Full wwPDB X-ray Structure Validation Report (i)

Apr 29, 2024 – 10:03 am BST

PDB ID	:	1DWV
Title	:	MURINE INDUCIBLE NITRIC OXIDE SYNTHASE OXYGENASE DIMER N-hydroxyarginine and 4-amino tetrahydrobiopterin
Authors	:	Crane, B.R.; Arvai, A.S.; Getzoff, E.D.; Stuehr, D.J.; Tainer, J.A.
Deposited on	:	1999-12-14
Resolution	:	2.35 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

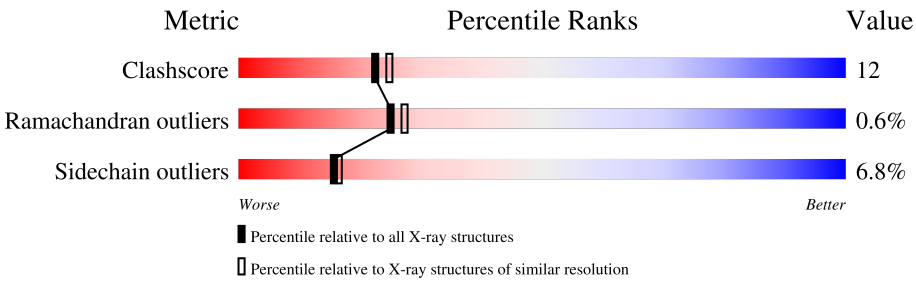
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)

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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	420	73% 24% •
1	B	420	75% 22% •

2 Entry composition (i)

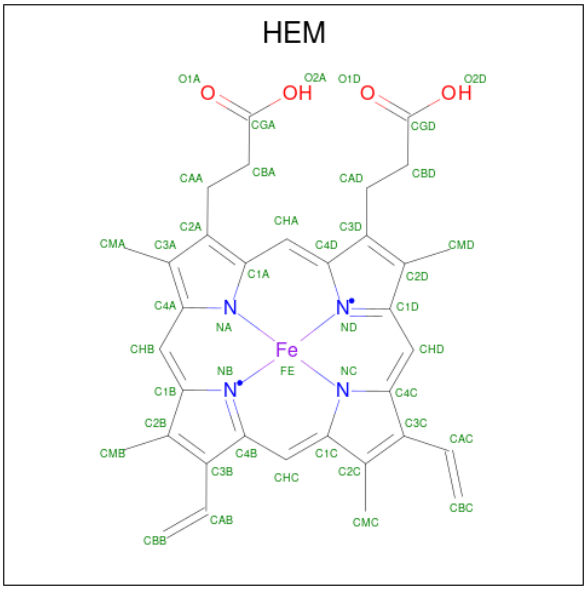
There are 7 unique types of molecules in this entry. The entry contains 7461 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 NITRIC OXIDE SYNTHASE.

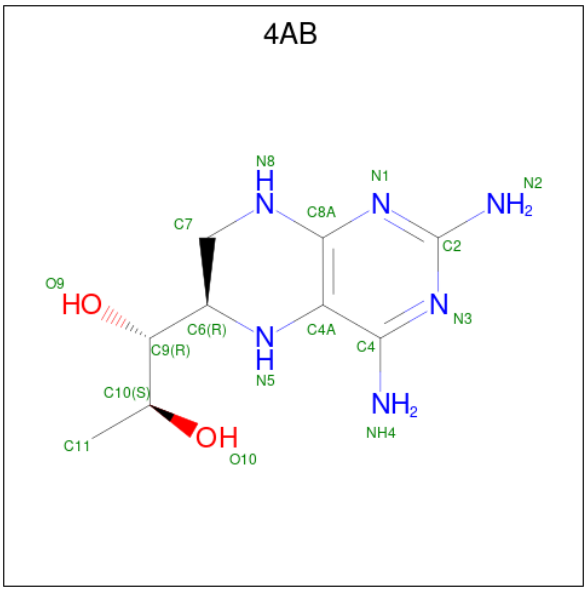
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	420	3424	2194	590	619	21	0	0	0
1	B	420	3424	2194	590	619	21	0	0	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is 2,4-DIAMINO-6-[2,3-DIHYDROXY-PROP-3-YL]-5,6,7,8-TETRAHYDROPTERIDINE (three-letter code: 4AB) (formula: $C_9H_{16}N_6O_2$).

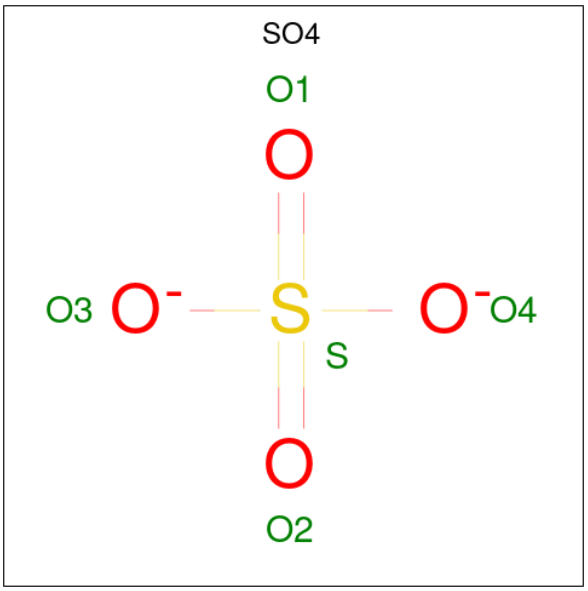


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	17	9	6	2	0	0
			Total	C	N	O		
3	B	1	17	9	6	2	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

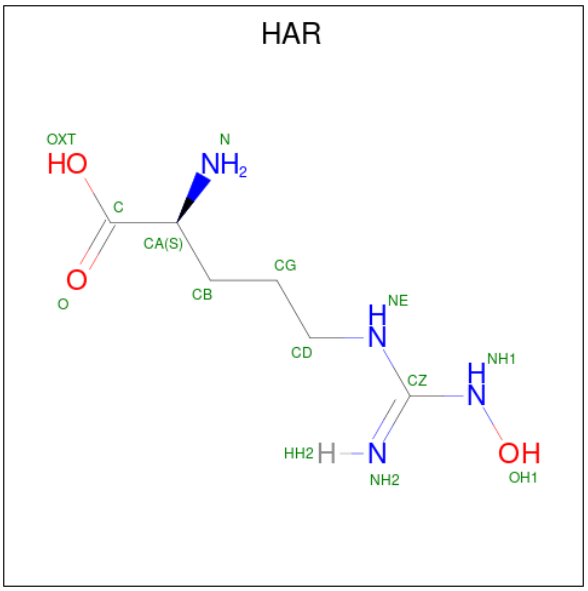
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0
			Total	Zn		
4	B	1	1	1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is N-OMEGA-HYDROXY-L-ARGININE (three-letter code: HAR) (formula: $C_6H_{14}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	13	6	4	3	0	0
			Total	C	N	O		
6	B	1	13	6	4	3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	209	209	209	0	0
			Total	O		
7	B	216	216	216	0	0

3 Residue-property plots (i)

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: NITRIC OXIDE SYNTHASE

Chain A: 73% 24% •

• Molecule 1: NITRIC OXIDE SYNTHASE

Chain B: 75% 22% •

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	212.98Å 212.98Å 114.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.35	Depositor
% Data completeness (in resolution range)	92.1 (30.00-2.35)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.247 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7461	wwPDB-VP
Average B, all atoms (Å^2)	60.0	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: 4AB, ZN, HEM, HAR, SO4

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	0.39	0/3524	0.64	1/4790 (0.0%)
1	B	0.39	0/3524	0.65	2/4790 (0.0%)
All	All	0.39	0/7048	0.64	3/9580 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	365	GLY	N-CA-C	-6.11	97.83	113.10
1	B	80	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	B	365	GLY	N-CA-C	-5.96	98.20	113.10

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	3424	0	3320	87	0
1	B	3424	0	3320	73	0
2	A	43	0	30	0	0
2	B	43	0	30	2	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	20	0	0	0	0
5	B	20	0	0	0	0
6	A	13	0	12	0	0
6	B	13	0	12	0	0
7	A	209	0	0	12	0
7	B	216	0	0	2	0
All	All	7461	0	6754	160	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 12.

All (160) 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:266:MET:SD	1:A:272:ARG:HD3	2.13	0.88
1:A:81:ILE:HD11	1:A:475:LEU:HD13	1.58	0.85
1:A:217:MET:HE2	1:A:305:ALA:HB2	1.60	0.83
1:A:141:ILE:HD11	1:A:163:VAL:HG21	1.61	0.82
1:B:77:GLN:HE21	1:B:77:GLN:HA	1.47	0.79
1:B:467:THR:CG2	1:B:469:VAL:HG22	2.18	0.74
1:A:81:ILE:HG21	7:A:2183:HOH:O	1.90	0.71
1:A:195:ILE:HG21	1:A:368:MET:HE3	1.73	0.70
1:B:177:LEU:O	1:B:181:ILE:HD13	1.89	0.69
1:B:356:LEU:H	1:B:356:LEU:HD23	1.58	0.69
1:B:301:LEU:HD13	1:B:315:ILE:HD11	1.75	0.68
1:A:407:ARG:HA	7:A:2159:HOH:O	1.96	0.66
1:B:175:LEU:CD2	1:B:356:LEU:HD11	2.26	0.66
1:B:459:VAL:HG22	1:B:469:VAL:HG23	1.81	0.63
1:B:175:LEU:HD22	1:B:356:LEU:HD11	1.81	0.62
1:A:438:MET:HE3	1:A:469:VAL:HA	1.81	0.62
1:A:252:ARG:HB2	1:A:304:GLN:HG2	1.80	0.62
1:B:141:ILE:HD11	1:B:163:VAL:HG21	1.81	0.62
1:A:81:ILE:HD13	7:A:2183:HOH:O	1.99	0.62
1:A:467:THR:CG2	1:A:469:VAL:HG22	2.31	0.61
1:A:221:ILE:HG21	1:A:301:LEU:HD21	1.83	0.61
1:B:148:PHE:CZ	1:B:152:LYS:HE2	2.35	0.61
1:A:438:MET:CE	1:A:469:VAL:HG12	2.31	0.60
1:B:209:ARG:O	1:B:242:PRO:HG3	2.02	0.60
1:B:467:THR:HG21	1:B:469:VAL:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ARG:HD3	7:B:2073:HOH:O	1.99	0.60
1:A:194:CYS:O	1:A:197:ARG:HD3	2.02	0.59
1:B:116:PRO:HG2	1:B:119:LEU:HB2	1.85	0.59
1:A:209:ARG:O	1:A:242:PRO:HG3	2.03	0.58
1:B:464:GLY:O	1:B:467:THR:HB	2.02	0.58
1:A:266:MET:SD	1:A:272:ARG:CD	2.89	0.58
1:B:304:GLN:HG3	1:B:304:GLN:O	2.03	0.58
1:B:272:ARG:NH1	1:B:295:ARG:HG3	2.19	0.57
1:B:99:THR:HG22	1:B:100:SER:N	2.20	0.57
1:A:465:SER:O	1:A:471:HIS:HE1	1.87	0.57
1:A:223:ARG:HD3	7:A:2073:HOH:O	2.03	0.57
1:B:186:MET:HB3	1:B:481:PRO:HG2	1.87	0.56
1:B:80:ARG:NH2	1:B:89:ILE:HD13	2.20	0.56
1:B:438:MET:CE	1:B:469:VAL:HG12	2.35	0.56
1:B:330:TYR:HD2	1:B:332:TRP:CZ2	2.25	0.55
1:A:438:MET:HE2	1:A:469:VAL:HG12	1.89	0.55
1:B:252:ARG:NH2	1:B:489:PRO:HD3	2.22	0.55
1:A:77:GLN:O	1:A:96:HIS:HE1	1.89	0.55
1:A:368:MET:HE2	1:A:433:ALA:CB	2.37	0.55
1:A:194:CYS:HB3	1:A:197:ARG:HD2	1.89	0.54
1:A:467:THR:HG21	1:A:469:VAL:HG22	1.90	0.54
1:A:273:GLY:HA2	1:A:295:ARG:O	2.07	0.54
1:B:258:LEU:HB2	1:B:345:ALA:HB3	1.90	0.53
1:B:348:ASN:HD22	1:B:348:ASN:H	1.55	0.53
1:B:221:ILE:HG21	1:B:301:LEU:HD21	1.90	0.53
1:A:257:GLN:HG3	1:A:260:ARG:HD3	1.89	0.53
1:A:348:ASN:HB2	7:A:2091:HOH:O	2.09	0.53
1:A:258:LEU:HB2	1:A:345:ALA:HB3	1.90	0.53
1:A:304:GLN:O	1:A:304:GLN:HG3	2.09	0.52
1:A:459:VAL:HG22	1:A:469:VAL:HG23	1.89	0.52
1:A:217:MET:CE	1:A:303:LEU:HB3	2.38	0.52
1:A:244:ARG:HD2	1:A:357:GLU:OE2	2.10	0.52
1:A:144:TYR:CZ	1:A:148:PHE:HZ	2.28	0.52
1:A:266:MET:HB3	1:A:267:PRO:HD2	1.92	0.52
1:B:305:ALA:O	1:B:308:GLN:HG2	2.10	0.52
1:B:215:GLN:HE21	1:B:219:GLN:NE2	2.08	0.52
1:B:445:TYR:CE1	1:B:450:GLY:HA2	2.45	0.52
1:B:81:ILE:HD11	1:B:475:LEU:HD22	1.92	0.51
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.45	0.51
1:A:190:ASN:O	1:A:192:PRO:HD3	2.11	0.51
1:A:386:LEU:HB2	7:A:2148:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.46	0.51
1:B:239:THR:O	1:B:361:CYS:HA	2.11	0.51
1:B:438:MET:HG3	1:B:468:PRO:HB2	1.93	0.51
1:A:301:LEU:HD13	1:A:315:ILE:HD11	1.93	0.51
1:A:410:THR:O	1:A:414:VAL:HG22	2.11	0.50
1:A:239:THR:O	1:A:361:CYS:HA	2.11	0.50
1:A:360:ALA:HA	7:A:2137:HOH:O	2.11	0.50
1:A:283:LEU:O	1:A:287:LEU:HG	2.12	0.50
1:A:348:ASN:HD22	1:A:348:ASN:H	1.59	0.50
1:B:285:ILE:HD12	1:B:291:PRO:HD3	1.92	0.50
1:B:327:HIS:ND1	1:B:328:PRO:HD2	2.27	0.50
1:B:434:SER:HB3	1:B:468:PRO:HD2	1.94	0.50
1:B:173:TYR:CE1	1:B:356:LEU:HD22	2.46	0.49
1:A:281:THR:O	1:A:285:ILE:HG12	2.12	0.49
1:A:348:ASN:H	1:A:348:ASN:ND2	2.09	0.49
1:A:264:TYR:CE2	1:A:293:TYR:HA	2.47	0.49
1:B:438:MET:HE2	1:B:469:VAL:HG12	1.94	0.49
1:B:348:ASN:H	1:B:348:ASN:ND2	2.10	0.49
1:A:368:MET:HE2	1:A:433:ALA:HB3	1.94	0.49
1:B:197:ARG:NH2	1:B:452:PRO:O	2.45	0.49
1:B:385:ILE:O	1:B:389:VAL:HG23	2.13	0.49
1:B:142:ASN:ND2	1:B:160:LEU:HD21	2.28	0.48
1:A:134:LEU:HB3	1:A:135:PRO:HD3	1.95	0.48
1:A:293:TYR:CD2	1:B:267:PRO:HB3	2.49	0.48
1:B:190:ASN:O	1:B:192:PRO:HD3	2.14	0.48
1:A:301:LEU:HD22	1:A:315:ILE:HG12	1.96	0.48
1:B:330:TYR:CD1	1:B:330:TYR:N	2.82	0.47
1:B:252:ARG:HB2	1:B:304:GLN:HG2	1.97	0.47
1:A:271:ILE:HG22	7:A:2099:HOH:O	2.15	0.47
1:A:438:MET:HE3	1:A:469:VAL:HG12	1.96	0.47
1:A:195:ILE:HD13	1:A:368:MET:HE1	1.96	0.47
1:B:348:ASN:HD22	1:B:348:ASN:N	2.10	0.47
1:B:188:TRP:O	1:B:197:ARG:HD2	2.15	0.46
1:A:116:PRO:HG2	1:A:119:LEU:HB2	1.97	0.46
1:A:102:PHE:CG	1:A:103:THR:N	2.80	0.46
1:A:252:ARG:NH2	1:A:489:PRO:HD3	2.29	0.46
1:B:488:GLU:HA	1:B:489:PRO:HD2	1.76	0.46
1:B:330:TYR:N	1:B:330:TYR:HD1	2.13	0.46
1:A:134:LEU:O	1:A:138:ILE:HG12	2.16	0.46
1:B:134:LEU:HB3	1:B:135:PRO:HD3	1.97	0.46
1:A:405:LYS:O	1:A:409:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ILE:HD11	1:B:291:PRO:HB3	1.98	0.45
1:A:348:ASN:HD22	1:A:348:ASN:N	2.14	0.45
1:A:407:ARG:HG2	7:A:2159:HOH:O	2.17	0.45
2:B:901:HEM:HBB2	2:B:901:HEM:HHC	1.99	0.45
1:B:386:LEU:HB2	7:B:2153:HOH:O	2.16	0.45
1:A:303:LEU:O	1:A:310:PRO:HA	2.17	0.45
1:A:342:ALA:HB1	1:A:425:VAL:HG11	1.99	0.45
1:A:217:MET:HE3	1:A:303:LEU:HB3	1.98	0.44
1:A:145:TYR:HA	1:A:148:PHE:HE1	1.81	0.44
1:A:145:TYR:HA	1:A:148:PHE:CE1	2.53	0.44
1:B:129:PRO:HG2	1:B:132:GLU:HG2	2.00	0.44
1:B:254:TRP:CZ3	1:B:490:TRP:HB3	2.53	0.44
1:B:378:CYS:SG	1:B:386:LEU:HD23	2.58	0.44
1:A:123:PRO:HD3	1:A:487:ILE:HD12	2.00	0.44
1:A:467:THR:HG23	1:A:468:PRO:HD2	2.00	0.44
1:B:99:THR:HG22	1:B:100:SER:H	1.83	0.44
1:A:321:LEU:HD12	7:A:2124:HOH:O	2.19	0.43
1:A:438:MET:HG3	1:A:468:PRO:HB2	2.01	0.43
1:A:214:ALA:HA	1:A:217:MET:HE3	2.00	0.43
1:A:488:GLU:HA	1:A:489:PRO:HD2	1.83	0.43
1:B:258:LEU:HD13	1:B:347:ALA:HB2	2.00	0.43
1:A:217:MET:HE1	1:A:303:LEU:HB3	2.01	0.43
1:B:410:THR:O	1:B:414:VAL:HG13	2.18	0.43
1:B:281:THR:O	1:B:285:ILE:HG12	2.19	0.42
1:A:467:THR:HG22	1:A:469:VAL:HG22	1.99	0.42
1:A:267:PRO:HB3	1:B:293:TYR:CD2	2.54	0.42
1:B:467:THR:HA	1:B:468:PRO:HD3	1.94	0.42
1:B:453:ALA:HB1	1:B:458:LEU:CD1	2.50	0.42
1:A:263:GLY:O	1:A:278:LEU:HD23	2.19	0.42
1:A:494:ILE:HG12	7:A:2194:HOH:O	2.19	0.42
1:B:254:TRP:CE2	1:B:489:PRO:HB2	2.55	0.42
1:A:258:LEU:HA	1:A:258:LEU:HD12	1.82	0.41
1:A:195:ILE:HG21	1:A:368:MET:CE	2.47	0.41
1:B:356:LEU:HD23	1:B:356:LEU:N	2.31	0.41
1:A:285:ILE:HD11	1:A:291:PRO:HB3	2.02	0.41
1:A:141:ILE:CD1	1:A:163:VAL:HG21	2.40	0.41
1:B:127:PRO:HG3	1:B:246:ASP:HA	2.02	0.41
1:B:191:ALA:O	1:B:197:ARG:NH1	2.54	0.41
1:A:227:TYR:CD1	1:A:227:TYR:C	2.94	0.41
1:B:241:PHE:HB3	1:B:242:PRO:HD2	2.02	0.41
1:A:94:LEU:HB2	1:A:450:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ARG:NH1	1:A:128:THR:OG1	2.54	0.41
1:A:464:GLY:O	1:A:467:THR:HB	2.21	0.41
1:B:386:LEU:HD13	1:B:404:TRP:CZ3	2.56	0.41
1:A:78:TYR:CD1	1:A:78:TYR:C	2.95	0.41
2:B:901:HEM:HMD2	2:B:901:HEM:HAD1	1.94	0.41
1:A:172:THR:OG1	1:A:173:TYR:N	2.53	0.40
1:B:252:ARG:HB2	1:B:304:GLN:CG	2.51	0.40
1:A:369:GLY:HA2	1:A:427:ILE:HD11	2.03	0.40
1:B:78:TYR:CD1	1:B:78:TYR:C	2.95	0.40
1:A:429:ASP:HA	7:A:2169:HOH:O	2.20	0.40
1:B:102:PHE:CG	1:B:103:THR:N	2.89	0.40
1:A:272:ARG:HH21	1:A:294:GLY:HA2	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	418/420 (100%)	389 (93%)	27 (6%)	2 (0%)	29	32
1	B	418/420 (100%)	390 (93%)	25 (6%)	3 (1%)	22	23
All	All	836/840 (100%)	779 (93%)	52 (6%)	5 (1%)	25	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	100	SER
1	A	100	SER
1	B	306	ASP
1	B	369	GLY
1	A	464	GLY

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	368/368 (100%)	340 (92%)	28 (8%)	13	13
1	B	368/368 (100%)	346 (94%)	22 (6%)	19	21
All	All	736/736 (100%)	686 (93%)	50 (7%)	16	16

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	78	TYR
1	A	114	MET
1	A	119	LEU
1	A	130	LEU
1	A	147	SER
1	A	150	GLU
1	A	157	LEU
1	A	161	GLU
1	A	170	THR
1	A	180	LEU
1	A	257	GLN
1	A	258	LEU
1	A	301	LEU
1	A	303	LEU
1	A	306	ASP
1	A	338	LEU
1	A	348	ASN
1	A	357	GLU
1	A	387	GLU
1	A	395	LEU
1	A	396	GLU
1	A	400	LEU
1	A	414	VAL
1	A	441	MET
1	A	474	MET
1	A	494	ILE

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Mol	Chain	Res	Type
1	A	496	GLN
1	B	77	GLN
1	B	78	TYR
1	B	93	THR
1	B	110	LEU
1	B	119	LEU
1	B	130	LEU
1	B	148	PHE
1	B	210	ASN
1	B	258	LEU
1	B	264	TYR
1	B	292	ARG
1	B	301	LEU
1	B	330	TYR
1	B	348	ASN
1	B	356	LEU
1	B	386	LEU
1	B	400	LEU
1	B	444	GLU
1	B	462	VAL
1	B	467	THR
1	B	474	MET
1	B	475	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	96	HIS
1	A	156	HIS
1	A	202	ASN
1	A	233	ASN
1	A	348	ASN
1	A	421	GLN
1	A	471	HIS
1	B	77	GLN
1	B	91	HIS
1	B	210	ASN
1	B	219	GLN
1	B	233	ASN
1	B	348	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	A	907	-	4,4,4	0.36	0	6,6,6	1.00	0
5	SO4	B	906	-	4,4,4	0.38	0	6,6,6	0.43	0
3	4AB	B	902	-	16,18,18	2.02	1 (6%)	11,26,26	1.67	3 (27%)
5	SO4	B	904	-	4,4,4	1.36	0	6,6,6	0.29	0
2	HEM	A	901	1	41,50,50	1.32	4 (9%)	45,82,82	1.40	8 (17%)
6	HAR	B	909	-	10,12,12	1.13	1 (10%)	11,14,14	0.76	0
2	HEM	B	901	1	41,50,50	1.37	5 (12%)	45,82,82	1.68	8 (17%)
5	SO4	A	906	-	4,4,4	0.78	0	6,6,6	0.39	0
5	SO4	B	905	-	4,4,4	0.27	0	6,6,6	0.99	0
5	SO4	B	907	-	4,4,4	1.61	1 (25%)	6,6,6	1.72	2 (33%)
3	4AB	A	902	-	16,18,18	1.61	1 (6%)	11,26,26	1.81	4 (36%)
5	SO4	A	904	-	4,4,4	1.49	0	6,6,6	0.45	0
6	HAR	A	909	-	10,12,12	1.13	1 (10%)	11,14,14	0.76	0
5	SO4	A	905	-	4,4,4	0.33	0	6,6,6	0.29	0

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	4AB	B	902	-	-	1/8/17/17	0/2/2/2
2	HEM	A	901	1	-	4/12/54/54	-
6	HAR	B	909	-	-	0/11/13/13	-
2	HEM	B	901	1	-	5/12/54/54	-
3	4AB	A	902	-	-	0/8/17/17	0/2/2/2
6	HAR	A	909	-	-	0/11/13/13	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	4AB	C7-C6	-7.21	1.45	1.52
3	A	902	4AB	C7-C6	-5.33	1.47	1.52
2	A	901	HEM	C3C-CAC	-3.54	1.40	1.47
2	B	901	HEM	C3C-CAC	-3.01	1.41	1.47
6	B	909	HAR	OH1-NH1	-2.52	1.33	1.40
2	B	901	HEM	CAB-C3B	-2.50	1.40	1.47
5	B	907	SO4	O2-S	2.37	1.58	1.46
2	A	901	HEM	C1B-NB	-2.36	1.36	1.40
6	A	909	HAR	OH1-NH1	-2.33	1.34	1.40
2	A	901	HEM	CAB-C3B	-2.29	1.41	1.47
2	B	901	HEM	CHD-C1D	-2.20	1.34	1.41
2	B	901	HEM	CHA-C4D	2.20	1.40	1.35
2	A	901	HEM	C3D-C2D	-2.17	1.32	1.36
2	B	901	HEM	C3D-C2D	-2.09	1.32	1.36

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	901	HEM	CAD-C3D-C2D	-3.66	121.07	127.88
2	B	901	HEM	C4B-CHC-C1C	3.66	127.38	122.56
2	A	901	HEM	C4C-CHD-C1D	3.63	127.35	122.56
2	B	901	HEM	C4C-CHD-C1D	3.61	127.32	122.56
2	B	901	HEM	CAD-C3D-C4D	3.45	130.69	124.66
2	B	901	HEM	CMD-C2D-C1D	3.29	130.06	125.04
2	A	901	HEM	CMC-C2C-C3C	3.22	130.71	124.68
2	A	901	HEM	C4A-C3A-C2A	-3.13	104.82	107.00
2	B	901	HEM	C2C-C3C-C4C	-3.06	104.76	106.90
3	A	902	4AB	C2-N3-C4	3.01	120.31	116.99
2	B	901	HEM	CMC-C2C-C3C	2.98	130.25	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	902	4AB	C2-N1-C8A	2.78	120.77	114.54
3	B	902	4AB	C2-N3-C4	2.65	119.92	116.99
2	A	901	HEM	CAD-C3D-C4D	2.58	129.16	124.66
5	B	907	SO4	O4-S-O3	-2.54	98.21	109.06
3	A	902	4AB	C2-N1-C8A	2.51	120.15	114.54
2	A	901	HEM	C4B-CHC-C1C	2.50	125.86	122.56
3	A	902	4AB	NH4-C4-N3	2.44	120.49	117.03
2	B	901	HEM	CAB-C3B-C2B	-2.40	120.70	128.60
5	B	907	SO4	O4-S-O1	-2.36	96.99	109.31
3	A	902	4AB	N3-C2-N1	-2.34	121.74	125.42
2	A	901	HEM	CMD-C2D-C1D	2.32	128.57	125.04
3	B	902	4AB	N3-C2-N1	-2.24	121.91	125.42
2	A	901	HEM	C4B-C3B-C2B	-2.21	105.36	107.11
2	A	901	HEM	C2C-C3C-C4C	-2.05	105.47	106.90

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	HEM	C4B-C3B-CAB-CBB
2	A	901	HEM	CAD-CBD-CGD-O2D
2	A	901	HEM	CAA-CBA-CGA-O1A
2	B	901	HEM	CAD-CBD-CGD-O2D
3	B	902	4AB	C7-C6-C9-O9
2	A	901	HEM	CAA-CBA-CGA-O2A
2	A	901	HEM	CAD-CBD-CGD-O1D
2	B	901	HEM	CAD-CBD-CGD-O1D
2	B	901	HEM	CAA-CBA-CGA-O2A
2	B	901	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

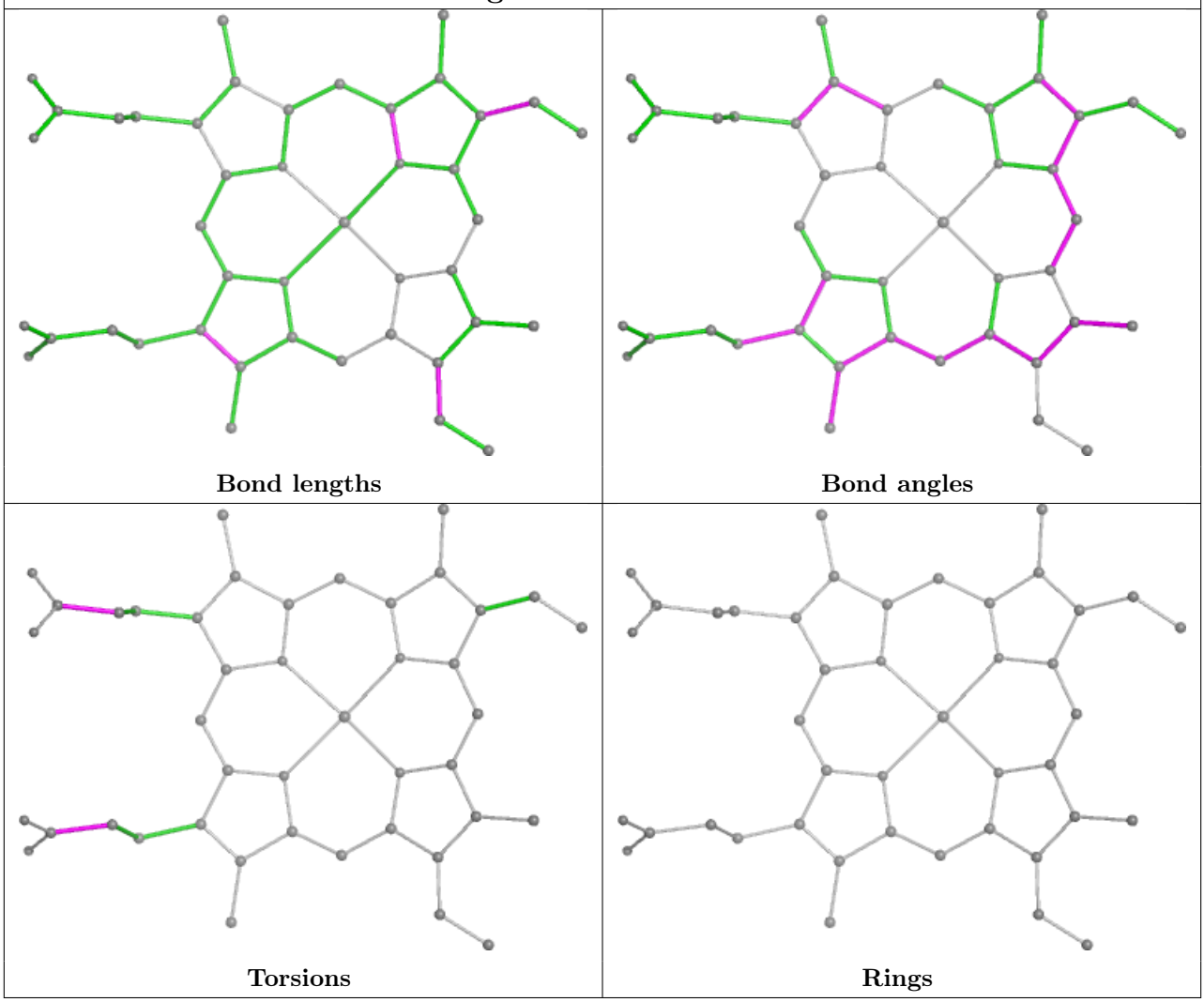
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	HEM	2	0

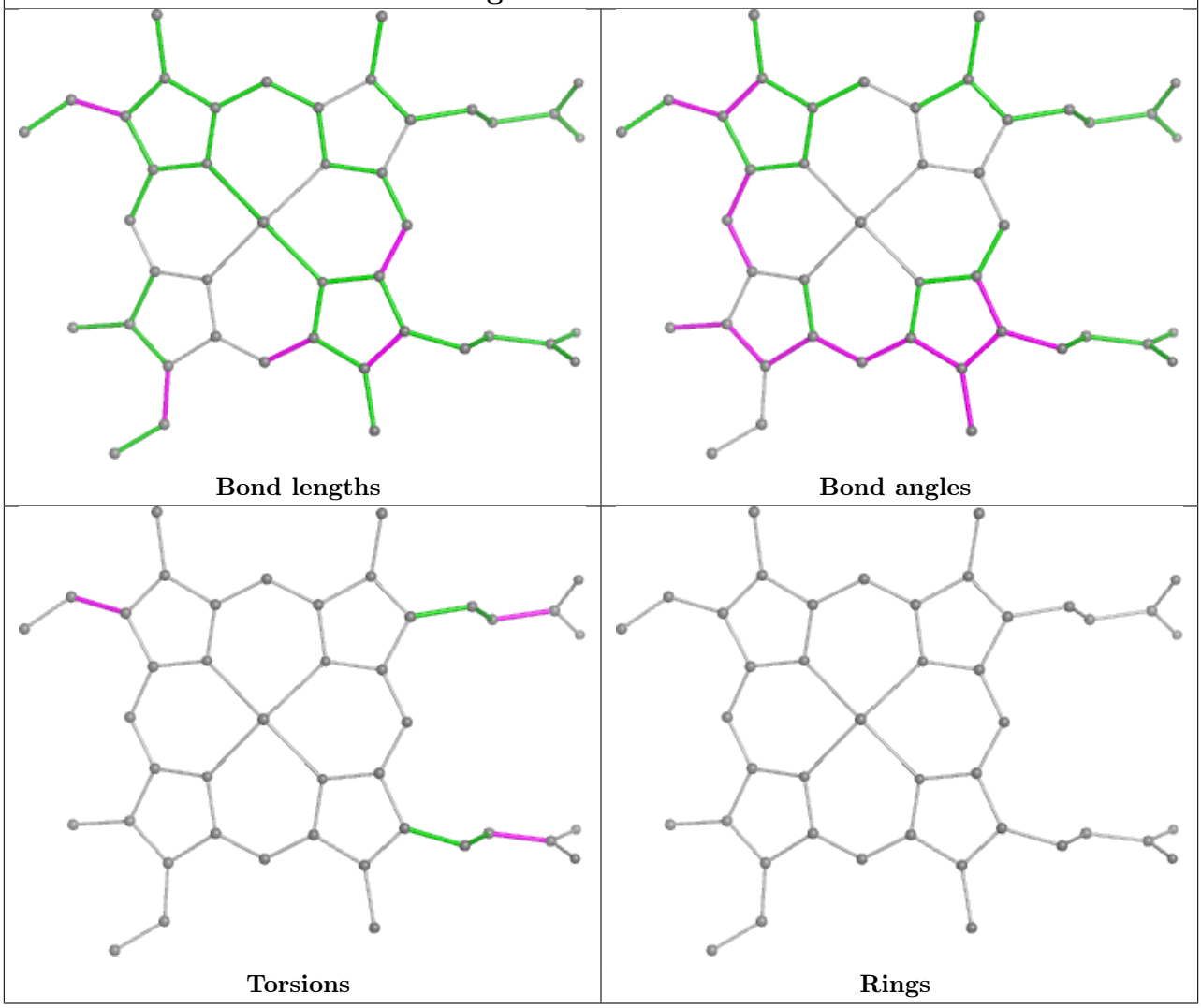
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 HEM A 901



Ligand HEM B 901



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.