



## Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 07:37 PM JST

PDB ID : 7DEG / pdb\_00007deg  
EMDB ID : EMD-30657  
Title : Cryo-EM structure of a heme-copper terminal oxidase dimer provides insights into its catalytic mechanism  
Authors : Fei, S.; Hartmut, M.; Yun, Z.; Guoliang, Z.; Shuangbo, Z.  
Deposited on : 2020-11-04  
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

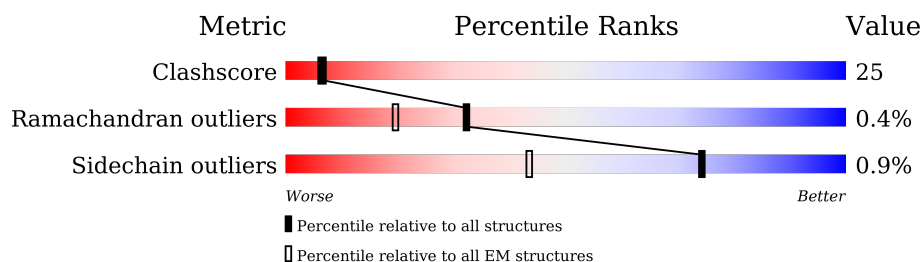
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	587	55% 43% ..
1	D	587	55% 42% ..
2	C	32	50% 47% .
2	F	32	50% 47% .
3	B	147	61% 39% .
3	E	147	61% 39% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	HAS	A	601	X	-	-	-
4	HAS	D	602	X	-	-	-
8	PGV	A	607	-	-	X	-
8	PGV	D	601	-	-	X	-
9	3PE	A	606	-	-	X	-
9	3PE	D	607	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12852 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 Cytochrome c oxidase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	581	Total	C	N	O	S	0	0
			4624	3131	715	762	16		
1	D	581	Total	C	N	O	S	0	0
			4624	3131	715	762	16		

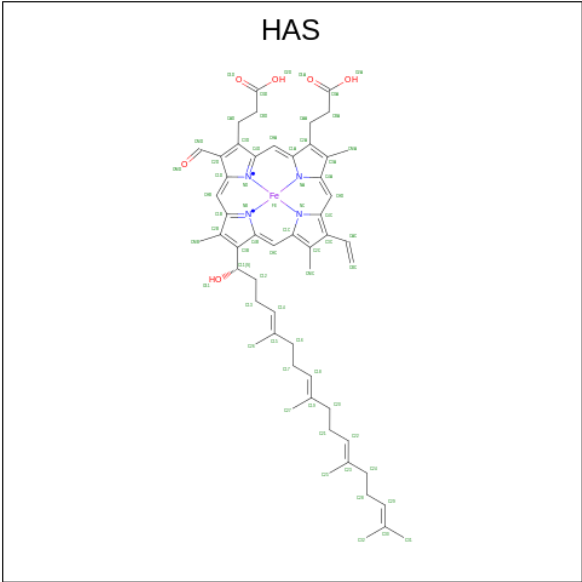
- Molecule 2 is a protein called Cytochrome oxidase subunit IIa.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	32	Total	C	N	O	S	0	0
			281	202	37	39	3		
2	F	32	Total	C	N	O	S	0	0
			281	202	37	39	3		

- Molecule 3 is a protein called Cytochrome oxidase subunit II.

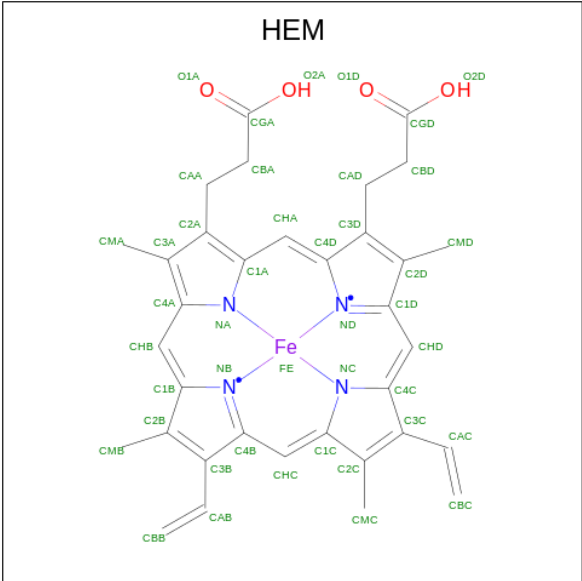
Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	147	Total	C	N	O	S	0	0
			1159	758	195	199	7		
3	E	147	Total	C	N	O	S	0	0
			1159	758	195	199	7		

- Molecule 4 is HEME-AS (CCD ID: HAS) (formula:  $C_{54}H_{64}FeN_4O_6$ ).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 65	C 54	Fe 1	N 4	O 6	0
4	D	1	Total 65	C 54	Fe 1	N 4	O 6	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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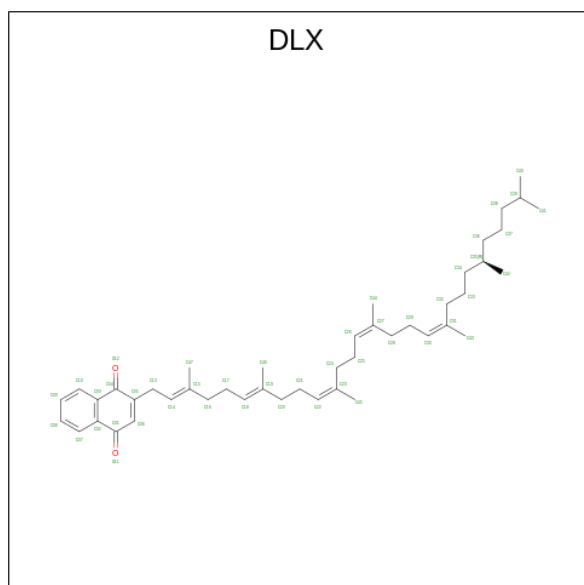
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Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 6 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

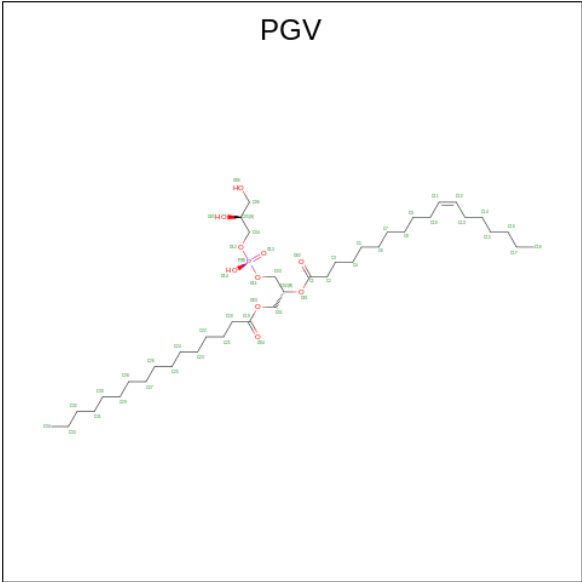
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Cu	0
			1	1	
6	D	1	Total	Cu	0
			1	1	

- Molecule 7 is 2-[(2 {E},6 {E},10 {Z},14 {Z},18 {Z},23 {R})-3,7,11,15,19,23,27-heptamethylotacosa-2,6,10,14,18-pentaenyl]naphthalene-1,4-dione (CCD ID: DLX) (formula: C<sub>45</sub>H<sub>66</sub>O<sub>2</sub>).



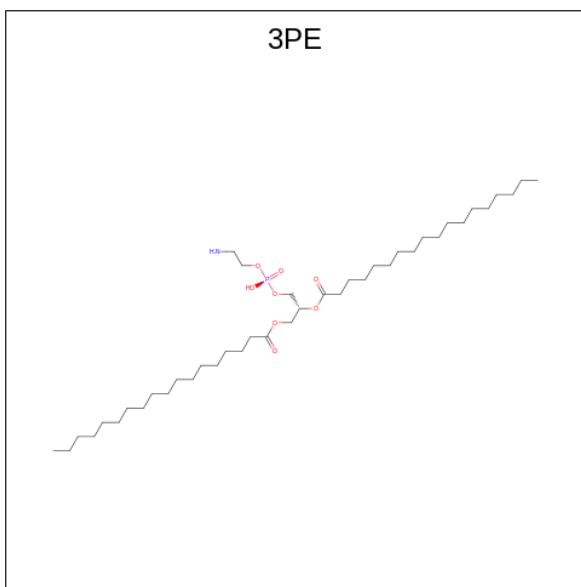
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			47	45	2	
7	D	1	Total	C	O	0
			47	45	2	

- Molecule 8 is (1R)-2-{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



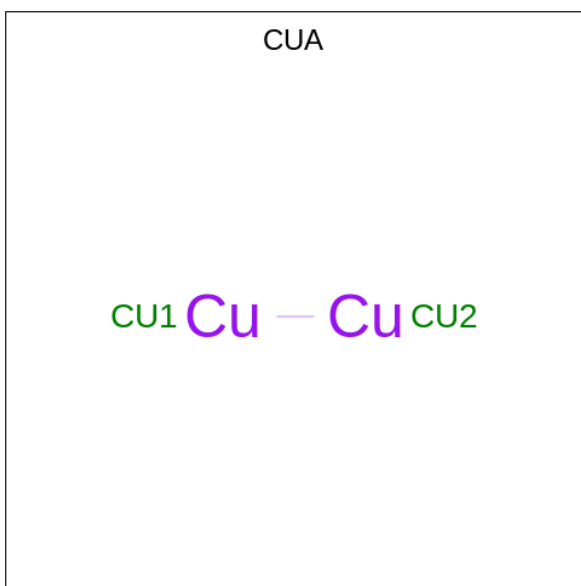
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	O	P	0
			51	40	10	1	
8	A	1	Total	C	O	P	0
			51	40	10	1	
8	C	1	Total	C	O	P	0
			51	40	10	1	
8	D	1	Total	C	O	P	0
			51	40	10	1	
8	D	1	Total	C	O	P	0
			51	40	10	1	
8	F	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 9 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
9	D	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 10 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu<sub>2</sub>).



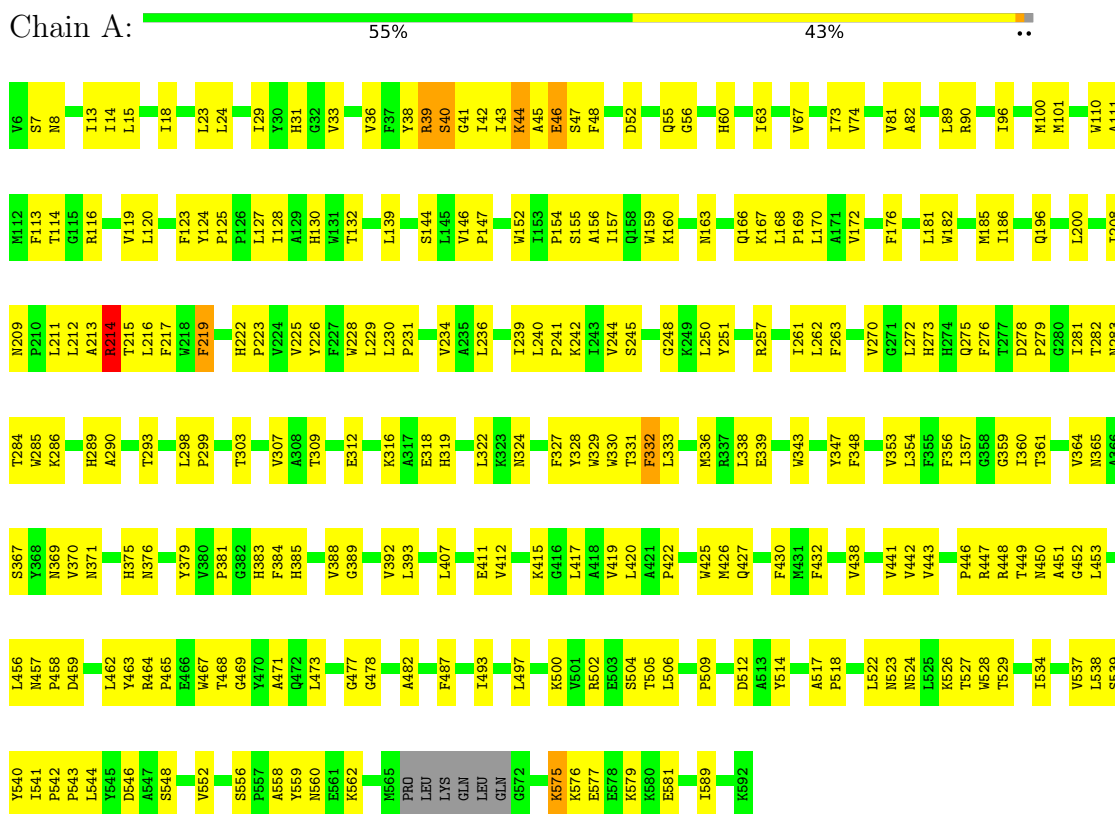
Mol	Chain	Residues	Atoms		AltConf
10	B	1	Total	Cu	0
			2	2	
10	E	1	Total	Cu	0
			2	2	



### 3 Residue-property plots

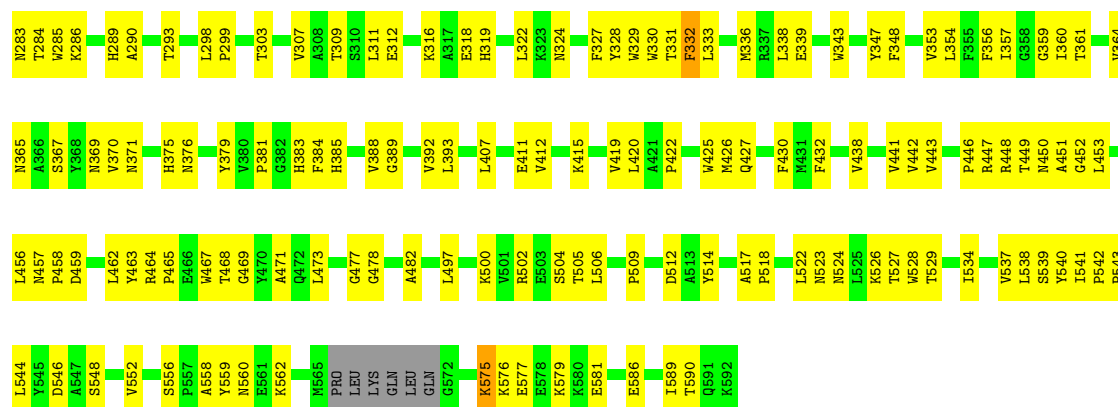
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

#### • Molecule 1: Cytochrome c oxidase subunit I

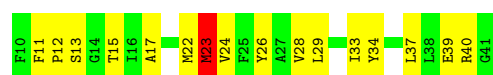


#### • Molecule 1: Cytochrome c oxidase subunit I





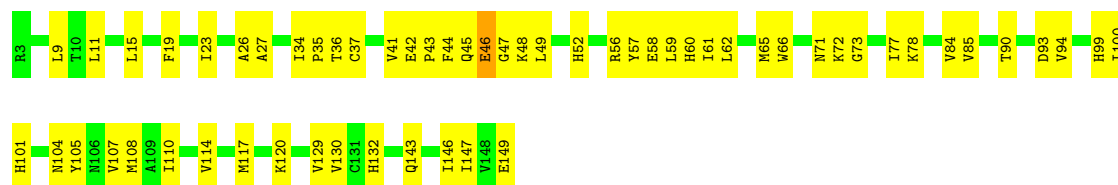
• Molecule 2: Cytochrome oxidase subunit IIa



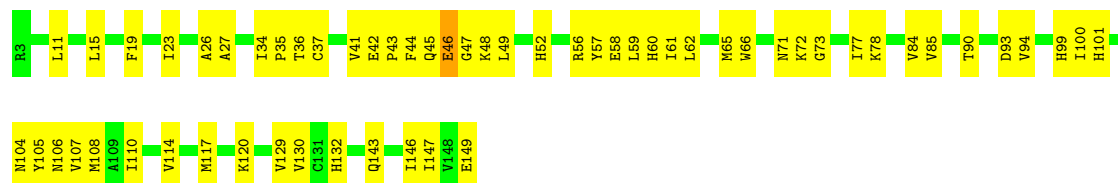
• Molecule 2: Cytochrome oxidase subunit IIa



• Molecule 3: Cytochrome oxidase subunit II



• Molecule 3: Cytochrome oxidase subunit II



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32982	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGV, DLX, 3PE, CU, HAS, HEM, CUA

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	0.81	1/4777 (0.0%)	0.65	0/6521
1	D	0.81	1/4777 (0.0%)	0.65	0/6521
2	C	0.74	0/294	0.60	0/397
2	F	0.74	0/294	0.60	0/397
3	B	0.72	0/1188	0.63	0/1607
3	E	0.72	0/1188	0.63	0/1607
All	All	0.79	2/12518 (0.0%)	0.65	0/17050

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	2
2	C	0	1
2	F	0	1
3	B	0	1
3	E	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	332	PHE	C-N	-5.09	1.22	1.34
1	A	332	PHE	C-N	-5.08	1.22	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	ARG	Peptide
1	A	512	ASP	Peptide
3	B	46	GLU	Peptide
2	C	23	MET	Peptide
1	D	214	ARG	Peptide
1	D	512	ASP	Peptide
3	E	46	GLU	Peptide
2	F	23	MET	Peptide

## 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	4624	0	4725	238	0
1	D	4624	0	4725	238	0
2	C	281	0	274	24	0
2	F	281	0	274	23	0
3	B	1159	0	1184	54	0
3	E	1159	0	1184	53	0
4	A	65	0	62	11	0
4	D	65	0	62	11	0
5	A	43	0	30	8	0
5	D	43	0	30	8	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	A	47	0	0	3	0
7	D	47	0	0	3	0
8	A	102	0	151	30	0
8	C	51	0	76	4	0
8	D	102	0	151	29	0
8	F	51	0	76	4	0
9	A	51	0	80	36	0
9	D	51	0	80	34	0
10	B	2	0	0	0	0
10	E	2	0	0	0	0
All	All	12852	0	13164	653	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 25.

All (653) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:PHE:O	9:D:607:3PE:C22	1.68	1.41
1:A:327:PHE:O	9:A:606:3PE:C22	1.68	1.39
1:D:40:SER:HB2	1:D:471:ALA:O	1.31	1.27
1:A:40:SER:HB2	1:A:471:ALA:O	1.31	1.22
3:B:48:LYS:HD2	3:B:77:ILE:HD11	1.48	0.96
3:E:48:LYS:HD2	3:E:77:ILE:HD11	1.48	0.93
1:A:446:PRO:HG2	1:A:449:THR:HG21	1.57	0.87
1:A:40:SER:CB	1:A:471:ALA:O	2.22	0.86
1:D:446:PRO:HG2	1:D:449:THR:HG21	1.57	0.86
1:D:40:SER:CB	1:D:471:ALA:O	2.22	0.85
3:E:52:HIS:HB2	3:E:56:ARG:HB2	1.60	0.83
9:A:606:3PE:H272	1:D:336:MET:CE	2.09	0.82
1:A:336:MET:CE	9:D:607:3PE:H272	2.09	0.82
3:B:52:HIS:HB2	3:B:56:ARG:HB2	1.60	0.82
8:A:607:PGV:H212	8:D:601:PGV:H212	1.62	0.81
3:E:42:GLU:HB3	3:E:114:VAL:HG21	1.63	0.81
3:B:42:GLU:HB3	3:B:114:VAL:HG21	1.63	0.80
1:A:427:GLN:HB2	8:A:607:PGV:H231	1.63	0.80
1:A:119:VAL:HG13	1:A:120:LEU:H	1.47	0.79
1:D:43:ILE:O	1:D:44:LYS:O	2.01	0.79
1:A:312:GLU:OE2	1:A:316:LYS:NZ	2.15	0.79
1:D:119:VAL:HG13	1:D:120:LEU:H	1.47	0.78
1:D:427:GLN:HB2	8:D:601:PGV:H231	1.65	0.78
1:D:312:GLU:OE2	1:D:316:LYS:NZ	2.15	0.78
1:D:168:LEU:O	1:D:257:ARG:NH2	2.17	0.77
1:A:464:ARG:NH2	3:B:143:GLN:OE1	2.18	0.77
8:D:601:PGV:C4	9:D:607:3PE:H2A1	2.15	0.77
1:A:43:ILE:O	1:A:44:LYS:O	2.01	0.76
1:D:464:ARG:NH2	3:E:143:GLN:OE1	2.18	0.76
9:A:606:3PE:H2A1	8:A:607:PGV:C4	2.15	0.76
9:D:607:3PE:H3B1	8:F:101:PGV:H201	1.66	0.76
9:A:606:3PE:H3B1	8:C:101:PGV:H201	1.66	0.76
8:A:607:PGV:H312	9:D:607:3PE:H2B1	1.68	0.75
9:A:606:3PE:H2B1	8:D:601:PGV:H312	1.68	0.75
1:A:365:ASN:O	1:A:371:ASN:ND2	2.20	0.75
3:B:65:MET:HB2	3:B:93:ASP:OD2	1.86	0.75
3:E:65:MET:HB2	3:E:93:ASP:OD2	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:529:THR:HG21	1:D:589:ILE:HG21	1.69	0.75
1:D:39:ARG:HG2	1:D:39:ARG:HH11	1.52	0.74
1:A:144:SER:HB2	1:A:182:TRP:CH2	2.22	0.74
1:A:529:THR:HG21	1:A:589:ILE:HG21	1.69	0.74
1:D:36:VAL:HG11	1:D:478:GLY:HA3	1.70	0.74
1:D:144:SER:HB2	1:D:182:TRP:CH2	2.22	0.74
1:A:39:ARG:HH11	1:A:39:ARG:HG2	1.52	0.74
1:D:73:ILE:HD12	1:D:231:PRO:HG2	1.70	0.73
1:D:411:GLU:HG2	1:D:412:VAL:H	1.54	0.73
1:D:39:ARG:HG2	1:D:39:ARG:NH1	2.03	0.73
1:A:360:ILE:HB	2:C:26:TYR:CD1	2.24	0.73
1:A:524:ASN:ND2	1:A:527:THR:OG1	2.22	0.73
1:D:360:ILE:HB	2:F:26:TYR:CD1	2.24	0.73
1:A:360:ILE:HG21	2:C:29:LEU:HD12	1.70	0.73
1:D:360:ILE:HG21	2:F:29:LEU:HD12	1.70	0.73
1:A:36:VAL:HG11	1:A:478:GLY:HA3	1.70	0.72
9:A:606:3PE:H3A1	8:C:101:PGV:H92	1.71	0.72
1:A:168:LEU:O	1:A:257:ARG:NH2	2.17	0.72
1:A:411:GLU:HG2	1:A:412:VAL:H	1.54	0.72
2:F:23:MET:HA	2:F:26:TYR:HB2	1.71	0.72
2:C:23:MET:HA	2:C:26:TYR:HB2	1.71	0.72
1:A:73:ILE:HD12	1:A:231:PRO:HG2	1.70	0.72
1:D:160:LYS:NZ	1:D:166:GLN:O	2.23	0.72
1:A:465:PRO:HB2	1:D:465:PRO:HB2	1.71	0.72
1:D:365:ASN:O	1:D:371:ASN:ND2	2.20	0.72
9:A:606:3PE:H292	8:D:601:PGV:C31	2.20	0.71
9:D:607:3PE:H3A1	8:F:101:PGV:H92	1.71	0.71
1:A:327:PHE:HB2	9:A:606:3PE:H2	1.73	0.71
1:D:81:VAL:HG22	1:D:172:VAL:HG23	1.73	0.71
1:D:524:ASN:ND2	1:D:527:THR:OG1	2.22	0.71
1:A:160:LYS:NZ	1:A:166:GLN:O	2.23	0.71
1:A:81:VAL:HG22	1:A:172:VAL:HG23	1.73	0.70
1:D:146:VAL:HG13	1:D:147:PRO:HD3	1.72	0.70
1:A:181:LEU:O	1:A:185:MET:HG3	1.91	0.70
8:A:607:PGV:C31	9:D:607:3PE:H292	2.20	0.70
9:A:606:3PE:H272	1:D:336:MET:HE1	1.74	0.70
1:A:544:LEU:HB3	1:A:575:LYS:HG3	1.74	0.70
8:A:607:PGV:H312	9:D:607:3PE:C2A	2.22	0.70
1:A:146:VAL:HG13	1:A:147:PRO:HD3	1.72	0.69
1:D:544:LEU:HB3	1:D:575:LYS:HG3	1.74	0.69
1:A:367:SER:O	1:A:370:VAL:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:100:ILE:HG12	3:E:129:VAL:HG22	1.75	0.69
1:D:181:LEU:O	1:D:185:MET:HG3	1.91	0.69
1:A:39:ARG:HG2	1:A:39:ARG:NH1	2.03	0.69
9:A:606:3PE:C2A	8:D:601:PGV:H312	2.22	0.69
1:D:327:PHE:HB2	9:D:607:3PE:H2	1.73	0.69
1:A:360:ILE:HB	2:C:26:TYR:CE1	2.28	0.69
8:A:607:PGV:H302	9:D:607:3PE:H292	1.74	0.69
3:B:100:ILE:HG12	3:B:129:VAL:HG22	1.75	0.69
1:D:367:SER:O	1:D:370:VAL:N	2.25	0.69
1:D:222:HIS:CD2	1:D:226:TYR:HE1	2.11	0.69
1:D:442:VAL:HG23	1:D:443:VAL:HG13	1.74	0.69
9:A:606:3PE:H292	8:D:601:PGV:H302	1.74	0.68
1:A:385:HIS:NE2	5:A:602:HEM:ND	2.42	0.68
1:A:222:HIS:CD2	1:A:226:TYR:HE1	2.11	0.68
1:A:442:VAL:HG23	1:A:443:VAL:HG13	1.74	0.68
3:E:45:GLN:HA	3:E:62:LEU:HD13	1.75	0.68
8:A:607:PGV:H312	9:D:607:3PE:C2B	2.24	0.68
1:D:90:ARG:HH12	1:D:155:SER:HB3	1.59	0.68
1:D:462:LEU:HD22	3:E:143:GLN:HG2	1.76	0.68
1:D:360:ILE:HB	2:F:26:TYR:CE1	2.28	0.67
1:D:385:HIS:NE2	5:D:603:HEM:ND	2.42	0.67
3:B:45:GLN:HA	3:B:62:LEU:HD13	1.75	0.67
1:D:231:PRO:HA	1:D:234:VAL:HG12	1.76	0.67
2:F:23:MET:HB2	3:E:15:LEU:HD22	1.77	0.67
1:A:128:ILE:HG12	1:A:558:ALA:HB1	1.77	0.67
1:A:276:PHE:HB3	3:B:34:ILE:HD11	1.77	0.67
1:A:336:MET:HE1	9:D:607:3PE:H272	1.77	0.67
1:A:125:PRO:HA	1:A:127:LEU:H	1.60	0.67
1:A:239:ILE:HG23	1:A:509:PRO:HG2	1.77	0.67
2:C:23:MET:HB2	3:B:15:LEU:HD22	1.77	0.67
1:D:128:ILE:HG12	1:D:558:ALA:HB1	1.77	0.67
1:A:449:THR:HG23	1:A:451:ALA:HB2	1.78	0.66
1:A:462:LEU:HD22	3:B:143:GLN:HG2	1.76	0.66
1:D:276:PHE:HB3	3:E:34:ILE:HD11	1.77	0.66
9:A:606:3PE:C2B	8:D:601:PGV:H312	2.24	0.66
1:A:231:PRO:HA	1:A:234:VAL:HG12	1.76	0.66
1:A:367:SER:HB3	3:B:23:ILE:HG21	1.77	0.66
1:D:367:SER:HB3	3:E:23:ILE:HG21	1.77	0.66
1:D:239:ILE:HG23	1:D:509:PRO:HG2	1.77	0.65
4:D:602:HAS:HMC1	4:D:602:HAS:HBC1	1.78	0.65
3:E:41:VAL:HG22	3:E:43:PRO:HD3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:449:THR:HG23	1:D:451:ALA:HB2	1.77	0.65
1:D:125:PRO:HA	1:D:127:LEU:H	1.60	0.65
3:E:47:GLY:HA3	3:E:60:HIS:HB2	1.78	0.65
1:A:90:ARG:HH12	1:A:155:SER:HB3	1.59	0.65
8:A:607:PGV:H02	8:D:601:PGV:H02	1.79	0.65
1:D:364:VAL:HG11	2:F:33:ILE:HD13	1.79	0.65
1:A:63:ILE:HA	1:A:67:VAL:HG22	1.80	0.64
4:A:601:HAS:HBC1	4:A:601:HAS:HMC1	1.78	0.64
1:D:55:GLN:NE2	1:D:113:PHE:O	2.30	0.64
3:B:47:GLY:HA3	3:B:60:HIS:HB2	1.78	0.64
1:D:343:TRP:HB2	1:D:419:VAL:HG22	1.78	0.64
3:B:41:VAL:HG22	3:B:43:PRO:HD3	1.78	0.64
1:D:338:LEU:O	1:D:339:GLU:HG2	1.97	0.64
1:A:343:TRP:HB2	1:A:419:VAL:HG22	1.78	0.64
1:A:55:GLN:NE2	1:A:113:PHE:O	2.30	0.64
3:B:71:ASN:O	3:B:73:GLY:N	2.31	0.64
1:A:364:VAL:HG11	2:C:33:ILE:HD13	1.79	0.64
3:E:56:ARG:HD2	3:E:84:VAL:HG13	1.80	0.63
1:A:338:LEU:O	1:A:339:GLU:HG2	1.97	0.63
1:D:63:ILE:HA	1:D:67:VAL:HG22	1.80	0.63
3:E:71:ASN:O	3:E:73:GLY:N	2.31	0.63
3:B:56:ARG:HD2	3:B:84:VAL:HG13	1.80	0.63
1:A:40:SER:HA	1:A:471:ALA:HB1	1.81	0.62
9:A:606:3PE:H2A1	8:A:607:PGV:H42	1.81	0.62
1:D:45:ALA:O	1:D:453:LEU:HD22	2.00	0.62
1:D:524:ASN:ND2	1:D:526:LYS:O	2.33	0.62
1:A:524:ASN:ND2	1:A:526:LYS:O	2.33	0.62
1:A:45:ALA:O	1:A:453:LEU:HD22	2.00	0.62
1:A:330:TRP:HA	1:A:333:LEU:HD12	1.82	0.62
1:D:33:VAL:HG21	1:D:482:ALA:HB2	1.81	0.62
9:A:606:3PE:H292	8:D:601:PGV:C30	2.29	0.62
9:A:606:3PE:C3A	8:C:101:PGV:H92	2.30	0.62
1:D:40:SER:HA	1:D:471:ALA:HB1	1.81	0.62
1:D:330:TRP:HA	1:D:333:LEU:HD12	1.82	0.62
2:F:22:MET:O	2:F:24:VAL:N	2.33	0.62
8:D:601:PGV:H41	9:D:607:3PE:H291	1.82	0.61
1:A:361:THR:HG23	1:A:379:TYR:CE2	2.35	0.61
9:A:606:3PE:H2B1	8:D:601:PGV:H331	1.82	0.61
8:A:607:PGV:C30	9:D:607:3PE:H292	2.29	0.61
1:D:46:GLU:O	1:D:46:GLU:HG2	2.00	0.61
1:A:46:GLU:O	1:A:46:GLU:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:ARG:NH2	1:D:278:ASP:OD1	2.28	0.61
2:C:22:MET:O	2:C:24:VAL:N	2.33	0.61
1:A:214:ARG:NH2	1:A:278:ASP:OD1	2.28	0.61
1:A:407:LEU:O	1:A:504:SER:OG	2.18	0.61
1:A:336:MET:SD	9:D:607:3PE:H272	2.41	0.61
1:D:361:THR:HG23	1:D:379:TYR:CE2	2.35	0.61
1:D:411:GLU:OE1	1:D:411:GLU:N	2.19	0.61
1:A:33:VAL:HG21	1:A:482:ALA:HB2	1.81	0.61
8:D:601:PGV:H42	9:D:607:3PE:H2A1	1.81	0.61
9:D:607:3PE:C3A	8:F:101:PGV:H92	2.31	0.60
1:A:125:PRO:HG3	1:A:213:ALA:HB3	1.83	0.60
8:A:607:PGV:H331	9:D:607:3PE:H2B1	1.82	0.60
1:A:411:GLU:OE1	1:A:411:GLU:N	2.19	0.60
5:A:602:HEM:HHC	5:A:602:HEM:HBB2	1.82	0.60
1:A:7:SER:OG	1:A:8:ASN:N	2.34	0.60
5:D:603:HEM:HBB2	5:D:603:HEM:HHC	1.82	0.60
1:D:7:SER:OG	1:D:8:ASN:N	2.34	0.60
1:D:500:LYS:NZ	1:D:502:ARG:O	2.34	0.60
3:B:93:ASP:OD1	3:B:94:VAL:N	2.35	0.60
1:A:120:LEU:HD23	1:A:448:ARG:CZ	2.32	0.60
9:A:606:3PE:H272	1:D:336:MET:SD	2.41	0.60
1:D:39:ARG:HH11	1:D:39:ARG:CG	2.14	0.60
1:A:415:LYS:O	1:A:419:VAL:HG23	2.02	0.60
1:D:415:LYS:O	1:D:419:VAL:HG23	2.02	0.60
1:A:500:LYS:NZ	1:A:502:ARG:O	2.34	0.59
9:A:606:3PE:H291	8:A:607:PGV:H41	1.83	0.59
1:A:279:PRO:HD2	3:B:110:ILE:HD12	1.83	0.59
1:D:120:LEU:HD23	1:D:448:ARG:CZ	2.32	0.59
1:D:125:PRO:HG3	1:D:213:ALA:HB3	1.83	0.59
1:D:329:TRP:O	1:D:330:TRP:HB2	2.02	0.59
1:D:560:ASN:HD22	1:D:562:LYS:H	1.50	0.59
8:A:605:PGV:H71	8:A:605:PGV:H21	1.85	0.59
8:A:607:PGV:H312	9:D:607:3PE:H292	1.84	0.59
1:D:124:TYR:OH	1:D:214:ARG:NH1	2.36	0.59
3:E:77:ILE:HG22	3:E:146:ILE:HA	1.84	0.59
1:A:329:TRP:O	1:A:330:TRP:HB2	2.02	0.58
1:A:124:TYR:OH	1:A:214:ARG:NH1	2.36	0.58
1:A:196:GLN:HE22	1:A:212:LEU:HD23	1.69	0.58
1:D:279:PRO:HD2	3:E:110:ILE:HD12	1.83	0.58
9:A:606:3PE:H292	8:D:601:PGV:H312	1.84	0.58
8:D:606:PGV:H21	8:D:606:PGV:H71	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:LEU:O	1:D:504:SER:OG	2.18	0.58
1:D:196:GLN:HE22	1:D:212:LEU:HD23	1.69	0.58
3:E:93:ASP:OD1	3:E:94:VAL:N	2.35	0.58
3:B:56:ARG:HD2	3:B:84:VAL:CG1	2.34	0.58
1:A:473:LEU:HD12	1:D:473:LEU:HD12	1.85	0.58
3:E:41:VAL:HG13	3:E:42:GLU:H	1.69	0.57
1:A:39:ARG:HH11	1:A:39:ARG:CG	2.14	0.57
9:A:606:3PE:H2B2	9:A:606:3PE:C26	2.35	0.57
9:A:606:3PE:C29	8:D:601:PGV:H312	2.34	0.57
3:B:77:ILE:HG22	3:B:146:ILE:HA	1.84	0.57
1:D:283:ASN:OD1	1:D:284:THR:N	2.36	0.57
1:A:14:ILE:O	1:A:18:ILE:HG12	2.04	0.57
1:A:560:ASN:HD22	1:A:562:LYS:H	1.50	0.57
9:D:607:3PE:C26	9:D:607:3PE:H2B2	2.34	0.57
1:A:152:TRP:HD1	1:A:176:PHE:HE1	1.53	0.57
1:D:14:ILE:O	1:D:18:ILE:HG12	2.04	0.57
8:A:607:PGV:H312	9:D:607:3PE:C29	2.34	0.57
1:D:152:TRP:HD1	1:D:176:PHE:HE1	1.53	0.57
3:E:58:GLU:OE2	3:E:60:HIS:NE2	2.37	0.57
1:D:353:VAL:HA	4:D:602:HAS:H323	1.86	0.57
3:B:58:GLU:OE2	3:B:60:HIS:NE2	2.37	0.57
1:D:389:GLY:O	1:D:425:TRP:NE1	2.38	0.57
1:A:353:VAL:HA	4:A:601:HAS:H323	1.86	0.56
1:D:38:TYR:OH	1:D:48:PHE:HB2	2.05	0.56
3:E:56:ARG:HD2	3:E:84:VAL:CG1	2.34	0.56
3:B:41:VAL:HG13	3:B:42:GLU:H	1.69	0.56
1:D:456:LEU:HD22	1:D:468:THR:HG22	1.88	0.56
3:E:46:GLU:OE1	3:E:72:LYS:HD3	2.06	0.56
1:D:537:VAL:HG13	1:D:579:LYS:HD2	1.87	0.56
1:A:241:PRO:O	1:A:248:GLY:HA3	2.06	0.56
1:A:251:TYR:HA	1:A:514:TYR:HB3	1.87	0.56
1:A:328:TYR:HB2	9:A:606:3PE:O12	2.06	0.56
1:A:283:ASN:OD1	1:A:284:THR:N	2.36	0.55
1:D:241:PRO:O	1:D:248:GLY:HA3	2.06	0.55
1:D:328:TYR:HB2	9:D:607:3PE:O12	2.06	0.55
1:D:47:SER:HA	1:D:52:ASP:HA	1.88	0.55
1:A:38:TYR:OH	1:A:48:PHE:HB2	2.05	0.55
1:A:244:VAL:HG12	1:A:245:SER:H	1.71	0.55
1:D:15:LEU:HG	1:D:407:LEU:HD11	1.89	0.55
8:D:601:PGV:H52	9:D:607:3PE:H2A2	1.89	0.55
1:A:215:THR:C	1:A:217:PHE:H	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:46:GLU:OE1	3:B:72:LYS:HD3	2.06	0.55
1:D:359:GLY:HA3	4:D:602:HAS:H161	1.89	0.55
1:A:359:GLY:HA3	4:A:601:HAS:H161	1.89	0.55
3:B:36:THR:OG1	3:B:37:CYS:N	2.40	0.55
1:D:244:VAL:HG12	1:D:245:SER:H	1.71	0.55
1:D:251:TYR:HA	1:D:514:TYR:HB3	1.87	0.55
1:A:456:LEU:HD22	1:A:468:THR:HG22	1.88	0.55
1:A:15:LEU:HG	1:A:407:LEU:HD11	1.89	0.55
1:D:450:ASN:O	1:D:452:GLY:N	2.40	0.55
1:A:43:ILE:O	1:A:44:LYS:C	2.45	0.55
1:A:450:ASN:O	1:A:452:GLY:N	2.40	0.55
3:E:36:THR:OG1	3:E:37:CYS:N	2.40	0.55
1:D:272:LEU:HD21	1:D:281:ILE:HG21	1.88	0.54
1:D:215:THR:C	1:D:217:PHE:H	2.10	0.54
1:A:537:VAL:HG13	1:A:579:LYS:HD2	1.87	0.54
1:D:116:ARG:HB3	1:D:130:HIS:HB2	1.90	0.54
1:D:119:VAL:HG22	1:D:123:PHE:HA	1.89	0.54
1:A:119:VAL:HG22	1:A:123:PHE:HA	1.90	0.54
1:D:214:ARG:NE	1:D:278:ASP:OD2	2.41	0.54
1:A:116:ARG:HB3	1:A:130:HIS:HB2	1.90	0.54
1:A:272:LEU:HD12	1:A:275:GLN:HE21	1.73	0.54
1:A:272:LEU:HD21	1:A:281:ILE:HG21	1.88	0.54
1:D:43:ILE:O	1:D:44:LYS:C	2.45	0.54
1:A:47:SER:HA	1:A:52:ASP:HA	1.88	0.54
9:A:606:3PE:H2A2	8:A:607:PGV:H52	1.90	0.54
1:D:356:PHE:CE2	2:F:22:MET:HG3	2.43	0.54
1:A:74:VAL:HG11	1:A:101:MET:SD	2.48	0.54
1:D:303:THR:O	1:D:307:VAL:HG12	2.07	0.54
2:F:22:MET:C	2:F:24:VAL:H	2.11	0.54
1:A:144:SER:HB2	1:A:182:TRP:HH2	1.73	0.53
1:A:168:LEU:HG	1:A:172:VAL:HG13	1.90	0.53
1:A:356:PHE:CE2	2:C:22:MET:HG3	2.43	0.53
1:D:539:SER:O	1:D:539:SER:OG	2.26	0.53
1:D:74:VAL:HG11	1:D:101:MET:SD	2.48	0.53
2:C:22:MET:C	2:C:24:VAL:H	2.11	0.53
1:A:214:ARG:NE	1:A:278:ASP:OD2	2.41	0.53
1:A:303:THR:O	1:A:307:VAL:HG12	2.07	0.53
3:E:52:HIS:ND1	3:E:56:ARG:HG3	2.24	0.53
1:D:411:GLU:O	1:D:412:VAL:HG23	2.09	0.53
1:A:240:LEU:HD13	1:A:348:PHE:HD2	1.74	0.53
1:A:393:LEU:HD22	5:A:602:HEM:HMC1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LEU:O	1:A:548:SER:OG	2.18	0.53
1:D:119:VAL:O	1:D:120:LEU:HB2	2.09	0.53
1:A:270:VAL:O	1:A:273:HIS:ND1	2.40	0.52
1:D:168:LEU:HG	1:D:172:VAL:HG13	1.90	0.52
1:D:240:LEU:HD13	1:D:348:PHE:HD2	1.74	0.52
1:A:411:GLU:O	1:A:412:VAL:HG23	2.09	0.52
3:B:65:MET:HG2	3:B:66:TRP:CE2	2.44	0.52
1:A:537:VAL:O	1:A:541:ILE:HG12	2.10	0.52
1:D:272:LEU:HD12	1:D:275:GLN:HE21	1.73	0.52
1:A:539:SER:O	1:A:539:SER:OG	2.26	0.52
1:A:389:GLY:O	1:A:425:TRP:NE1	2.38	0.52
1:D:144:SER:HB2	1:D:182:TRP:HH2	1.72	0.52
1:D:537:VAL:O	1:D:541:ILE:HG12	2.10	0.52
1:A:96:ILE:HD11	1:A:146:VAL:HG21	1.92	0.52
1:A:119:VAL:O	1:A:120:LEU:HB2	2.09	0.52
1:A:524:ASN:HD22	1:A:527:THR:HG1	1.57	0.52
3:E:65:MET:HG2	3:E:66:TRP:CE2	2.44	0.52
1:A:219:PHE:CD1	1:A:540:TYR:HE2	2.28	0.51
8:A:605:PGV:O02	8:A:605:PGV:H042	2.10	0.51
3:E:99:HIS:HB2	3:E:132:HIS:CD2	2.45	0.51
3:B:99:HIS:HB2	3:B:132:HIS:CD2	2.45	0.51
1:D:219:PHE:CD1	1:D:540:TYR:HE2	2.28	0.51
3:B:52:HIS:ND1	3:B:56:ARG:HG3	2.24	0.51
1:D:270:VAL:O	1:D:273:HIS:ND1	2.40	0.51
9:D:607:3PE:C2B	9:D:607:3PE:H261	2.40	0.51
1:A:163:ASN:HD22	1:A:166:GLN:HB3	1.75	0.51
3:B:59:LEU:HG	3:B:61:ILE:HG23	1.92	0.51
1:D:289:HIS:O	1:D:293:THR:OG1	2.24	0.51
1:D:309:THR:HG23	2:F:12:PRO:HB3	1.92	0.51
3:E:46:GLU:HA	3:E:72:LYS:NZ	2.26	0.51
1:A:167:LYS:HD3	1:A:518:PRO:HA	1.92	0.51
3:B:46:GLU:HA	3:B:72:LYS:NZ	2.26	0.51
1:D:167:LYS:HD3	1:D:518:PRO:HA	1.92	0.51
8:D:601:PGV:C4	9:D:607:3PE:C2A	2.87	0.51
9:A:606:3PE:H2B1	8:D:601:PGV:C33	2.40	0.51
1:A:322:LEU:HD11	1:A:332:PHE:CD2	2.46	0.51
8:A:607:PGV:C33	9:D:607:3PE:H2B1	2.40	0.51
3:E:46:GLU:HA	3:E:72:LYS:HZ3	1.76	0.51
1:A:276:PHE:CZ	1:A:290:ALA:HB2	2.46	0.51
8:A:607:PGV:H201	8:A:607:PGV:H32	1.93	0.51
8:D:601:PGV:H32	8:D:601:PGV:H201	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:606:PGV:O02	8:D:606:PGV:H042	2.10	0.51
1:A:154:PRO:C	1:A:156:ALA:H	2.14	0.50
9:A:606:3PE:C2B	9:A:606:3PE:H261	2.40	0.50
1:D:163:ASN:HD22	1:D:166:GLN:HB3	1.75	0.50
1:D:577:GLU:O	1:D:581:GLU:HB2	2.11	0.50
1:A:110:TRP:CE3	1:A:111:ALA:HB2	2.47	0.50
1:A:577:GLU:O	1:A:581:GLU:HB2	2.11	0.50
1:D:46:GLU:O	1:D:47:SER:HB3	2.11	0.50
1:D:393:LEU:HD22	5:D:603:HEM:HMC1	1.91	0.50
1:D:322:LEU:HD11	1:D:332:PHE:CD2	2.46	0.50
1:D:546:ASP:C	1:D:548:SER:H	2.14	0.50
1:D:41:GLY:O	1:D:44:LYS:HE3	2.12	0.50
1:A:41:GLY:O	1:A:44:LYS:HE3	2.12	0.50
1:A:119:VAL:HG13	1:A:120:LEU:N	2.23	0.50
1:A:222:HIS:CD2	1:A:273:HIS:HE1	2.30	0.50
1:D:96:ILE:HD11	1:D:146:VAL:HG21	1.92	0.50
1:D:182:TRP:HA	1:D:185:MET:SD	2.52	0.50
1:D:371:ASN:HD21	4:D:602:HAS:HBD2	1.77	0.50
3:E:59:LEU:HG	3:E:61:ILE:HG23	1.92	0.50
1:A:309:THR:HG23	2:C:12:PRO:HB3	1.92	0.50
9:A:606:3PE:C2A	8:A:607:PGV:C4	2.87	0.50
3:E:44:PHE:CD1	3:E:90:THR:HB	2.47	0.50
1:A:347:TYR:CD2	1:A:422:PRO:HG3	2.47	0.50
1:D:110:TRP:CE3	1:D:111:ALA:HB2	2.46	0.50
1:A:46:GLU:O	1:A:47:SER:HB3	2.11	0.50
1:A:159:TRP:CH2	1:A:169:PRO:HD3	2.47	0.50
3:B:44:PHE:CD1	3:B:90:THR:HB	2.47	0.50
1:D:124:TYR:CZ	1:D:214:ARG:NH1	2.80	0.50
1:A:546:ASP:C	1:A:548:SER:H	2.14	0.50
1:D:159:TRP:CH2	1:D:169:PRO:HD3	2.47	0.49
1:D:276:PHE:CZ	1:D:290:ALA:HB2	2.46	0.49
1:A:124:TYR:CZ	1:A:214:ARG:NH1	2.80	0.49
2:C:11:PHE:O	2:C:13:SER:N	2.46	0.49
1:D:347:TYR:CD2	1:D:422:PRO:HG3	2.47	0.49
1:D:441:VAL:O	2:F:40:ARG:NH1	2.46	0.49
1:D:154:PRO:C	1:D:156:ALA:H	2.14	0.49
1:A:542:PRO:HB2	1:A:543:PRO:HD3	1.95	0.49
1:D:230:LEU:HD21	1:D:263:PHE:CD2	2.48	0.49
1:D:309:THR:OG1	2:F:15:THR:HG21	2.13	0.49
1:D:371:ASN:O	1:D:375:HIS:HB2	2.13	0.49
1:A:167:LYS:HD2	1:A:523:ASN:HD21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:TRP:HA	1:A:185:MET:SD	2.52	0.49
1:A:371:ASN:O	1:A:375:HIS:HB2	2.13	0.49
1:D:240:LEU:HB3	1:D:241:PRO:HD3	1.95	0.49
1:D:446:PRO:HD3	1:D:467:TRP:CH2	2.48	0.49
1:A:230:LEU:HD21	1:A:263:PHE:CD2	2.48	0.49
1:D:170:LEU:HD23	1:D:250:LEU:HD21	1.95	0.48
1:D:542:PRO:HB2	1:D:543:PRO:HD3	1.95	0.48
1:A:170:LEU:HD23	1:A:250:LEU:HD21	1.95	0.48
1:A:371:ASN:HD21	4:A:601:HAS:HBD2	1.77	0.48
1:D:167:LYS:HD2	1:D:523:ASN:HD21	1.78	0.48
1:D:524:ASN:HD22	1:D:527:THR:HG1	1.59	0.48
3:E:19:PHE:O	3:E:23:ILE:HG23	2.13	0.48
1:A:240:LEU:HB3	1:A:241:PRO:HD3	1.95	0.48
1:A:289:HIS:O	1:A:293:THR:OG1	2.24	0.48
1:A:446:PRO:HD3	1:A:467:TRP:CH2	2.48	0.48
1:A:559:TYR:CZ	3:B:93:ASP:HB2	2.49	0.48
1:D:222:HIS:CD2	1:D:273:HIS:HE1	2.30	0.48
1:A:324:ASN:ND2	1:A:324:ASN:O	2.47	0.48
1:A:441:VAL:O	2:C:40:ARG:NH1	2.46	0.48
3:B:19:PHE:O	3:B:23:ILE:HG23	2.13	0.48
1:A:276:PHE:HZ	1:A:290:ALA:HB2	1.78	0.48
1:D:388:VAL:CG2	4:D:602:HAS:HAC	2.44	0.48
2:F:11:PHE:O	2:F:13:SER:N	2.46	0.48
1:A:309:THR:OG1	2:C:15:THR:HG21	2.13	0.48
1:A:31:HIS:CE1	1:A:56:GLY:HA3	2.49	0.48
1:D:324:ASN:O	1:D:324:ASN:ND2	2.47	0.48
1:D:276:PHE:HZ	1:D:290:ALA:HB2	1.78	0.48
1:A:388:VAL:CG2	4:A:601:HAS:HAC	2.44	0.48
1:A:130:HIS:CE1	1:A:132:THR:HG23	2.49	0.47
1:A:354:LEU:HD11	1:A:426:MET:HA	1.96	0.47
1:A:376:ASN:HD22	3:B:108:MET:HE1	1.79	0.47
1:D:31:HIS:CE1	1:D:56:GLY:HA3	2.49	0.47
1:A:327:PHE:CB	9:A:606:3PE:H2	2.43	0.47
1:A:152:TRP:CD1	1:A:176:PHE:HE1	2.32	0.47
1:D:60:HIS:NE2	5:D:603:HEM:C4D	2.77	0.47
1:D:354:LEU:HD11	1:D:426:MET:HA	1.96	0.47
1:D:559:TYR:CZ	3:E:93:ASP:HB2	2.48	0.47
1:D:130:HIS:CE1	1:D:132:THR:HG23	2.49	0.47
1:A:384:PHE:HE1	5:A:602:HEM:C3D	2.33	0.46
1:A:464:ARG:HG2	1:A:467:TRP:CE2	2.50	0.46
3:E:72:LYS:HA	3:E:72:LYS:HD2	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:HIS:NE2	5:A:602:HEM:C4D	2.77	0.46
1:A:282:THR:HG22	1:A:283:ASN:O	2.15	0.46
1:D:152:TRP:CD1	1:D:176:PHE:HE1	2.32	0.46
1:D:384:PHE:HE1	5:D:603:HEM:C3D	2.33	0.46
1:A:432:PHE:HB2	1:A:477:GLY:HA3	1.98	0.46
1:D:327:PHE:CB	9:D:607:3PE:H2	2.44	0.46
1:D:430:PHE:CE2	8:D:601:PGV:H91	2.50	0.46
1:A:534:ILE:O	1:A:538:LEU:HG	2.16	0.46
2:C:37:LEU:HD12	3:B:104:ASN:HD22	1.80	0.46
1:D:43:ILE:O	1:D:43:ILE:HG13	2.16	0.46
1:D:464:ARG:HG2	1:D:467:TRP:CE2	2.50	0.46
2:F:37:LEU:HD12	3:E:104:ASN:HD22	1.81	0.46
8:A:605:PGV:H172	8:A:605:PGV:H141	1.79	0.46
1:D:534:ILE:HD13	1:D:534:ILE:HA	1.78	0.46
1:A:430:PHE:CE2	8:A:607:PGV:H91	2.50	0.46
1:D:281:ILE:HB	1:D:286:LYS:HE3	1.98	0.46
8:D:601:PGV:H41	9:D:607:3PE:H2A1	1.96	0.46
1:A:230:LEU:HD23	1:A:230:LEU:HA	1.60	0.46
1:D:230:LEU:HD23	1:D:230:LEU:HA	1.60	0.46
1:D:376:ASN:HD22	3:E:108:MET:HE1	1.80	0.46
2:F:39:GLU:O	2:F:39:GLU:HG2	2.16	0.46
9:A:606:3PE:H2B2	9:A:606:3PE:H261	1.98	0.46
1:D:125:PRO:HG3	1:D:213:ALA:CB	2.46	0.46
1:D:318:GLU:HG3	1:D:319:HIS:CD2	2.51	0.46
1:A:43:ILE:O	1:A:43:ILE:HG13	2.16	0.45
1:D:534:ILE:O	1:D:538:LEU:HG	2.16	0.45
1:D:544:LEU:HD12	1:D:579:LYS:NZ	2.31	0.45
1:A:276:PHE:CD1	1:A:286:LYS:HB3	2.51	0.45
9:A:606:3PE:C2A	8:A:607:PGV:H52	2.46	0.45
1:D:432:PHE:HB2	1:D:477:GLY:HA3	1.98	0.45
1:D:576:LYS:HD2	1:D:576:LYS:HA	1.59	0.45
8:D:601:PGV:H52	9:D:607:3PE:C2A	2.45	0.45
3:E:35:PRO:HG2	3:E:107:VAL:HG22	1.98	0.45
3:E:45:GLN:O	3:E:46:GLU:HG2	2.16	0.45
1:A:196:GLN:OE1	1:A:213:ALA:HB2	2.17	0.45
1:A:576:LYS:HD2	1:A:576:LYS:HA	1.59	0.45
1:D:282:THR:HG22	1:D:283:ASN:O	2.15	0.45
1:A:420:LEU:HD12	9:D:607:3PE:H331	1.97	0.45
3:B:45:GLN:O	3:B:46:GLU:HG2	2.16	0.45
1:D:293:THR:HG22	4:D:602:HAS:HMB2	1.98	0.45
2:F:26:TYR:C	2:F:28:VAL:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:PRO:HG3	1:A:213:ALA:CB	2.46	0.45
1:A:465:PRO:HG2	1:D:465:PRO:HG2	1.98	0.45
1:A:505:THR:OG1	1:A:506:LEU:N	2.50	0.45
1:D:457:ASN:C	1:D:459:ASP:H	2.20	0.45
1:A:457:ASN:C	1:A:459:ASP:H	2.20	0.45
1:D:276:PHE:CD1	1:D:286:LYS:HB3	2.51	0.45
3:E:42:GLU:CB	3:E:114:VAL:HG21	2.42	0.45
1:A:469:GLY:HA3	1:D:469:GLY:HA3	1.97	0.45
3:E:48:LYS:O	3:E:49:LEU:HD23	2.17	0.45
1:A:360:ILE:HD13	2:C:26:TYR:CG	2.52	0.45
9:A:606:3PE:H331	1:D:420:LEU:HD12	1.98	0.45
1:A:228:TRP:HB3	1:A:392:VAL:HG11	1.99	0.45
1:D:196:GLN:OE1	1:D:213:ALA:HB2	2.17	0.45
1:D:388:VAL:HG23	4:D:602:HAS:HAC	1.99	0.45
1:A:336:MET:CE	9:D:607:3PE:C27	2.88	0.44
9:A:606:3PE:H322	9:A:606:3PE:H32	1.87	0.44
1:D:24:LEU:HD12	1:D:24:LEU:HA	1.69	0.44
1:D:327:PHE:CZ	2:F:17:ALA:HB1	2.52	0.44
1:D:360:ILE:HD13	2:F:26:TYR:CG	2.52	0.44
1:A:186:ILE:HD13	1:A:186:ILE:HA	1.64	0.44
1:A:281:ILE:HB	1:A:286:LYS:HE3	1.98	0.44
1:A:388:VAL:HG23	4:A:601:HAS:HAC	1.99	0.44
2:C:39:GLU:O	2:C:39:GLU:HG2	2.16	0.44
3:B:35:PRO:HG2	3:B:107:VAL:HG22	1.98	0.44
1:D:236:LEU:HB3	1:D:307:VAL:HG21	2.00	0.44
2:F:23:MET:SD	3:E:11:LEU:HB3	2.58	0.44
1:A:33:VAL:CG2	1:A:482:ALA:HB2	2.48	0.44
1:A:327:PHE:CZ	2:C:17:ALA:HB1	2.52	0.44
1:A:540:TYR:HA	1:A:543:PRO:HD2	1.99	0.44
1:A:544:LEU:HD12	1:A:579:LYS:NZ	2.31	0.44
4:A:601:HAS:H251	4:A:601:HAS:H282	1.76	0.44
9:A:606:3PE:C2A	8:A:607:PGV:H41	2.48	0.44
8:A:607:PGV:C31	9:D:607:3PE:H261	2.48	0.44
8:D:601:PGV:H252	8:D:601:PGV:H282	1.56	0.44
1:A:293:THR:HG22	4:A:601:HAS:HMB2	1.98	0.44
8:D:601:PGV:H41	9:D:607:3PE:C2A	2.48	0.44
1:A:497:LEU:HA	1:A:497:LEU:HD23	1.69	0.44
9:A:606:3PE:H261	8:D:601:PGV:C31	2.48	0.44
3:B:78:LYS:HA	3:B:147:ILE:O	2.18	0.44
1:A:29:ILE:HG23	5:A:602:HEM:CBB	2.48	0.44
1:A:318:GLU:HG3	1:A:319:HIS:CD2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:SER:HB2	1:A:370:VAL:HB	2.00	0.44
1:D:211:LEU:HD13	3:E:110:ILE:HD13	2.00	0.44
1:D:228:TRP:HB3	1:D:392:VAL:HG11	1.99	0.44
1:D:505:THR:OG1	1:D:506:LEU:N	2.50	0.44
3:B:42:GLU:CB	3:B:114:VAL:HG21	2.42	0.43
1:D:100:MET:HG2	1:D:139:LEU:HD21	2.00	0.43
1:D:119:VAL:HG13	1:D:120:LEU:N	2.23	0.43
1:D:261:ILE:HD13	1:D:261:ILE:HA	1.85	0.43
1:A:215:THR:HG22	1:A:216:LEU:H	1.83	0.43
1:A:236:LEU:HB3	1:A:307:VAL:HG21	2.00	0.43
2:C:23:MET:SD	3:B:11:LEU:HB3	2.58	0.43
3:B:57:TYR:HB2	3:B:85:VAL:HG12	2.00	0.43
1:D:33:VAL:CG2	1:D:482:ALA:HB2	2.48	0.43
3:E:61:ILE:HD13	3:E:61:ILE:HG21	1.72	0.43
1:A:100:MET:HG2	1:A:139:LEU:HD21	2.00	0.43
1:A:211:LEU:HD13	3:B:110:ILE:HD13	2.00	0.43
1:D:215:THR:HG22	1:D:216:LEU:H	1.83	0.43
1:A:354:LEU:HA	1:A:354:LEU:HD23	1.77	0.43
1:A:544:LEU:HD23	1:A:544:LEU:HA	1.74	0.43
2:C:26:TYR:C	2:C:28:VAL:H	2.20	0.43
1:D:29:ILE:HG23	5:D:603:HEM:CBB	2.48	0.43
3:E:78:LYS:HA	3:E:147:ILE:O	2.18	0.43
1:A:24:LEU:HA	1:A:24:LEU:HD12	1.69	0.43
1:D:540:TYR:HA	1:D:543:PRO:HD2	1.99	0.43
1:D:438:VAL:O	1:D:442:VAL:HG22	2.19	0.43
1:A:329:TRP:C	1:A:331:THR:H	2.22	0.43
1:D:497:LEU:HD23	1:D:497:LEU:HA	1.69	0.43
1:A:285:TRP:CE2	1:A:542:PRO:HB3	2.54	0.43
1:D:586:GLU:O	1:D:590:THR:OG1	2.27	0.43
8:F:101:PGV:H291	8:F:101:PGV:H322	1.81	0.43
1:A:369:ASN:HD21	3:B:27:ALA:N	2.16	0.43
2:C:37:LEU:CD1	3:B:104:ASN:HD22	2.32	0.43
3:B:72:LYS:HD2	3:B:72:LYS:HA	1.63	0.43
1:D:114:THR:OG1	1:D:116:ARG:HD3	2.19	0.43
1:D:329:TRP:C	1:D:331:THR:H	2.22	0.43
1:A:15:LEU:HD23	1:A:15:LEU:HA	1.69	0.43
3:B:48:LYS:O	3:B:49:LEU:HD23	2.17	0.43
3:B:78:LYS:HE2	3:B:149:GLU:HB2	2.01	0.43
1:D:15:LEU:HA	1:D:15:LEU:HD23	1.69	0.43
1:D:285:TRP:CE2	1:D:542:PRO:HB3	2.54	0.43
1:D:369:ASN:HD21	3:E:27:ALA:N	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:LEU:HD13	5:D:603:HEM:HBC2	2.01	0.43
1:D:465:PRO:O	1:D:468:THR:HG23	2.19	0.43
2:F:37:LEU:CD1	3:E:104:ASN:HD22	2.32	0.43
3:E:78:LYS:HE2	3:E:149:GLU:HB2	2.01	0.43
1:A:229:LEU:HD22	4:A:601:HAS:HMC2	2.00	0.42
9:A:606:3PE:C27	1:D:336:MET:CE	2.89	0.42
1:D:357:ILE:HG21	7:D:605:DLX:C44	2.49	0.42
1:D:360:ILE:HD13	2:F:26:TYR:CB	2.49	0.42
1:A:114:THR:OG1	1:A:116:ARG:HD3	2.19	0.42
1:A:360:ILE:HD13	2:C:26:TYR:CB	2.49	0.42
9:A:606:3PE:H2B2	9:A:606:3PE:H281	1.87	0.42
1:D:229:LEU:HD22	4:D:602:HAS:HMC2	2.00	0.42
1:D:522:LEU:O	1:D:523:ASN:HB2	2.19	0.42
1:A:357:ILE:HG21	7:A:604:DLX:C44	2.49	0.42
1:A:458:PRO:HA	1:A:463:TYR:CE1	2.54	0.42
1:A:465:PRO:O	1:A:468:THR:HG23	2.19	0.42
1:D:270:VAL:HG22	1:D:273:HIS:CE1	2.55	0.42
1:D:458:PRO:HA	1:D:463:TYR:CE1	2.54	0.42
1:D:524:ASN:O	1:D:528:TRP:HD1	2.02	0.42
4:D:602:HAS:H271	4:D:602:HAS:H212	1.70	0.42
1:A:393:LEU:HD13	5:A:602:HEM:HBC2	2.01	0.42
2:C:34:TYR:OH	3:B:26:ALA:HB2	2.20	0.42
1:D:82:ALA:HB2	1:D:89:LEU:HG	2.01	0.42
1:D:214:ARG:HG2	1:D:275:GLN:OE1	2.19	0.42
1:D:367:SER:HB2	1:D:370:VAL:HB	2.00	0.42
9:D:607:3PE:H2B2	9:D:607:3PE:H281	1.87	0.42
1:A:214:ARG:HG2	1:A:275:GLN:OE1	2.19	0.42
1:A:427:GLN:CB	8:A:607:PGV:H251	2.49	0.42
1:A:438:VAL:O	1:A:442:VAL:HG22	2.18	0.42
3:B:120:LYS:HB3	3:B:120:LYS:HE2	1.74	0.42
1:D:311:LEU:HD23	1:D:311:LEU:HA	1.74	0.42
1:D:506:LEU:HD12	1:D:506:LEU:HA	1.88	0.42
1:A:167:LYS:HB2	1:A:167:LYS:HE3	1.70	0.42
1:A:208:ILE:HG22	1:A:556:SER:O	2.20	0.42
1:A:522:LEU:O	1:A:523:ASN:HB2	2.19	0.42
9:A:606:3PE:H2A1	8:A:607:PGV:H41	1.96	0.42
3:B:101:HIS:CE1	3:B:130:VAL:HG11	2.55	0.42
1:D:200:LEU:HD22	1:D:208:ILE:HB	2.02	0.42
1:D:242:LYS:HB3	1:D:509:PRO:HB2	2.01	0.42
2:F:22:MET:C	2:F:24:VAL:N	2.73	0.42
3:E:120:LYS:HE2	3:E:120:LYS:HB3	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LEU:HD12	1:A:181:LEU:HA	1.77	0.42
1:D:209:ASN:OD1	1:D:552:VAL:HG11	2.20	0.42
3:E:57:TYR:HB2	3:E:85:VAL:HG12	2.00	0.42
3:E:78:LYS:HE3	3:E:149:GLU:OE1	2.20	0.42
3:E:101:HIS:CE1	3:E:130:VAL:HG11	2.55	0.42
1:A:517:ALA:HA	1:A:518:PRO:HD3	1.90	0.42
3:B:105:TYR:CE1	3:B:117:MET:HB3	2.55	0.42
1:D:23:LEU:HD23	1:D:23:LEU:HA	1.74	0.42
4:D:602:HAS:H282	4:D:602:HAS:H251	1.76	0.42
1:A:144:SER:O	1:A:147:PRO:HD2	2.20	0.41
1:A:200:LEU:HD22	1:A:208:ILE:HB	2.02	0.41
1:A:270:VAL:HG22	1:A:273:HIS:CE1	2.55	0.41
4:A:601:HAS:H262	4:A:601:HAS:H132	1.80	0.41
1:D:541:ILE:HB	1:D:542:PRO:HD3	2.02	0.41
1:D:544:LEU:O	1:D:548:SER:OG	2.18	0.41
1:A:261:ILE:HD13	1:A:261:ILE:HA	1.85	0.41
1:A:298:LEU:N	1:A:299:PRO:HD2	2.36	0.41
1:A:524:ASN:O	1:A:528:TRP:HD1	2.02	0.41
8:C:101:PGV:H322	8:C:101:PGV:H291	1.81	0.41
1:A:215:THR:C	1:A:217:PHE:N	2.73	0.41
1:D:110:TRP:CZ3	1:D:111:ALA:HB2	2.56	0.41
1:D:278:ASP:O	1:D:286:LYS:NZ	2.42	0.41
4:D:602:HAS:H262	4:D:602:HAS:H132	1.80	0.41
1:A:361:THR:HG22	1:A:383:HIS:HB2	2.03	0.41
4:A:601:HAS:H271	4:A:601:HAS:H212	1.70	0.41
1:D:60:HIS:CD2	5:D:603:HEM:C4D	3.09	0.41
1:D:361:THR:HG22	1:D:383:HIS:HB2	2.03	0.41
1:D:473:LEU:HD23	1:D:473:LEU:HA	1.81	0.41
2:F:34:TYR:OH	3:E:26:ALA:HB2	2.20	0.41
1:A:82:ALA:HB2	1:A:89:LEU:HG	2.01	0.41
1:A:242:LYS:HB3	1:A:509:PRO:HB2	2.01	0.41
1:A:381:PRO:HD3	1:A:447:ARG:HD2	2.02	0.41
8:A:607:PGV:H31	8:A:607:PGV:H62	1.87	0.41
3:B:78:LYS:HE3	3:B:149:GLU:OE1	2.20	0.41
1:D:208:ILE:HG22	1:D:556:SER:O	2.20	0.41
1:D:215:THR:C	1:D:217:PHE:N	2.73	0.41
1:D:381:PRO:HD3	1:D:447:ARG:HD2	2.02	0.41
3:E:105:TYR:CE1	3:E:117:MET:HB3	2.55	0.41
1:A:244:VAL:HG12	1:A:245:SER:N	2.34	0.41
1:A:60:HIS:CD2	5:A:602:HEM:C4D	3.09	0.41
1:D:153:ILE:HD13	1:D:153:ILE:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:GLN:CB	8:D:601:PGV:H251	2.51	0.41
1:A:209:ASN:OD1	1:A:552:VAL:HG11	2.20	0.41
1:A:357:ILE:HG13	7:A:604:DLX:C28	2.51	0.41
3:B:9:LEU:HA	3:B:9:LEU:HD12	1.76	0.41
1:D:298:LEU:N	1:D:299:PRO:HD2	2.36	0.41
1:D:420:LEU:HD23	1:D:420:LEU:HA	1.84	0.41
1:A:13:ILE:HD13	1:A:13:ILE:HA	1.83	0.41
1:A:23:LEU:HA	1:A:23:LEU:HD23	1.74	0.41
1:D:219:PHE:CD1	1:D:540:TYR:CE2	3.09	0.41
1:D:517:ALA:HA	1:D:518:PRO:HD3	1.90	0.41
1:A:282:THR:HB	1:A:285:TRP:CD1	2.56	0.41
2:C:22:MET:C	2:C:24:VAL:N	2.73	0.41
1:D:144:SER:O	1:D:147:PRO:HD2	2.20	0.41
1:D:167:LYS:HB2	1:D:167:LYS:HE3	1.70	0.41
1:A:110:TRP:CZ3	1:A:111:ALA:HB2	2.56	0.40
1:A:185:MET:HG2	1:A:223:PRO:HB2	2.02	0.40
1:A:457:ASN:O	1:A:459:ASP:N	2.54	0.40
7:A:604:DLX:C29	8:A:607:PGV:H131	2.52	0.40
2:C:15:THR:H	2:C:15:THR:HG23	1.60	0.40
1:D:13:ILE:HD13	1:D:13:ILE:HA	1.83	0.40
1:D:282:THR:HB	1:D:285:TRP:CD1	2.56	0.40
1:D:357:ILE:HG13	7:D:605:DLX:C28	2.51	0.40
1:D:457:ASN:O	1:D:459:ASP:N	2.54	0.40
1:A:473:LEU:HA	1:A:473:LEU:HD23	1.81	0.40
3:B:84:VAL:HB	3:B:120:LYS:HE2	2.03	0.40
1:A:541:ILE:HB	1:A:542:PRO:HD3	2.02	0.40
3:B:41:VAL:HG13	3:B:42:GLU:N	2.35	0.40
1:D:244:VAL:HG12	1:D:245:SER:N	2.34	0.40
8:D:601:PGV:H131	7:D:605:DLX:C29	2.50	0.40
3:E:106:ASN:OD1	3:E:132:HIS:NE2	2.52	0.40
1:A:120:LEU:HA	1:A:120:LEU:HD12	1.71	0.40
1:A:219:PHE:CD1	1:A:540:TYR:CE2	3.09	0.40
1:A:493:ILE:HD13	1:A:493:ILE:HA	1.85	0.40
1:D:65:VAL:HB	1:D:228:TRP:CH2	2.56	0.40
1:D:225:VAL:HA	1:D:228:TRP:CE3	2.56	0.40
1:A:157:ILE:HD13	1:A:157:ILE:HA	1.89	0.40
1:A:225:VAL:HA	1:A:228:TRP:CE3	2.56	0.40
1:A:262:LEU:HD23	1:A:299:PRO:HD3	2.03	0.40
1:A:417:LEU:HD12	1:A:487:PHE:CD1	2.57	0.40
3:B:61:ILE:HD13	3:B:61:ILE:HG21	1.72	0.40
1:D:85:LEU:HD13	1:D:155:SER:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:LEU:HD21	1:D:558:ALA:HB2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	577/587 (98%)	482 (84%)	93 (16%)	2 (0%)	37	66
1	D	577/587 (98%)	481 (83%)	94 (16%)	2 (0%)	37	66
2	C	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	3	18
2	F	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	3	18
3	B	145/147 (99%)	118 (81%)	27 (19%)	0	100	100
3	E	145/147 (99%)	118 (81%)	27 (19%)	0	100	100
All	All	1504/1532 (98%)	1249 (83%)	249 (17%)	6 (0%)	32	60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	LYS
1	D	44	LYS
1	A	46	GLU
1	D	46	GLU
2	C	23	MET
2	F	23	MET

### 5.3.2 Protein sidechains [i](#)

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	486/492 (99%)	480 (99%)	6 (1%)	67	80
1	D	486/492 (99%)	480 (99%)	6 (1%)	67	80
2	C	28/28 (100%)	28 (100%)	0	100	100
2	F	28/28 (100%)	28 (100%)	0	100	100
3	B	125/125 (100%)	125 (100%)	0	100	100
3	E	125/125 (100%)	125 (100%)	0	100	100
All	All	1278/1290 (99%)	1266 (99%)	12 (1%)	74	86

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	40	SER
1	A	42	ILE
1	A	214	ARG
1	A	219	PHE
1	A	575	LYS
1	D	39	ARG
1	D	40	SER
1	D	42	ILE
1	D	214	ARG
1	D	219	PHE
1	D	575	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	275	GLN
1	A	341	ASN
1	A	369	ASN
1	A	371	ASN
1	A	375	HIS
1	A	376	ASN
1	A	472	GLN
1	A	524	ASN

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Mol	Chain	Res	Type
1	A	560	ASN
1	D	94	GLN
1	D	341	ASN
1	D	369	ASN
1	D	371	ASN
1	D	375	HIS
1	D	376	ASN
1	D	472	GLN
1	D	524	ASN
1	D	560	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	HAS	D	602	2,1	69,72,72	3.18	26 (37%)	73,109,109	3.59	41 (56%)
4	HAS	A	601	2,1	69,72,72	3.18	26 (37%)	73,109,109	3.59	41 (56%)
5	HEM	D	603	1	41,50,50	1.60	6 (14%)	45,82,82	1.46	6 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	PGV	A	605	-	50,50,50	0.87	2 (4%)	53,56,56	1.10	5 (9%)
8	PGV	C	101	-	50,50,50	0.91	2 (4%)	53,56,56	1.09	4 (7%)
8	PGV	D	606	-	50,50,50	0.87	2 (4%)	53,56,56	1.10	5 (9%)
8	PGV	A	607	8	50,50,50	0.94	2 (4%)	53,56,56	1.15	3 (5%)
8	PGV	D	601	8	50,50,50	0.94	2 (4%)	53,56,56	1.15	3 (5%)
8	PGV	F	101	-	50,50,50	0.91	2 (4%)	53,56,56	1.09	4 (7%)
9	3PE	A	606	-	50,50,50	0.26	0	53,55,55	0.30	0
9	3PE	D	607	-	50,50,50	0.26	0	53,55,55	0.31	0
10	CUA	E	600	3	0,1,1	-	-	-	-	-
10	CUA	B	600	3	0,1,1	-	-	-	-	-
5	HEM	A	602	1	41,50,50	1.60	6 (14%)	45,82,82	1.47	6 (13%)
7	DLX	D	605	2,1	48,48,48	3.23	12 (25%)	59,61,61	3.24	22 (37%)
7	DLX	A	604	2,1	48,48,48	3.24	12 (25%)	59,61,61	3.24	22 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HAS	D	602	2,1	1/1/8/18	23/40/82/82	-
4	HAS	A	601	2,1	1/1/8/18	23/40/82/82	-
5	HEM	D	603	1	-	2/12/54/54	-
8	PGV	A	605	-	-	16/55/55/55	-
8	PGV	C	101	-	-	21/55/55/55	-
8	PGV	D	606	-	-	16/55/55/55	-
8	PGV	A	607	8	-	28/55/55/55	-
8	PGV	D	601	8	-	28/55/55/55	-
8	PGV	F	101	-	-	21/55/55/55	-
9	3PE	A	606	-	-	28/54/54/54	-
9	3PE	D	607	-	-	28/54/54/54	-
5	HEM	A	602	1	-	2/12/54/54	-
7	DLX	D	605	2,1	-	28/41/57/57	0/2/2/2
7	DLX	A	604	2,1	-	28/41/57/57	0/2/2/2

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	602	HAS	CHD-C4A	9.83	1.49	1.35
4	A	601	HAS	CHD-C4A	9.83	1.48	1.35
7	A	604	DLX	C26-C27	8.47	1.53	1.33
7	A	604	DLX	C30-C31	8.45	1.53	1.33
7	D	605	DLX	C30-C31	8.45	1.53	1.33
7	D	605	DLX	C26-C27	8.45	1.53	1.33
4	A	601	HAS	C22-C23	8.01	1.52	1.33
4	D	602	HAS	C22-C23	8.01	1.52	1.33
7	D	605	DLX	C22-C23	7.99	1.52	1.33
7	A	604	DLX	C22-C23	7.98	1.52	1.33
4	D	602	HAS	C18-C19	7.97	1.52	1.33
4	A	601	HAS	C18-C19	7.93	1.52	1.33
7	A	604	DLX	C14-C15	7.86	1.51	1.33
7	D	605	DLX	C14-C15	7.83	1.51	1.33
4	A	601	HAS	C14-C15	7.81	1.51	1.33
4	D	602	HAS	C14-C15	7.79	1.51	1.33
7	A	604	DLX	C18-C19	7.74	1.51	1.33
7	D	605	DLX	C18-C19	7.73	1.51	1.33
4	D	602	HAS	C29-C30	7.34	1.53	1.32
4	A	601	HAS	C29-C30	7.32	1.53	1.32
4	A	601	HAS	O1D-CGD	6.35	1.43	1.22
4	D	602	HAS	O1D-CGD	6.35	1.43	1.22
4	A	601	HAS	O1A-CGA	6.15	1.42	1.22
4	D	602	HAS	O1A-CGA	6.15	1.42	1.22
7	D	605	DLX	O12-C04	6.03	1.36	1.23
7	A	604	DLX	O12-C04	6.03	1.36	1.23
5	A	602	HEM	C3C-C2C	-5.92	1.32	1.40
5	D	603	HEM	C3C-C2C	-5.92	1.32	1.40
4	A	601	HAS	CHC-C4B	5.77	1.49	1.35
4	D	602	HAS	CHC-C4B	5.75	1.49	1.35
7	A	604	DLX	O11-C01	5.64	1.36	1.24
7	D	605	DLX	O11-C01	5.64	1.36	1.24
7	A	604	DLX	C05-C04	-5.28	1.37	1.48
7	D	605	DLX	C05-C04	-5.26	1.37	1.48
4	A	601	HAS	CHB-C1D	5.23	1.49	1.38
4	D	602	HAS	CHB-C1D	5.23	1.49	1.38
7	D	605	DLX	C03-C04	-5.19	1.38	1.48
4	D	602	HAS	CHA-C1A	5.18	1.48	1.38
4	A	601	HAS	CHA-C1A	5.17	1.48	1.38
7	A	604	DLX	C02-C01	-5.15	1.39	1.48
7	D	605	DLX	C02-C01	-5.15	1.39	1.48
7	A	604	DLX	C03-C04	-5.14	1.38	1.48
4	A	601	HAS	CHB-C1B	4.40	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	602	HAS	CHB-C1B	4.40	1.49	1.39
8	A	607	PGV	O01-C1	4.37	1.46	1.34
8	D	601	PGV	O01-C1	4.37	1.46	1.34
8	C	101	PGV	O01-C1	4.17	1.46	1.34
8	F	101	PGV	O01-C1	4.17	1.46	1.34
8	C	101	PGV	O03-C19	4.16	1.45	1.33
8	F	101	PGV	O03-C19	4.16	1.45	1.33
8	A	607	PGV	O03-C19	4.04	1.45	1.33
8	D	601	PGV	O03-C19	4.04	1.45	1.33
4	A	601	HAS	CHA-C4D	4.03	1.48	1.39
4	D	602	HAS	CHA-C4D	4.03	1.48	1.39
4	D	602	HAS	C1D-ND	-3.89	1.33	1.40
4	A	601	HAS	C1D-ND	-3.88	1.33	1.40
8	A	605	PGV	O03-C19	3.81	1.44	1.33
8	D	606	PGV	O03-C19	3.81	1.44	1.33
8	A	605	PGV	O01-C1	3.79	1.45	1.34
8	D	606	PGV	O01-C1	3.79	1.45	1.34
4	D	602	HAS	O2D-CGD	3.74	1.43	1.30
4	A	601	HAS	O2D-CGD	3.71	1.43	1.30
4	D	602	HAS	O2A-CGA	3.61	1.42	1.30
4	A	601	HAS	O2A-CGA	3.61	1.42	1.30
4	A	601	HAS	C1A-NA	-3.60	1.32	1.39
4	D	602	HAS	C1A-NA	-3.60	1.32	1.39
4	A	601	HAS	C3C-C2C	-3.39	1.35	1.40
4	D	602	HAS	C3C-C2C	-3.36	1.35	1.40
4	A	601	HAS	C4B-NB	-3.26	1.34	1.40
4	D	602	HAS	C4B-NB	-3.26	1.34	1.40
4	D	602	HAS	C4C-CHD	3.25	1.50	1.41
4	A	601	HAS	C4C-CHD	3.25	1.50	1.41
4	A	601	HAS	FE-NA	3.24	2.08	1.95
4	D	602	HAS	C4A-NA	-3.23	1.33	1.39
4	A	601	HAS	C4A-NA	-3.23	1.33	1.39
4	D	602	HAS	FE-NA	3.22	2.08	1.95
4	A	601	HAS	C1C-CHC	3.08	1.49	1.41
4	D	602	HAS	C1C-CHC	3.08	1.49	1.41
5	A	602	HEM	C3B-C2B	-2.82	1.31	1.37
5	D	603	HEM	C3B-C2B	-2.81	1.31	1.37
7	A	604	DLX	C06-C01	-2.58	1.39	1.44
7	D	605	DLX	C06-C01	-2.58	1.39	1.44
5	D	603	HEM	C3D-C2D	-2.56	1.31	1.36
5	A	602	HEM	C3D-C2D	-2.52	1.31	1.36
5	A	602	HEM	C2A-C3A	-2.46	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	603	HEM	C2A-C3A	-2.44	1.30	1.37
5	A	602	HEM	CAB-C3B	2.36	1.53	1.47
5	D	603	HEM	CAB-C3B	2.36	1.53	1.47
5	A	602	HEM	C3C-CAC	2.34	1.52	1.47
4	D	602	HAS	C4D-ND	-2.31	1.34	1.38
5	D	603	HEM	C3C-CAC	2.31	1.52	1.47
4	A	601	HAS	C4D-ND	-2.30	1.34	1.38
4	A	601	HAS	C1B-NB	-2.17	1.34	1.38
4	D	602	HAS	C1B-NB	-2.15	1.34	1.38
4	D	602	HAS	FE-NB	2.15	2.09	1.97
4	A	601	HAS	FE-NB	2.14	2.08	1.97
4	A	601	HAS	C4B-C3B	2.12	1.48	1.44
7	D	605	DLX	C28-C27	2.08	1.55	1.51
7	A	604	DLX	C28-C27	2.08	1.55	1.51
4	D	602	HAS	C4B-C3B	2.06	1.48	1.44

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	605	DLX	C13-C14-C15	-10.03	110.10	126.79
7	A	604	DLX	C13-C14-C15	-10.02	110.10	126.79
7	A	604	DLX	C16-C15-C14	-7.09	106.78	121.12
4	D	602	HAS	C17-C18-C19	-7.08	110.61	127.66
7	D	605	DLX	C16-C15-C14	-7.08	106.80	121.12
4	A	601	HAS	C17-C18-C19	-7.07	110.63	127.66
4	A	601	HAS	C21-C22-C23	-6.92	111.00	127.66
4	D	602	HAS	C21-C22-C23	-6.92	111.01	127.66
7	D	605	DLX	C20-C19-C18	-6.75	107.46	121.12
7	A	604	DLX	C20-C19-C18	-6.72	107.51	121.12
7	D	605	DLX	C17-C18-C19	-6.72	111.48	127.66
7	A	604	DLX	C17-C18-C19	-6.71	111.50	127.66
4	A	601	HAS	C16-C15-C14	-6.68	107.59	121.12
4	D	602	HAS	C16-C15-C14	-6.67	107.63	121.12
7	A	604	DLX	C25-C26-C27	-6.59	111.79	127.66
7	D	605	DLX	C25-C26-C27	-6.58	111.81	127.66
4	D	602	HAS	C24-C23-C22	-6.49	107.98	121.12
4	A	601	HAS	C24-C23-C22	-6.47	108.02	121.12
4	A	601	HAS	CHA-C1A-NA	6.47	131.44	124.44
7	A	604	DLX	C21-C22-C23	-6.46	112.10	127.66
4	D	602	HAS	CHA-C1A-NA	6.46	131.43	124.44
7	D	605	DLX	C21-C22-C23	-6.45	112.13	127.66
4	A	601	HAS	C13-C14-C15	-6.22	112.69	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	602	HAS	C13-C14-C15	-6.20	112.72	127.66
4	A	601	HAS	CHB-C1B-NB	6.15	131.10	124.42
4	D	602	HAS	CHB-C1B-NB	6.15	131.09	124.42
4	D	602	HAS	O2A-CGA-O1A	-6.07	108.18	123.30
4	A	601	HAS	O2A-CGA-O1A	-6.05	108.22	123.30
4	A	601	HAS	CHA-C4D-ND	5.97	130.91	124.42
4	D	602	HAS	CHA-C4D-ND	5.94	130.87	124.42
7	A	604	DLX	C46-C19-C18	-5.90	108.54	123.68
7	D	605	DLX	C46-C19-C18	-5.89	108.56	123.68
4	D	602	HAS	C20-C19-C18	-5.86	109.25	121.12
4	A	601	HAS	C20-C19-C18	-5.86	109.27	121.12
7	D	605	DLX	C29-C30-C31	-5.82	113.64	127.66
7	A	604	DLX	C29-C30-C31	-5.81	113.67	127.66
7	D	605	DLX	C24-C23-C22	-5.72	109.55	121.12
7	A	604	DLX	C24-C23-C22	-5.70	109.58	121.12
4	D	602	HAS	O2D-CGD-O1D	-5.66	109.19	123.30
4	A	601	HAS	O2D-CGD-O1D	-5.64	109.24	123.30
4	D	602	HAS	CHB-C1D-ND	5.62	131.31	124.37
4	A	601	HAS	CHB-C1D-ND	5.59	131.26	124.37
7	A	604	DLX	C44-C27-C26	-5.34	109.97	123.68
7	D	605	DLX	C44-C27-C26	-5.34	109.99	123.68
4	D	602	HAS	C27-C19-C18	-5.28	110.12	123.68
4	A	601	HAS	C27-C19-C18	-5.27	110.15	123.68
4	A	601	HAS	CHD-C4A-NA	5.26	130.12	124.43
4	D	602	HAS	CHD-C4A-NA	5.23	130.09	124.43
4	A	601	HAS	CHA-C4D-C3D	-5.18	117.22	124.84
4	D	602	HAS	CHA-C4D-C3D	-5.18	117.23	124.84
4	D	602	HAS	CHA-C1A-C2A	-5.07	116.73	124.94
7	A	604	DLX	C43-C31-C30	-5.05	110.72	123.68
7	D	605	DLX	C43-C31-C30	-5.05	110.72	123.68
4	A	601	HAS	CHA-C1A-C2A	-5.05	116.76	124.94
8	A	607	PGV	O01-C1-C2	5.00	122.27	111.50
8	D	601	PGV	O01-C1-C2	5.00	122.27	111.50
4	D	602	HAS	C2D-C3D-C4D	-4.85	103.03	106.49
4	A	601	HAS	C1A-CHA-C4D	-4.83	115.64	126.06
4	D	602	HAS	C1A-CHA-C4D	-4.83	115.64	126.06
4	A	601	HAS	C2D-C3D-C4D	-4.81	103.06	106.49
4	A	601	HAS	C26-C15-C14	-4.79	111.38	123.68
4	D	602	HAS	C26-C15-C14	-4.79	111.39	123.68
7	A	604	DLX	C32-C31-C30	-4.78	111.44	121.12
7	D	605	DLX	C32-C31-C30	-4.77	111.47	121.12
7	D	605	DLX	C45-C23-C22	-4.74	111.52	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	604	DLX	C45-C23-C22	-4.73	111.53	123.68
8	C	101	PGV	O01-C1-C2	4.55	121.32	111.50
8	F	101	PGV	O01-C1-C2	4.55	121.30	111.50
5	A	602	HEM	CAD-CBD-CGD	-4.55	103.82	113.60
5	D	603	HEM	CAD-CBD-CGD	-4.54	103.83	113.60
8	A	605	PGV	O01-C1-C2	4.51	121.23	111.50
8	D	606	PGV	O01-C1-C2	4.51	121.23	111.50
4	A	601	HAS	C1B-CHB-C1D	-4.48	115.68	125.96
4	D	602	HAS	C1B-CHB-C1D	-4.48	115.68	125.96
7	A	604	DLX	C47-C15-C14	-4.43	112.31	123.68
7	D	605	DLX	C47-C15-C14	-4.41	112.36	123.68
4	A	601	HAS	O1D-CGD-CBD	-4.26	109.41	123.08
4	D	602	HAS	O1D-CGD-CBD	-4.26	109.41	123.08
4	A	601	HAS	O1A-CGA-CBA	-4.25	109.43	123.08
4	D	602	HAS	O1A-CGA-CBA	-4.25	109.43	123.08
4	A	601	HAS	C25-C23-C22	-4.16	113.00	123.68
4	D	602	HAS	C25-C23-C22	-4.15	113.03	123.68
4	A	601	HAS	CHB-C1B-C2B	-4.08	118.60	124.98
4	D	602	HAS	CHB-C1B-C2B	-4.08	118.60	124.98
4	D	602	HAS	C32-C30-C29	-4.04	110.98	122.65
4	A	601	HAS	C32-C30-C29	-4.03	111.01	122.65
4	A	601	HAS	CHC-C4B-NB	3.76	129.03	124.38
4	D	602	HAS	CHC-C4B-NB	3.73	128.99	124.38
4	A	601	HAS	CAA-C2A-C3A	3.70	134.77	127.88
4	D	602	HAS	CAA-C2A-C3A	3.69	134.76	127.88
4	A	601	HAS	C28-C29-C30	-3.69	115.13	127.75
4	D	602	HAS	C28-C29-C30	-3.69	115.13	127.75
4	D	602	HAS	CMC-C2C-C3C	3.64	131.49	124.68
4	A	601	HAS	CMC-C2C-C3C	3.62	131.45	124.68
5	A	602	HEM	CBA-CAA-C2A	-3.46	106.72	112.62
5	D	603	HEM	CBA-CAA-C2A	-3.46	106.72	112.62
7	D	605	DLX	C28-C27-C26	-3.31	114.43	121.12
7	A	604	DLX	C28-C27-C26	-3.30	114.43	121.12
4	A	601	HAS	C26-C15-C16	-3.11	110.05	115.27
4	D	602	HAS	C26-C15-C16	-3.08	110.08	115.27
8	A	605	PGV	O03-C19-C20	3.05	121.49	111.91
8	D	606	PGV	O03-C19-C20	3.05	121.47	111.91
5	D	603	HEM	CAA-CBA-CGA	-3.03	105.27	113.76
5	A	602	HEM	CAA-CBA-CGA	-3.02	105.30	113.76
4	A	601	HAS	OMD-CMD-C2D	-2.96	119.00	125.69
4	D	602	HAS	OMD-CMD-C2D	-2.93	119.07	125.69
4	D	602	HAS	CAD-CBD-CGD	-2.92	107.31	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	602	HAS	C31-C30-C29	-2.92	114.20	122.65
4	A	601	HAS	C31-C30-C29	-2.92	114.21	122.65
4	A	601	HAS	CAD-CBD-CGD	-2.90	107.36	113.60
8	F	101	PGV	O03-C19-C20	2.89	120.96	111.91
8	C	101	PGV	O03-C19-C20	2.88	120.96	111.91
5	A	602	HEM	C3B-C2B-C1B	2.88	108.62	106.49
8	A	607	PGV	O03-C19-C20	2.83	120.78	111.91
8	D	601	PGV	O03-C19-C20	2.83	120.78	111.91
5	D	603	HEM	C3B-C2B-C1B	2.83	108.58	106.49
7	D	605	DLX	C45-C23-C24	-2.79	110.58	115.27
7	A	604	DLX	C45-C23-C24	-2.77	110.61	115.27
4	A	601	HAS	C13-C12-C11	-2.75	110.22	114.35
4	A	601	HAS	C4B-NB-C1B	2.74	107.91	105.07
4	D	602	HAS	C4B-NB-C1B	2.74	107.90	105.07
4	D	602	HAS	C13-C12-C11	-2.72	110.27	114.35
4	D	602	HAS	C1D-ND-C4D	2.69	107.85	105.07
4	A	601	HAS	C1D-ND-C4D	2.68	107.84	105.07
4	D	602	HAS	CMC-C2C-C1C	-2.56	124.52	128.46
4	A	601	HAS	CMC-C2C-C1C	-2.56	124.53	128.46
4	A	601	HAS	CAA-C2A-C1A	-2.48	120.22	124.89
5	A	602	HEM	CHC-C4B-C3B	2.47	128.35	124.57
7	D	605	DLX	C43-C31-C32	-2.46	111.13	115.27
7	A	604	DLX	C43-C31-C32	-2.46	111.13	115.27
4	D	602	HAS	CAA-C2A-C1A	-2.46	120.25	124.89
5	D	603	HEM	CHC-C4B-C3B	2.45	128.32	124.57
8	C	101	PGV	C02-O01-C1	-2.44	111.78	117.79
8	F	101	PGV	C02-O01-C1	-2.44	111.78	117.79
4	A	601	HAS	C32-C30-C31	-2.43	109.25	114.60
8	D	601	PGV	C21-C20-C19	-2.42	104.82	113.62
8	A	607	PGV	C21-C20-C19	-2.41	104.84	113.62
4	D	602	HAS	C32-C30-C31	-2.40	109.29	114.60
5	D	603	HEM	CMC-C2C-C3C	2.39	129.15	124.68
5	A	602	HEM	CMC-C2C-C3C	2.38	129.13	124.68
7	A	604	DLX	C03-C04-C05	2.37	119.83	116.62
7	D	605	DLX	C03-C04-C05	2.36	119.83	116.62
7	D	605	DLX	O12-C04-C05	-2.35	119.46	121.96
4	A	601	HAS	C1D-C2D-C3D	2.34	108.97	107.11
4	D	602	HAS	C1D-C2D-C3D	2.33	108.96	107.11
8	A	605	PGV	O03-C19-O04	-2.31	117.75	123.59
7	A	604	DLX	O12-C04-C05	-2.30	119.50	121.96
8	D	606	PGV	O03-C19-O04	-2.30	117.79	123.59
7	A	604	DLX	C13-C05-C04	2.29	118.74	116.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	605	DLX	C13-C05-C04	2.28	118.73	116.88
8	A	605	PGV	C02-O01-C1	-2.28	112.19	117.79
8	D	606	PGV	C02-O01-C1	-2.26	112.23	117.79
8	D	606	PGV	O01-C1-O02	-2.22	118.33	123.70
8	A	605	PGV	O01-C1-O02	-2.20	118.37	123.70
7	D	605	DLX	C47-C15-C16	-2.16	111.64	115.27
7	A	604	DLX	C47-C15-C16	-2.15	111.65	115.27
4	A	601	HAS	C25-C23-C24	-2.14	111.68	115.27
4	D	602	HAS	C25-C23-C24	-2.14	111.68	115.27
7	A	604	DLX	C13-C05-C06	-2.10	120.53	123.30
7	D	605	DLX	C13-C05-C06	-2.09	120.56	123.30
8	C	101	PGV	O01-C1-O02	-2.05	118.74	123.70
8	F	101	PGV	O01-C1-O02	-2.05	118.75	123.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	601	HAS	NA
4	D	602	HAS	NA

All (292) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	HAS	C3A-C2A-CAA-CBA
4	A	601	HAS	C1D-C2D-CMD-OMD
4	A	601	HAS	C13-C14-C15-C26
4	A	601	HAS	C14-C15-C16-C17
4	A	601	HAS	C17-C18-C19-C20
4	A	601	HAS	C18-C19-C20-C21
4	A	601	HAS	C19-C20-C21-C22
4	A	601	HAS	C21-C22-C23-C24
4	A	601	HAS	C28-C29-C30-C32
4	D	602	HAS	C3A-C2A-CAA-CBA
4	D	602	HAS	C1D-C2D-CMD-OMD
4	D	602	HAS	C13-C14-C15-C26
4	D	602	HAS	C14-C15-C16-C17
4	D	602	HAS	C17-C18-C19-C20
4	D	602	HAS	C18-C19-C20-C21
4	D	602	HAS	C19-C20-C21-C22
4	D	602	HAS	C21-C22-C23-C24
4	D	602	HAS	C28-C29-C30-C32
7	A	604	DLX	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
7	A	604	DLX	C25-C26-C27-C28
7	A	604	DLX	C21-C22-C23-C45
7	A	604	DLX	C21-C22-C23-C24
7	A	604	DLX	C17-C18-C19-C46
7	A	604	DLX	C13-C14-C15-C16
7	D	605	DLX	C29-C30-C31-C32
7	D	605	DLX	C25-C26-C27-C28
7	D	605	DLX	C21-C22-C23-C45
7	D	605	DLX	C21-C22-C23-C24
7	D	605	DLX	C17-C18-C19-C46
7	D	605	DLX	C13-C14-C15-C16
8	A	605	PGV	C03-O11-P-O13
8	A	605	PGV	C03-O11-P-O14
8	A	605	PGV	C04-O12-P-O13
8	A	605	PGV	O02-C1-O01-C02
8	A	605	PGV	C2-C1-O01-C02
8	A	607	PGV	C04-O12-P-O11
8	A	607	PGV	C04-O12-P-O13
8	C	101	PGV	C04-O12-P-O13
8	D	601	PGV	C04-O12-P-O11
8	D	601	PGV	C04-O12-P-O13
8	D	606	PGV	C03-O11-P-O13
8	D	606	PGV	C03-O11-P-O14
8	D	606	PGV	C04-O12-P-O13
8	D	606	PGV	O02-C1-O01-C02
8	D	606	PGV	C2-C1-O01-C02
8	F	101	PGV	C04-O12-P-O13
9	A	606	3PE	C1-O11-P-O12
9	A	606	3PE	C11-O13-P-O11
9	A	606	3PE	C11-O13-P-O14
9	A	606	3PE	O13-C11-C12-N
9	A	606	3PE	C22-C21-O21-C2
9	D	607	3PE	C1-O11-P-O12
9	D	607	3PE	C11-O13-P-O11
9	D	607	3PE	C11-O13-P-O14
9	D	607	3PE	O13-C11-C12-N
9	D	607	3PE	C22-C21-O21-C2
9	A	606	3PE	O32-C31-O31-C3
9	D	607	3PE	O32-C31-O31-C3
9	A	606	3PE	C32-C31-O31-C3
9	D	607	3PE	C32-C31-O31-C3
8	C	101	PGV	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
8	F	101	PGV	O04-C19-O03-C01
9	A	606	3PE	O22-C21-O21-C2
9	D	607	3PE	O22-C21-O21-C2
8	C	101	PGV	C20-C19-O03-C01
8	F	101	PGV	C20-C19-O03-C01
4	A	601	HAS	C27-C19-C20-C21
4	D	602	HAS	C27-C19-C20-C21
7	A	604	DLX	C22-C23-C24-C25
7	D	605	DLX	C22-C23-C24-C25
8	A	607	PGV	O04-C19-O03-C01
8	D	601	PGV	O04-C19-O03-C01
4	A	601	HAS	C1A-C2A-CAA-CBA
4	A	601	HAS	C4D-C3D-CAD-CBD
4	D	602	HAS	C1A-C2A-CAA-CBA
4	D	602	HAS	C4D-C3D-CAD-CBD
4	A	601	HAS	C21-C22-C23-C25
4	D	602	HAS	C21-C22-C23-C25
7	A	604	DLX	C29-C30-C31-C43
7	D	605	DLX	C29-C30-C31-C43
7	A	604	DLX	C17-C18-C19-C20
7	D	605	DLX	C17-C18-C19-C20
8	A	607	PGV	C20-C19-O03-C01
8	D	601	PGV	C20-C19-O03-C01
4	A	601	HAS	C2D-C3D-CAD-CBD
4	D	602	HAS	C2D-C3D-CAD-CBD
7	A	604	DLX	C43-C31-C32-C33
7	A	604	DLX	C46-C19-C20-C21
7	D	605	DLX	C43-C31-C32-C33
7	D	605	DLX	C46-C19-C20-C21
4	A	601	HAS	C22-C23-C24-C28
4	D	602	HAS	C22-C23-C24-C28
4	A	601	HAS	C28-C29-C30-C31
4	D	602	HAS	C28-C29-C30-C31
7	A	604	DLX	C42-C35-C36-C37
7	D	605	DLX	C42-C35-C36-C37
8	A	607	PGV	C19-C20-C21-C22
8	D	601	PGV	C19-C20-C21-C22
7	A	604	DLX	C25-C26-C27-C44
7	D	605	DLX	C25-C26-C27-C44
9	A	606	3PE	C21-C22-C23-C24
9	D	607	3PE	C21-C22-C23-C24
9	A	606	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
9	D	607	3PE	C31-C32-C33-C34
4	A	601	HAS	C23-C24-C28-C29
4	D	602	HAS	C23-C24-C28-C29
8	A	607	PGV	O12-C04-C05-O05
8	D	601	PGV	O12-C04-C05-O05
7	A	604	DLX	C35-C36-C37-C38
7	A	604	DLX	C32-C33-C34-C35
7	D	605	DLX	C35-C36-C37-C38
7	D	605	DLX	C32-C33-C34-C35
8	A	605	PGV	C03-O11-P-O12
8	D	606	PGV	C03-O11-P-O12
8	C	101	PGV	C7-C8-C9-C10
8	F	101	PGV	C7-C8-C9-C10
9	A	606	3PE	C28-C29-C2A-C2B
9	D	607	3PE	C28-C29-C2A-C2B
8	A	607	PGV	O12-C04-C05-C06
8	D	601	PGV	O12-C04-C05-C06
9	A	606	3PE	C22-C23-C24-C25
9	D	607	3PE	C22-C23-C24-C25
8	A	605	PGV	C4-C5-C6-C7
8	D	606	PGV	C4-C5-C6-C7
8	A	607	PGV	C28-C29-C30-C31
8	D	601	PGV	C28-C29-C30-C31
8	A	607	PGV	C30-C31-C32-C33
8	D	601	PGV	C30-C31-C32-C33
8	A	605	PGV	C3-C4-C5-C6
8	A	607	PGV	C13-C14-C15-C16
8	D	601	PGV	C13-C14-C15-C16
8	D	606	PGV	C3-C4-C5-C6
8	A	605	PGV	C7-C8-C9-C10
8	D	601	PGV	C24-C25-C26-C27
8	D	606	PGV	C7-C8-C9-C10
9	A	606	3PE	C27-C28-C29-C2A
9	D	607	3PE	C27-C28-C29-C2A
8	A	607	PGV	C24-C25-C26-C27
8	A	607	PGV	C04-C05-C06-O06
8	D	601	PGV	C04-C05-C06-O06
9	A	606	3PE	C38-C39-C3A-C3B
9	D	607	3PE	C38-C39-C3A-C3B
9	A	606	3PE	C36-C37-C38-C39
9	D	607	3PE	C36-C37-C38-C39
8	C	101	PGV	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
8	F	101	PGV	C28-C29-C30-C31
7	A	604	DLX	C44-C27-C28-C29
7	D	605	DLX	C44-C27-C28-C29
8	A	607	PGV	O05-C05-C06-O06
8	D	601	PGV	O05-C05-C06-O06
9	A	606	3PE	C33-C34-C35-C36
9	D	607	3PE	C33-C34-C35-C36
7	A	604	DLX	C37-C38-C39-C40
7	D	605	DLX	C37-C38-C39-C40
9	D	607	3PE	C39-C3A-C3B-C3C
9	A	606	3PE	C39-C3A-C3B-C3C
8	C	101	PGV	C19-C20-C21-C22
8	F	101	PGV	C19-C20-C21-C22
7	A	604	DLX	C26-C27-C28-C29
7	D	605	DLX	C26-C27-C28-C29
8	D	601	PGV	C25-C26-C27-C28
8	A	607	PGV	C25-C26-C27-C28
9	A	606	3PE	C37-C38-C39-C3A
9	D	607	3PE	C37-C38-C39-C3A
7	A	604	DLX	C27-C28-C29-C30
7	D	605	DLX	C27-C28-C29-C30
8	A	605	PGV	O01-C02-C03-O11
7	A	604	DLX	C04-C05-C13-C14
7	D	605	DLX	C04-C05-C13-C14
8	A	607	PGV	C15-C16-C17-C18
8	D	601	PGV	C15-C16-C17-C18
7	A	604	DLX	C19-C20-C21-C22
7	D	605	DLX	C19-C20-C21-C22
8	D	606	PGV	O01-C02-C03-O11
8	F	101	PGV	C12-C13-C14-C15
9	A	606	3PE	C35-C36-C37-C38
9	A	606	3PE	C2C-C2D-C2E-C2F
9	D	607	3PE	C35-C36-C37-C38
9	D	607	3PE	C2C-C2D-C2E-C2F
7	A	604	DLX	C34-C35-C36-C37
7	D	605	DLX	C34-C35-C36-C37
8	D	601	PGV	C5-C6-C7-C8
9	A	606	3PE	C2A-C2B-C2C-C2D
9	D	607	3PE	C2A-C2B-C2C-C2D
8	A	607	PGV	C5-C6-C7-C8
8	C	101	PGV	C12-C13-C14-C15
8	C	101	PGV	C01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
8	F	101	PGV	C01-C02-C03-O11
8	D	601	PGV	C1-C2-C3-C4
8	A	607	PGV	C1-C2-C3-C4
8	A	607	PGV	C2-C1-O01-C02
8	A	607	PGV	C9-C10-C11-C12
8	D	601	PGV	C9-C10-C11-C12
8	A	607	PGV	O03-C01-C02-C03
8	C	101	PGV	O03-C01-C02-C03
8	D	601	PGV	O03-C01-C02-C03
8	F	101	PGV	O03-C01-C02-C03
8	D	601	PGV	C2-C1-O01-C02
8	C	101	PGV	C2-C3-C4-C5
8	F	101	PGV	C2-C3-C4-C5
4	A	601	HAS	C3D-C2D-CMD-OMD
4	D	602	HAS	C3D-C2D-CMD-OMD
8	C	101	PGV	C4-C5-C6-C7
8	A	607	PGV	O01-C02-C03-O11
8	D	601	PGV	O01-C02-C03-O11
8	F	101	PGV	C4-C5-C6-C7
9	A	606	3PE	C3E-C3F-C3G-C3H
9	D	607	3PE	C3E-C3F-C3G-C3H
8	A	607	PGV	O02-C1-O01-C02
8	D	601	PGV	O02-C1-O01-C02
7	A	604	DLX	C37-C38-C39-C41
7	D	605	DLX	C37-C38-C39-C41
8	A	605	PGV	C9-C10-C11-C12
8	D	606	PGV	C9-C10-C11-C12
8	C	101	PGV	C5-C6-C7-C8
8	C	101	PGV	C24-C25-C26-C27
8	F	101	PGV	C5-C6-C7-C8
8	F	101	PGV	C24-C25-C26-C27
8	A	607	PGV	C3-C4-C5-C6
8	D	601	PGV	C3-C4-C5-C6
8	A	607	PGV	C01-C02-C03-O11
8	D	601	PGV	C01-C02-C03-O11
9	A	606	3PE	C2-C1-O11-P
9	D	607	3PE	C2-C1-O11-P
8	C	101	PGV	C04-O12-P-O11
8	F	101	PGV	C04-O12-P-O11
8	A	605	PGV	C01-C02-C03-O11
8	D	606	PGV	C01-C02-C03-O11
8	A	605	PGV	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
8	D	606	PGV	C11-C10-C9-C8
9	A	606	3PE	C24-C25-C26-C27
9	D	607	3PE	C24-C25-C26-C27
8	C	101	PGV	O01-C02-C03-O11
8	F	101	PGV	O01-C02-C03-O11
8	A	607	PGV	O03-C01-C02-O01
8	D	601	PGV	O03-C01-C02-O01
8	A	605	PGV	C11-C12-C13-C14
8	D	606	PGV	C11-C12-C13-C14
8	A	605	PGV	C25-C26-C27-C28
8	D	606	PGV	C25-C26-C27-C28
4	A	601	HAS	C15-C16-C17-C18
4	D	602	HAS	C15-C16-C17-C18
7	A	604	DLX	C36-C37-C38-C39
7	D	605	DLX	C36-C37-C38-C39
4	A	601	HAS	C11-C12-C13-C14
4	D	602	HAS	C11-C12-C13-C14
8	A	605	PGV	C04-O12-P-O11
8	C	101	PGV	C03-O11-P-O12
8	D	606	PGV	C04-O12-P-O11
8	F	101	PGV	C03-O11-P-O12
7	A	604	DLX	C47-C15-C16-C17
7	D	605	DLX	C47-C15-C16-C17
8	A	607	PGV	C11-C12-C13-C14
8	D	601	PGV	C11-C12-C13-C14
4	A	601	HAS	CAD-CBD-CGD-O1D
4	D	602	HAS	CAD-CBD-CGD-O1D
4	A	601	HAS	CAA-CBA-CGA-O2A
4	D	602	HAS	CAA-CBA-CGA-O2A
9	D	607	3PE	C26-C27-C28-C29
9	A	606	3PE	C26-C27-C28-C29
8	C	101	PGV	O03-C01-C02-O01
8	F	101	PGV	O03-C01-C02-O01
5	A	602	HEM	CAD-CBD-CGD-O1D
5	D	603	HEM	CAD-CBD-CGD-O1D
8	C	101	PGV	C26-C27-C28-C29
8	F	101	PGV	C26-C27-C28-C29
8	C	101	PGV	C20-C21-C22-C23
8	F	101	PGV	C20-C21-C22-C23
9	A	606	3PE	C1-O11-P-O13
9	D	607	3PE	C1-O11-P-O13
8	C	101	PGV	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
8	C	101	PGV	C11-C12-C13-C14
8	F	101	PGV	C9-C10-C11-C12
8	F	101	PGV	C11-C12-C13-C14
4	A	601	HAS	CAA-CBA-CGA-O1A
4	D	602	HAS	CAA-CBA-CGA-O1A
9	D	607	3PE	C29-C2A-C2B-C2C
9	A	606	3PE	C29-C2A-C2B-C2C
7	A	604	DLX	C28-C29-C30-C31
7	D	605	DLX	C28-C29-C30-C31
5	A	602	HEM	CAD-CBD-CGD-O2D
5	D	603	HEM	CAD-CBD-CGD-O2D
9	A	606	3PE	C1-O11-P-O14
9	D	607	3PE	C1-O11-P-O14
8	A	607	PGV	C03-C02-O01-C1
8	D	601	PGV	C03-C02-O01-C1
7	A	604	DLX	C06-C05-C13-C14
7	D	605	DLX	C06-C05-C13-C14
7	A	604	DLX	C23-C24-C25-C26
7	D	605	DLX	C23-C24-C25-C26
8	A	607	PGV	O03-C19-C20-C21
8	D	601	PGV	O03-C19-C20-C21

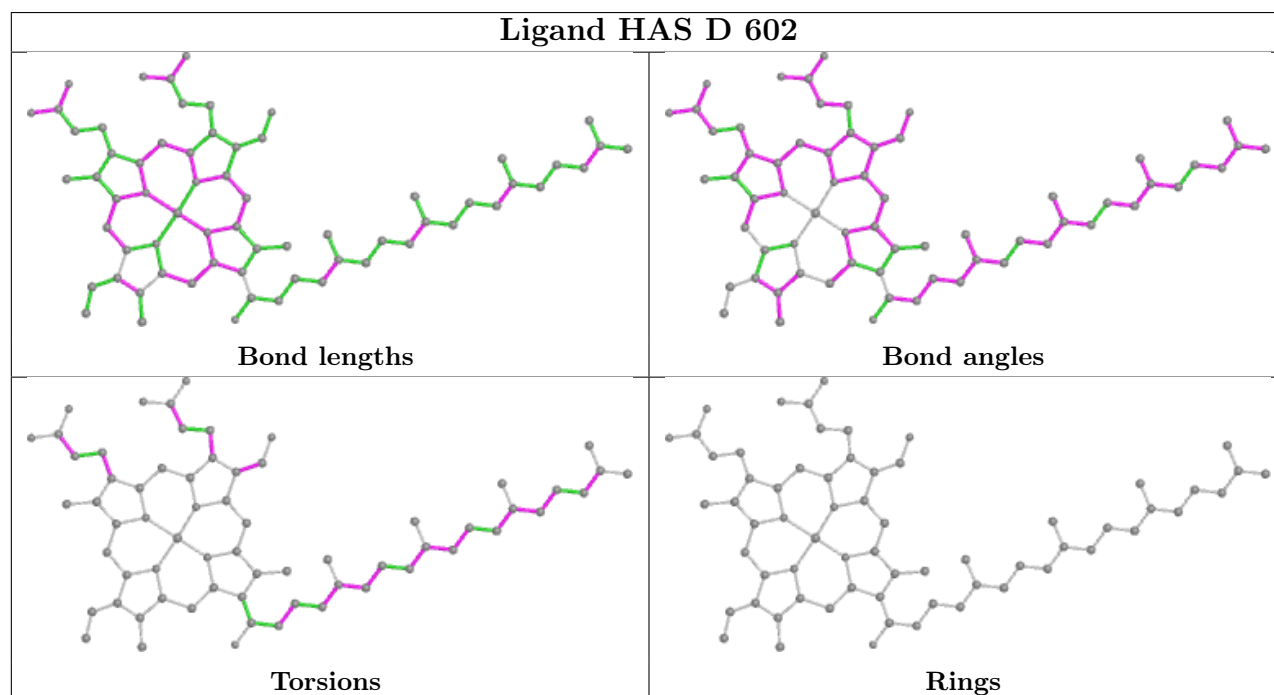
There are no ring outliers.

14 monomers are involved in 133 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	602	HAS	11	0
4	A	601	HAS	11	0
5	D	603	HEM	8	0
8	A	605	PGV	3	0
8	C	101	PGV	4	0
8	D	606	PGV	2	0
8	A	607	PGV	27	0
8	D	601	PGV	27	0
8	F	101	PGV	4	0
9	A	606	3PE	36	0
9	D	607	3PE	34	0
5	A	602	HEM	8	0
7	D	605	DLX	3	0
7	A	604	DLX	3	0

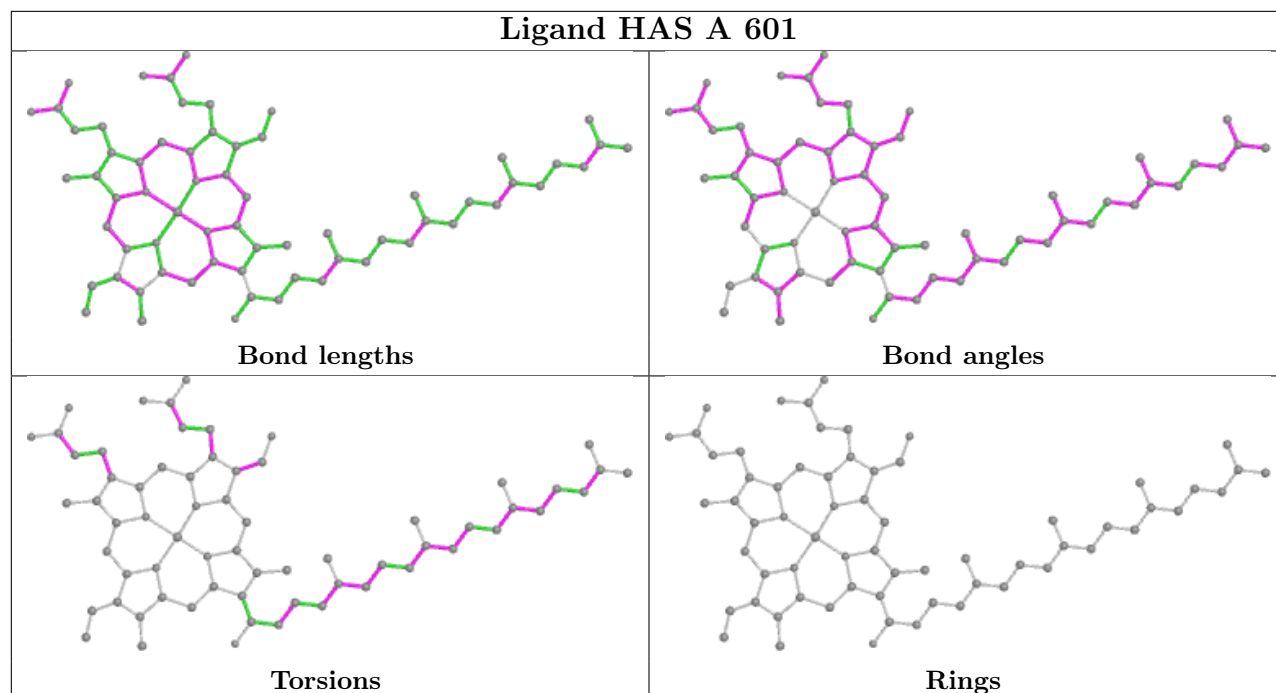
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

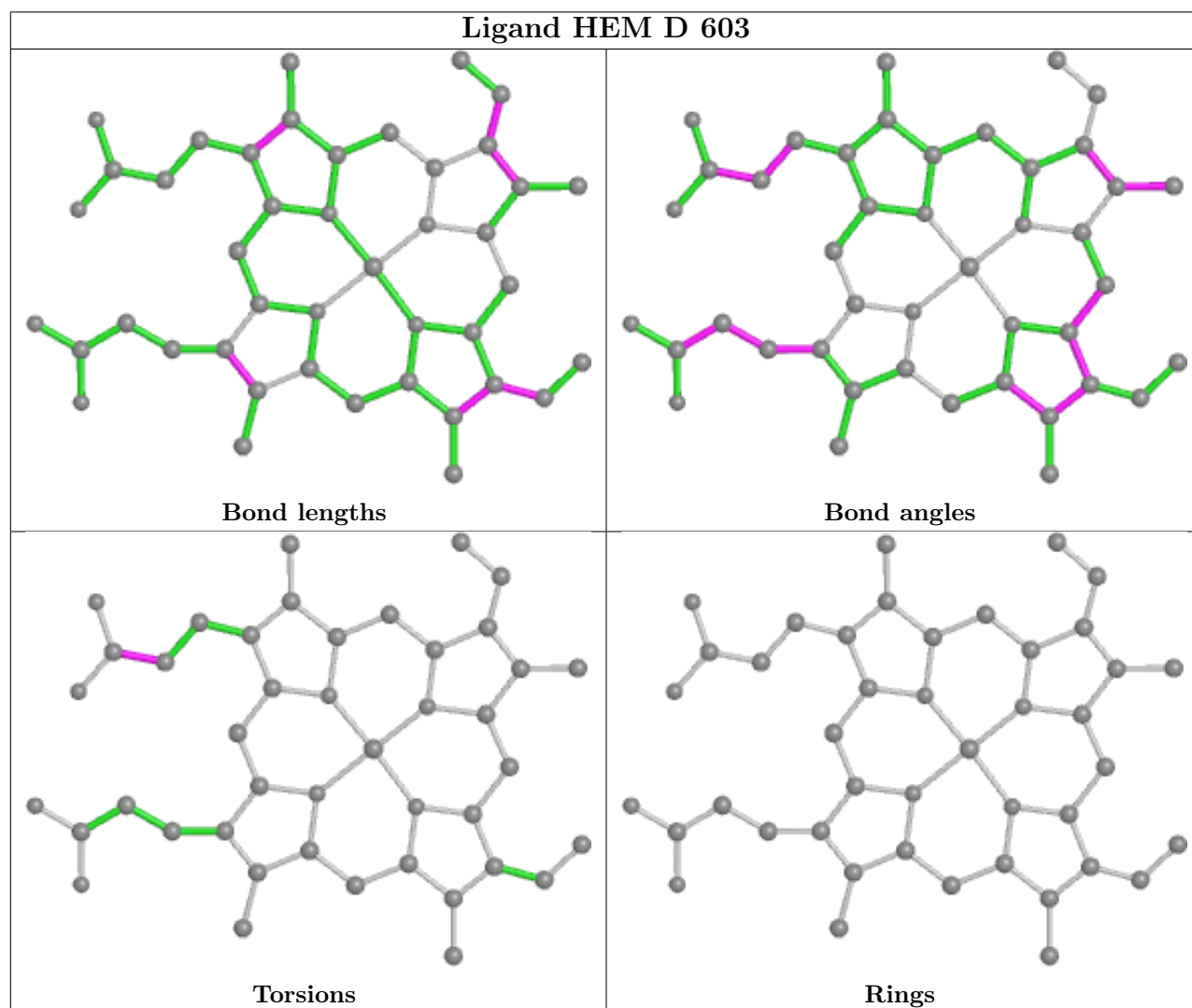


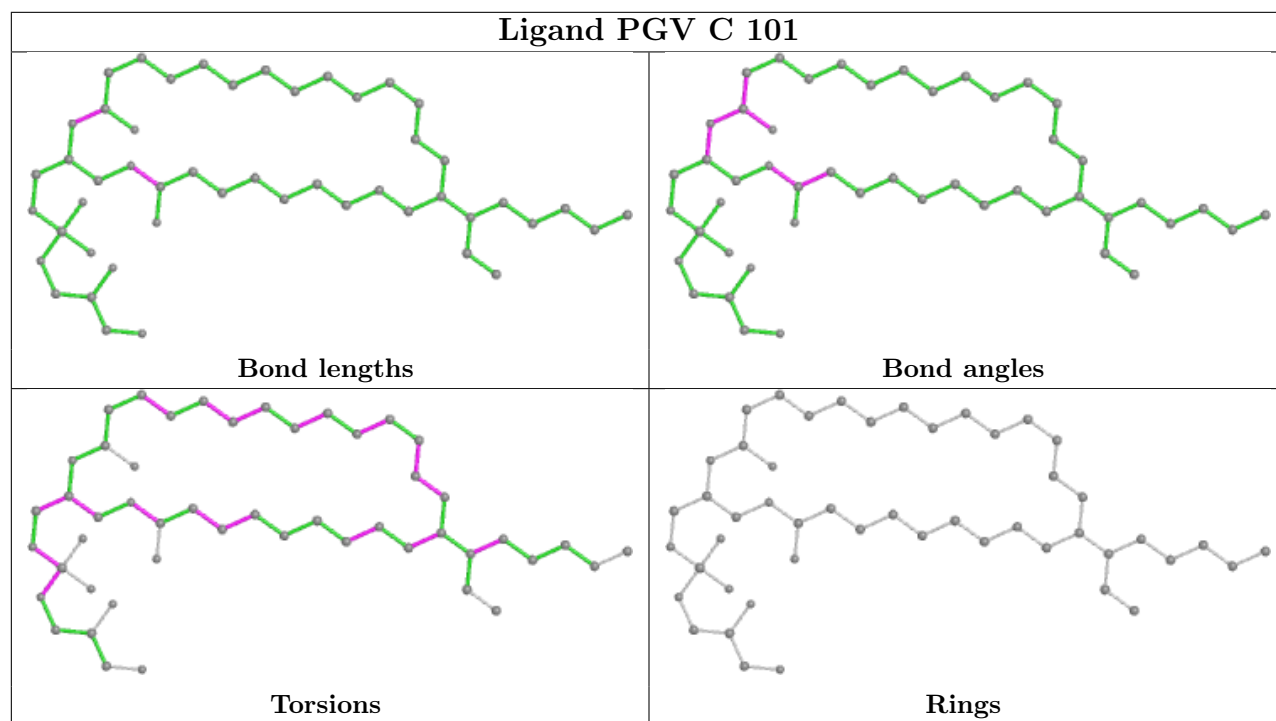
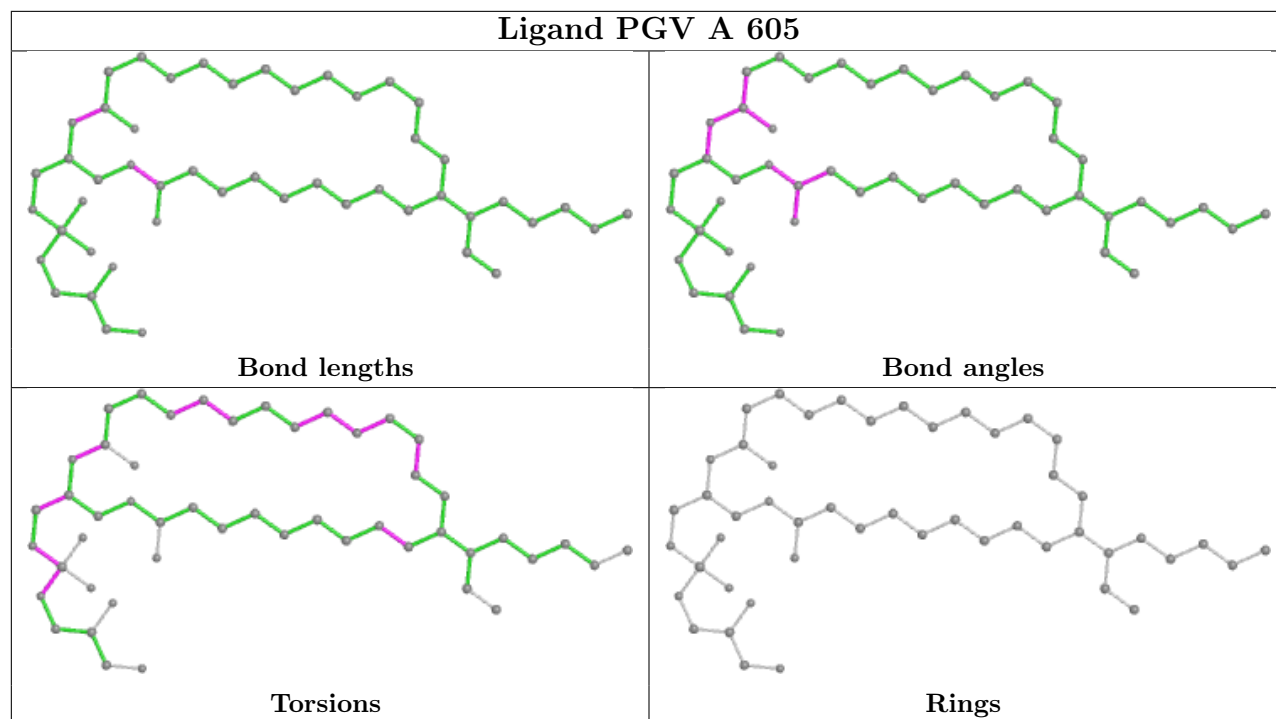


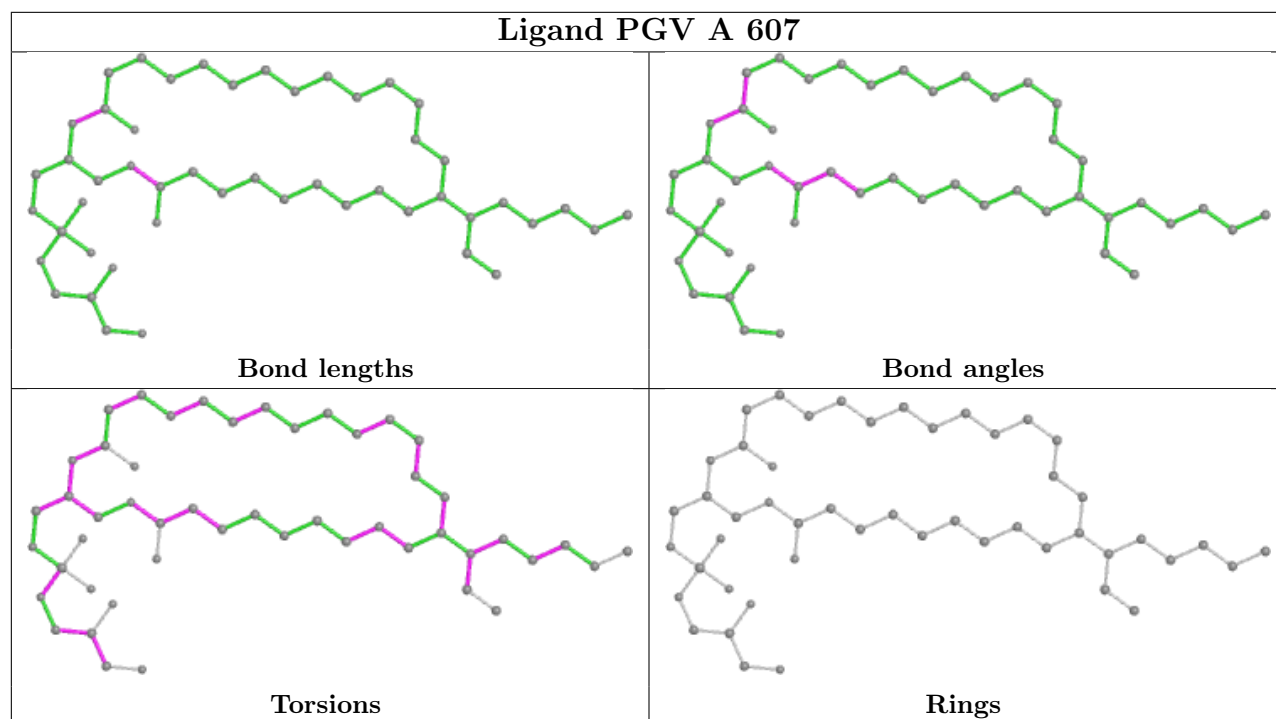
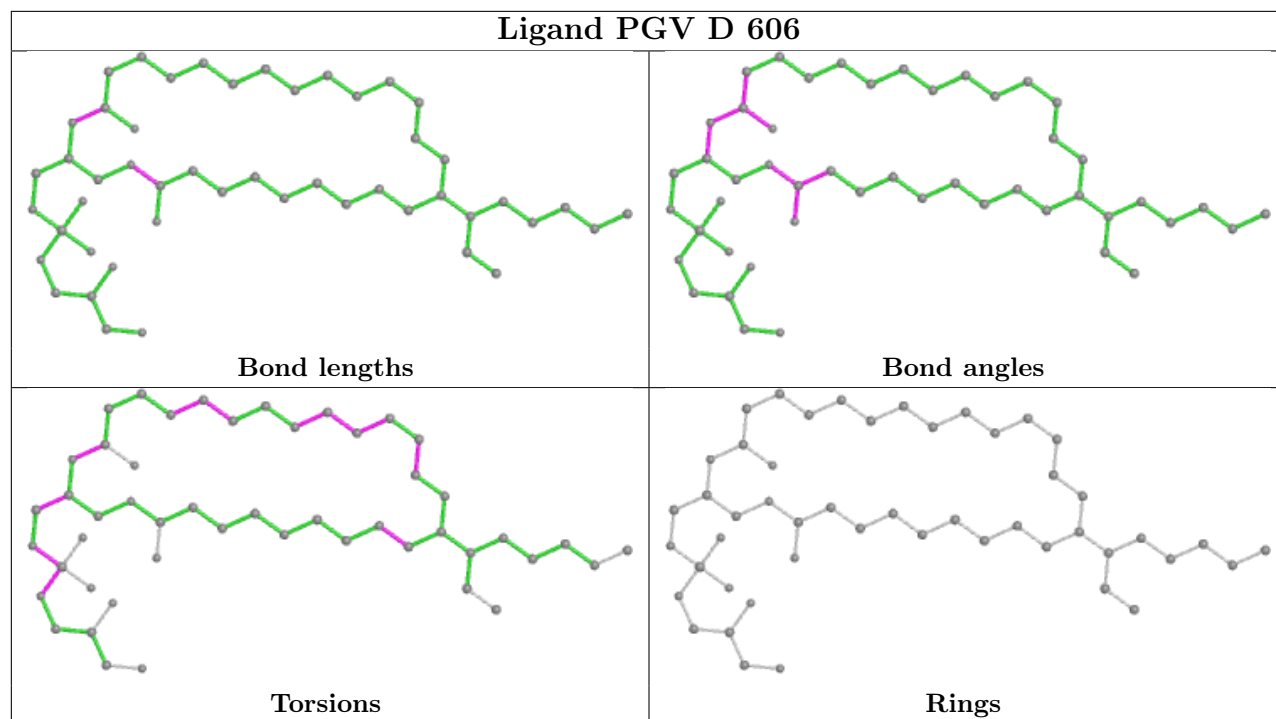
## Ligand HAS A 601

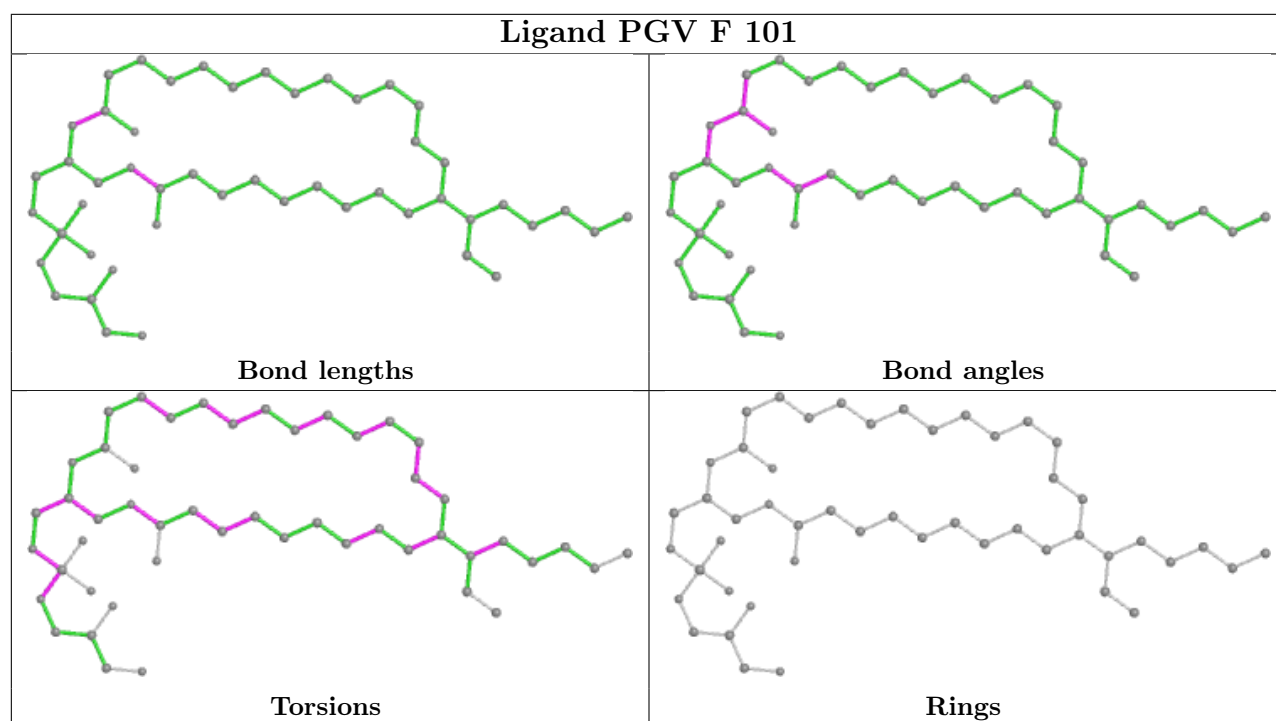
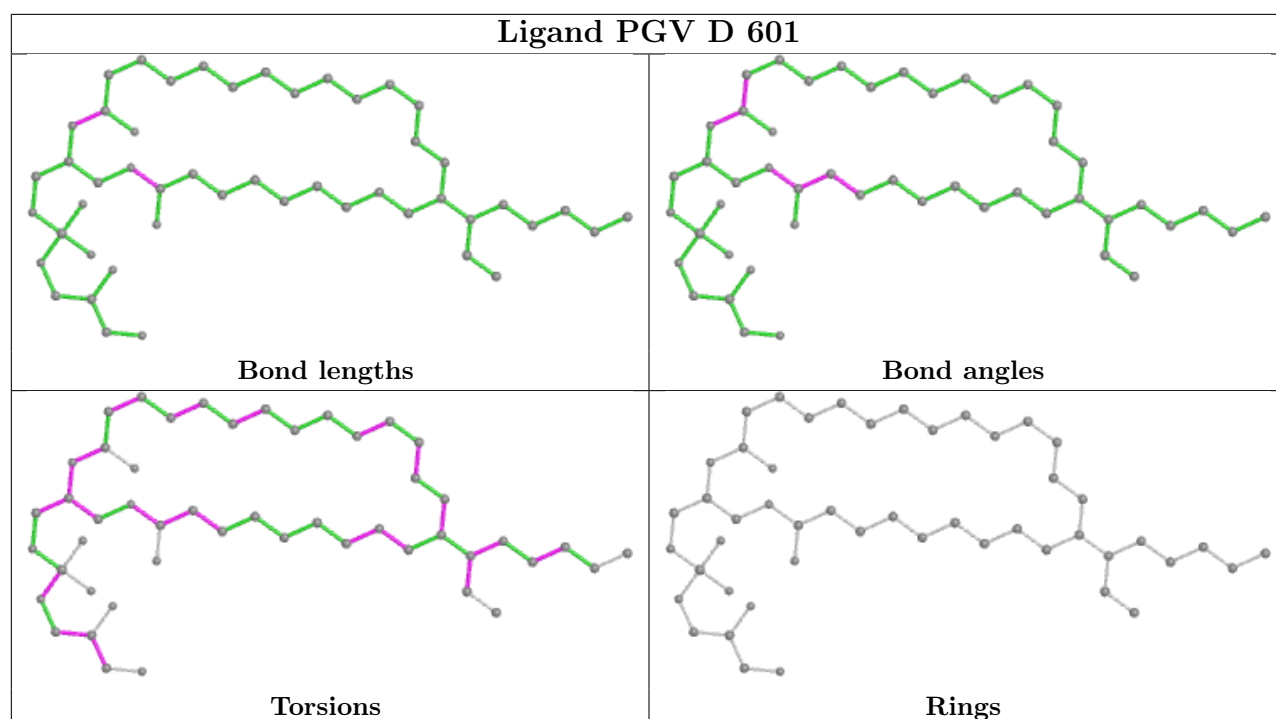


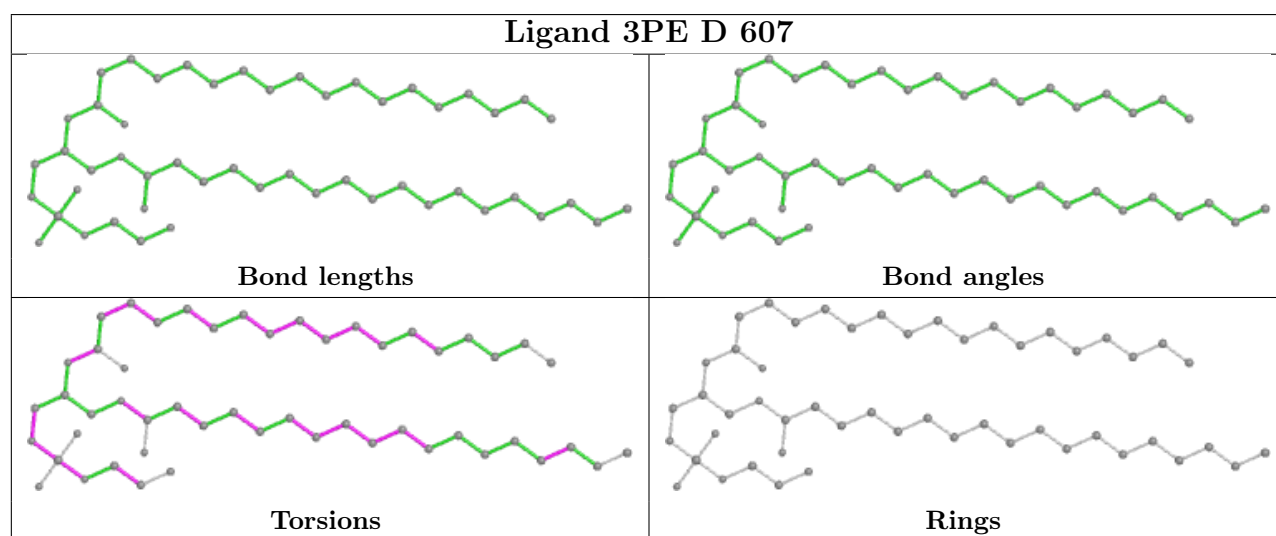
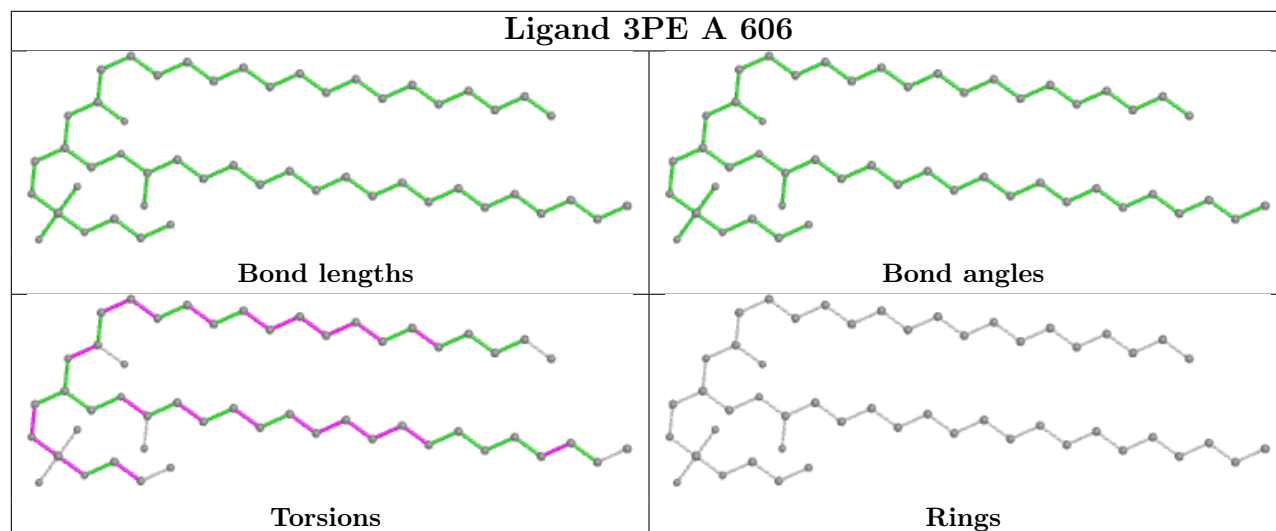
## Ligand HEM D 603

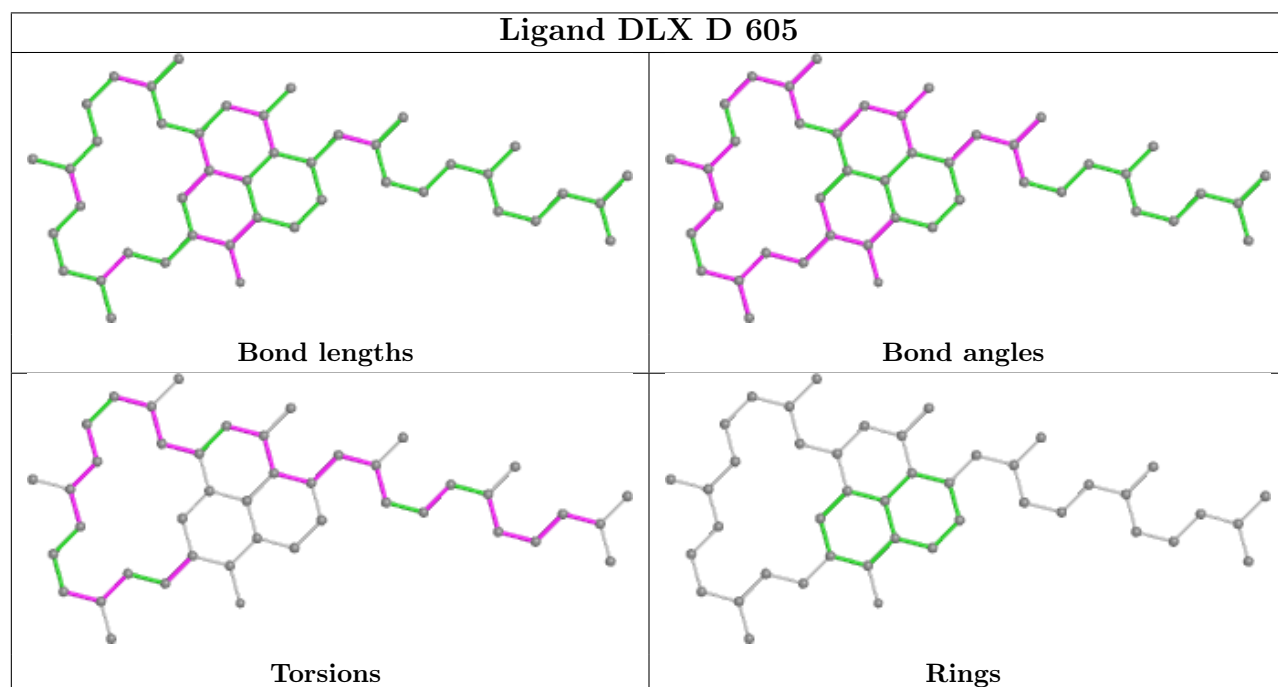
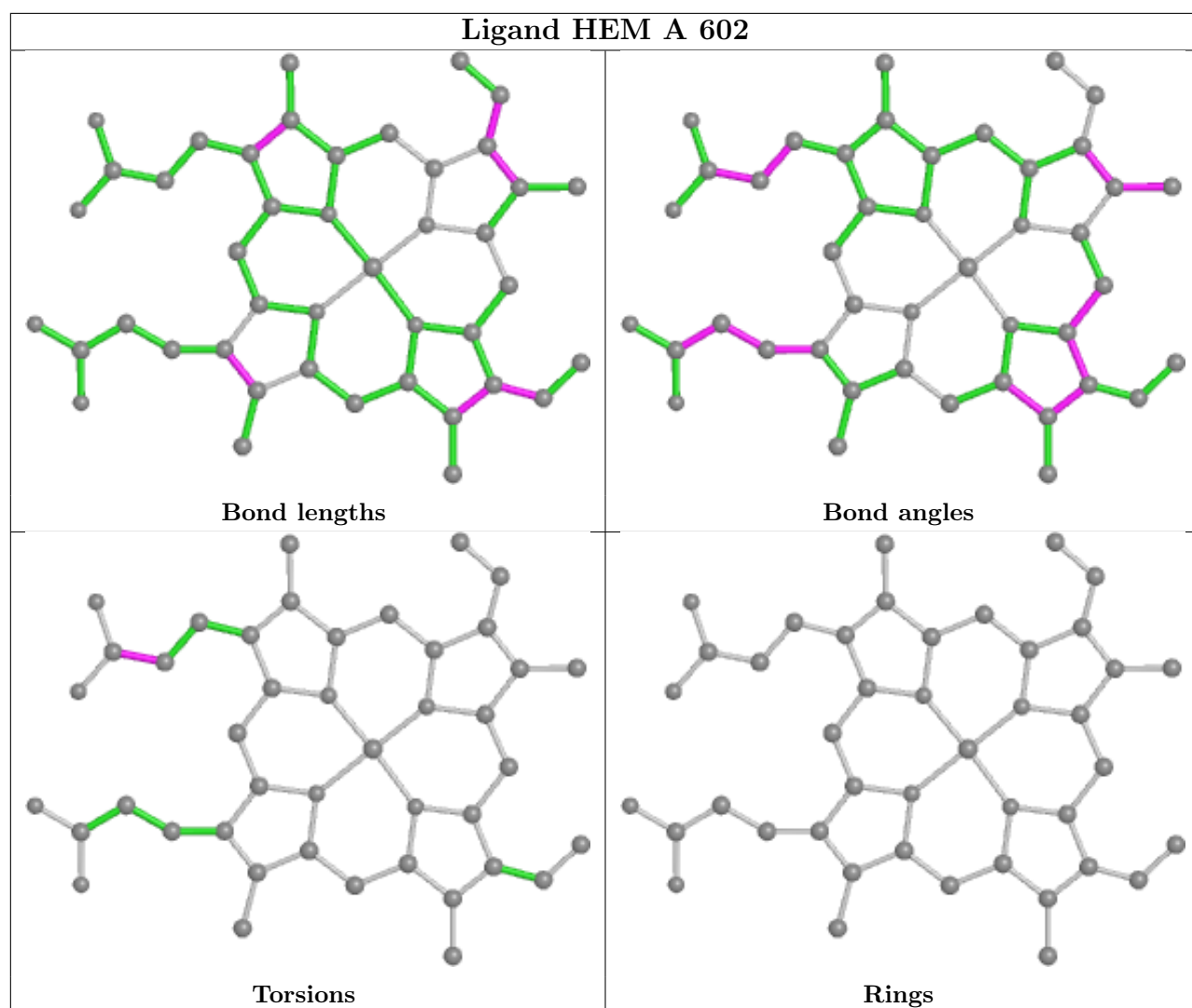


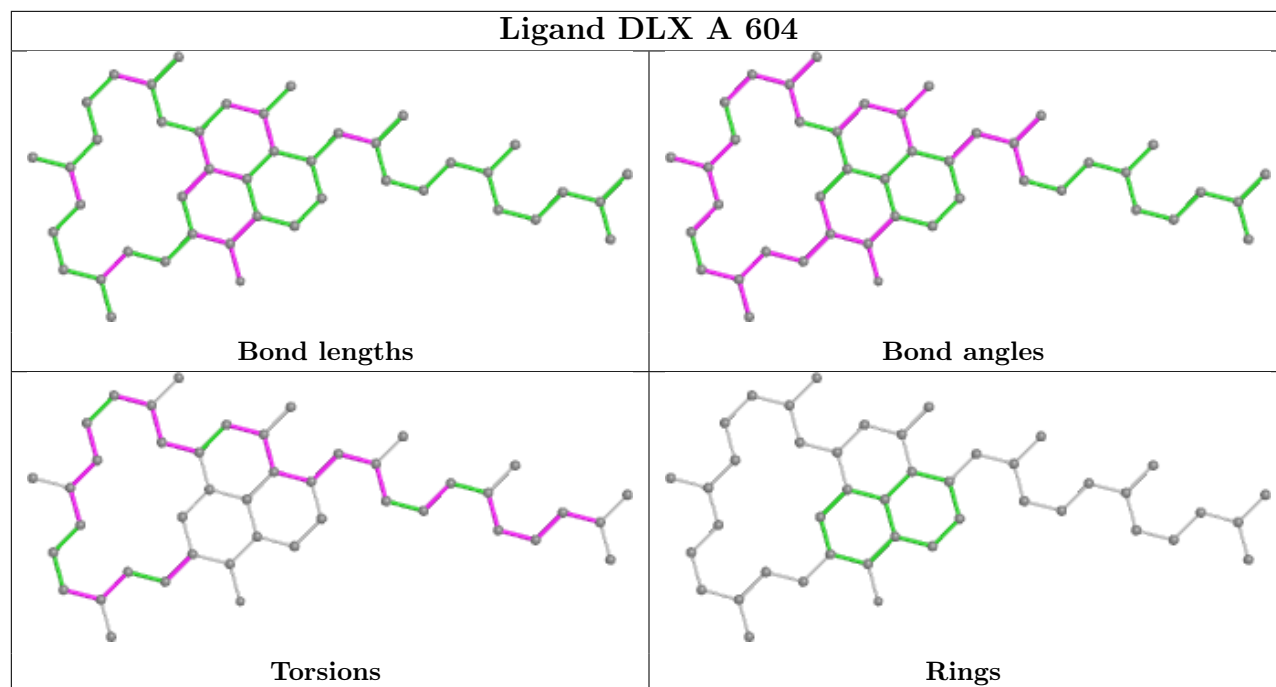












## 5.7 Other polymers [i](#)

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

This section contains visualisations of the EMDB entry EMD-30657. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

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



## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

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

## 9 Map-model fit ⓘ

This section was not generated.