



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2023 – 12:50 PM EDT

PDB ID : 1IT3  
Title : Hagfish CO ligand hemoglobin  
Authors : Mito, M.; Chong, K.T.; Park, S.-Y.; Tame, J.R.  
Deposited on : 2002-01-05  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

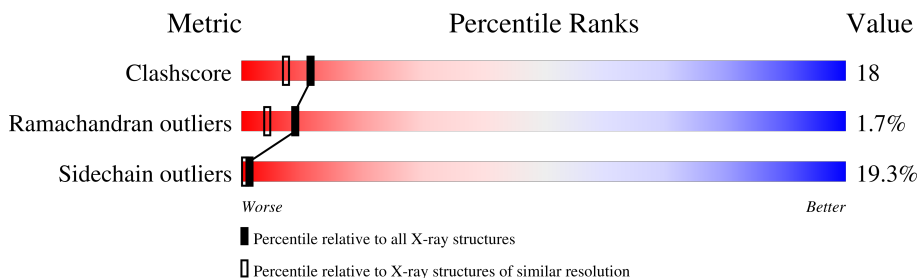
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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  $\leq 5\%$

Note EDS was not executed.

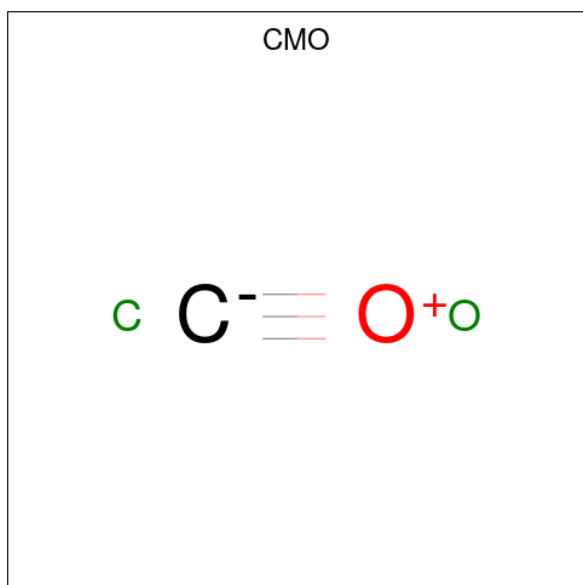
Mol	Chain	Length	Quality of chain
1	A	146	
1	B	146	
1	C	146	
1	D	146	



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

- Molecule 3 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3	A	1	Total	C	O	0	0
			2	1	1		
3	B	1	Total	C	O	0	0
			2	1	1		
3	C	1	Total	C	O	0	0
			2	1	1		
3	D	1	Total	C	O	0	0
			2	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	67	Total	O	0	0
			67	67		
4	B	58	Total	O	0	0
			58	58		
4	C	60	Total	O	0	0
			60	60		

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	D	85	Total	O	0	0
			85	85		

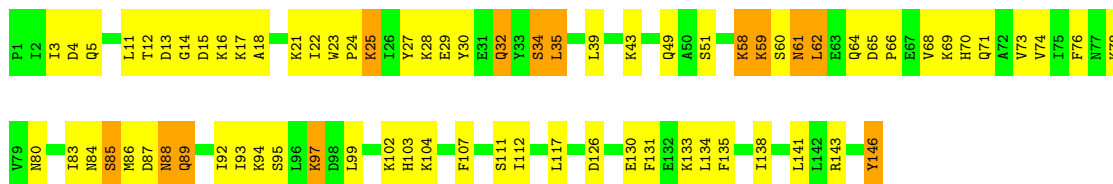
### 3 Residue-property plots

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.

Note EDS was not executed.

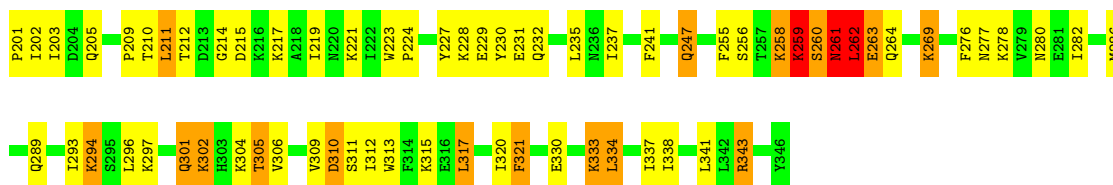
- Molecule 1: hemoglobin

Chain A: 



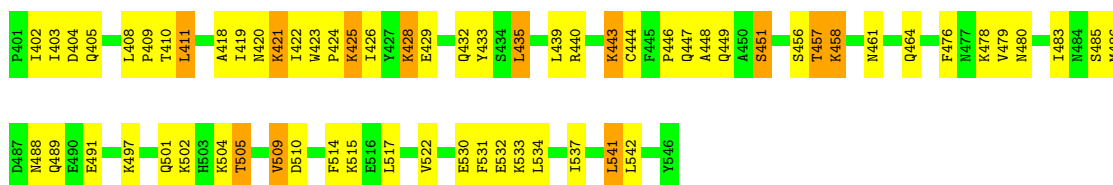
- Molecule 1: hemoglobin

Chain B: 



- Molecule 1: hemoglobin

Chain C: 



- Molecule 1: hemoglobin

Chain D: 



T688	M684	S695	N688	Q689	E690	E691	I692	I693	K694	S695	L696	K697	K708	V709	D710	L717	I720	F721	V722	E730	L734	I738	L741	L742	R743	Y746
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.97Å 150.64Å 51.94Å 90.00° 106.37° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	84.1 (20.00-2.10)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.196 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.37	0/1216	0.55	0/1637
1	B	0.38	0/1216	0.54	0/1637
1	C	0.40	0/1216	0.58	0/1637
1	D	0.39	0/1216	0.59	0/1637
All	All	0.39	0/4864	0.57	0/6548

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1190	0	1223	62	0
1	B	1190	0	1221	47	0
1	C	1190	0	1221	38	0
1	D	1190	0	1221	38	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
2	C	43	0	30	1	0
2	D	43	0	30	2	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	67	0	0	3	0
4	B	58	0	0	3	0
4	C	60	0	0	2	0
4	D	85	0	0	5	0
All	All	5210	0	5006	175	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 18.

All (175) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:PRO:HA	1:A:69:LYS:HD2	1.34	1.05
1:A:12:THR:HG22	1:A:14:GLY:H	1.29	0.95
1:B:223:TRP:HE1	1:B:280:ASN:HD22	1.03	0.95
1:D:612:THR:HG22	1:D:614:GLY:H	1.30	0.95
1:C:440:ARG:HA	1:C:443:LYS:HD3	1.48	0.95
1:A:23:TRP:HE1	1:A:80:ASN:HD22	1.11	0.91
1:B:201:PRO:HA	1:D:647:GLN:NE2	1.86	0.89
1:A:12:THR:HG22	1:A:14:GLY:N	1.88	0.88
1:B:223:TRP:HE1	1:B:280:ASN:ND2	1.71	0.87
1:A:65:ASP:HB3	1:A:68:VAL:HB	1.61	0.82
1:C:423:TRP:HE1	1:C:480:ASN:HD22	1.29	0.81
1:D:623:TRP:HE1	1:D:680:ASN:HD22	1.28	0.79
1:B:259:LYS:HA	1:B:262:LEU:HD21	1.66	0.78
1:A:12:THR:O	1:A:16:LYS:HG3	1.83	0.78
1:C:429:GLU:HB3	1:C:432:GLN:HE21	1.49	0.78
1:A:23:TRP:HE1	1:A:80:ASN:ND2	1.81	0.77
1:A:12:THR:CG2	1:A:14:GLY:H	1.98	0.75
1:D:612:THR:HG22	1:D:614:GLY:N	2.01	0.75
1:A:30:TYR:O	1:A:34:SER:HB3	1.88	0.73
1:A:18:ALA:HB3	1:A:130:GLU:HG2	1.72	0.70
1:A:12:THR:HG23	4:B:349:HOH:O	1.93	0.67
1:C:428:LYS:HD2	1:C:429:GLU:HG3	1.76	0.67
1:A:5:GLN:NE2	1:A:143:ARG:HH21	1.92	0.67
1:A:59:LYS:HA	1:A:62:LEU:HD22	1.75	0.67
1:B:201:PRO:HA	1:D:647:GLN:HE21	1.60	0.66
1:A:58:LYS:HG2	1:A:58:LYS:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:664:GLN:HB3	4:D:218:HOH:O	1.96	0.65
1:C:479:VAL:O	1:C:483:ILE:HG13	1.97	0.65
1:B:223:TRP:HB3	1:B:224:PRO:HD3	1.80	0.63
1:B:309:VAL:CG1	2:B:347:HEM:HAC	2.29	0.62
1:B:209:PRO:HG2	1:B:337:ILE:HG13	1.83	0.61
1:B:294:LYS:HZ2	1:B:294:LYS:HB3	1.66	0.60
1:D:629:GLU:HG3	4:D:90:HOH:O	2.01	0.60
1:B:215:ASP:O	1:B:219:ILE:HD12	2.02	0.60
1:D:651:SER:HB3	1:D:709:VAL:HG22	1.83	0.60
1:B:212:THR:HG22	1:B:214:GLY:H	1.67	0.59
1:A:27:TYR:HB2	1:D:607:PRO:HD3	1.85	0.59
1:B:263:GLU:HB3	4:B:359:HOH:O	2.02	0.59
1:A:102:LYS:HB3	1:A:107:PHE:CE1	2.36	0.58
1:C:432:GLN:HG2	4:C:10:HOH:O	2.03	0.58
1:C:440:ARG:HA	1:C:443:LYS:CD	2.29	0.58
1:A:66:PRO:HB2	1:C:501:GLN:HG2	1.85	0.57
1:C:422:ILE:O	1:C:425:LYS:HG2	2.05	0.57
1:A:65:ASP:O	1:A:69:LYS:HG3	2.04	0.56
1:A:66:PRO:CB	1:C:501:GLN:HG2	2.36	0.56
1:A:89:GLN:HG3	1:B:310:ASP:OD1	2.05	0.56
1:D:682:ILE:HG23	1:D:692:ILE:HD12	1.87	0.56
1:B:293:ILE:O	1:B:297:LYS:HB2	2.05	0.56
1:D:689:GLN:O	1:D:693:ILE:HG13	2.05	0.56
1:C:440:ARG:HG3	1:C:443:LYS:HE2	1.88	0.56
1:A:117:LEU:O	1:A:117:LEU:HD23	2.06	0.55
1:B:317:LEU:HD12	2:B:347:HEM:HMC1	1.88	0.55
1:A:35:LEU:HD22	1:A:39:LEU:HG	1.88	0.55
1:D:682:ILE:HD11	1:D:696:LEU:HD21	1.88	0.55
1:C:458:LYS:HG2	1:C:461:ASN:HB2	1.89	0.54
1:C:410:THR:O	1:C:533:LYS:HE2	2.07	0.54
1:A:84:ASN:ND2	1:D:603:ILE:HG13	2.23	0.54
1:A:70:HIS:O	1:A:74:VAL:HG23	2.07	0.53
1:B:294:LYS:HB3	1:B:294:LYS:NZ	2.23	0.53
1:D:709:VAL:HG21	2:D:747:HEM:HHD	1.91	0.53
1:B:282:ILE:HD11	1:B:296:LEU:HD21	1.91	0.52
1:D:631:GLU:HB2	4:D:17:HOH:O	2.08	0.52
1:A:5:GLN:NE2	1:A:143:ARG:NH2	2.56	0.52
1:B:309:VAL:HG11	2:B:347:HEM:HAC	1.91	0.52
1:C:402:ILE:HG13	1:C:532:GLU:HG2	1.90	0.52
1:B:227:TYR:OH	1:B:277:ASN:ND2	2.43	0.52
1:B:211:LEU:HD23	1:B:286:MET:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:HIS:HA	1:A:107:PHE:HD1	1.75	0.52
4:A:204:HOH:O	1:D:601:PRO:HB3	2.10	0.52
1:D:670:HIS:O	1:D:674:VAL:HG23	2.09	0.52
1:B:309:VAL:HG13	2:B:347:HEM:HAC	1.93	0.51
1:A:71:GLN:HE22	2:A:147:HEM:HBD1	1.75	0.51
1:C:488:ASN:OD1	1:C:491:GLU:HB2	2.10	0.51
1:C:429:GLU:CB	1:C:432:GLN:HE21	2.22	0.51
1:C:418:ALA:HB3	1:C:530:GLU:HG2	1.92	0.51
1:C:435:LEU:HD22	1:C:439:LEU:HG	1.91	0.50
1:B:259:LYS:HA	1:B:262:LEU:CD2	2.38	0.50
1:B:311:SER:HB2	1:B:343:ARG:CG	2.42	0.50
1:D:730:GLU:H	1:D:730:GLU:CD	2.14	0.49
1:C:537:ILE:O	1:C:541:LEU:HB2	2.12	0.49
1:A:88:ASN:C	1:A:88:ASN:HD22	2.15	0.49
1:C:423:TRP:N	1:C:424:PRO:CD	2.75	0.49
1:B:334:LEU:O	1:B:338:ILE:HG13	2.12	0.49
1:C:448:ALA:O	1:C:451:SER:HB2	2.12	0.49
1:B:247:GLN:HG3	1:B:313:TRP:CH2	2.48	0.49
1:A:49:GLN:NE2	1:A:59:LYS:NZ	2.61	0.48
1:A:111:SER:HB3	1:A:146:TYR:CD2	2.47	0.48
1:A:103:HIS:HA	1:A:107:PHE:CD1	2.48	0.48
1:B:202:ILE:O	1:B:315:LYS:HE2	2.13	0.48
1:A:83:ILE:HA	1:A:86:MET:HG3	1.95	0.48
1:B:210:THR:C	1:B:333:LYS:HZ1	2.15	0.48
1:A:4:ASP:HB2	1:A:143:ARG:HD3	1.96	0.48
1:B:269:LYS:HE2	4:B:401:HOH:O	2.13	0.48
1:B:258:LYS:HG3	1:B:260:SER:HB2	1.94	0.47
1:C:422:ILE:O	1:C:426:ILE:HG12	2.14	0.47
1:D:691:GLU:HA	1:D:694:LYS:HE2	1.95	0.47
1:B:241:PHE:HA	1:B:320:ILE:HD13	1.97	0.47
1:B:255:PHE:O	1:B:255:PHE:HD1	1.96	0.47
1:A:93:ILE:O	1:A:97:LYS:HB2	2.14	0.47
1:D:612:THR:O	1:D:616:LYS:HG2	2.15	0.47
1:D:618:ALA:HB3	1:D:730:GLU:HG2	1.96	0.47
1:A:58:LYS:HG2	1:A:60:SER:H	1.80	0.47
1:D:602:ILE:HD11	1:D:722:VAL:HG21	1.97	0.46
1:D:643:LYS:HA	1:D:659:LYS:HZ3	1.79	0.46
1:A:64:GLN:O	1:A:69:LYS:HE3	2.14	0.46
1:C:432:GLN:HG3	1:C:433:TYR:H	1.80	0.46
1:B:312:ILE:N	1:B:312:ILE:HD13	2.30	0.46
1:A:32:GLN:NE2	4:A:188:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:TYR:HB2	1:A:76:PHE:CE2	2.52	0.45
1:B:203:ILE:HG23	1:B:205:GLN:H	1.80	0.45
1:B:311:SER:HB2	1:B:343:ARG:HG2	1.99	0.45
1:D:689:GLN:H	1:D:689:GLN:HG2	1.62	0.45
1:B:255:PHE:O	1:B:255:PHE:CD1	2.70	0.45
1:B:258:LYS:HB2	1:B:258:LYS:HE2	1.69	0.45
1:B:293:ILE:HG23	1:B:297:LYS:HE3	1.99	0.44
1:D:682:ILE:HD13	1:D:738:ILE:HG12	1.99	0.44
1:A:112:ILE:HG22	1:A:112:ILE:O	2.17	0.44
1:C:403:ILE:CG2	1:C:404:ASP:N	2.80	0.44
1:B:302:LYS:HE3	1:B:306:VAL:HG21	2.00	0.44
1:B:237:ILE:HG12	1:B:321:PHE:HA	2.00	0.44
1:B:263:GLU:O	1:B:263:GLU:HG2	2.17	0.44
1:A:69:LYS:HG3	1:A:69:LYS:H	1.63	0.44
1:C:409:PRO:HD2	1:C:537:ILE:HG13	1.98	0.44
1:D:618:ALA:HA	4:D:256:HOH:O	2.18	0.44
1:A:95:SER:HB2	4:A:172:HOH:O	2.18	0.43
1:A:49:GLN:NE2	1:A:59:LYS:HZ2	2.16	0.43
1:A:111:SER:HB2	1:A:143:ARG:HG2	1.99	0.43
1:B:201:PRO:HA	1:D:647:GLN:HE22	1.78	0.43
1:D:641:PHE:HA	1:D:720:ILE:HD12	2.01	0.43
1:A:12:THR:CG2	1:A:13:ASP:N	2.81	0.43
1:A:24:PRO:HA	1:A:27:TYR:CE2	2.53	0.43
1:A:87:ASP:HB3	1:B:312:ILE:HG13	2.01	0.43
1:C:419:ILE:C	1:C:421:LYS:H	2.22	0.43
1:C:443:LYS:HG2	1:C:444:CYS:N	2.33	0.43
1:D:693:ILE:CG2	1:D:697:LYS:HE3	2.49	0.43
1:B:261:ASN:OD1	1:B:261:ASN:N	2.48	0.42
1:C:411:LEU:HD12	1:C:411:LEU:HA	1.93	0.42
1:C:514:PHE:CD2	1:C:542:LEU:HD13	2.54	0.42
1:A:61:ASN:O	1:A:61:ASN:CG	2.56	0.42
1:B:212:THR:HG22	1:B:214:GLY:N	2.33	0.42
1:D:689:GLN:HE21	1:D:689:GLN:HB3	1.65	0.42
1:D:690:GLU:HG3	4:D:260:HOH:O	2.19	0.42
1:A:22:ILE:O	1:A:25:LYS:HG2	2.19	0.42
1:A:111:SER:HB3	1:A:146:TYR:CE2	2.55	0.42
1:B:301:GLN:OE1	1:B:305:THR:HG21	2.19	0.42
1:C:504:LYS:HE3	1:C:505:THR:HG22	2.00	0.42
1:D:665:ASP:HB3	1:D:668:VAL:HG23	2.02	0.42
1:A:22:ILE:HD12	1:A:131:PHE:HE1	1.83	0.42
1:C:522:VAL:HG22	1:C:531:PHE:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:608:LEU:HD11	1:D:741:LEU:HD22	2.01	0.42
1:A:117:LEU:HD23	1:A:117:LEU:C	2.39	0.42
1:B:227:TYR:O	1:B:230:TYR:HB3	2.20	0.42
1:D:635:LEU:HD22	1:D:639:LEU:HG	2.02	0.42
1:A:135:PHE:HA	1:A:138:ILE:HB	2.03	0.41
1:C:446:PRO:O	1:C:449:GLN:HB2	2.19	0.41
1:D:709:VAL:CG1	1:D:710:ASP:N	2.83	0.41
1:C:483:ILE:O	1:C:486:MET:HG3	2.20	0.41
1:A:32:GLN:O	1:A:32:GLN:HG2	2.21	0.41
1:A:58:LYS:O	1:A:60:SER:N	2.52	0.41
1:C:403:ILE:HG23	1:C:405:GLN:H	1.85	0.41
1:C:509:VAL:HG21	2:C:547:HEM:CAC	2.51	0.41
1:C:514:PHE:HB2	4:C:6:HOH:O	2.21	0.41
1:D:652:PHE:CE1	2:D:747:HEM:HAC	2.56	0.41
1:B:228:LYS:HB3	1:B:229:GLU:OE1	2.21	0.40
1:D:612:THR:CG2	1:D:613:ASP:N	2.84	0.40
1:A:25:LYS:HG2	1:A:25:LYS:H	1.48	0.40
1:A:84:ASN:ND2	1:D:603:ILE:HA	2.36	0.40
1:A:85:SER:O	1:A:92:ILE:HD11	2.20	0.40
1:A:89:GLN:HE21	1:A:89:GLN:HB3	1.61	0.40
1:C:403:ILE:CG2	1:C:405:GLN:O	2.70	0.40
1:A:15:ASP:OD2	1:A:133:LYS:HE2	2.21	0.40
1:A:78:LYS:HE3	2:A:147:HEM:HMA3	2.02	0.40
1:C:432:GLN:HG3	1:C:433:TYR:N	2.36	0.40
1:A:62:LEU:O	1:A:68:VAL:HG11	2.21	0.40
1:A:99:LEU:HA	1:A:102:LYS:HZ2	1.85	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 X-ray entries followed by that with respect to entries of similar resolution.

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	144/146 (99%)	136 (94%)	7 (5%)	1 (1%)	22	18
1	B	144/146 (99%)	136 (94%)	5 (4%)	3 (2%)	7	3
1	C	144/146 (99%)	138 (96%)	3 (2%)	3 (2%)	7	3
1	D	144/146 (99%)	137 (95%)	4 (3%)	3 (2%)	7	3
All	All	576/584 (99%)	547 (95%)	19 (3%)	10 (2%)	9	4

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	262	LEU
1	D	662	LEU
1	A	59	LYS
1	B	261	ASN
1	C	456	SER
1	C	457	THR
1	D	659	LYS
1	B	259	LYS
1	C	420	ASN
1	D	656	SER

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	136/136 (100%)	110 (81%)	26 (19%)	1	0
1	B	136/136 (100%)	104 (76%)	32 (24%)	1	0
1	C	136/136 (100%)	111 (82%)	25 (18%)	1	1
1	D	136/136 (100%)	114 (84%)	22 (16%)	2	1
All	All	544/544 (100%)	439 (81%)	105 (19%)	1	0

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	11	LEU
1	A	17	LYS
1	A	21	LYS
1	A	25	LYS
1	A	28	LYS
1	A	29	GLU
1	A	32	GLN
1	A	34	SER
1	A	35	LEU
1	A	43	LYS
1	A	51	SER
1	A	58	LYS
1	A	61	ASN
1	A	62	LEU
1	A	73	VAL
1	A	85	SER
1	A	88	ASN
1	A	89	GLN
1	A	94	LYS
1	A	97	LYS
1	A	104	LYS
1	A	126	ASP
1	A	134	LEU
1	A	141	LEU
1	A	146	TYR
1	B	211	LEU
1	B	217	LYS
1	B	221	LYS
1	B	231	GLU
1	B	232	GLN
1	B	235	LEU
1	B	247	GLN
1	B	256	SER
1	B	258	LYS
1	B	259	LYS
1	B	260	SER
1	B	261	ASN
1	B	262	LEU
1	B	263	GLU
1	B	264	GLN
1	B	269	LYS
1	B	276	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	278	LYS
1	B	289	GLN
1	B	294	LYS
1	B	301	GLN
1	B	302	LYS
1	B	304	LYS
1	B	305	THR
1	B	310	ASP
1	B	317	LEU
1	B	321	PHE
1	B	330	GLU
1	B	333	LYS
1	B	334	LEU
1	B	341	LEU
1	B	343	ARG
1	C	408	LEU
1	C	411	LEU
1	C	421	LYS
1	C	425	LYS
1	C	428	LYS
1	C	435	LEU
1	C	443	LYS
1	C	447	GLN
1	C	451	SER
1	C	457	THR
1	C	458	LYS
1	C	464	GLN
1	C	476	PHE
1	C	478	LYS
1	C	485	SER
1	C	489	GLN
1	C	497	LYS
1	C	502	LYS
1	C	505	THR
1	C	509	VAL
1	C	510	ASP
1	C	515	LYS
1	C	517	LEU
1	C	534	LEU
1	C	541	LEU
1	D	603	ILE
1	D	611	LEU

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Mol	Chain	Res	Type
1	D	616	LYS
1	D	617	LYS
1	D	621	LYS
1	D	625	LYS
1	D	629	GLU
1	D	632	GLN
1	D	635	LEU
1	D	640	ARG
1	D	643	LYS
1	D	657	THR
1	D	661	ASN
1	D	684	ASN
1	D	685	SER
1	D	688	ASN
1	D	689	GLN
1	D	708	LYS
1	D	717	LEU
1	D	734	LEU
1	D	741	LEU
1	D	743	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	32	GLN
1	A	49	GLN
1	A	71	GLN
1	A	80	ASN
1	A	84	ASN
1	A	88	ASN
1	A	89	GLN
1	B	247	GLN
1	B	277	ASN
1	B	280	ASN
1	C	432	GLN
1	C	436	ASN
1	C	464	GLN
1	C	480	ASN
1	C	501	GLN
1	D	632	GLN
1	D	647	GLN

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Mol	Chain	Res	Type
1	D	680	ASN
1	D	688	ASN
1	D	689	GLN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	CMO	A	148	2	0,1,1	-	-	-		
3	CMO	B	348	2	0,1,1	-	-	-		
2	HEM	D	747	1,3	41,50,50	1.53	8 (19%)	45,82,82	0.97	2 (4%)
2	HEM	B	347	1,3	41,50,50	1.36	5 (12%)	45,82,82	0.90	0
2	HEM	C	547	1,3	41,50,50	1.54	9 (21%)	45,82,82	1.12	1 (2%)
3	CMO	C	548	2	0,1,1	-	-	-		
2	HEM	A	147	1,3	41,50,50	1.43	7 (17%)	45,82,82	0.95	1 (2%)
3	CMO	D	748	2	0,1,1	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	547	1,3	-	6/12/54/54	-
2	HEM	A	147	1,3	-	3/12/54/54	-
2	HEM	D	747	1,3	-	5/12/54/54	-
2	HEM	B	347	1,3	-	4/12/54/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	747	HEM	C3C-CAC	-4.67	1.38	1.47
2	C	547	HEM	C3C-CAC	-4.30	1.39	1.47
2	C	547	HEM	C3C-C2C	-3.76	1.35	1.40
2	A	147	HEM	C3C-CAC	-3.60	1.40	1.47
2	D	747	HEM	C4A-NA	3.41	1.43	1.36
2	B	347	HEM	C3C-CAC	-3.30	1.41	1.47
2	C	547	HEM	CHA-C4D	3.09	1.42	1.35
2	D	747	HEM	C1A-NA	2.96	1.42	1.36
2	B	347	HEM	CHB-C1B	2.93	1.42	1.35
2	B	347	HEM	CAB-C3B	-2.93	1.39	1.47
2	B	347	HEM	C1A-NA	2.86	1.42	1.36
2	D	747	HEM	CAB-C3B	-2.75	1.40	1.47
2	A	147	HEM	CHA-C4D	2.74	1.42	1.35
2	B	347	HEM	C4A-NA	2.72	1.41	1.36
2	A	147	HEM	CAB-C3B	-2.71	1.40	1.47
2	D	747	HEM	CHA-C4D	2.64	1.41	1.35
2	C	547	HEM	CAB-C3B	-2.58	1.40	1.47
2	D	747	HEM	C3C-C2C	-2.55	1.36	1.40
2	A	147	HEM	CHB-C1B	2.51	1.41	1.35
2	C	547	HEM	CHB-C1B	2.45	1.41	1.35
2	D	747	HEM	CBB-CAB	2.39	1.42	1.30
2	C	547	HEM	C4A-NA	2.36	1.41	1.36
2	D	747	HEM	CHB-C1B	2.33	1.40	1.35
2	A	147	HEM	C1A-NA	2.30	1.40	1.36
2	C	547	HEM	CBB-CAB	2.29	1.41	1.30
2	A	147	HEM	C4A-NA	2.28	1.40	1.36
2	C	547	HEM	C1A-NA	2.21	1.40	1.36
2	A	147	HEM	CBB-CAB	2.10	1.40	1.30
2	C	547	HEM	C2C-C1C	2.04	1.47	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	547	HEM	CBA-CAA-C2A	2.89	117.56	112.62
2	A	147	HEM	CMB-C2B-C1B	2.89	129.44	125.04
2	D	747	HEM	CAD-C3D-C2D	-2.50	123.23	127.88
2	D	747	HEM	CAD-C3D-C4D	2.19	128.48	124.66

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	347	HEM	C2B-C3B-CAB-CBB
2	B	347	HEM	C4B-C3B-CAB-CBB
2	A	147	HEM	C2B-C3B-CAB-CBB
2	D	747	HEM	C3D-CAD-CBD-CGD
2	C	547	HEM	C2B-C3B-CAB-CBB
2	D	747	HEM	C2B-C3B-CAB-CBB
2	C	547	HEM	CAD-CBD-CGD-O2D
2	D	747	HEM	CAD-CBD-CGD-O1D
2	D	747	HEM	CAD-CBD-CGD-O2D
2	B	347	HEM	CAD-CBD-CGD-O2D
2	C	547	HEM	CAD-CBD-CGD-O1D
2	B	347	HEM	CAD-CBD-CGD-O1D
2	C	547	HEM	CAA-CBA-CGA-O1A
2	A	147	HEM	C4B-C3B-CAB-CBB
2	C	547	HEM	C4B-C3B-CAB-CBB
2	D	747	HEM	C4B-C3B-CAB-CBB
2	C	547	HEM	CAA-CBA-CGA-O2A
2	A	147	HEM	CAA-CBA-CGA-O2A

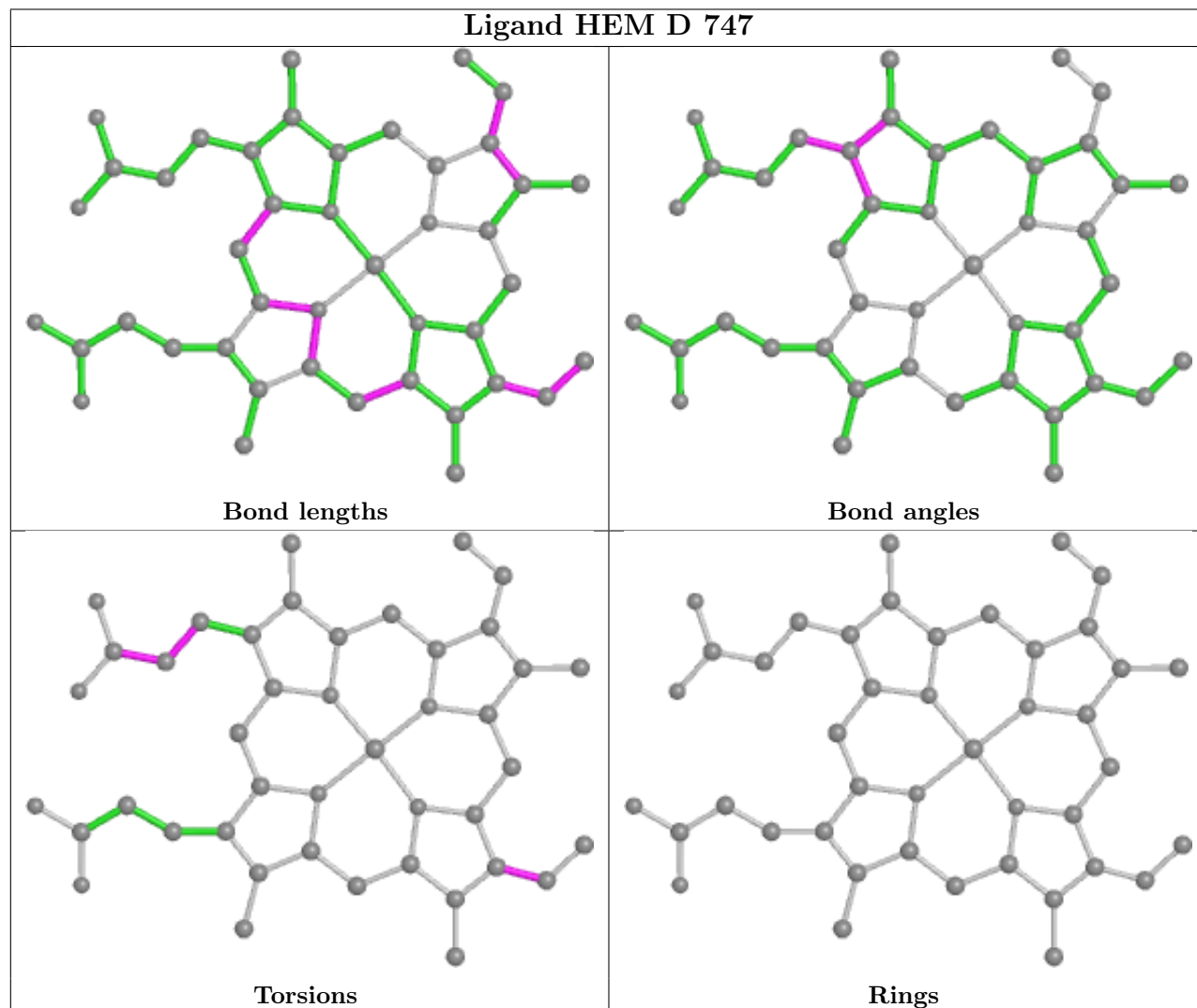
There are no ring outliers.

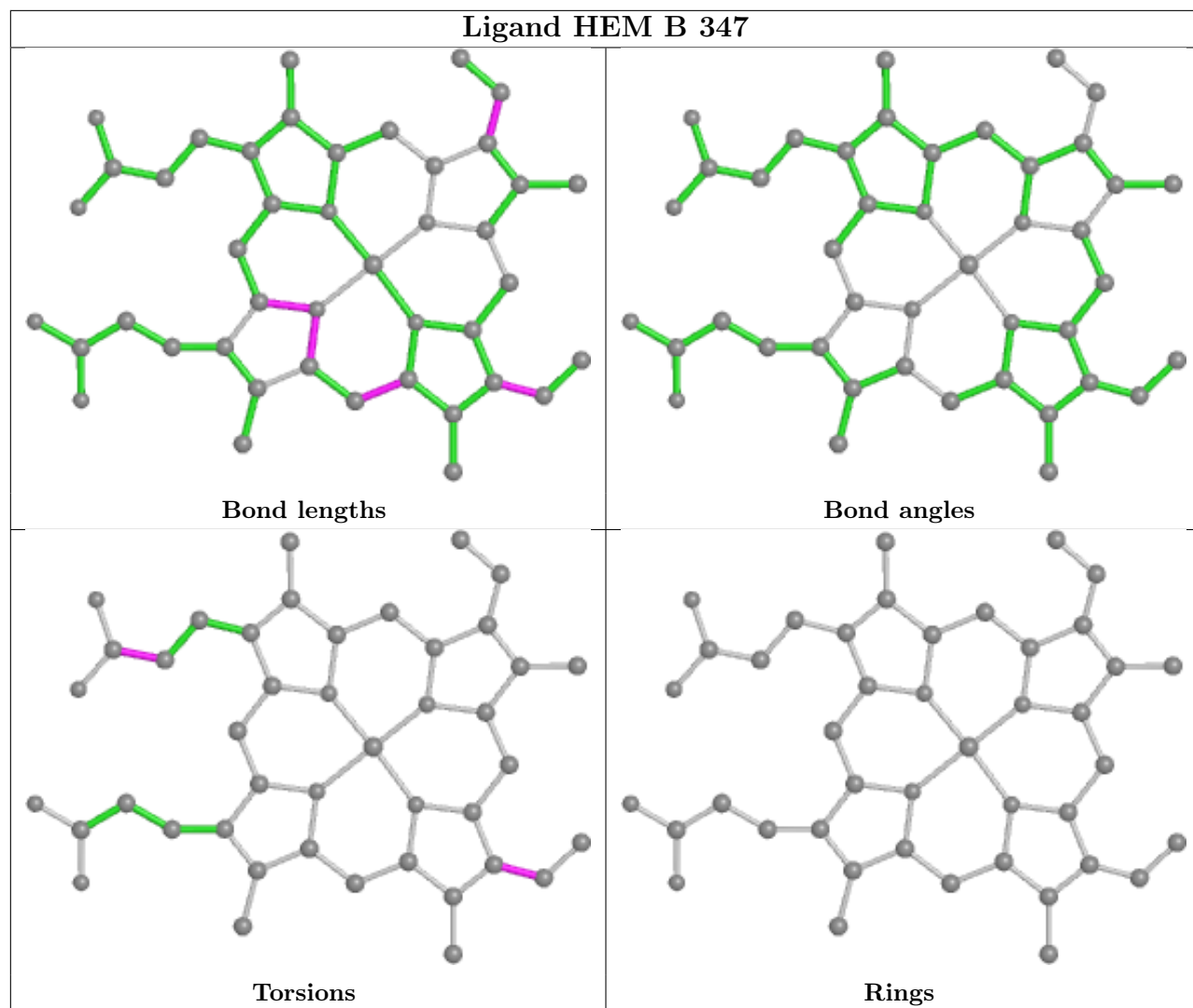
4 monomers are involved in 9 short contacts:

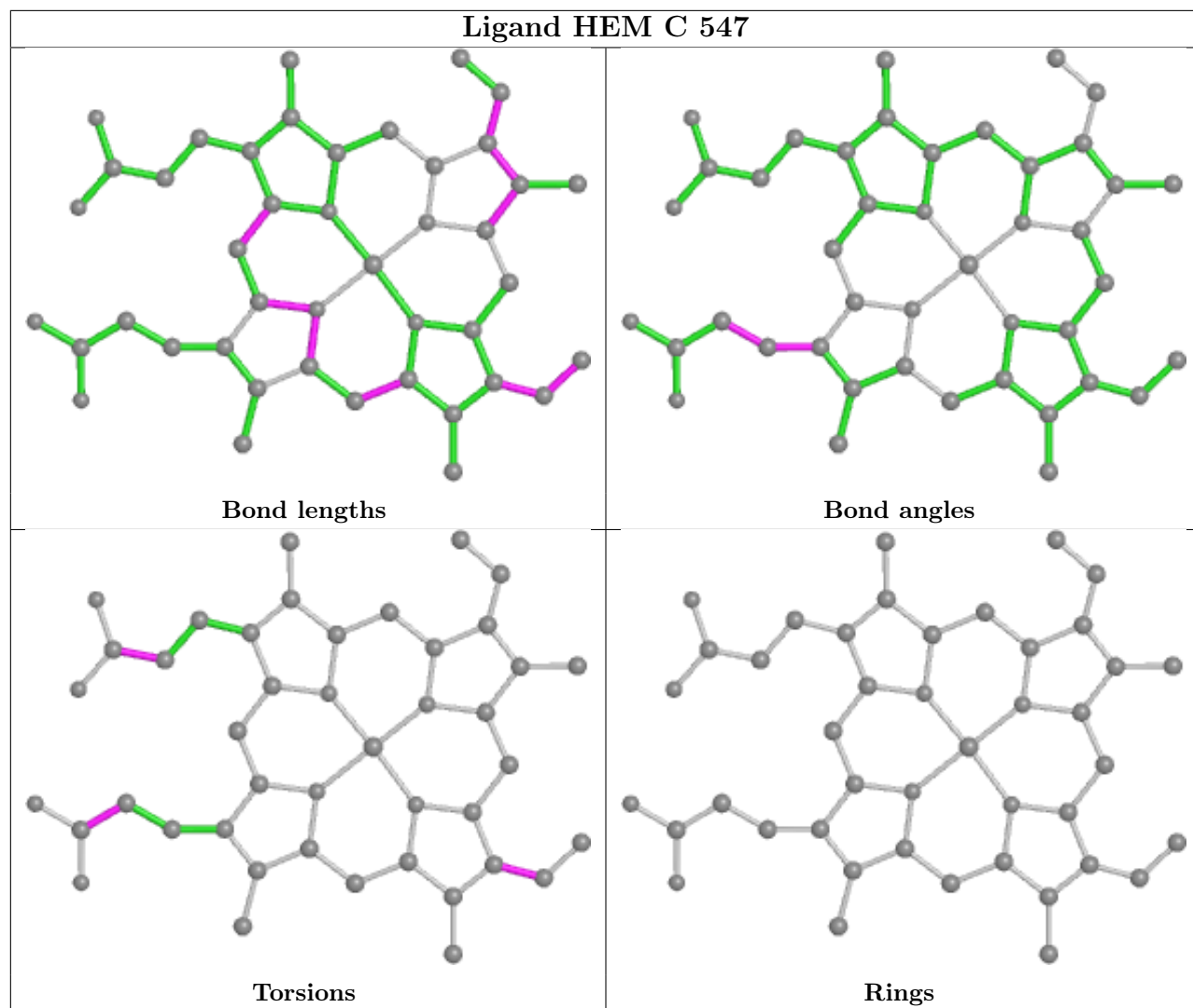
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	747	HEM	2	0
2	B	347	HEM	4	0
2	C	547	HEM	1	0
2	A	147	HEM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

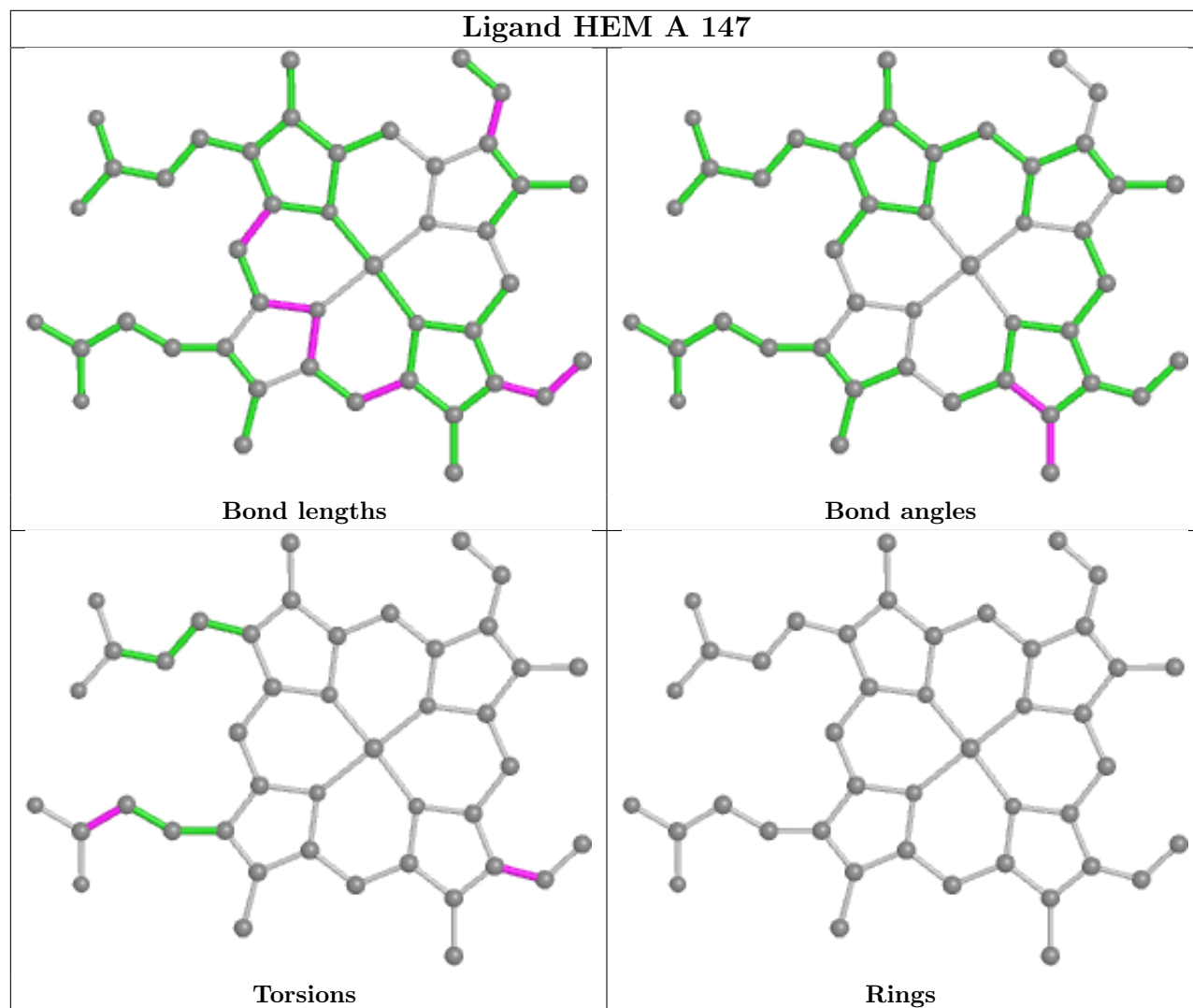
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 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 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.