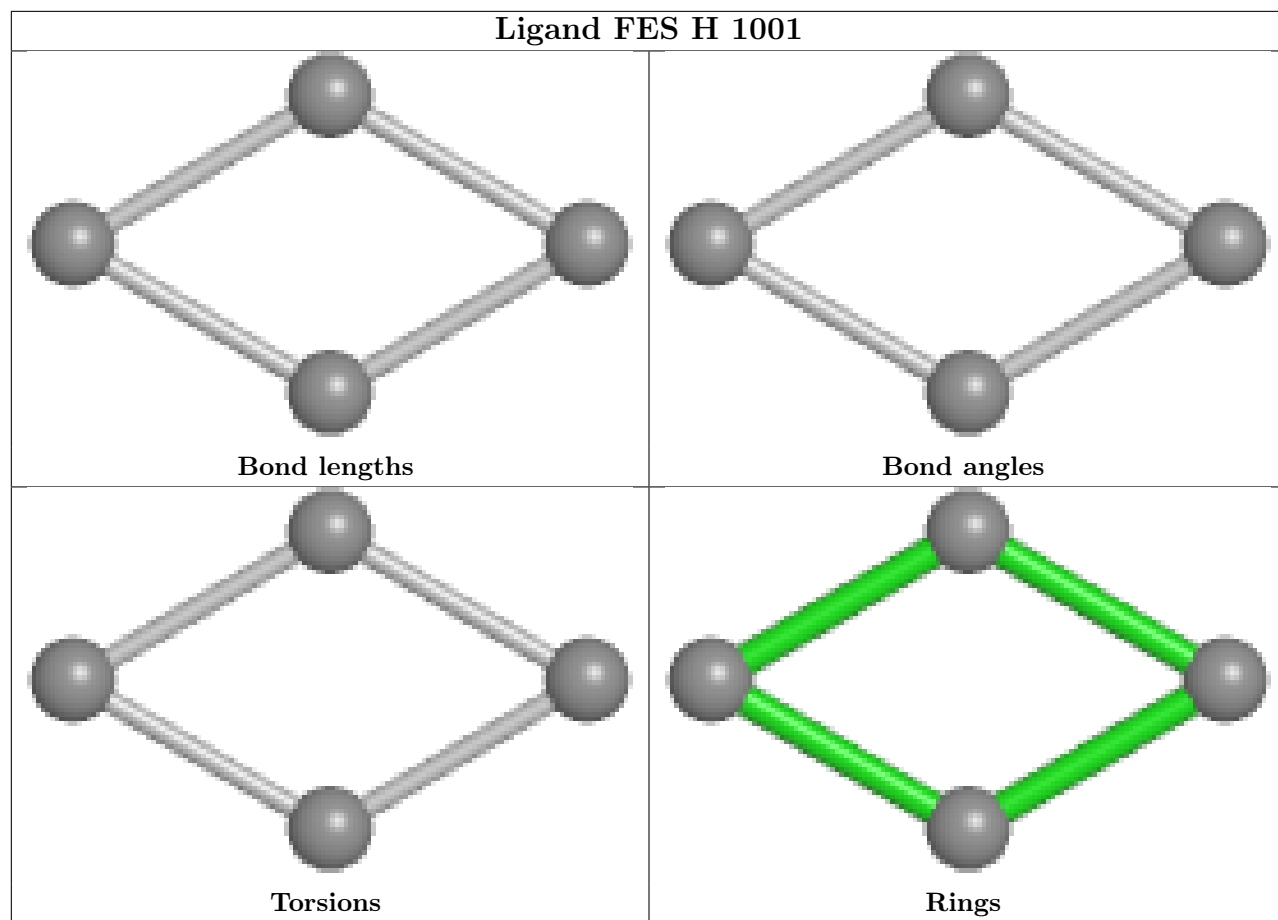


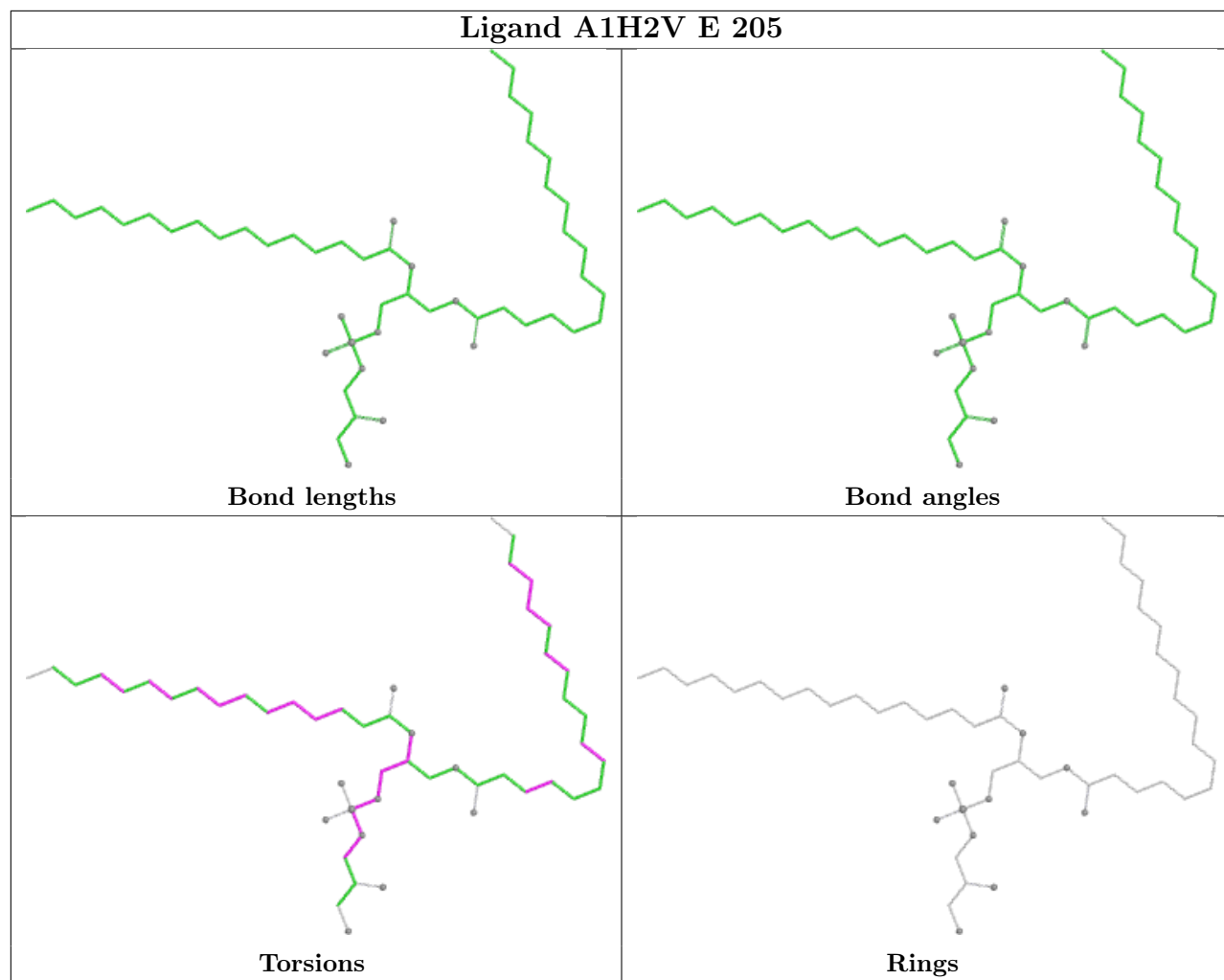


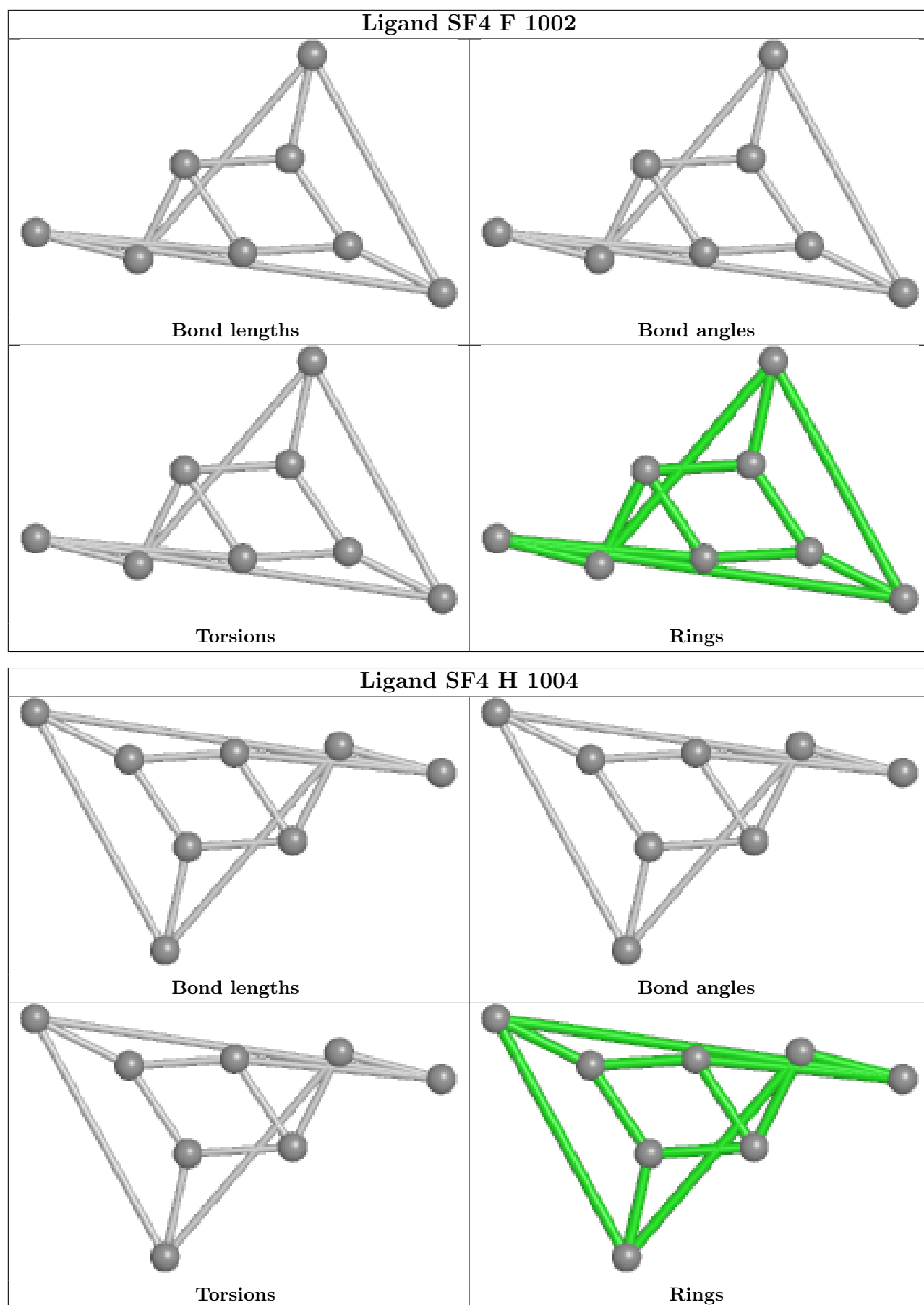


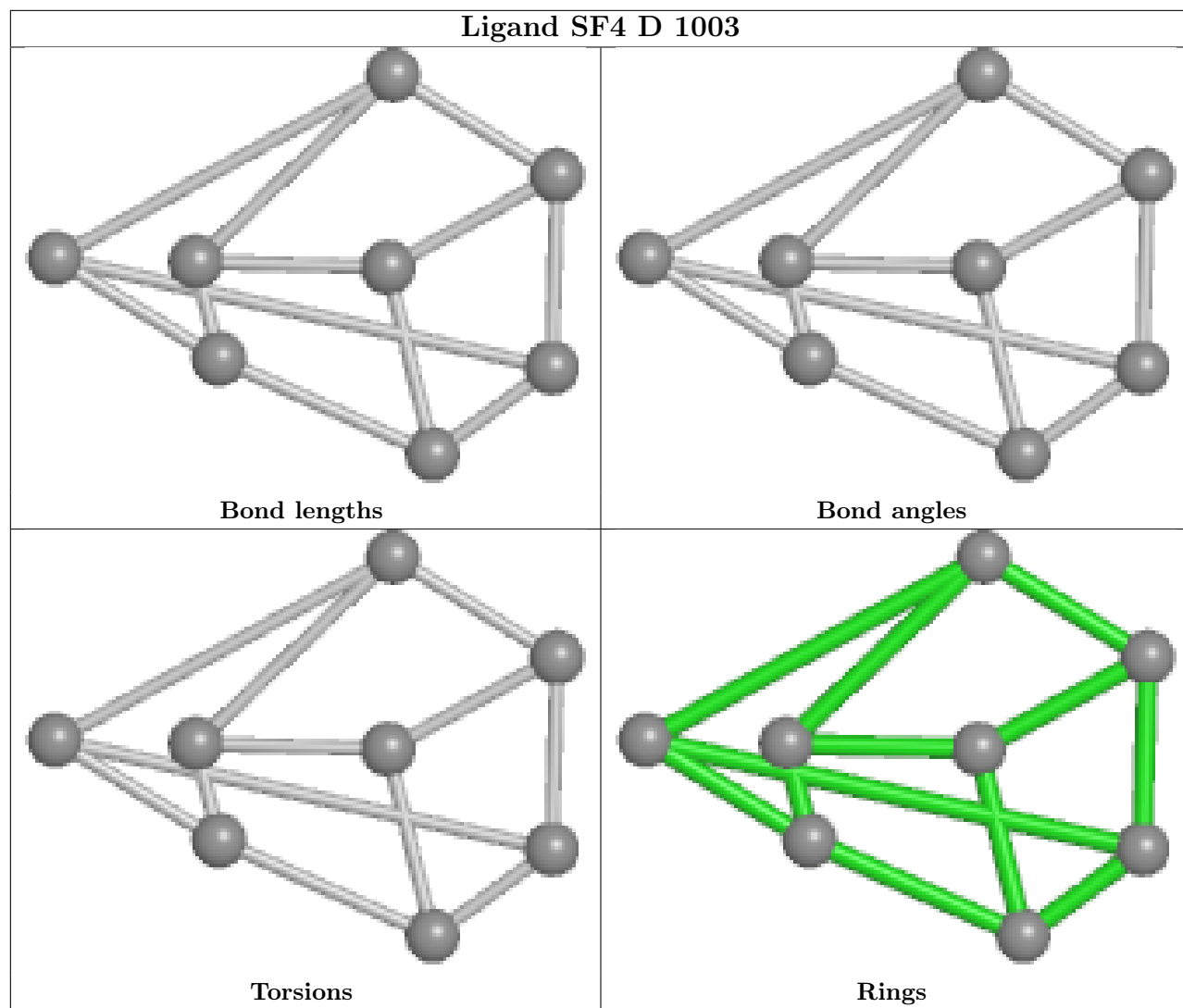


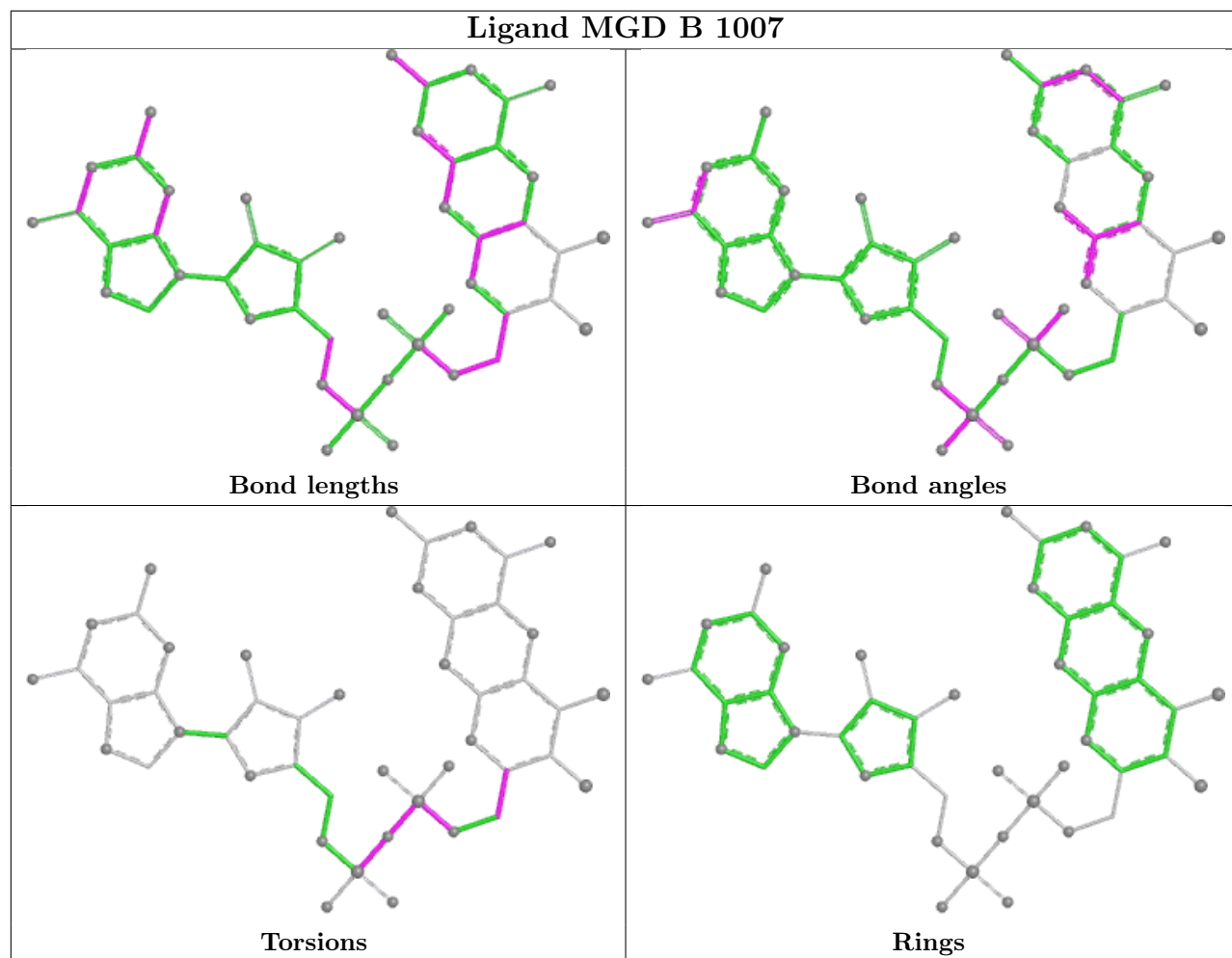


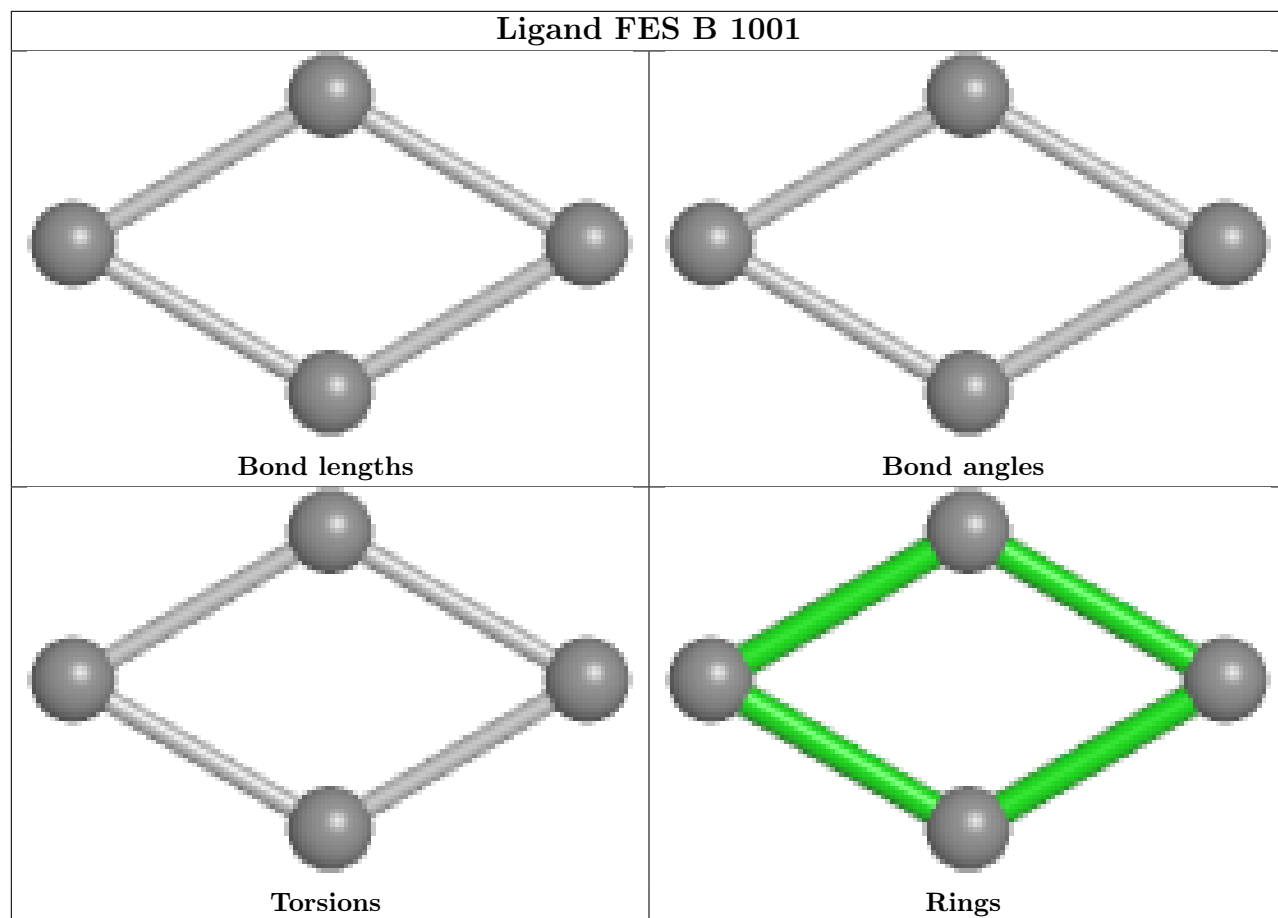


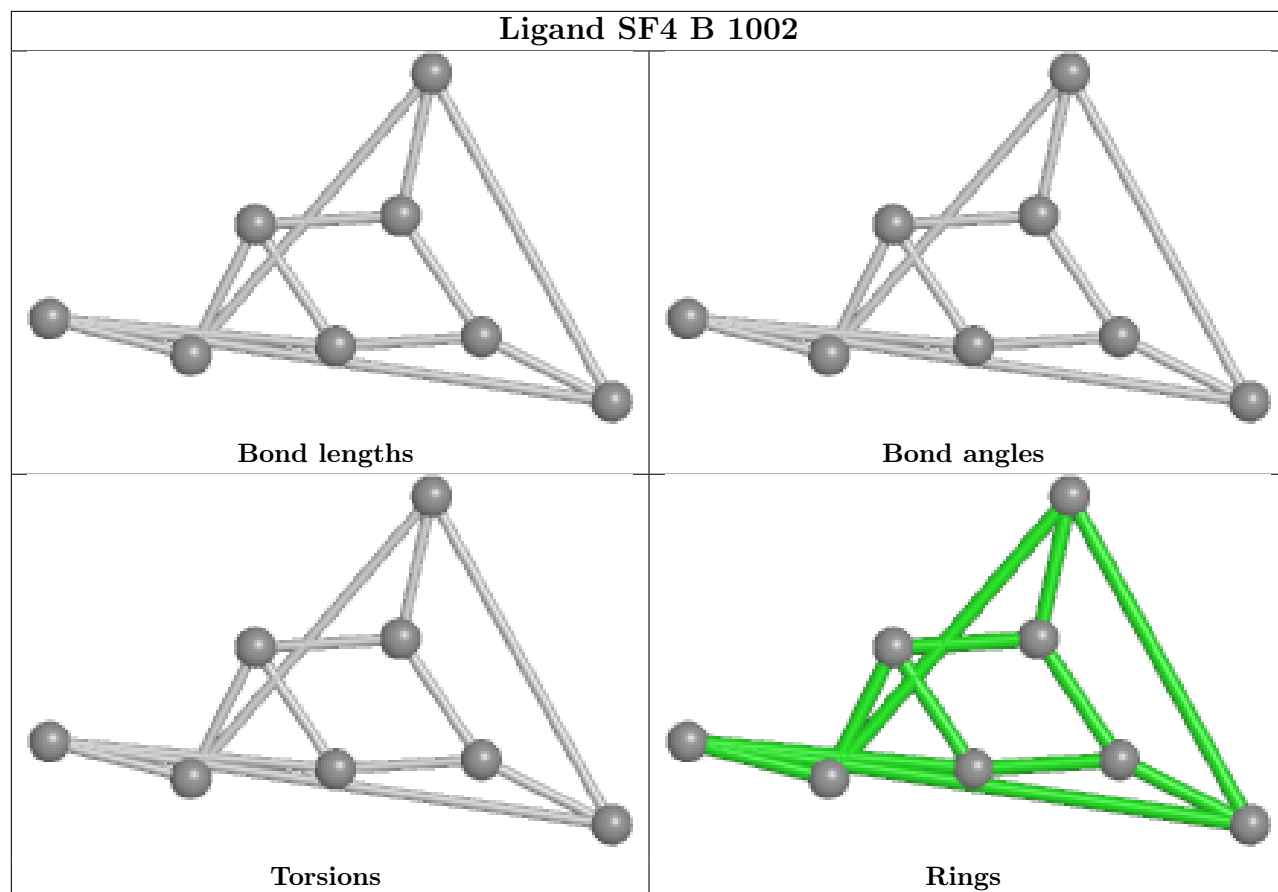


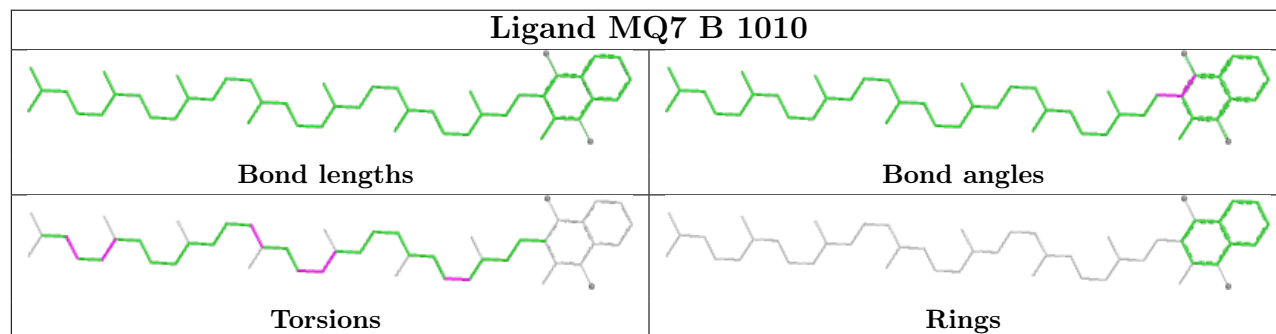
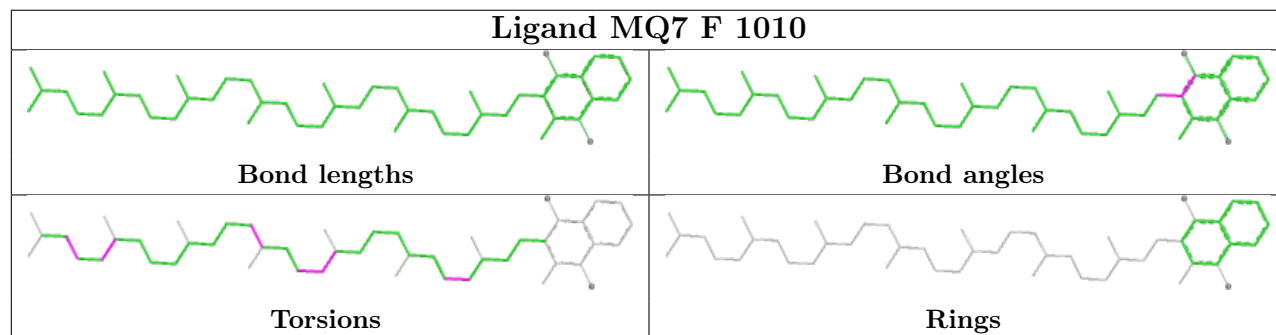
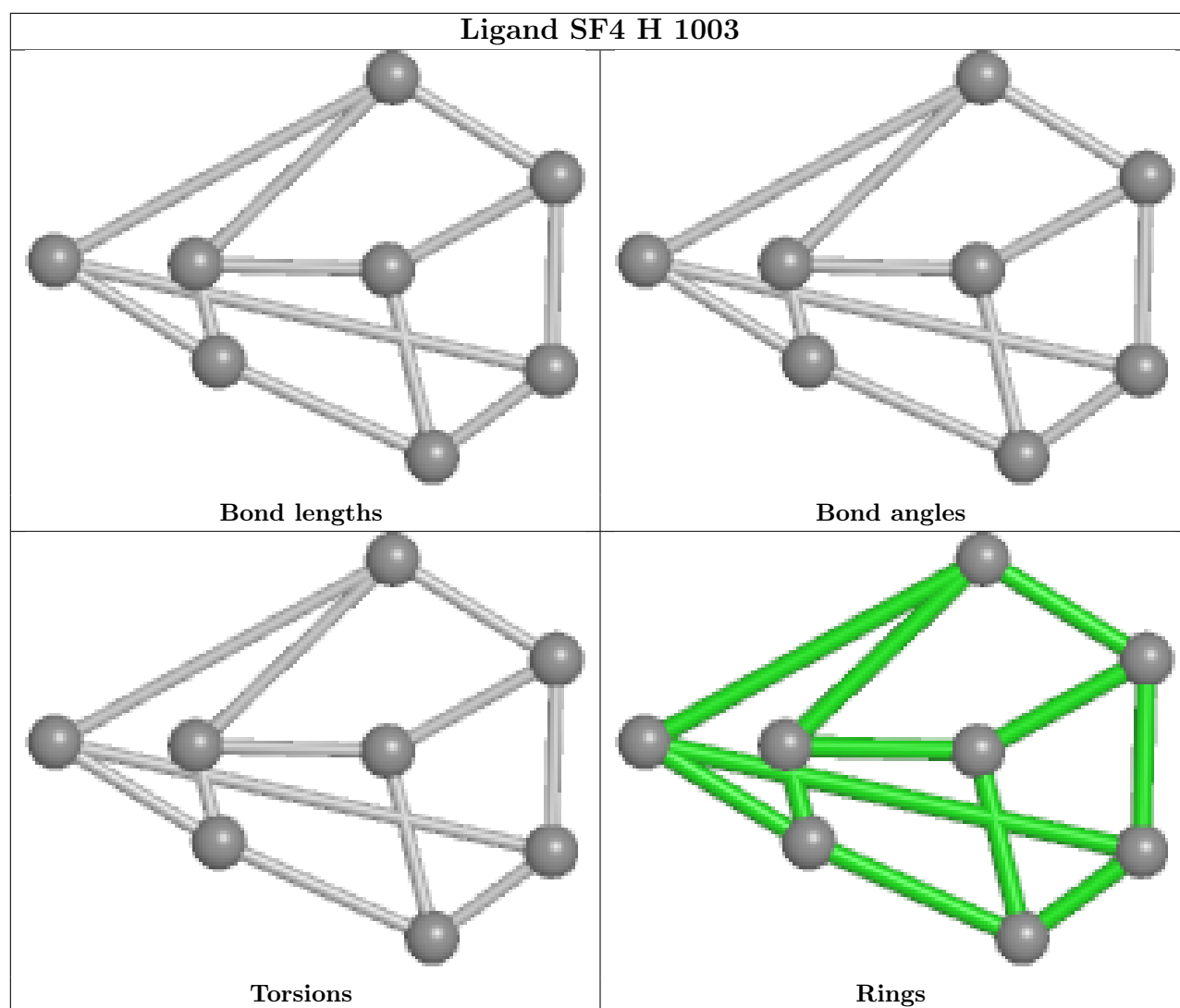


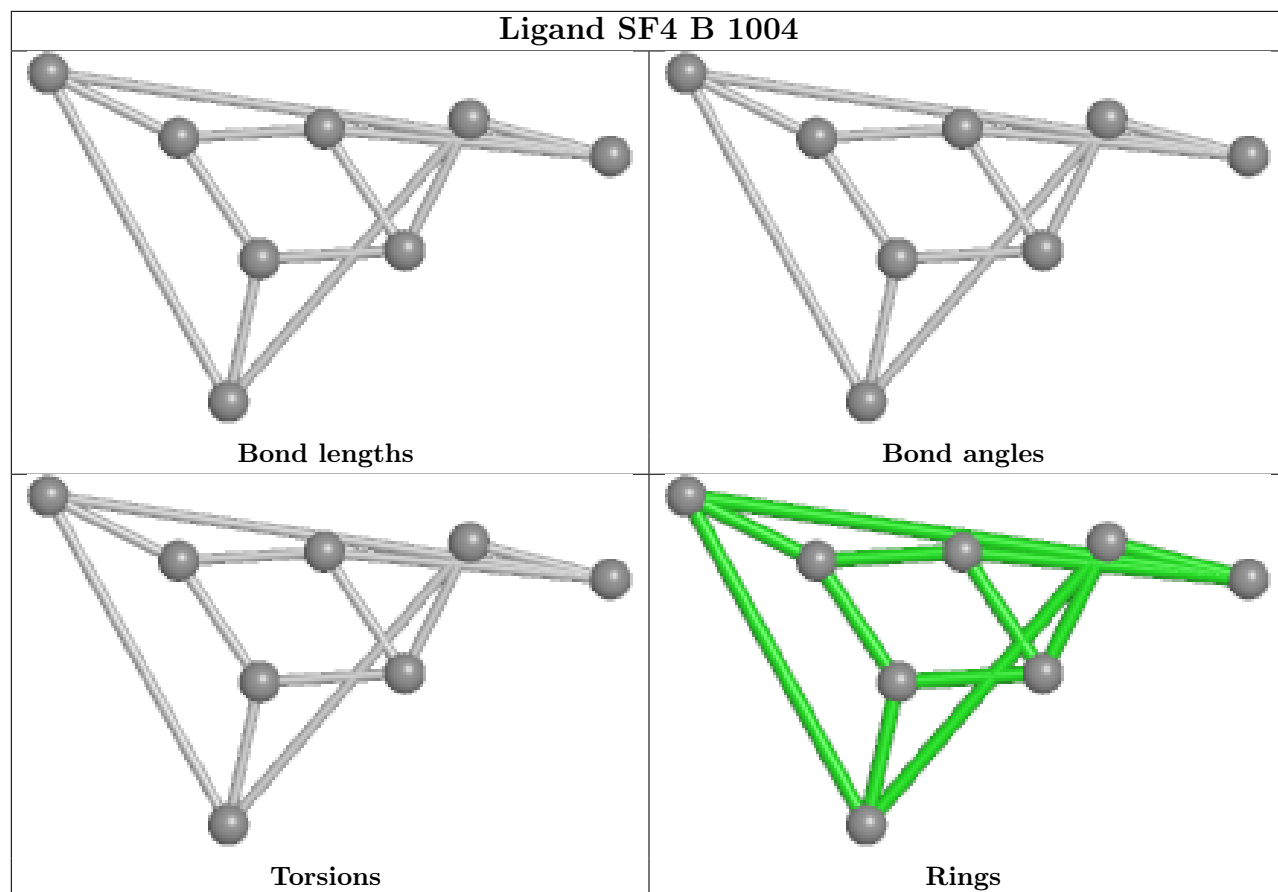


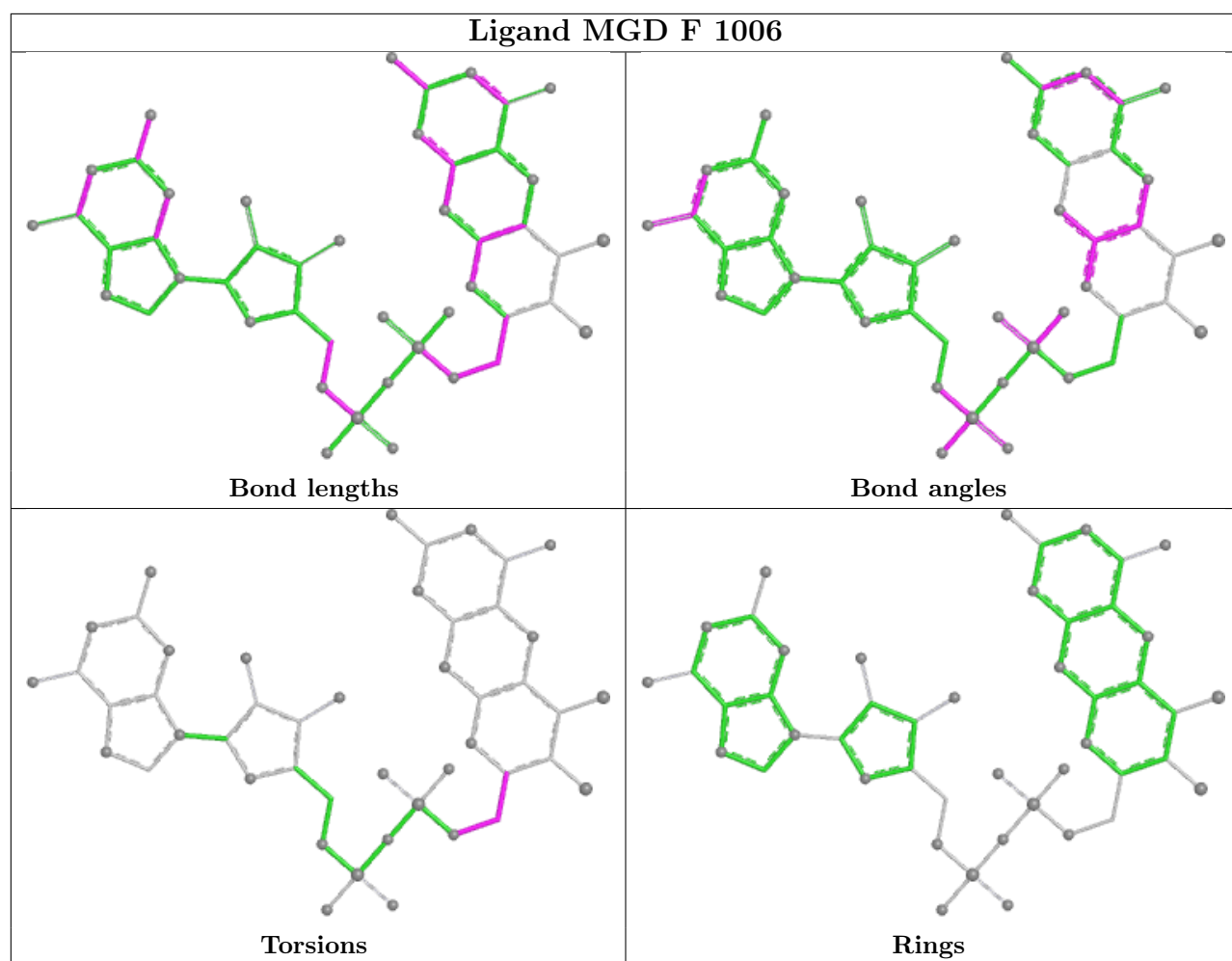


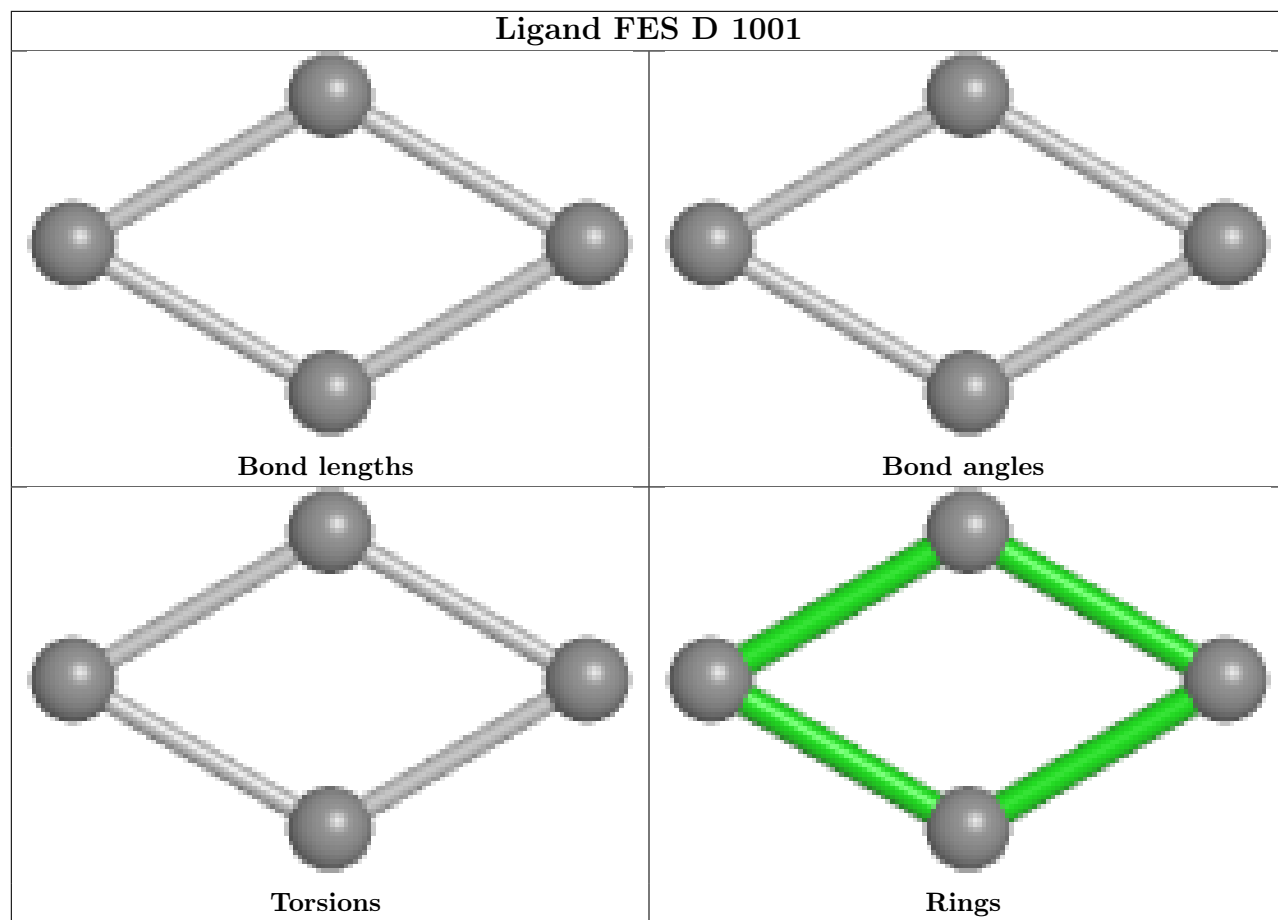


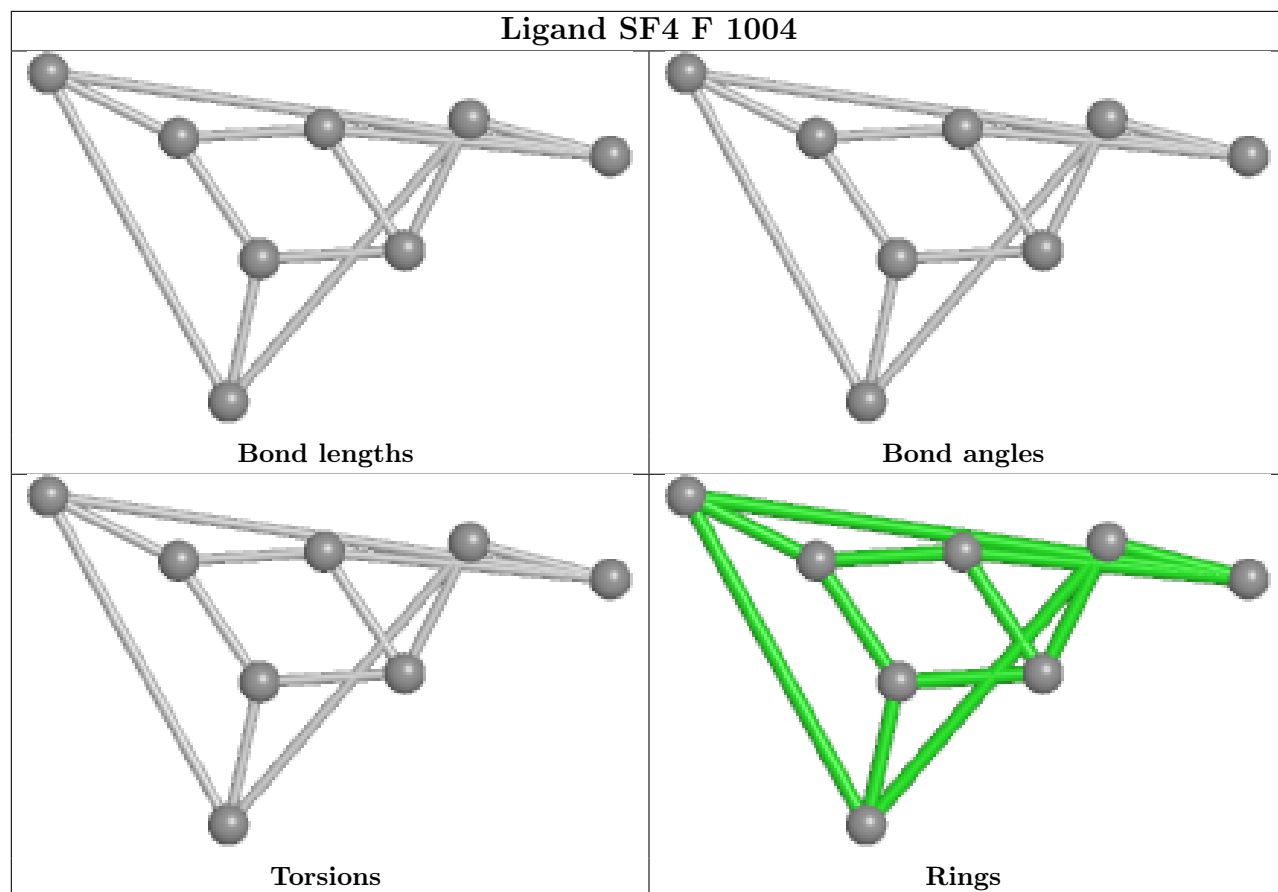


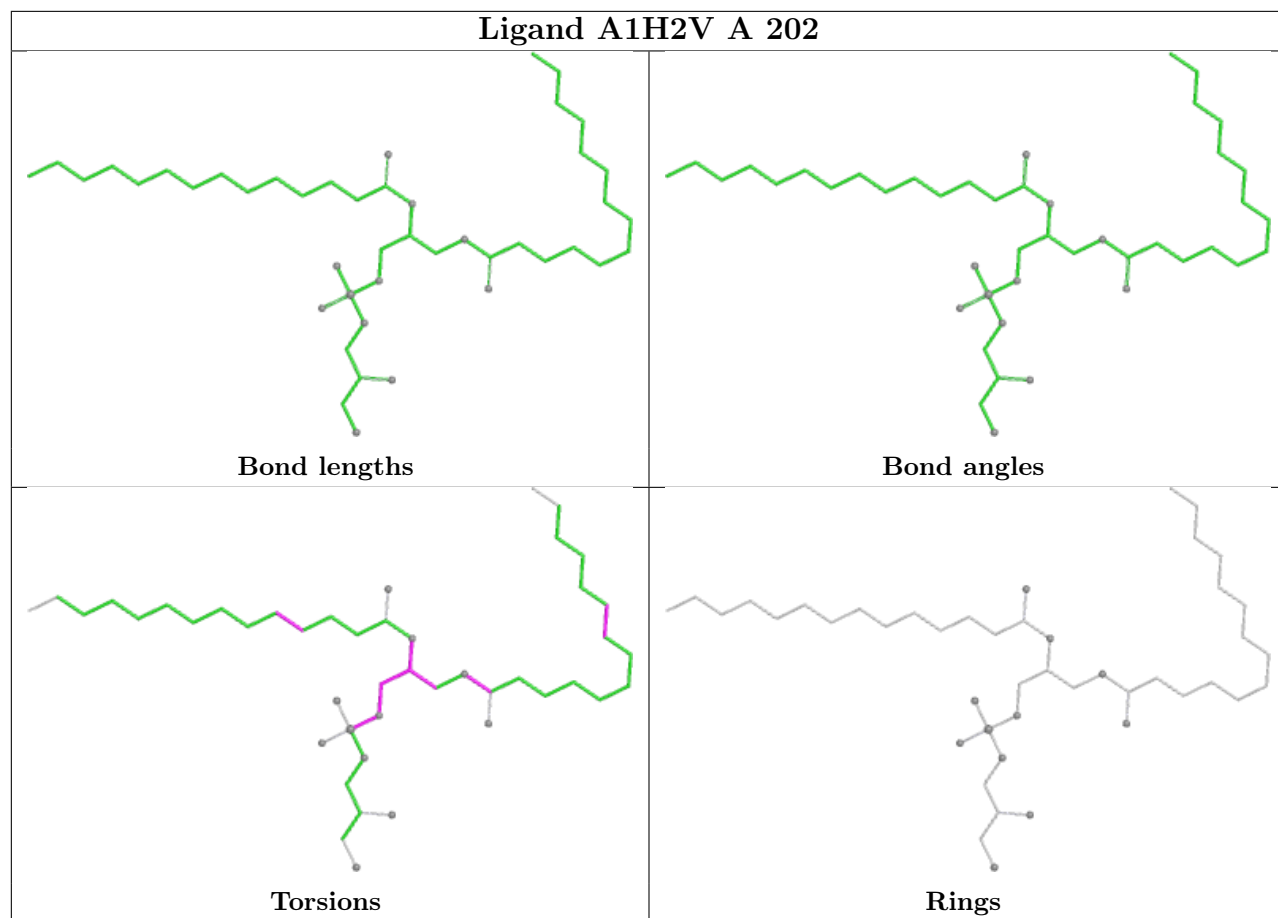


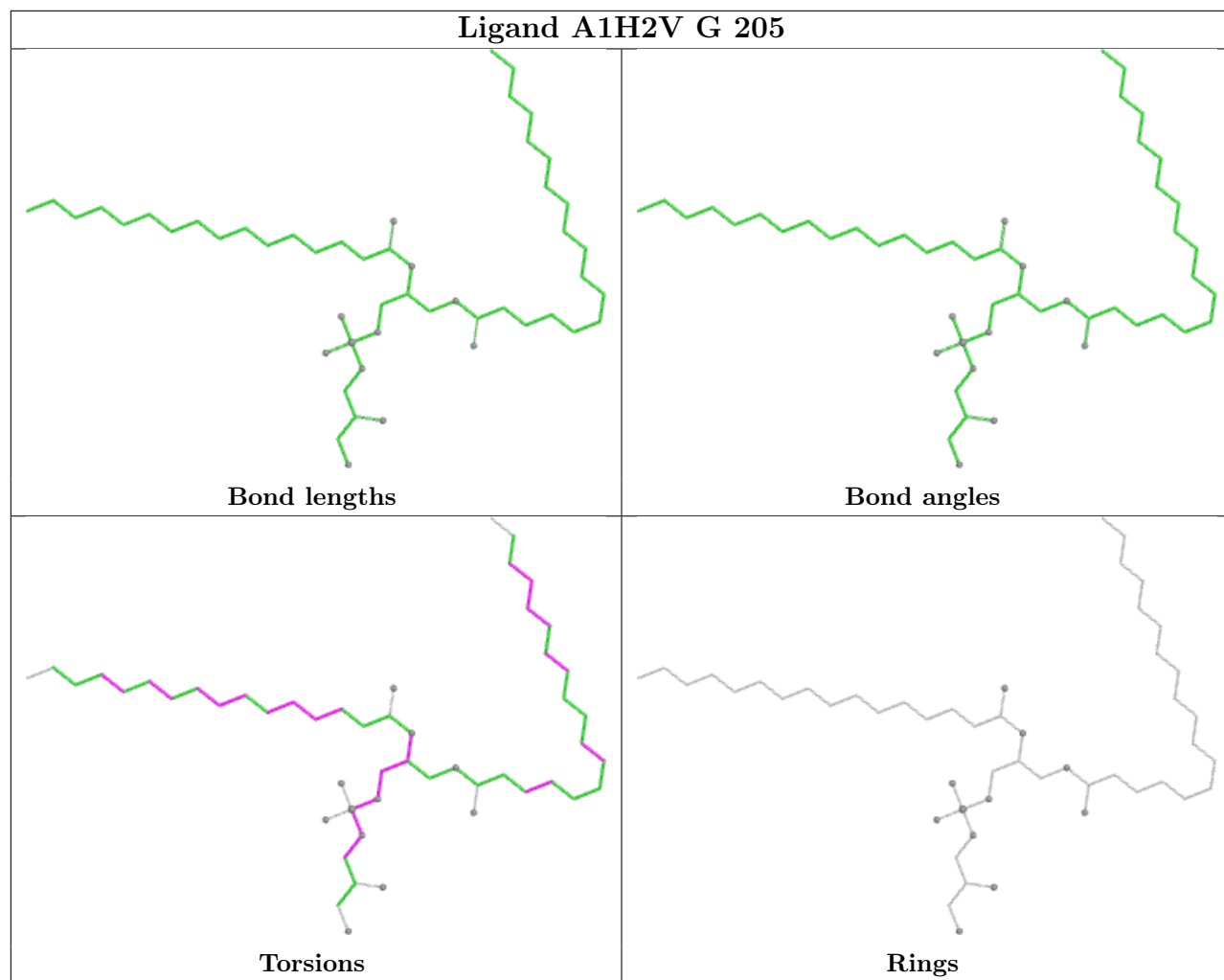


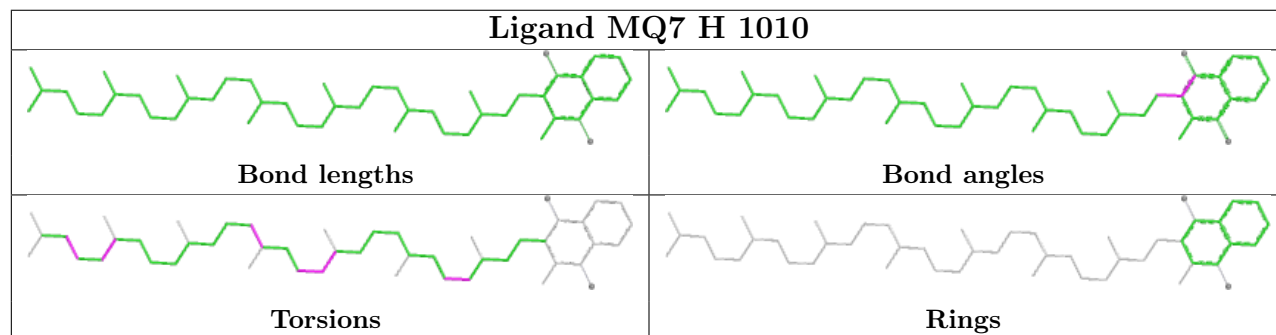
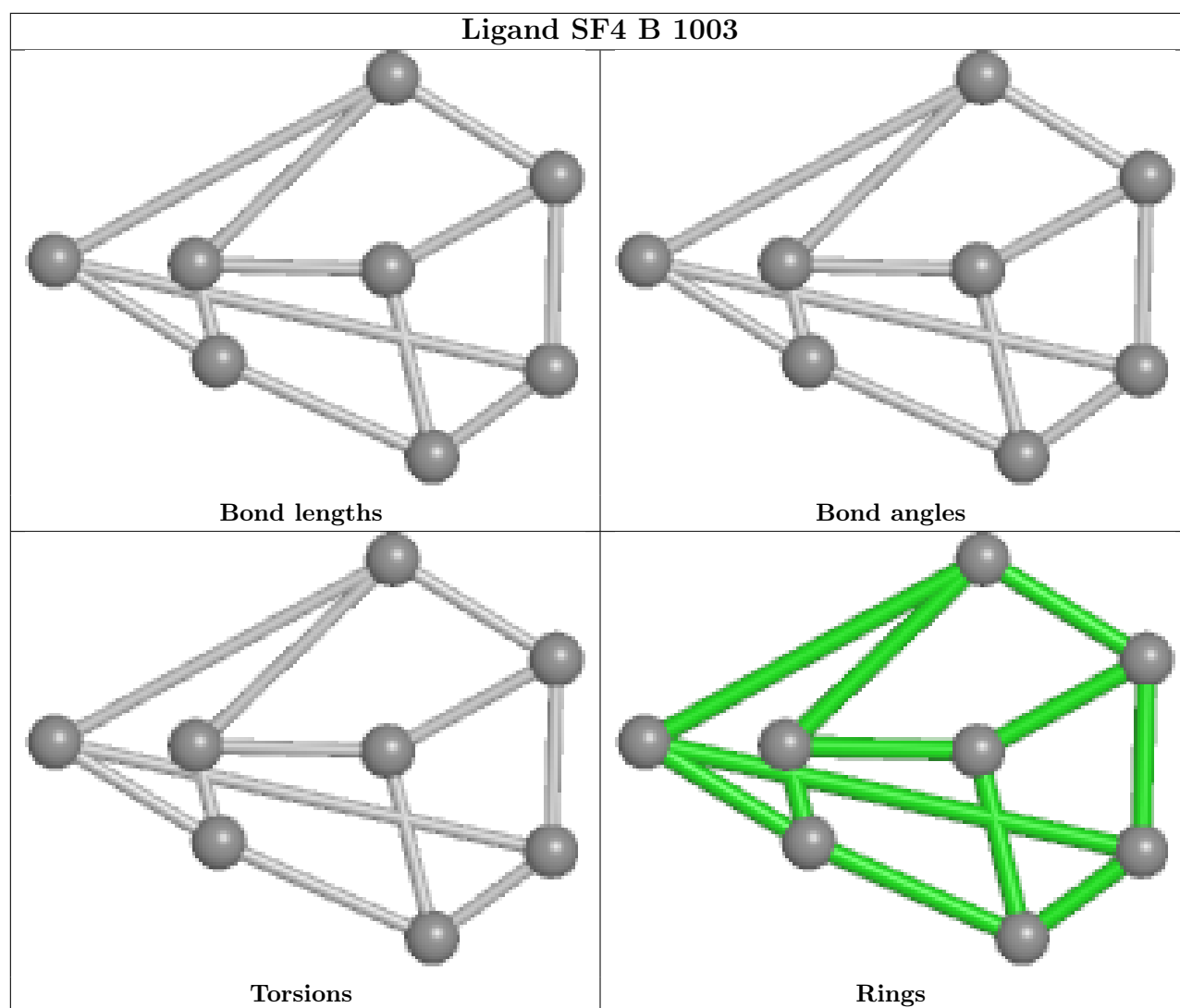


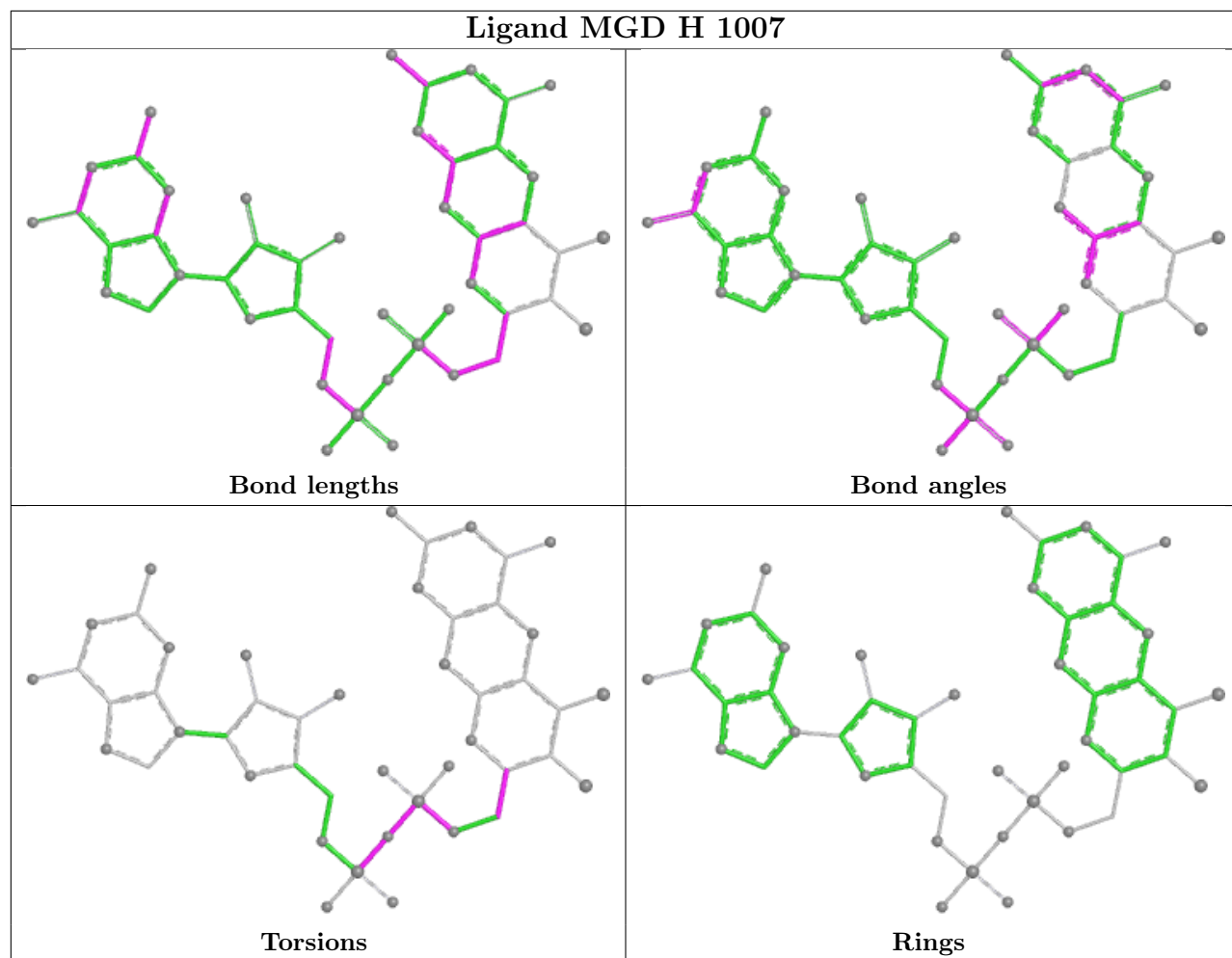


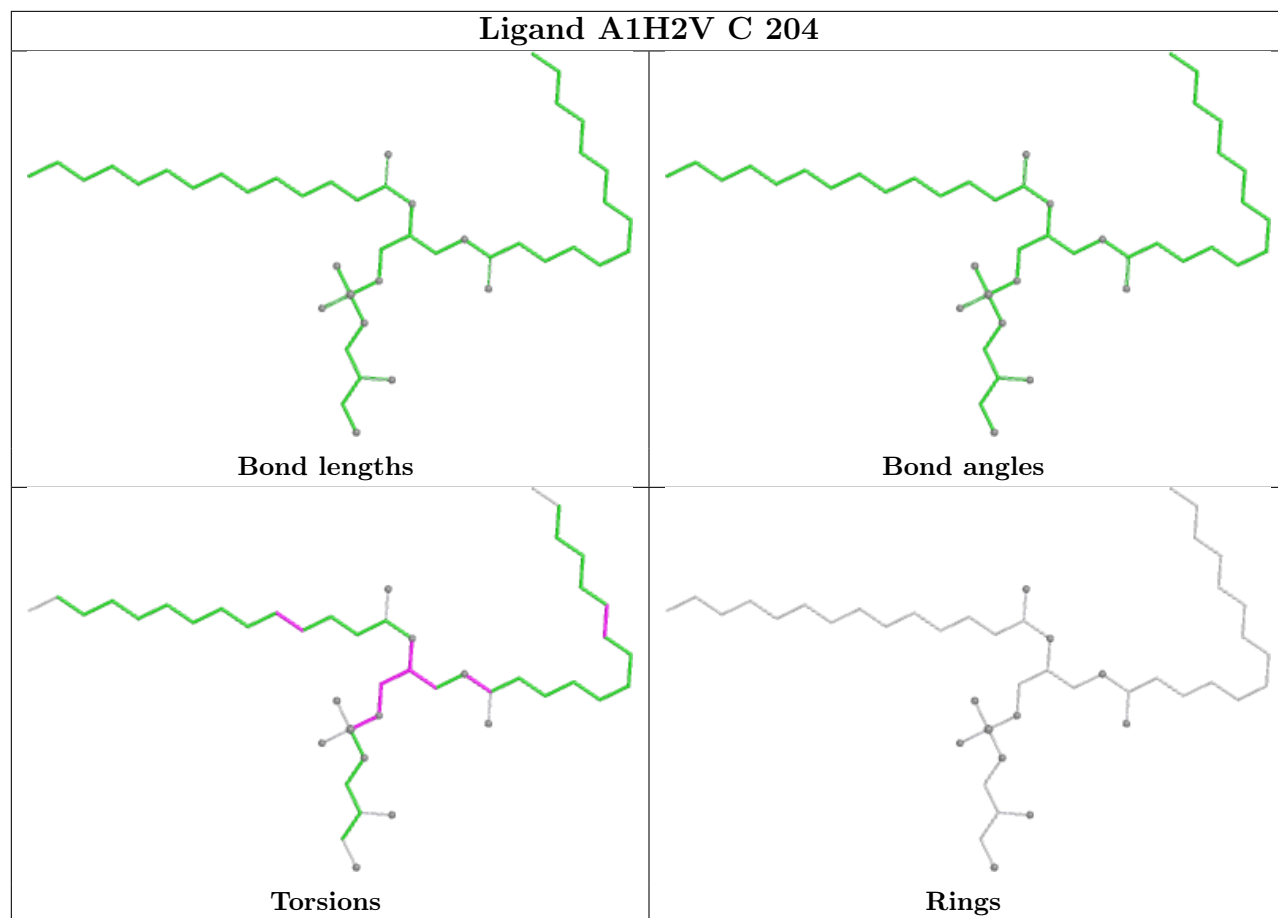


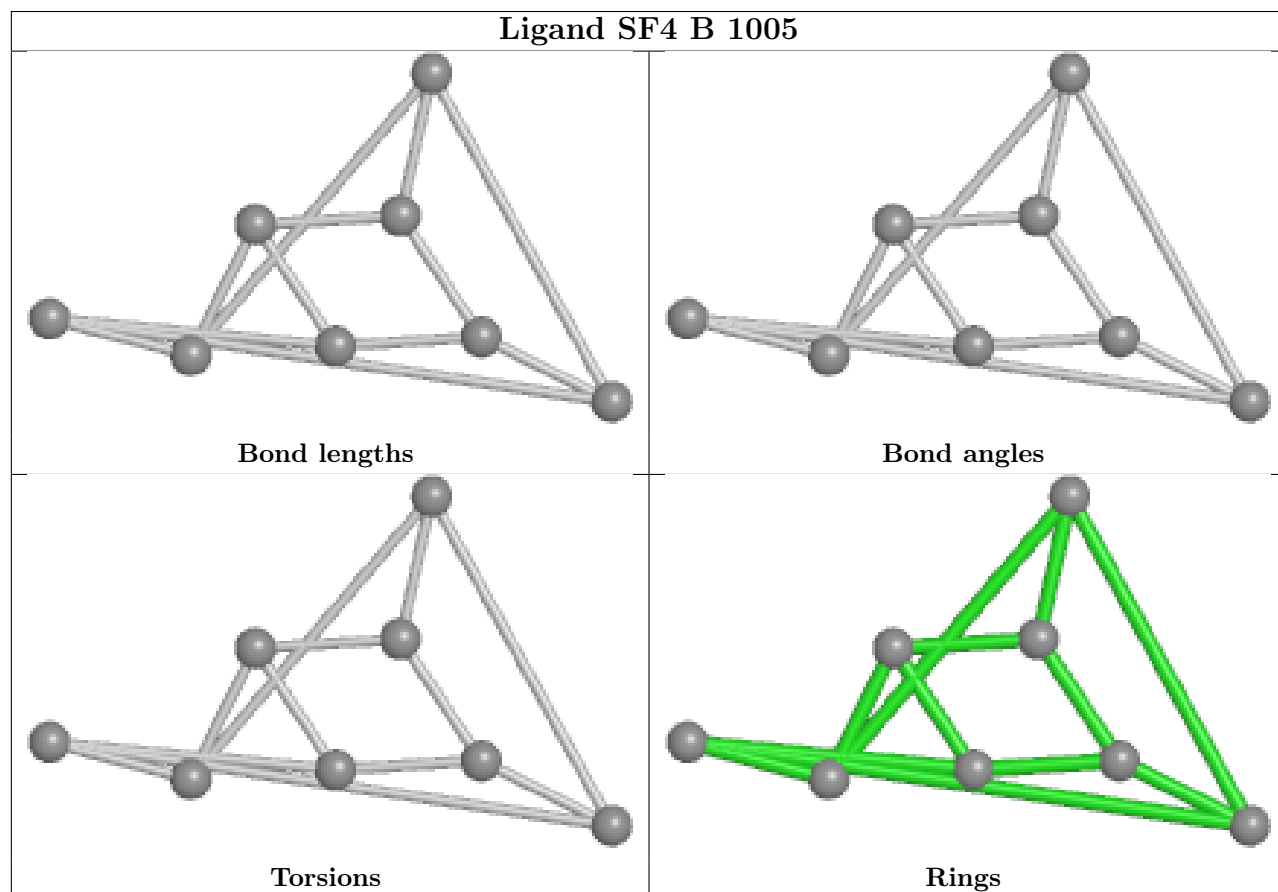
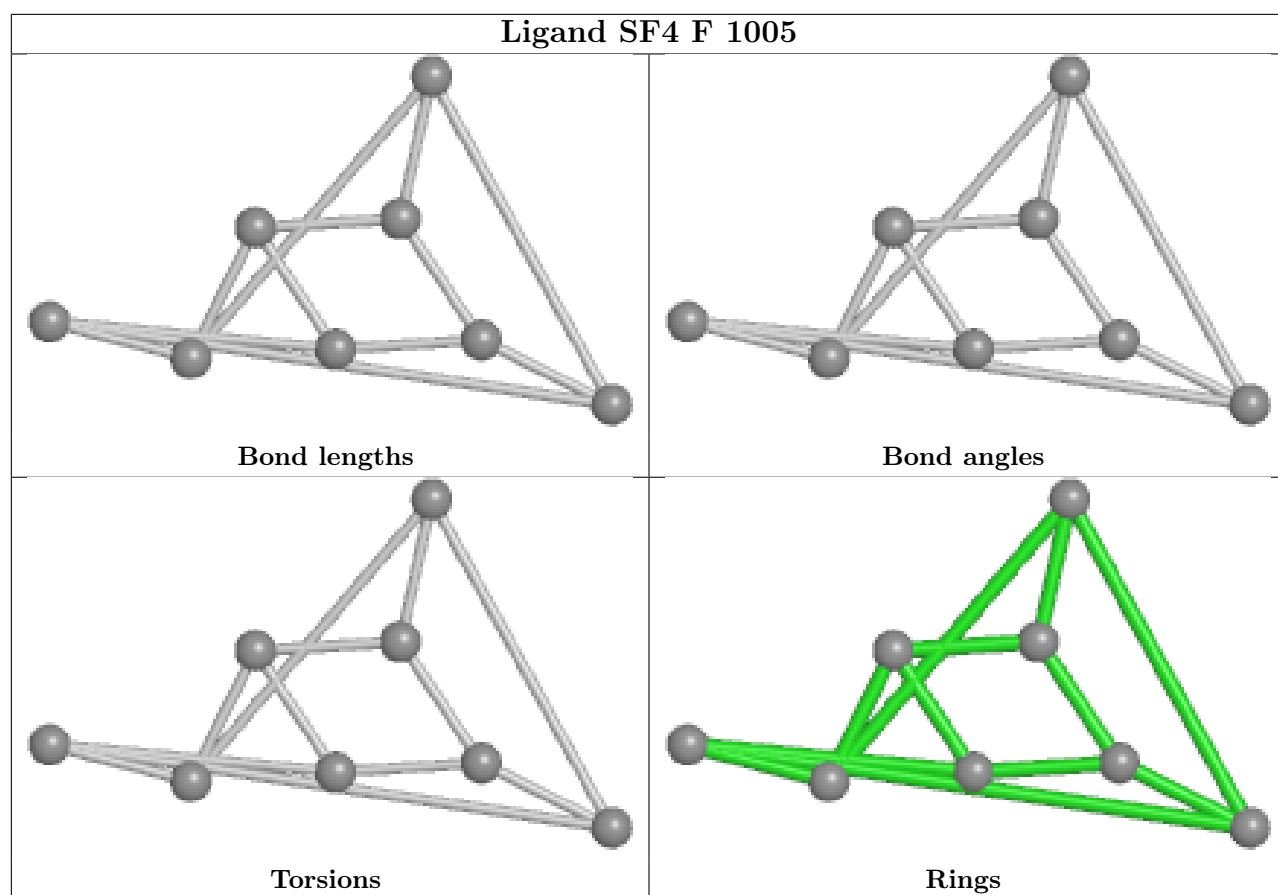




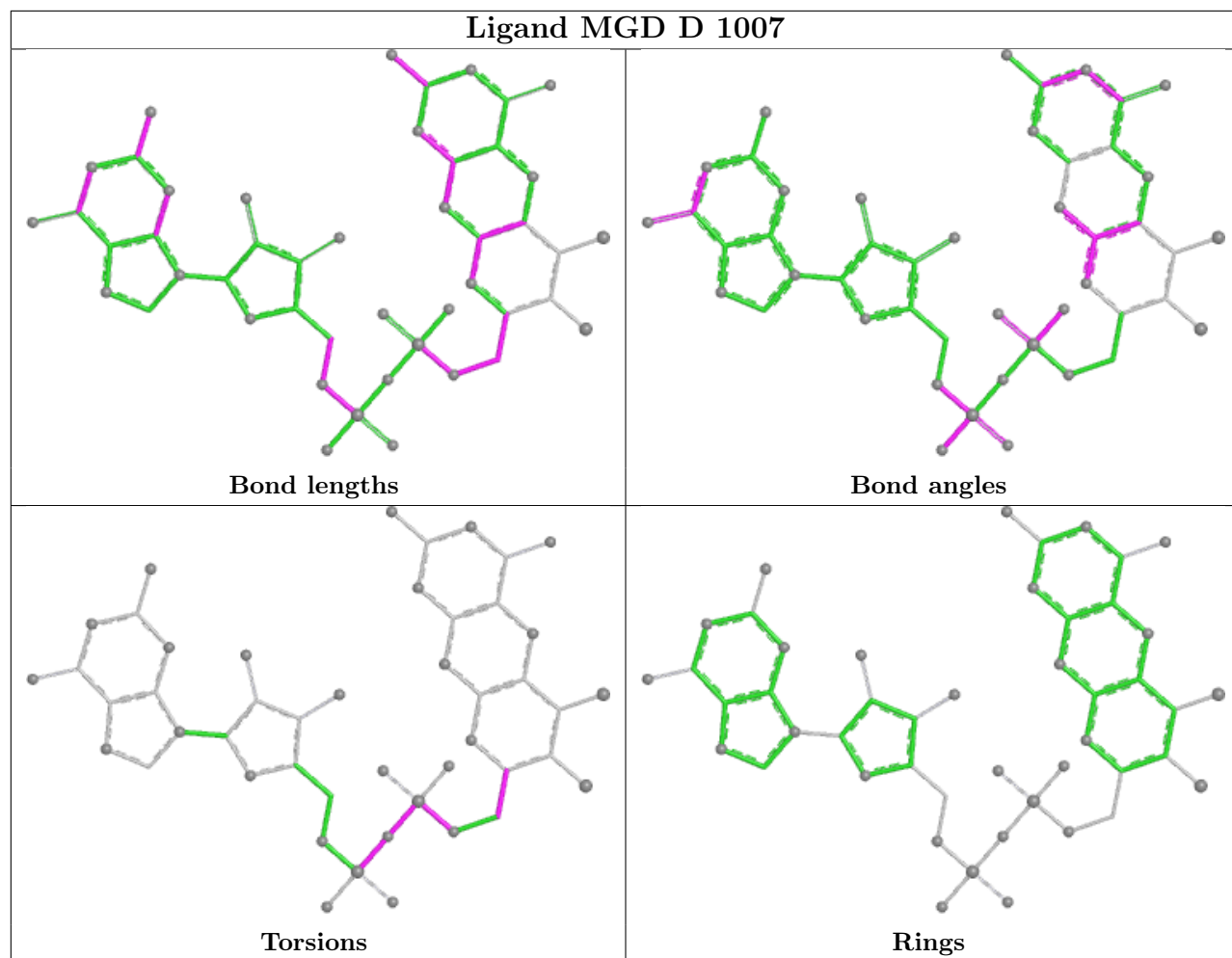


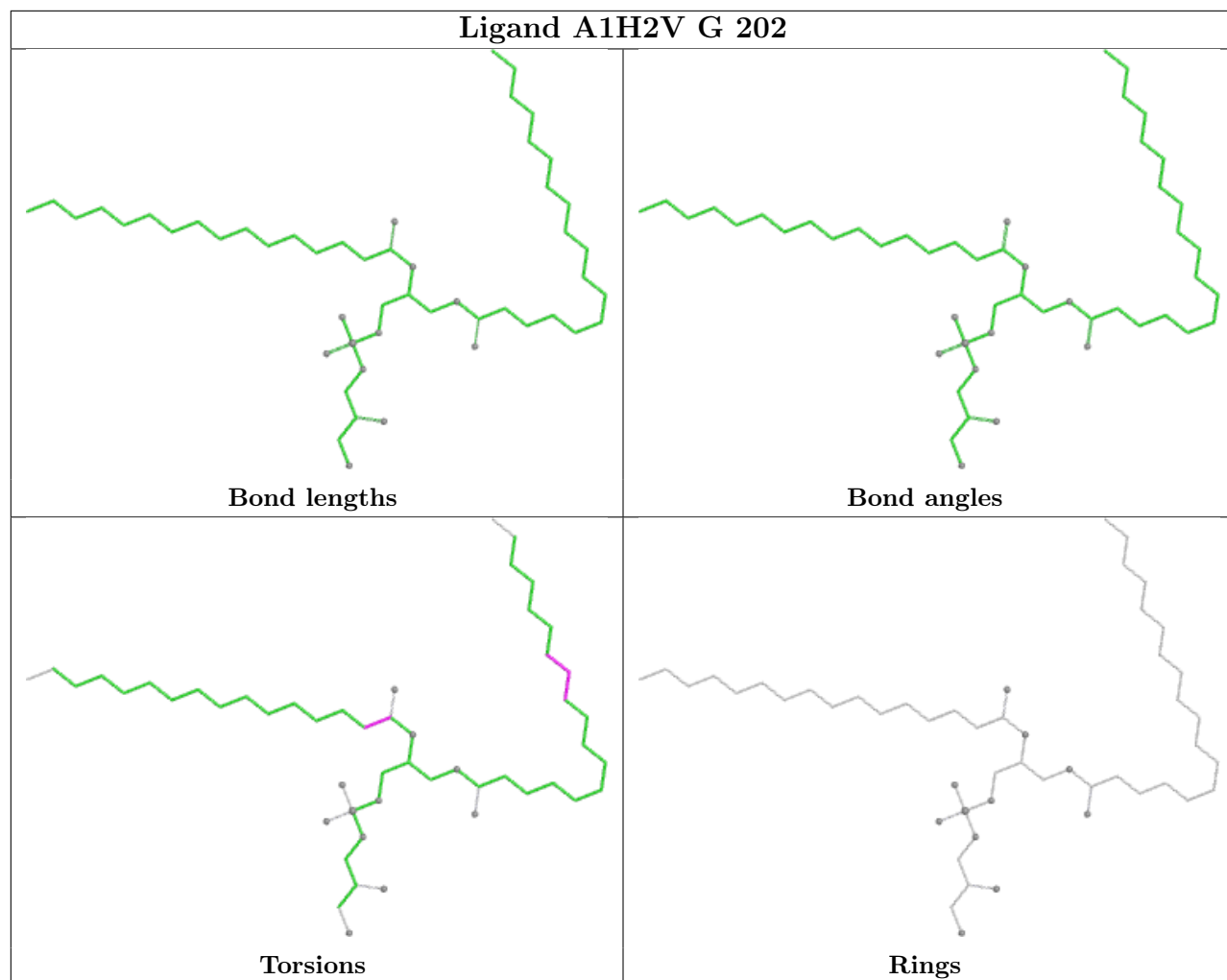


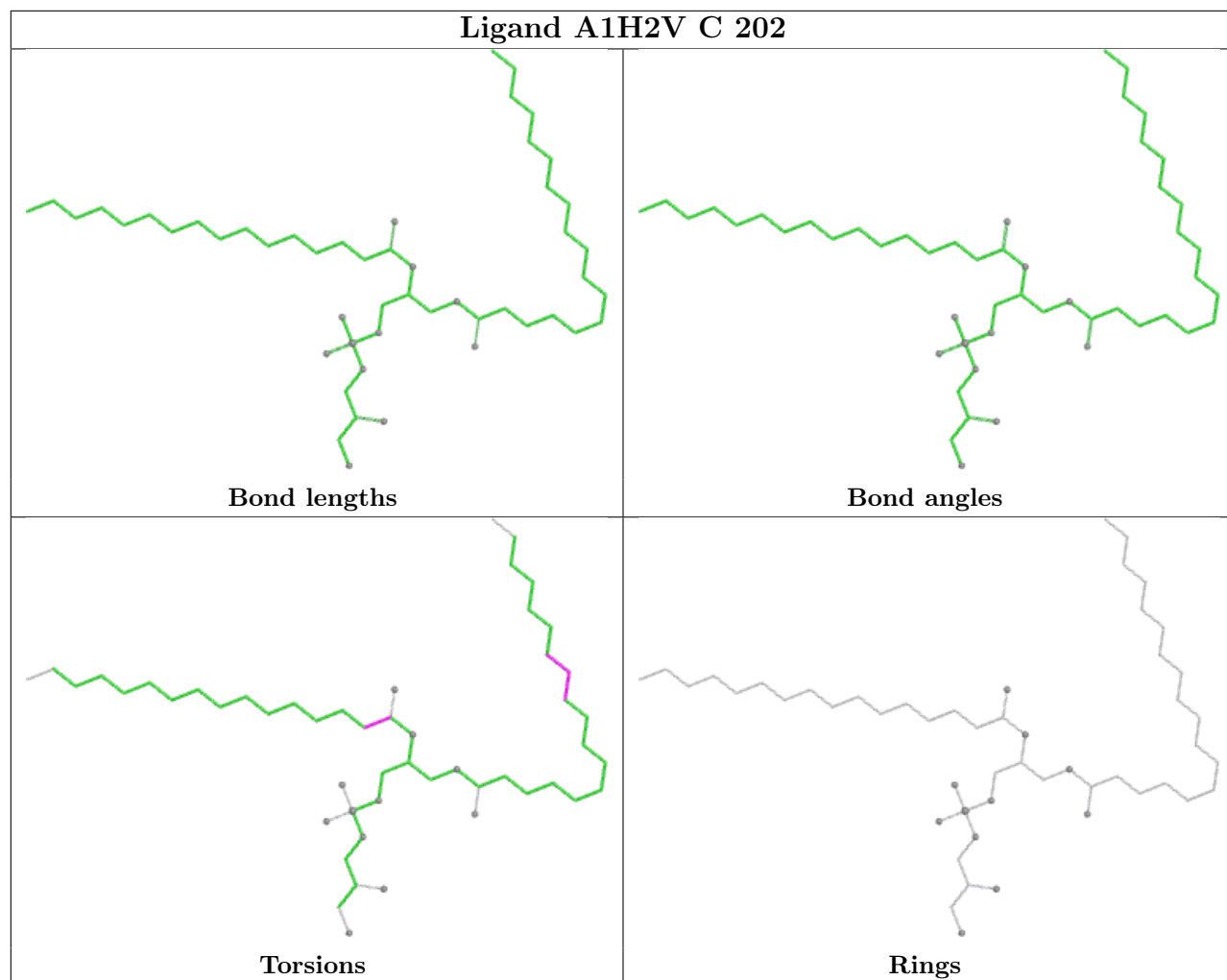


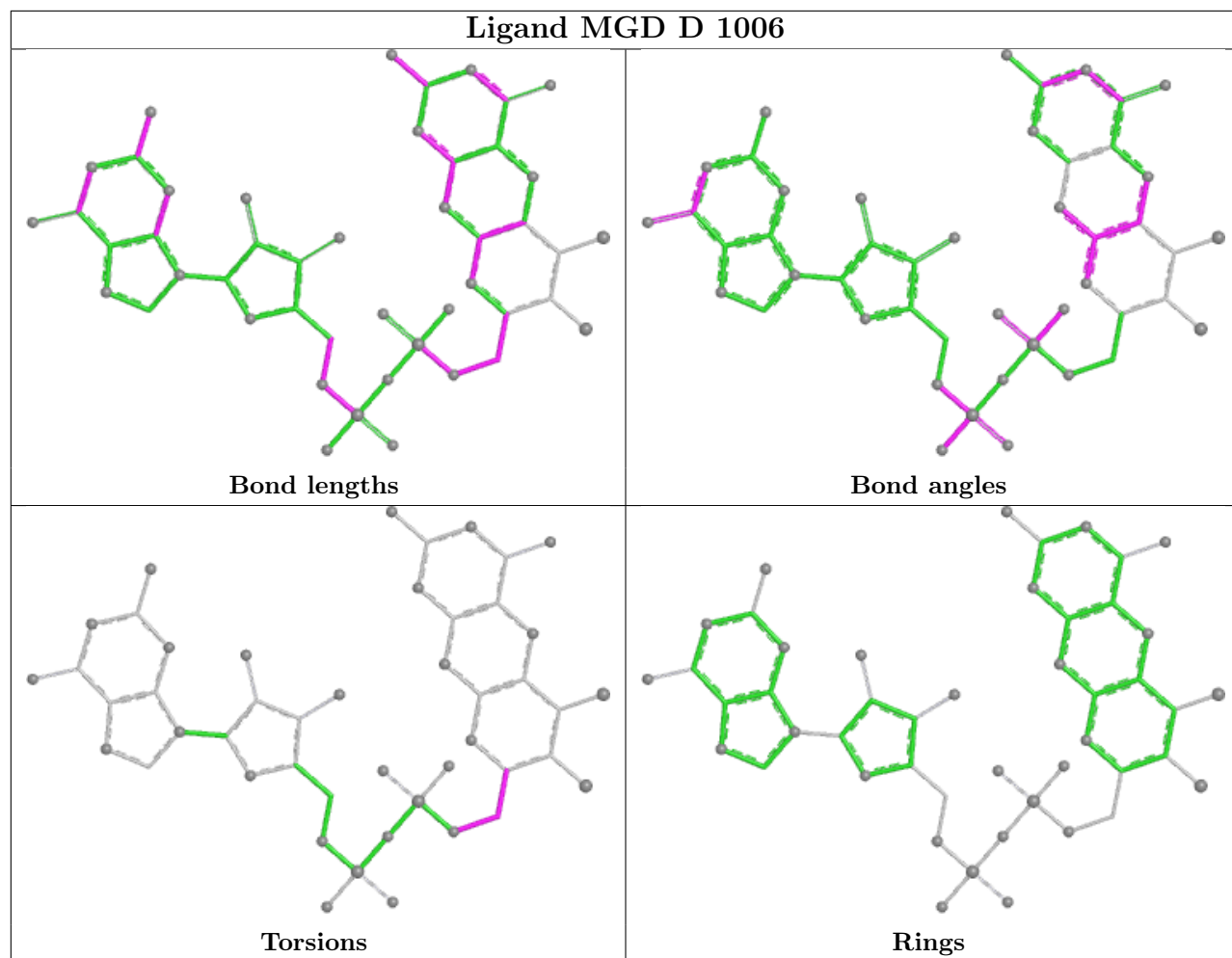


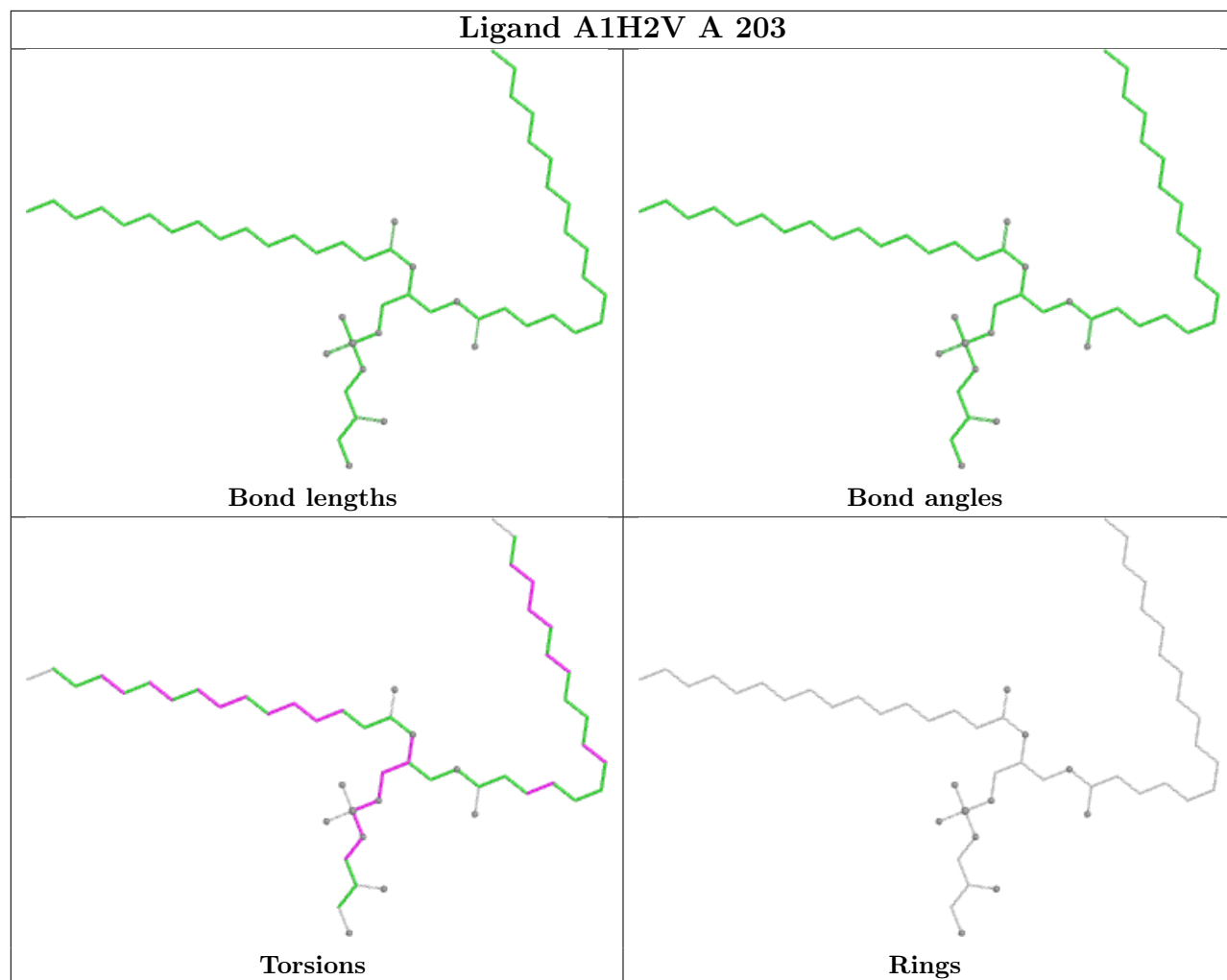
Ligand MGD D 1007

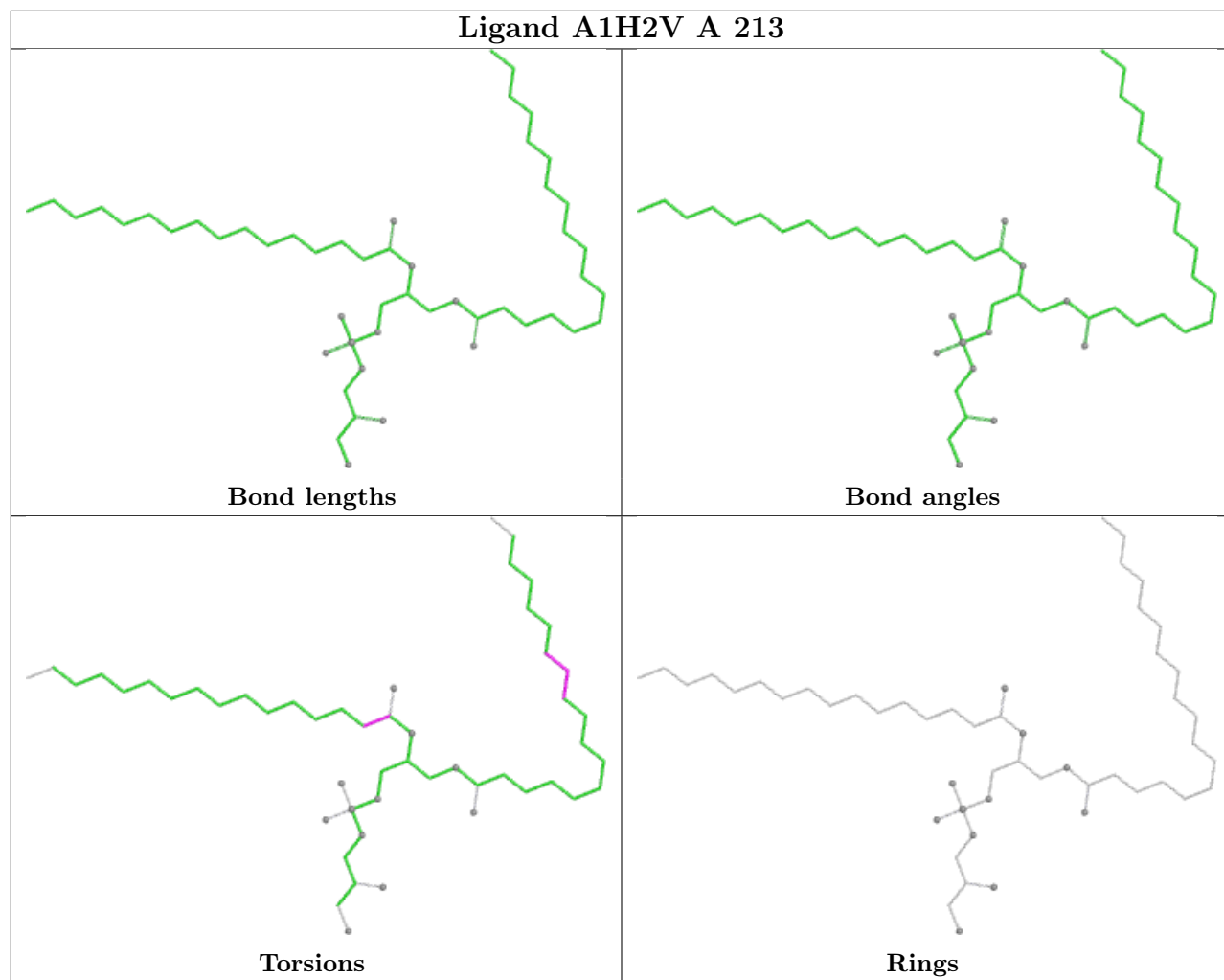


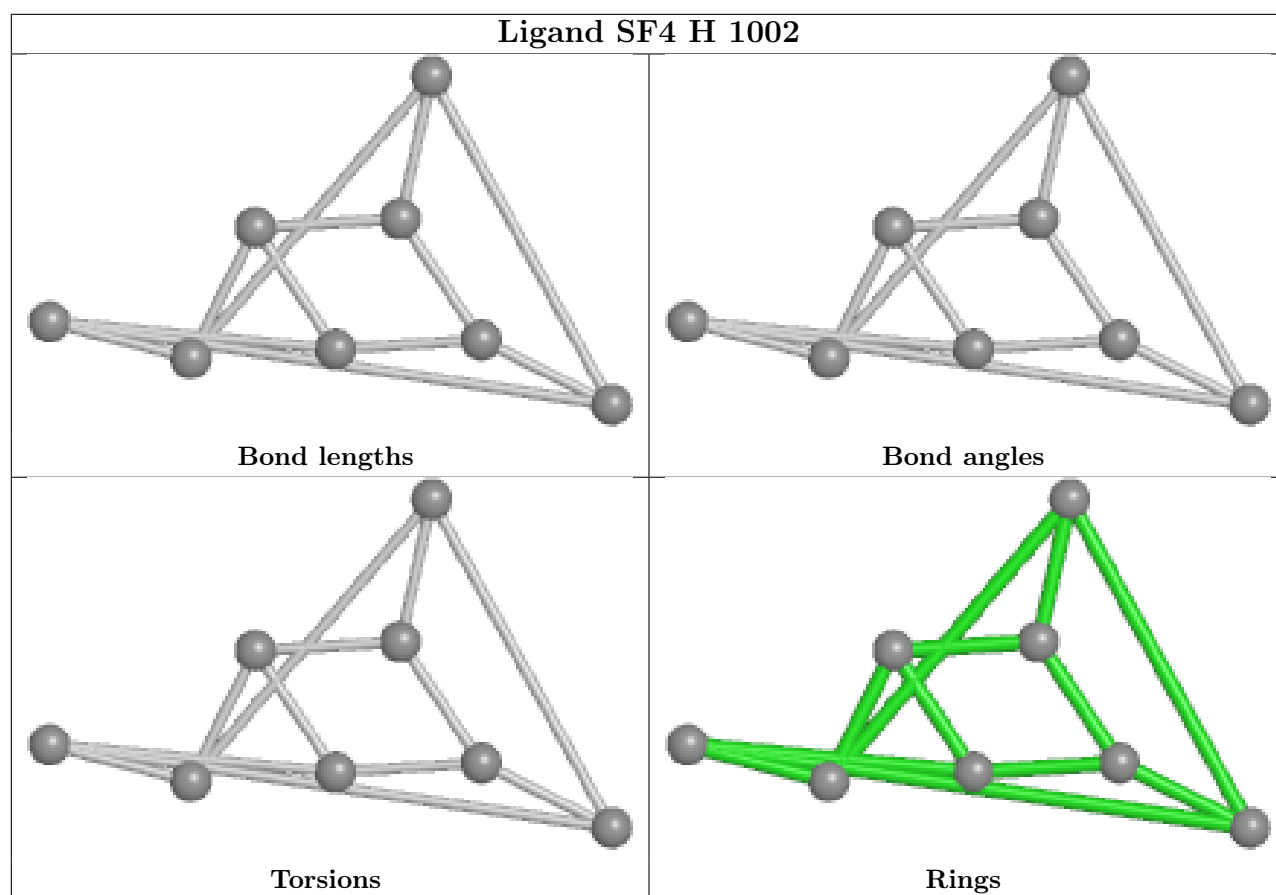












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

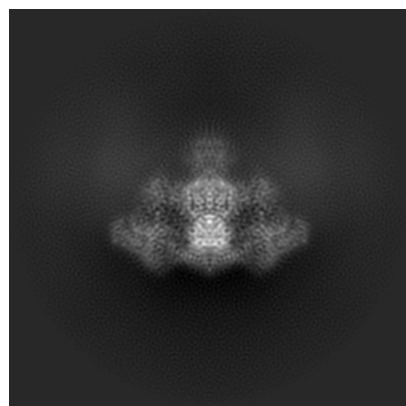
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19452. These allow visual inspection of the internal detail of the map and identification of artifacts.

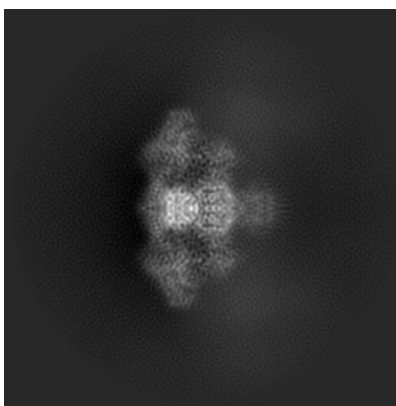
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

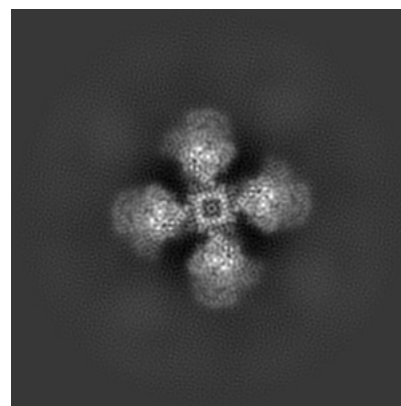
6.1.1 Primary map



X

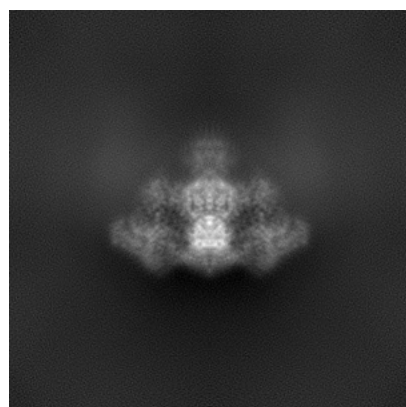


Y

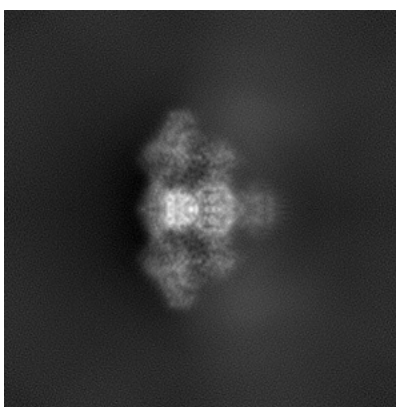


Z

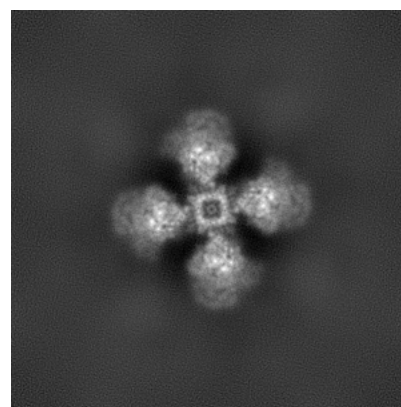
6.1.2 Raw map



X



Y

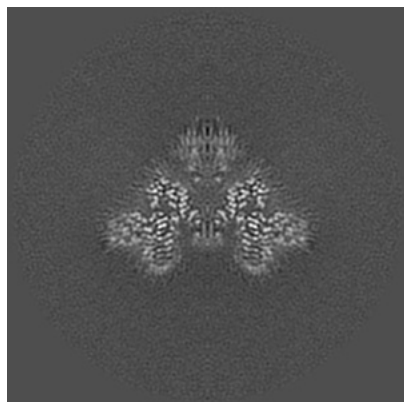


Z

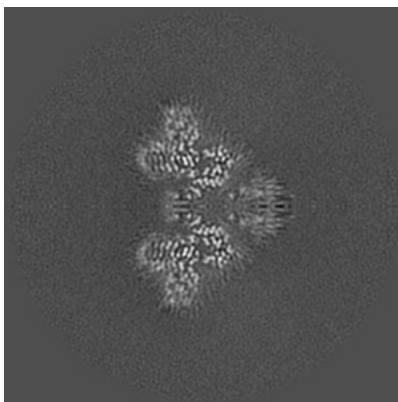
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

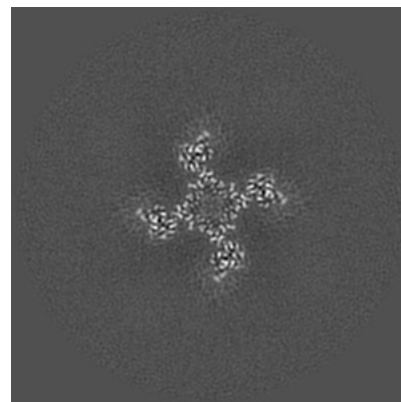
6.2.1 Primary map



X Index: 160

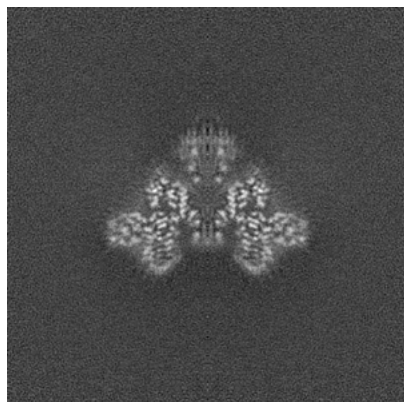


Y Index: 160

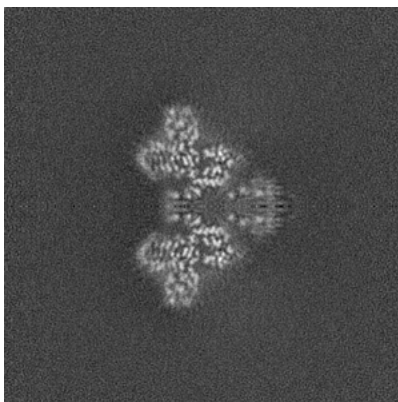


Z Index: 160

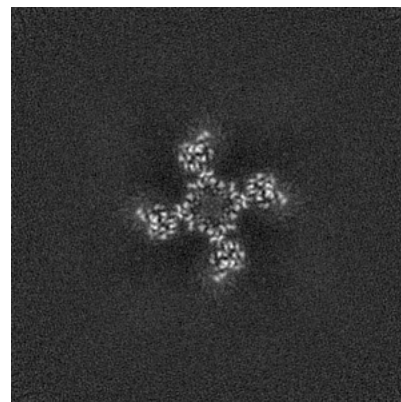
6.2.2 Raw map



X Index: 160



Y Index: 160

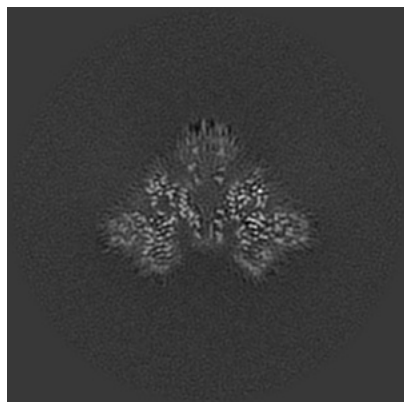


Z Index: 160

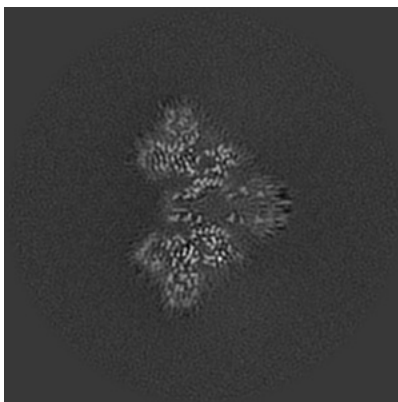
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

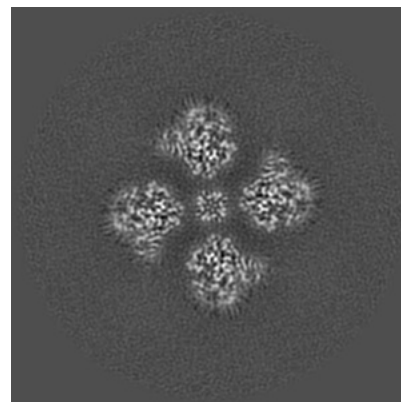
6.3.1 Primary map



X Index: 159

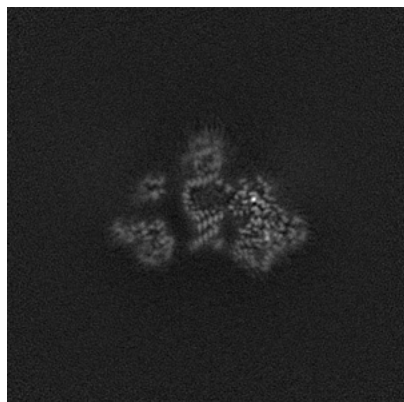


Y Index: 159

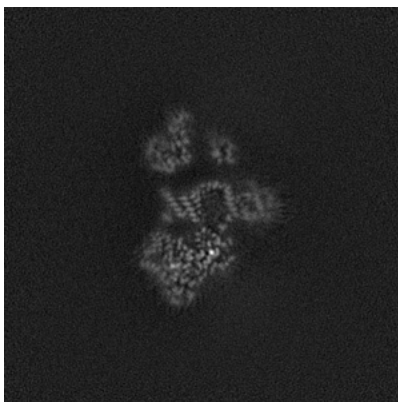


Z Index: 139

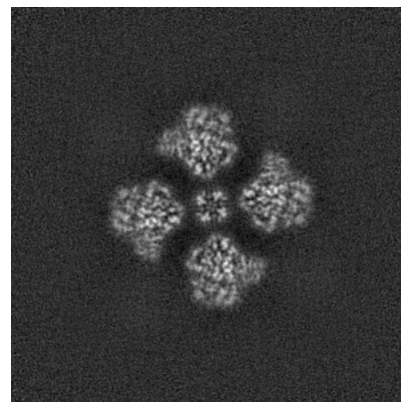
6.3.2 Raw map



X Index: 150



Y Index: 150

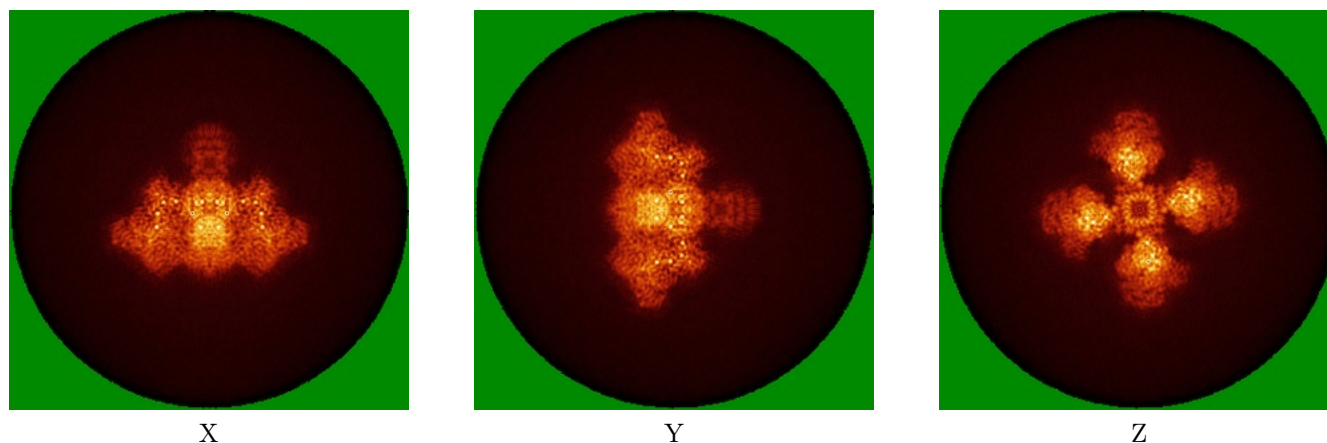


Z Index: 140

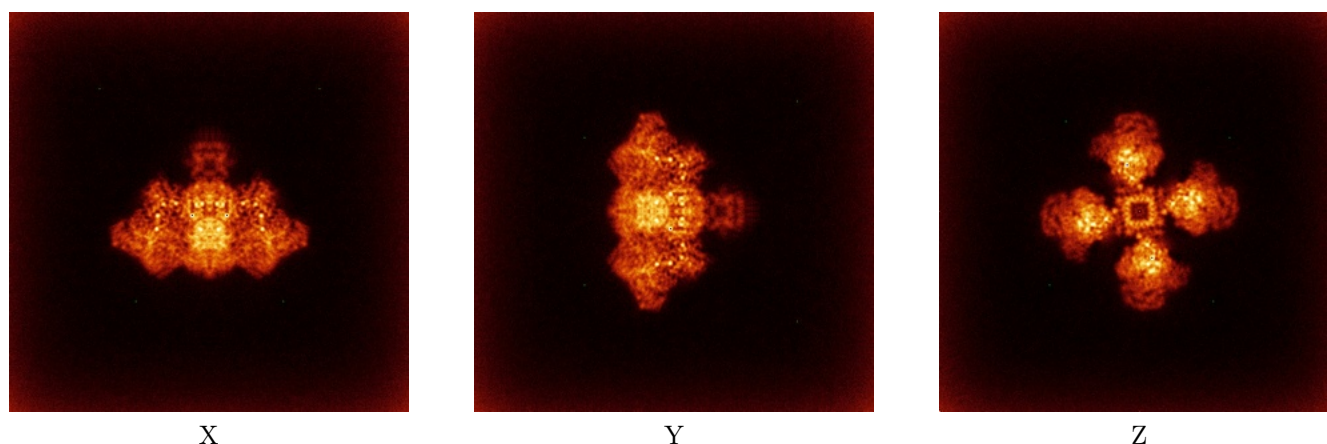
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw 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.

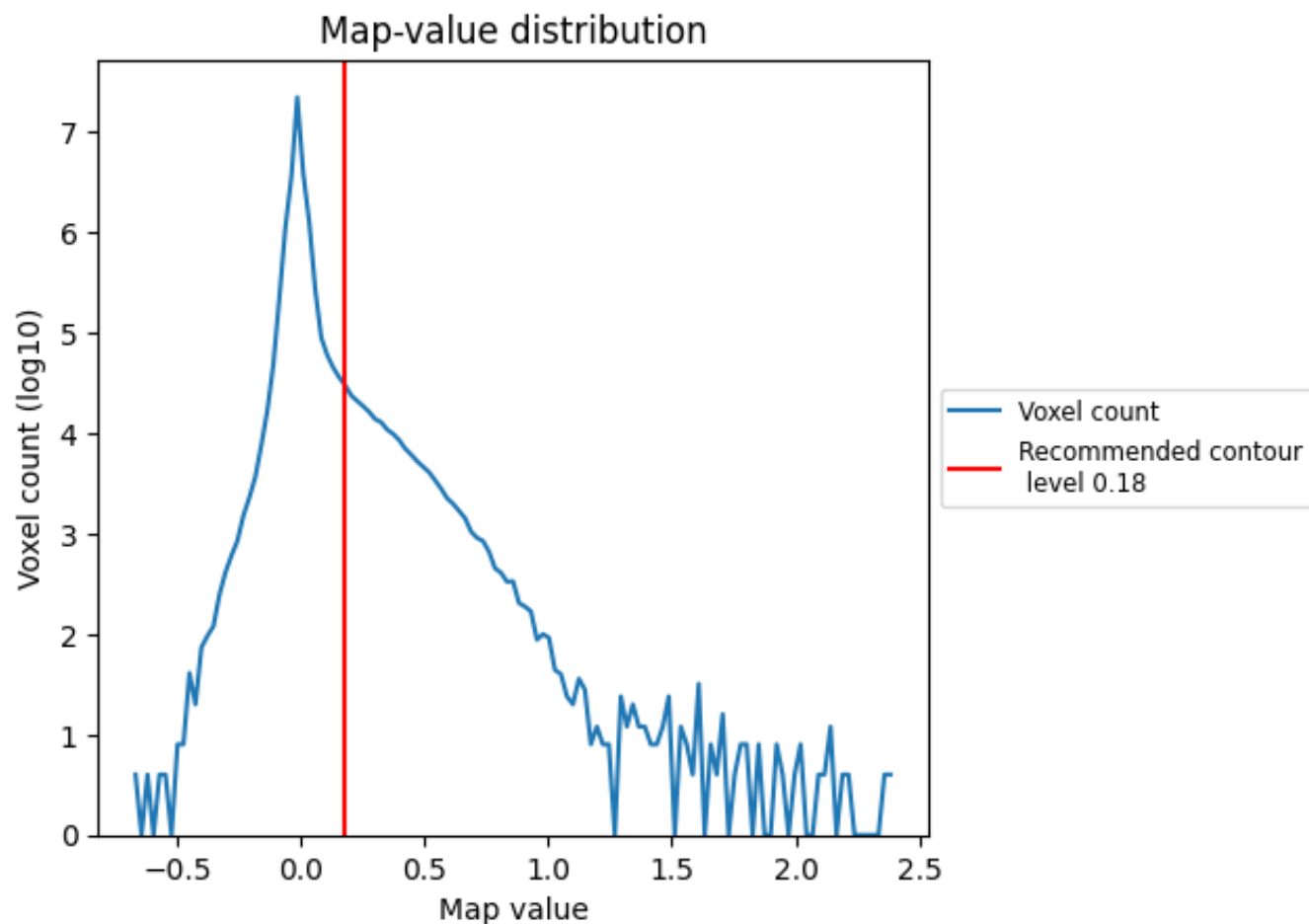
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

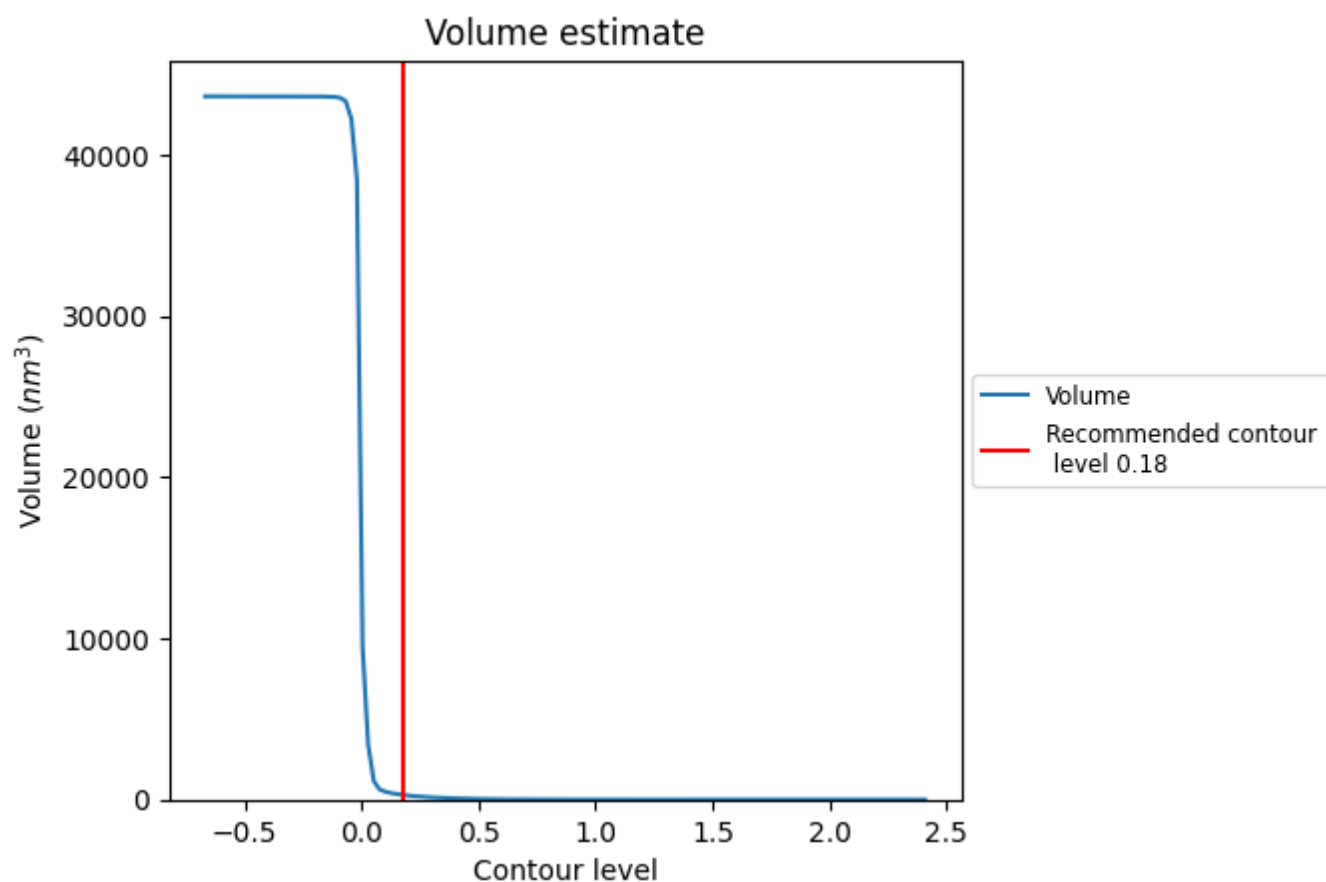
This section contains the results of statistical analysis of the map.

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.

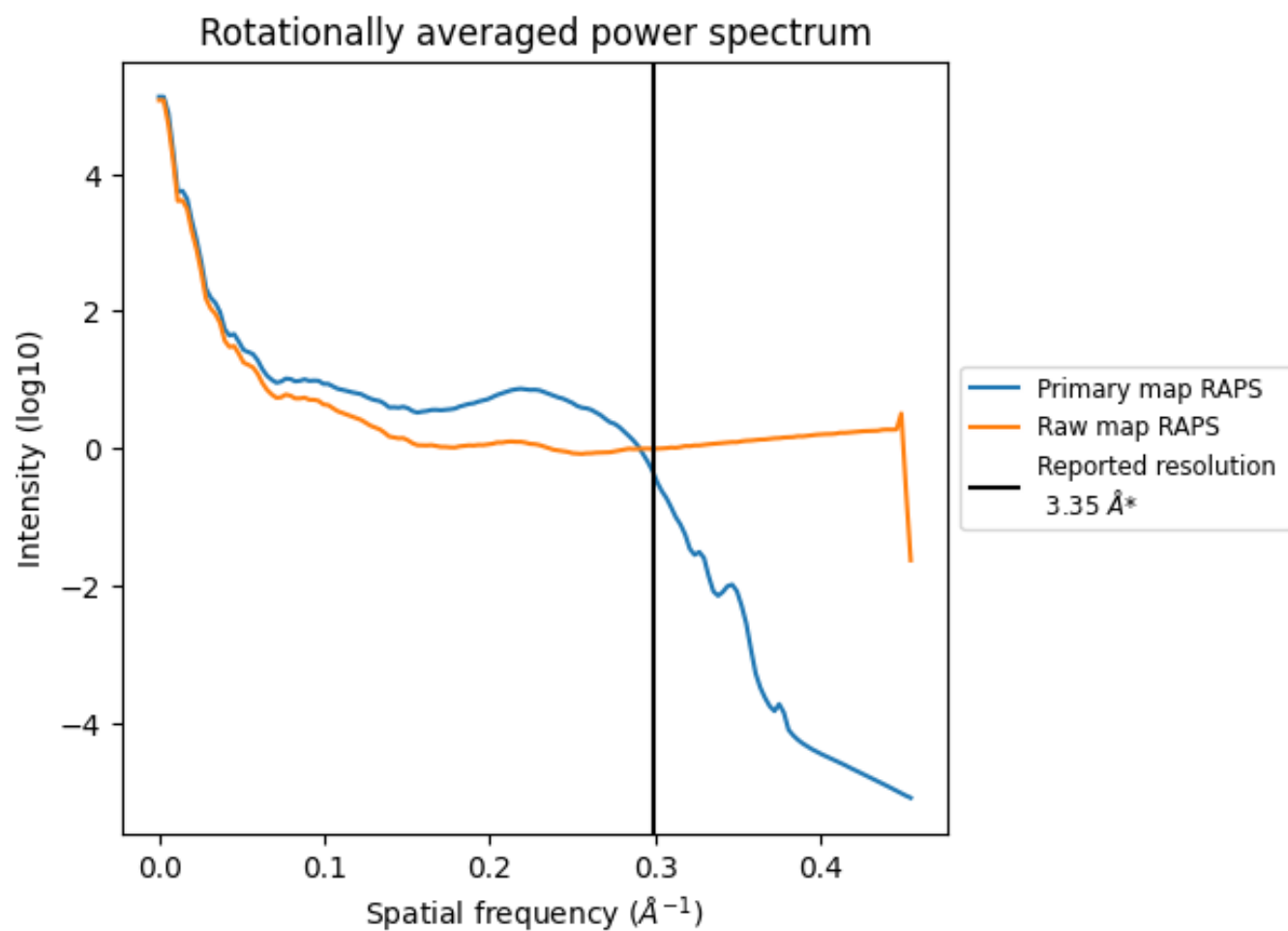
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 282 nm³; this corresponds to an approximate mass of 254 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

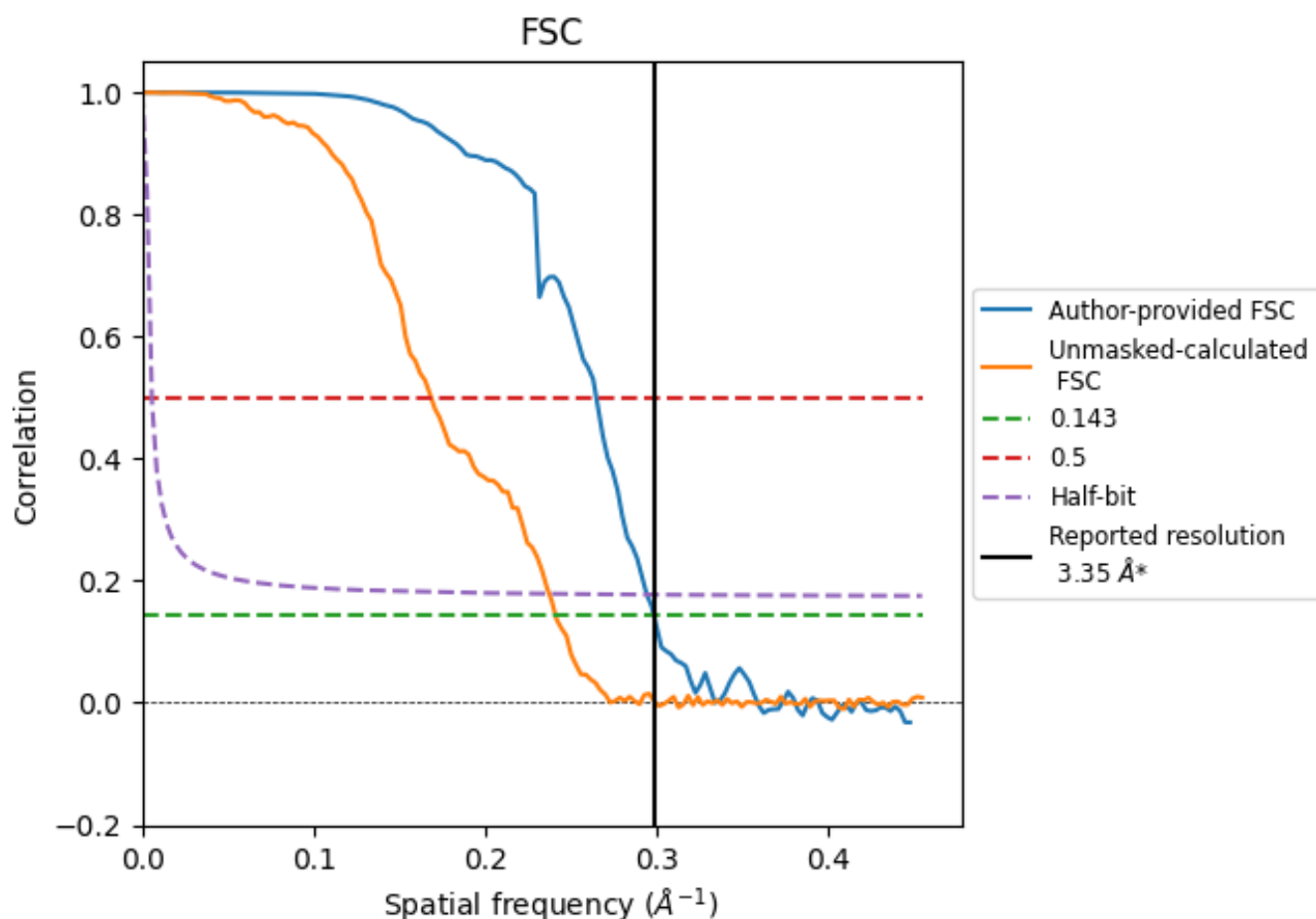


*Reported resolution corresponds to spatial frequency of $0.299 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.299 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

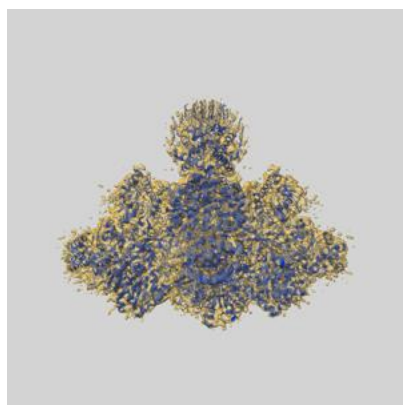
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	3.35	3.78	3.40
Unmasked-calculated*	4.15	5.94	4.22

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 3.35 by more than 10 %

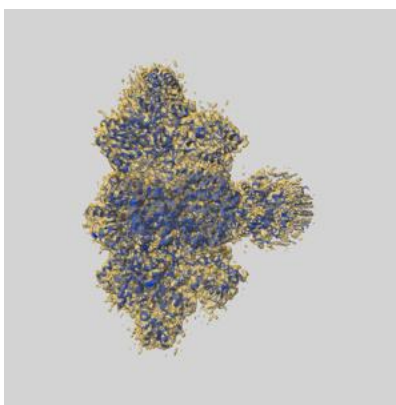
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19452 and PDB model 8RR0. Per-residue inclusion information can be found in section [3](#) on page [15](#).

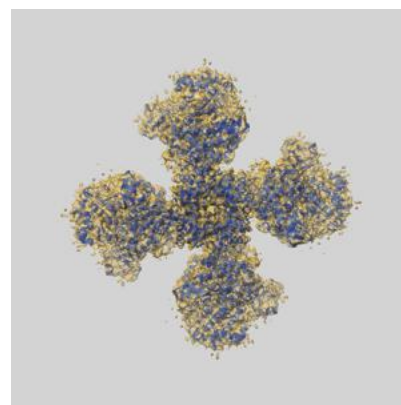
9.1 Map-model overlay [i](#)



X



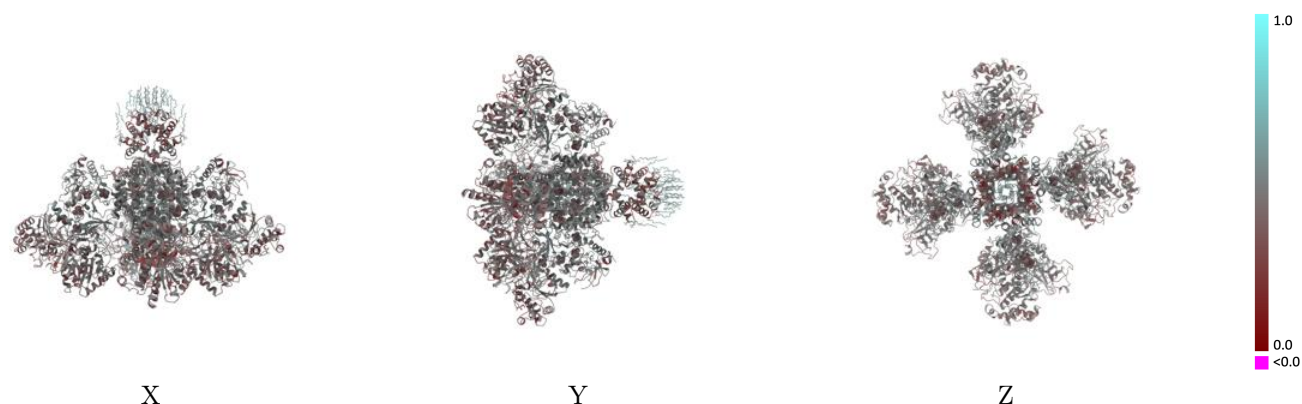
Y



Z

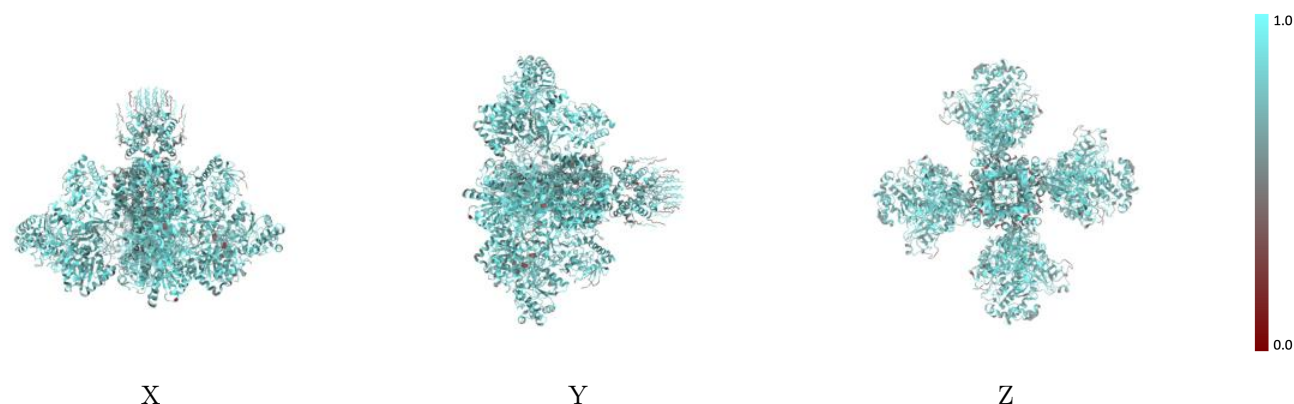
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



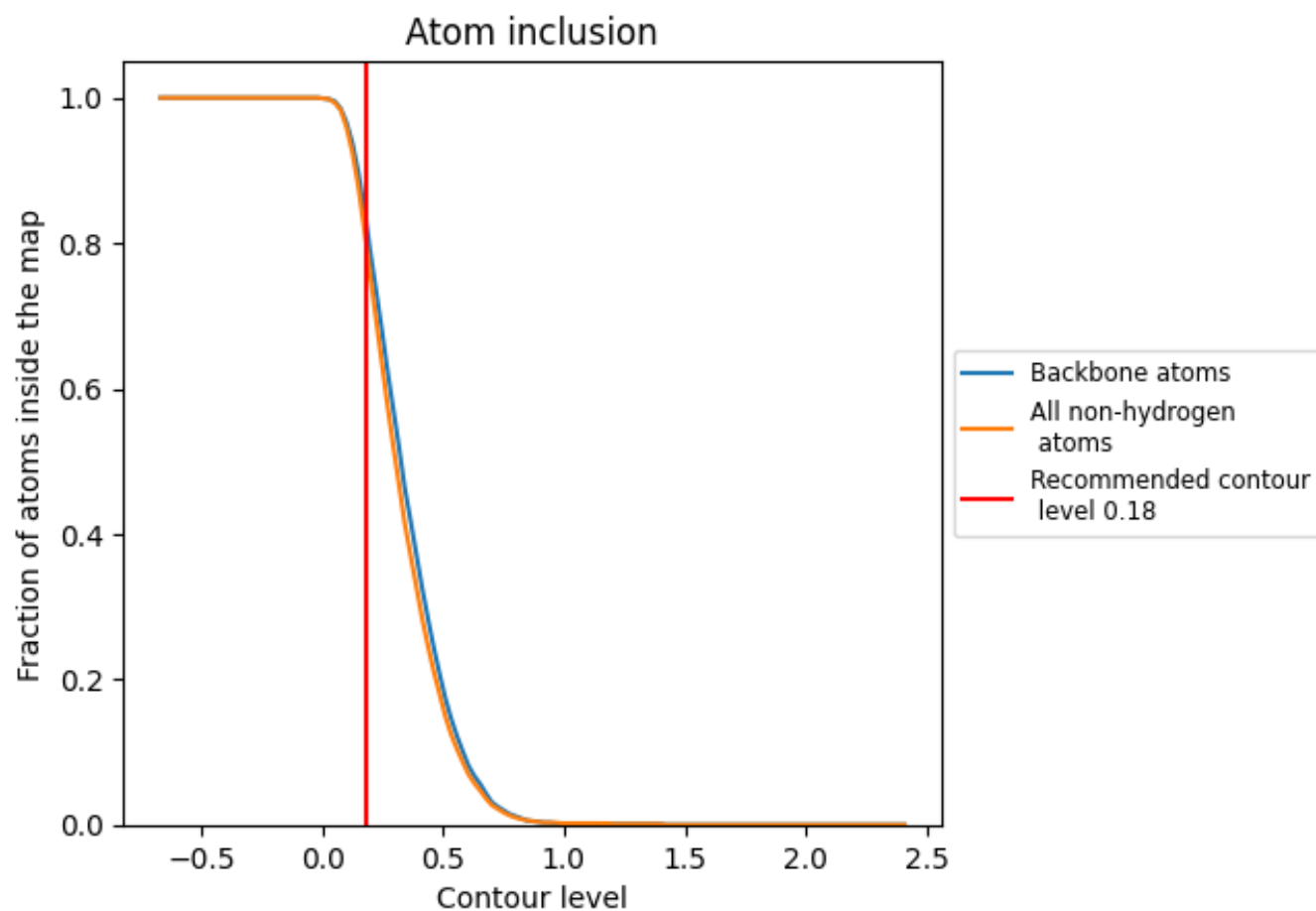
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8040	0.4440
A	0.7150	0.4420
B	0.8240	0.4440
C	0.7150	0.4450
D	0.8240	0.4450
E	0.7150	0.4440
F	0.8240	0.4440
G	0.7140	0.4420
H	0.8240	0.4430

1.0

0.0

<0.0