



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:53 AM UTC

PDB ID : 1JWJ / pdb_00001jwj
Title : Murine Inducible Nitric Oxide Synthase Oxygenase Dimer (Delta 65) with W457F Mutation at Tetrahydrobiopterin Binding Site
Authors : Aoyagi, M.; Arvai, A.S.; Ghosh, S.; Stuehr, D.J.; Tainer, J.A.; Getzoff, E.D.
Deposited on : 2001-09-04
Resolution : 2.60 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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

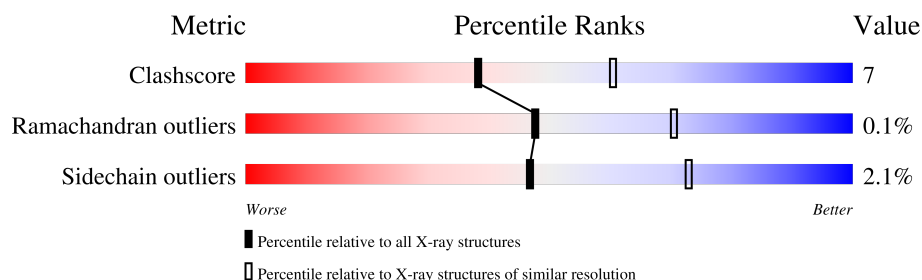
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	433	
1	B	433	

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
5	GOL	A	3102	-	-	X	-
5	GOL	B	3105	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7252 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.

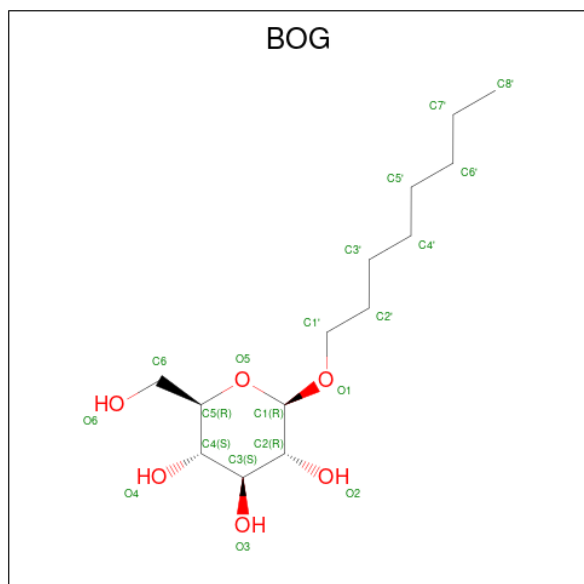
- Molecule 1 is a protein called Nitric Oxide Synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3354	2152	578	604	20			
1	B	411	Total	C	N	O	S	0	0	0
			3344	2147	576	602	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	457	PHE	TRP	engineered mutation	UNP P29477
B	457	PHE	TRP	engineered mutation	UNP P29477

- Molecule 2 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



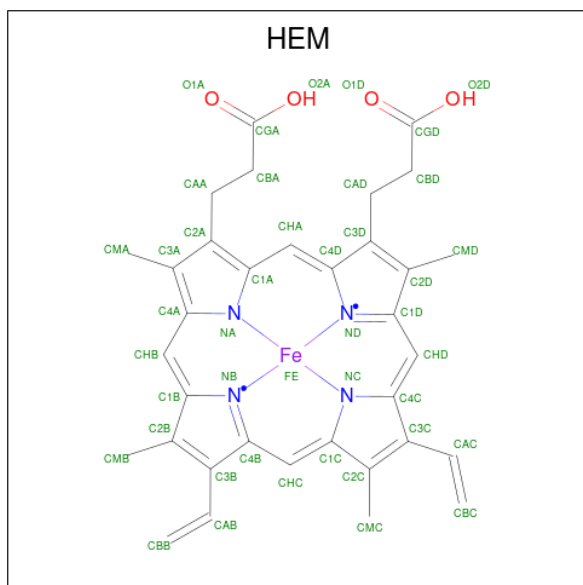
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		

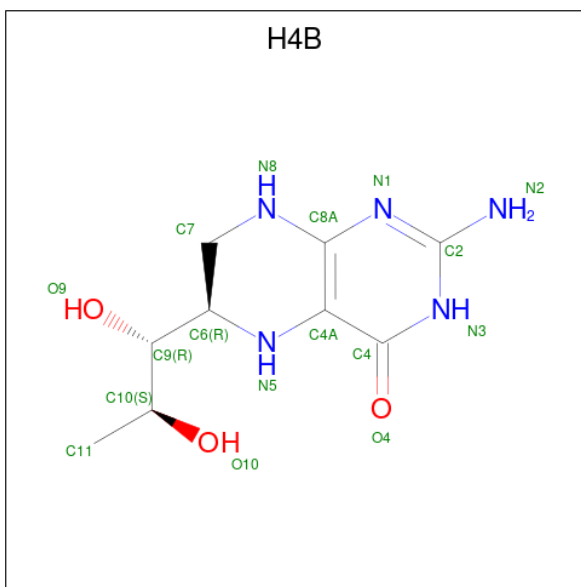
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			20	14	6		

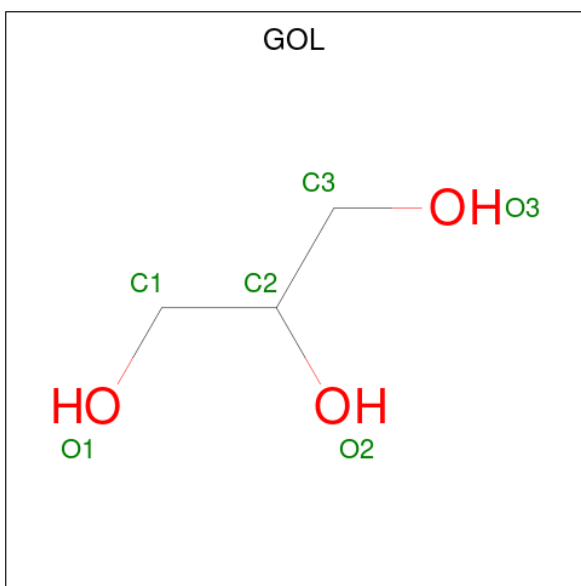
- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	9	5	3		
4	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



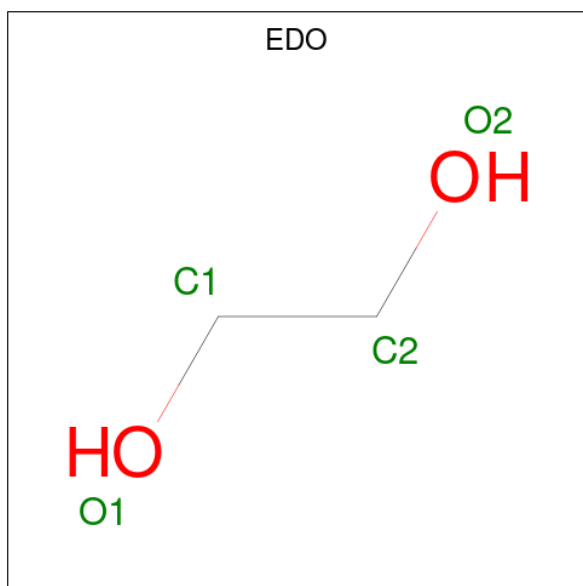
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	159	Total 159	O 159	0	0
7	B	173	Total 173	O 173	0	0

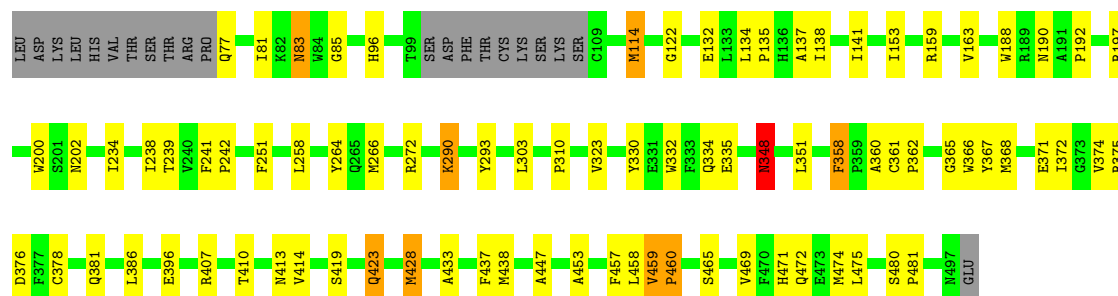
3 Residue-property plots [i](#)

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.

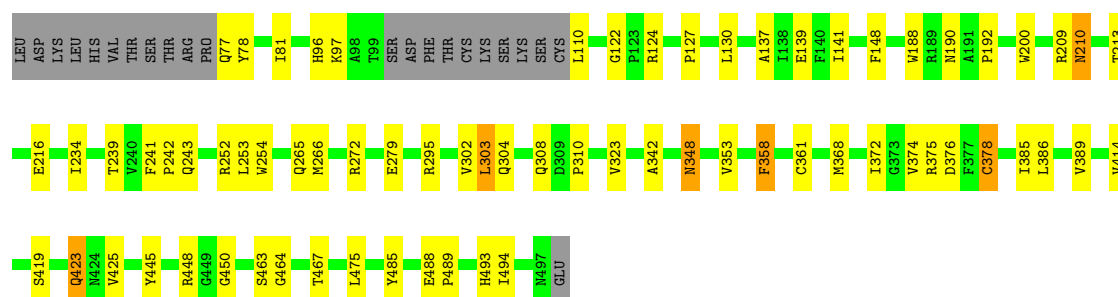
• Molecule 1: Nitric Oxide Synthase

Chain A:  76% 17% • 5%



• Molecule 1: Nitric Oxide Synthase

Chain B:  79% 15% • 5%



4 Data and refinement statistics

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	213.60Å 213.60Å 116.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.41 – 2.60	Depositor
% Data completeness (in resolution range)	96.9 (49.41-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7252	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, GOL, H4B, BOG, HEM

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	0.42	0/3451	0.94	19/4691 (0.4%)
1	B	0.42	0/3441	0.94	13/4678 (0.3%)
All	All	0.42	0/6892	0.94	32/9369 (0.3%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	ASN	N-CA-C	6.93	121.04	112.59
1	A	153	ILE	N-CA-C	6.83	118.40	110.62
1	B	386	LEU	N-CA-C	6.80	118.34	111.07
1	A	365	GLY	N-CA-C	-6.69	100.13	110.77
1	B	368	MET	N-CA-C	-6.61	98.43	109.07
1	B	348	ASN	N-CA-C	6.58	120.62	112.59
1	B	234	ILE	N-CA-C	6.52	118.83	109.51
1	A	368	MET	N-CA-C	-6.50	97.93	108.52
1	B	378	CYS	N-CA-C	6.43	121.40	113.50
1	A	358	PHE	CA-C-N	6.27	125.89	119.56
1	A	358	PHE	C-N-CA	6.27	125.89	119.56
1	B	303	LEU	N-CA-C	6.22	119.38	109.24
1	A	386	LEU	N-CA-C	6.16	118.50	111.11
1	B	358	PHE	CA-C-N	5.69	125.37	119.56
1	B	358	PHE	C-N-CA	5.69	125.37	119.56
1	A	234	ILE	N-CA-C	5.65	117.59	109.51
1	B	485	TYR	N-CA-C	-5.63	103.27	110.53
1	B	253	LEU	N-CA-C	-5.56	99.46	108.52
1	B	375	ARG	N-CA-C	5.56	117.20	111.03
1	A	122	GLY	N-CA-C	5.43	118.52	112.00
1	A	378	CYS	N-CA-C	5.40	120.03	113.38
1	A	367	TYR	N-CA-C	5.32	118.00	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	ARG	N-CA-C	5.32	119.25	112.87
1	A	447	ALA	N-CA-C	5.23	116.98	111.28
1	A	290	LYS	CA-C-N	5.22	125.39	119.90
1	A	290	LYS	C-N-CA	5.22	125.39	119.90
1	B	122	GLY	CA-C-N	5.12	126.25	119.84
1	B	122	GLY	C-N-CA	5.12	126.25	119.84
1	A	459	VAL	CA-C-N	5.09	125.63	120.38
1	A	459	VAL	C-N-CA	5.09	125.63	120.38
1	A	460	PRO	CA-C-N	5.01	124.73	119.82
1	A	460	PRO	C-N-CA	5.01	124.73	119.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3354	0	3250	52	0
1	B	3344	0	3239	41	0
2	A	20	0	28	0	0
2	B	20	0	28	0	0
3	A	43	0	30	0	0
3	B	43	0	30	1	0
4	A	17	0	15	0	0
4	B	17	0	15	0	0
5	A	18	0	23	4	0
5	B	36	0	45	8	0
6	B	8	0	12	0	0
7	A	159	0	0	4	0
7	B	173	0	0	1	0
All	All	7252	0	6715	94	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 7.

All (94) 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:83:ASN:HD22	1:A:85:GLY:H	1.30	0.79
1:A:407:ARG:HA	7:A:1383:HOH:O	1.81	0.79
1:A:81:ILE:HD11	1:A:475:LEU:HD13	1.65	0.78
1:B:493:HIS:HA	5:B:3104:GOL:H11	1.70	0.73
1:A:323:VAL:HG13	1:A:423:GLN:HG3	1.71	0.71
1:B:419:SER:O	1:B:423:GLN:HG2	1.92	0.69
1:B:494:ILE:H	5:B:3104:GOL:H11	1.56	0.69
1:B:97:LYS:HE3	5:B:3105:GOL:H11	1.76	0.67
1:B:414:VAL:HG13	5:B:3108:GOL:O3	1.96	0.66
1:A:266:MET:HE1	1:A:293:TYR:HD1	1.61	0.65
1:A:428:MET:HE2	1:A:433:ALA:HA	1.79	0.64
1:A:134:LEU:O	1:A:138:ILE:HG12	2.00	0.61
1:A:366:TRP:HE1	5:A:3102:GOL:H11	1.66	0.60
1:A:419:SER:O	1:A:423:GLN:HG2	2.03	0.58
3:B:901:HEM:HMC2	3:B:901:HEM:HBC2	1.86	0.58
1:A:453:ALA:HB3	1:A:474:MET:HB3	1.85	0.58
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.39	0.57
1:A:190:ASN:O	1:A:192:PRO:HD3	2.04	0.57
1:B:374:VAL:O	1:B:378:CYS:HB2	2.06	0.56
1:A:83:ASN:HD22	1:A:83:ASN:C	2.13	0.56
1:A:407:ARG:HD2	7:A:1485:HOH:O	2.06	0.54
1:A:428:MET:SD	5:A:3102:GOL:H12	2.47	0.54
1:B:448:ARG:HH21	5:B:3105:GOL:C3	2.21	0.54
1:A:83:ASN:ND2	1:A:85:GLY:H	2.02	0.53
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.45	0.52
1:B:295:ARG:HD2	7:B:1612:HOH:O	2.10	0.52
1:B:445:TYR:CE2	1:B:450:GLY:HA2	2.45	0.52
1:B:385:ILE:O	1:B:389:VAL:HG23	2.10	0.51
1:B:361:CYS:SG	1:B:361:CYS:O	2.69	0.51
1:A:264:TYR:HB2	1:A:266:MET:HE3	1.91	0.51
1:B:266:MET:HE2	1:B:272:ARG:NH2	2.25	0.50
1:B:137:ALA:O	1:B:141:ILE:HG12	2.11	0.50
1:A:137:ALA:O	1:A:141:ILE:HG12	2.10	0.50
1:A:366:TRP:NE1	5:A:3102:GOL:H11	2.26	0.50
1:A:410:THR:O	1:A:414:VAL:HG23	2.11	0.50
1:B:372:ILE:HA	1:B:376:ASP:OD2	2.11	0.50
1:A:132:GLU:O	1:A:135:PRO:HD2	2.13	0.49
1:B:493:HIS:HA	5:B:3104:GOL:C1	2.41	0.49
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.48	0.49
1:B:190:ASN:O	1:B:192:PRO:HD3	2.12	0.49
1:A:134:LEU:HB3	1:A:135:PRO:HD3	1.95	0.48
1:A:465:SER:O	1:A:471:HIS:HE1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ILE:HD11	1:B:475:LEU:HG	1.95	0.48
1:B:252:ARG:NH2	1:B:489:PRO:HD3	2.29	0.47
1:A:480:SER:HA	1:A:481:PRO:C	2.39	0.47
1:B:210:ASN:N	1:B:210:ASN:HD22	2.12	0.47
1:B:210:ASN:HD22	1:B:210:ASN:H	1.61	0.47
1:B:323:VAL:HG13	1:B:423:GLN:HG3	1.97	0.47
1:A:264:TYR:HB2	1:A:266:MET:CE	2.45	0.46
1:A:251:PHE:O	1:A:360:ALA:HB2	2.15	0.46
1:B:239:THR:O	1:B:361:CYS:HA	2.15	0.46
1:A:437:PHE:CE2	1:A:458:LEU:HD13	2.50	0.46
1:B:78:TYR:C	1:B:78:TYR:CD1	2.93	0.46
1:A:114:MET:HE3	1:A:457:PHE:HZ	1.80	0.46
1:B:303:LEU:O	1:B:310:PRO:HA	2.15	0.46
1:B:213:THR:OG1	1:B:216:GLU:HG3	2.15	0.46
1:A:348:ASN:HB2	7:A:1556:HOH:O	2.16	0.46
1:B:148:PHE:N	1:B:148:PHE:CD2	2.84	0.45
1:B:110:LEU:HD12	1:B:110:LEU:N	2.31	0.45
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.47	0.45
1:B:448:ARG:HH21	5:B:3105:GOL:H31	1.80	0.45
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.47	0.45
1:B:77:GLN:O	1:B:96:HIS:HE1	1.99	0.45
1:A:239:THR:O	1:A:361:CYS:HA	2.17	0.45
1:A:469:VAL:HG13	1:A:474:MET:HE1	1.99	0.45
1:A:290:LYS:HD3	1:A:290:LYS:HA	1.89	0.44
1:A:303:LEU:O	1:A:310:PRO:HA	2.17	0.44
1:A:159:ARG:O	1:A:163:VAL:HG23	2.17	0.44
1:B:241:PHE:HB3	1:B:242:PRO:HD2	1.99	0.44
1:A:372:ILE:HA	1:A:376:ASP:OD2	2.18	0.44
1:A:366:TRP:HE1	5:A:3102:GOL:C1	2.30	0.44
1:A:238:ILE:HG13	1:A:362:PRO:O	2.18	0.43
1:A:374:VAL:HG22	1:A:413:ASN:HD21	1.83	0.43
1:B:124:ARG:HH11	1:B:127:PRO:HA	1.83	0.43
1:A:114:MET:HE3	1:A:457:PHE:CZ	2.53	0.43
1:B:254:TRP:HB2	1:B:302:VAL:HB	2.01	0.43
1:B:97:LYS:HE3	5:B:3105:GOL:C1	2.46	0.43
1:A:202:ASN:HB2	7:A:1551:HOH:O	2.19	0.42
1:A:438:MET:HE1	1:A:472:GLN:OE1	2.19	0.42
1:B:342:ALA:HB1	1:B:425:VAL:HG11	2.01	0.42
1:A:258:LEU:HD23	1:A:258:LEU:HA	1.92	0.42
1:A:332:TRP:O	1:A:335:GLU:HB2	2.19	0.42
1:B:488:GLU:HA	1:B:489:PRO:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:GLU:O	1:A:375:ARG:HB2	2.20	0.41
1:A:361:CYS:SG	1:A:361:CYS:O	2.79	0.41
1:B:209:ARG:O	1:B:242:PRO:HG3	2.21	0.41
1:B:463:SER:O	1:B:467:THR:HG23	2.21	0.41
1:A:396:GLU:H	1:A:396:GLU:HG2	1.66	0.41
1:A:330:TYR:HB3	1:A:332:TRP:CE2	2.56	0.41
1:A:77:GLN:O	1:A:96:HIS:HE1	2.04	0.40
1:A:334:GLN:HE21	1:A:335:GLU:HG3	1.86	0.40
1:B:304:GLN:HG3	1:B:308:GLN:O	2.21	0.40
1:A:459:VAL:HA	1:A:460:PRO:HD3	1.93	0.40
1:A:351:LEU:HB3	1:A:358:PHE:HB2	2.04	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	408/433 (94%)	383 (94%)	25 (6%)	0	100	100
1	B	407/433 (94%)	383 (94%)	23 (6%)	1 (0%)	43	66
All	All	815/866 (94%)	766 (94%)	48 (6%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	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	358/381 (94%)	351 (98%)	7 (2%)	48	74
1	B	356/381 (93%)	348 (98%)	8 (2%)	45	72
All	All	714/762 (94%)	699 (98%)	15 (2%)	47	73

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	114	MET
1	A	272	ARG
1	A	348	ASN
1	A	381	GLN
1	A	423	GLN
1	A	428	MET
1	B	130	LEU
1	B	139	GLU
1	B	210	ASN
1	B	265	GLN
1	B	279	GLU
1	B	348	ASN
1	B	353	VAL
1	B	423	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	96	HIS
1	A	115	ASN
1	A	204	GLN
1	A	210	ASN
1	A	215	GLN
1	A	219	GLN
1	A	231	ASN
1	A	249	HIS
1	A	308	GLN
1	A	334	GLN
1	A	348	ASN

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Mol	Chain	Res	Type
1	A	381	GLN
1	A	413	ASN
1	A	471	HIS
1	A	486	GLN
1	B	91	HIS
1	B	96	HIS
1	B	115	ASN
1	B	210	ASN
1	B	215	GLN
1	B	219	GLN
1	B	334	GLN
1	B	348	ASN
1	B	418	HIS
1	B	423	GLN
1	B	486	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BOG	A	3000	-	20,20,20	0.68	1 (5%)	25,25,25	0.64	0
5	GOL	B	3106	-	5,5,5	0.84	0	5,5,5	0.60	0
6	EDO	B	3112	-	3,3,3	0.61	0	2,2,2	0.46	0
3	HEM	B	901	1	50,50,50	1.31	6 (12%)	67,82,82	1.17	5 (7%)
5	GOL	B	3105	-	5,5,5	0.89	0	5,5,5	0.62	0
2	BOG	B	3100	-	20,20,20	0.58	0	25,25,25	0.63	0
4	H4B	A	802	-	17,18,18	2.43	4 (23%)	14,26,26	1.98	5 (35%)
5	GOL	B	3110	-	5,5,5	0.84	0	5,5,5	0.71	0
4	H4B	B	902	-	17,18,18	2.67	4 (23%)	14,26,26	1.92	5 (35%)
5	GOL	A	3101	-	5,5,5	0.76	0	5,5,5	0.62	0
3	HEM	A	801	1	50,50,50	1.43	7 (14%)	67,82,82	1.17	5 (7%)
5	GOL	B	3107	-	5,5,5	0.87	0	5,5,5	0.67	0
5	GOL	B	3108	-	5,5,5	0.92	0	5,5,5	0.67	0
5	GOL	B	3104	-	5,5,5	0.89	0	5,5,5	0.67	0
6	EDO	B	3111	-	3,3,3	0.62	0	2,2,2	0.53	0
5	GOL	A	3103	-	5,5,5	1.05	0	5,5,5	0.72	0
5	GOL	A	3102	-	5,5,5	0.91	0	5,5,5	0.64	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
2	BOG	A	3000	-	-	1/11/31/31	0/1/1/1
5	GOL	B	3106	-	-	2/4/4/4	-
6	EDO	B	3112	-	-	0/1/1/1	-
3	HEM	B	901	1	-	2/14/54/54	-
5	GOL	B	3105	-	-	2/4/4/4	-
2	BOG	B	3100	-	-	2/11/31/31	0/1/1/1
4	H4B	A	802	-	-	0/8/17/17	0/2/2/2
5	GOL	B	3110	-	-	0/4/4/4	-
4	H4B	B	902	-	-	0/8/17/17	0/2/2/2
5	GOL	A	3101	-	-	4/4/4/4	-
3	HEM	A	801	1	-	2/14/54/54	-
5	GOL	B	3107	-	-	2/4/4/4	-
5	GOL	B	3108	-	-	2/4/4/4	-
5	GOL	B	3104	-	-	0/4/4/4	-
6	EDO	B	3111	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	3103	-	-	4/4/4/4	-
5	GOL	A	3102	-	-	2/4/4/4	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	902	H4B	C7-N8	-7.01	1.39	1.46
4	B	902	H4B	C7-C6	-6.93	1.45	1.52
4	A	802	H4B	C7-C6	-6.92	1.45	1.52
4	A	802	H4B	C7-N8	-5.57	1.40	1.46
3	A	801	HEM	FE-NB	4.36	2.08	1.94
3	B	901	HEM	CAC-C3C	-3.56	1.37	1.47
3	B	901	HEM	FE-ND	3.29	2.05	1.94
4	B	902	H4B	C4A-C8A	3.03	1.43	1.38
3	A	801	HEM	FE-ND	2.79	2.03	1.94
3	A	801	HEM	CAB-C3B	-2.69	1.40	1.47
4	A	802	H4B	C4-N3	-2.63	1.33	1.38
3	A	801	HEM	CAC-C3C	-2.60	1.40	1.47
4	B	902	H4B	C4-N3	-2.59	1.34	1.38
4	A	802	H4B	C4A-C8A	2.55	1.43	1.38
3	A	801	HEM	FE-NC	2.53	2.03	1.95
3	B	901	HEM	FE-NC	2.50	2.03	1.95
3	B	901	HEM	FE-NB	2.48	2.02	1.94
2	A	3000	BOG	O1-C1	2.37	1.44	1.40
3	B	901	HEM	CAB-C3B	-2.32	1.41	1.47
3	A	801	HEM	C3B-C4B	2.24	1.49	1.44
3	A	801	HEM	FE-NA	2.15	2.02	1.95
3	B	901	HEM	FE-NA	2.01	2.01	1.95

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	802	H4B	C2-N1-C8A	4.30	120.95	113.36
4	B	902	H4B	C2-N1-C8A	4.24	120.84	113.36
4	A	802	H4B	O4-C4-C4A	-3.84	118.01	127.26
3	B	901	HEM	C4B-C3B-C2B	-3.72	103.86	107.28
3	A	801	HEM	CMD-C2D-C1D	3.66	130.75	125.03
4	B	902	H4B	O4-C4-C4A	-3.61	118.55	127.26
3	B	901	HEM	CMD-C2D-C1D	3.06	129.81	125.03
4	A	802	H4B	C4A-C4-N3	2.88	120.03	112.13
3	B	901	HEM	C3B-C2B-C1B	2.77	108.49	106.41
4	B	902	H4B	C4A-C4-N3	2.70	119.55	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	HEM	C4C-C3C-C2C	-2.60	104.56	106.81
3	B	901	HEM	C3B-C4B-NB	2.49	111.26	109.47
4	A	802	H4B	C2-N3-C4	-2.32	120.91	125.11
4	B	902	H4B	C4-C4A-N5	2.22	122.32	116.27
4	B	902	H4B	C2-N3-C4	-2.22	121.09	125.11
4	A	802	H4B	C4-C4A-N5	2.21	122.29	116.27
3	A	801	HEM	C4B-C3B-C2B	-2.14	105.31	107.28
3	A	801	HEM	CBD-CAD-C3D	-2.14	106.63	112.53
3	B	901	HEM	CHC-C4B-NB	-2.08	122.19	124.42
3	A	801	HEM	CHD-C4C-C3C	-2.08	121.70	125.21

There are no chirality outliers.

All (25) torsion outliers are listed below:

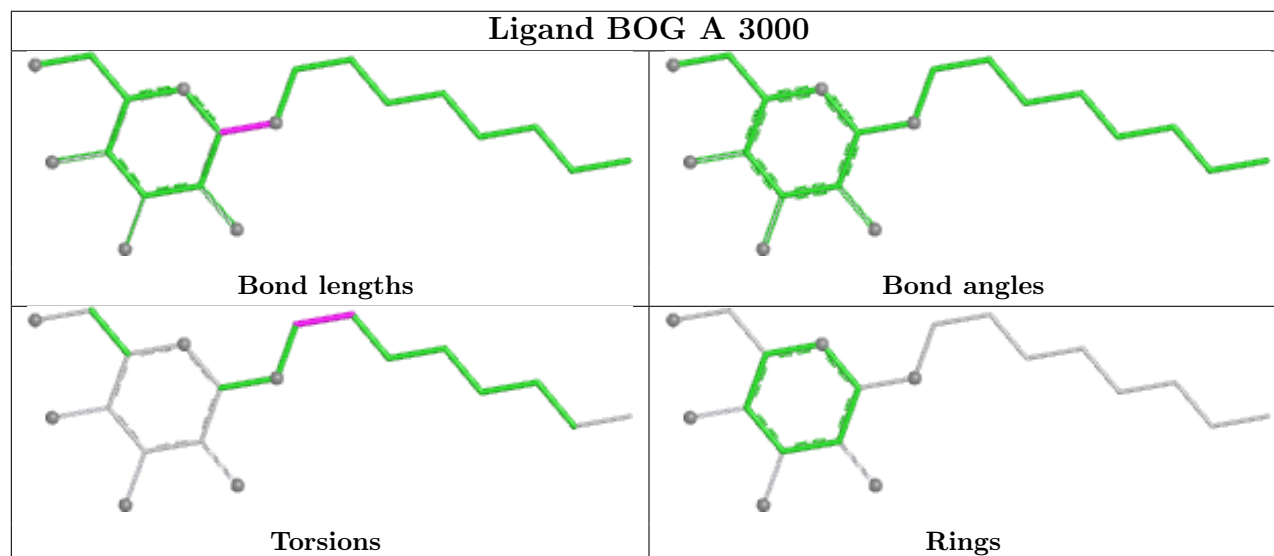
Mol	Chain	Res	Type	Atoms
5	A	3103	GOL	O1-C1-C2-O2
5	A	3103	GOL	O1-C1-C2-C3
5	A	3103	GOL	C1-C2-C3-O3
5	A	3101	GOL	O1-C1-C2-C3
5	A	3101	GOL	C1-C2-C3-O3
5	B	3106	GOL	C1-C2-C3-O3
5	B	3108	GOL	O1-C1-C2-O2
5	A	3102	GOL	O1-C1-C2-C3
5	B	3105	GOL	C1-C2-C3-O3
5	B	3107	GOL	C1-C2-C3-O3
5	B	3108	GOL	O1-C1-C2-C3
5	A	3102	GOL	O1-C1-C2-O2
5	A	3101	GOL	O1-C1-C2-O2
5	A	3101	GOL	O2-C2-C3-O3
5	B	3105	GOL	O2-C2-C3-O3
5	B	3106	GOL	O2-C2-C3-O3
5	A	3103	GOL	O2-C2-C3-O3
2	A	3000	BOG	O1-C1'-C2'-C3'
5	B	3107	GOL	O2-C2-C3-O3
3	A	801	HEM	CAA-CBA-CGA-O1A
3	A	801	HEM	CAA-CBA-CGA-O2A
2	B	3100	BOG	O5-C5-C6-O6
3	B	901	HEM	CAA-CBA-CGA-O1A
2	B	3100	BOG	C4-C5-C6-O6
3	B	901	HEM	CAA-CBA-CGA-O2A

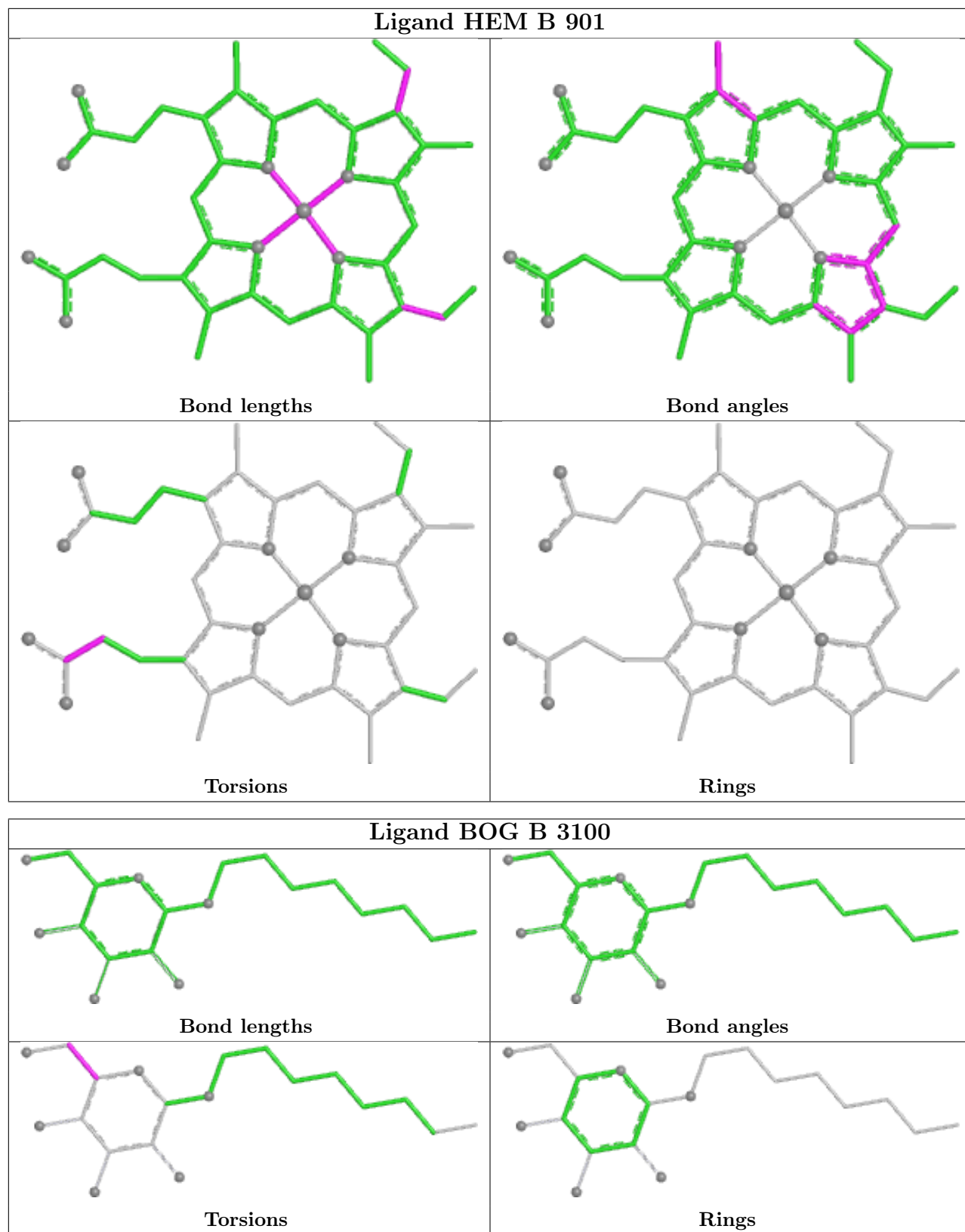
There are no ring outliers.

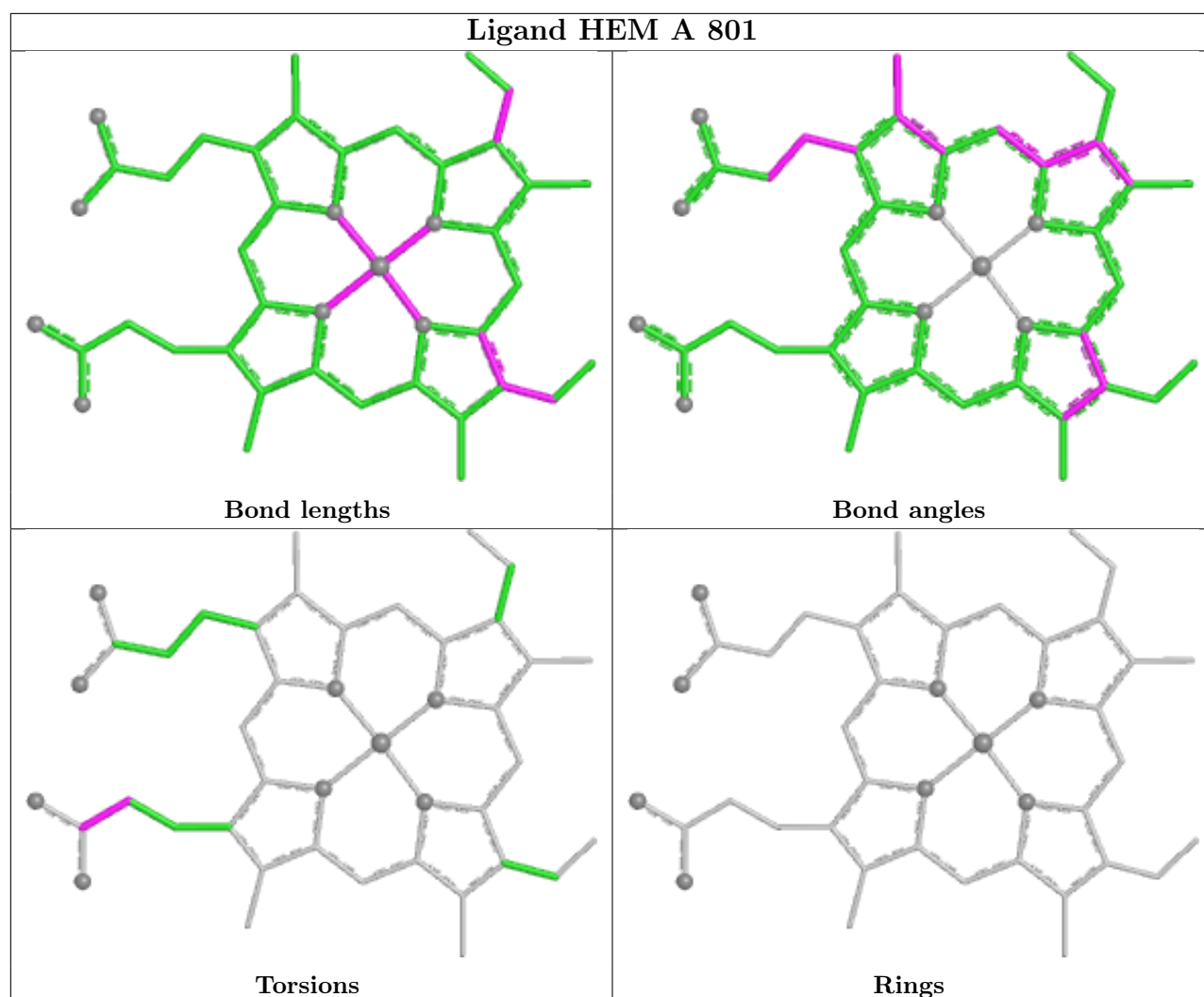
5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	HEM	1	0
5	B	3105	GOL	4	0
5	B	3108	GOL	1	0
5	B	3104	GOL	3	0
5	A	3102	GOL	4	0

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







5.7 Other polymers [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.