



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2026 – 04:31 am BST

PDB ID : 1OG2 / pdb_00001og2
Title : Structure of human cytochrome P450 CYP2C9
Authors : Williams, P.A.; Cosme, J.; Ward, A.; Angove, H.C.; Matak Vinkovic, D.; Jhoti, H.
Deposited on : 2003-04-23
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	:	1.8.4, CSD as541be (2020)
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)	:	2.50

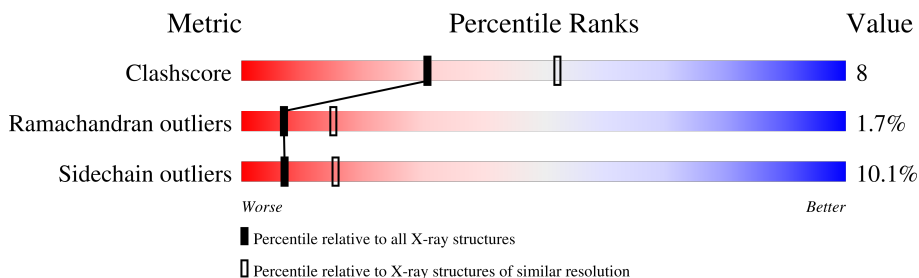
1 Overall quality at a glance

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	475	
1	B	475	

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
2	HEC	A	501	X	-	-	-
2	HEC	B	501	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7619 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 CYTOCHROME P450 2C9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	1
			3693	2384	617	669	23			
1	B	462	Total	C	N	O	S	0	0	1
			3693	2384	617	669	23			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	GLU	LYS	engineered mutation	UNP P11712
A	215	VAL	ILE	engineered mutation	UNP P11712
A	216	TYR	CYS	engineered mutation	UNP P11712
A	220	PRO	SER	engineered mutation	UNP P11712
A	221	ALA	PRO	engineered mutation	UNP P11712
A	222	LEU	ILE	engineered mutation	UNP P11712
A	223	LEU	ILE	engineered mutation	UNP P11712
B	206	GLU	LYS	engineered mutation	UNP P11712
B	215	VAL	ILE	engineered mutation	UNP P11712
B	216	TYR	CYS	engineered mutation	UNP P11712
B	220	PRO	SER	engineered mutation	UNP P11712
B	221	ALA	PRO	engineered mutation	UNP P11712
B	222	LEU	ILE	engineered mutation	UNP P11712
B	223	LEU	ILE	engineered mutation	UNP P11712

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).

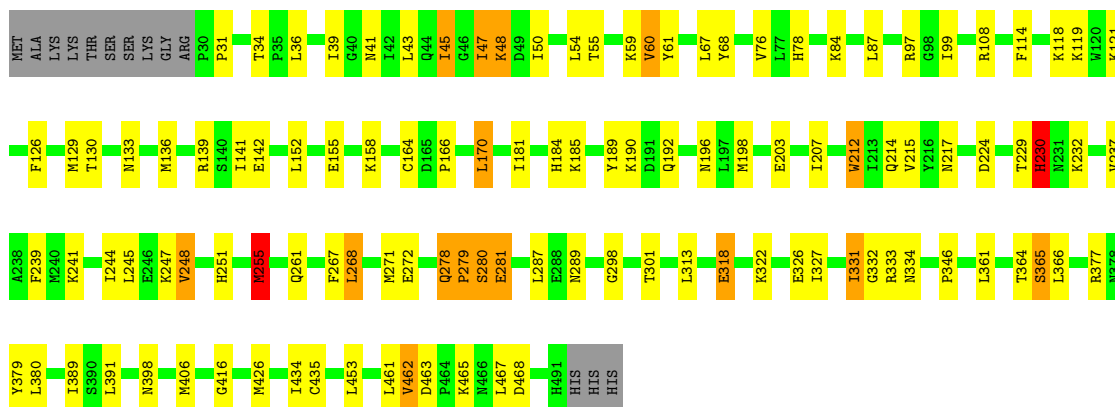
3 Residue-property plots

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.

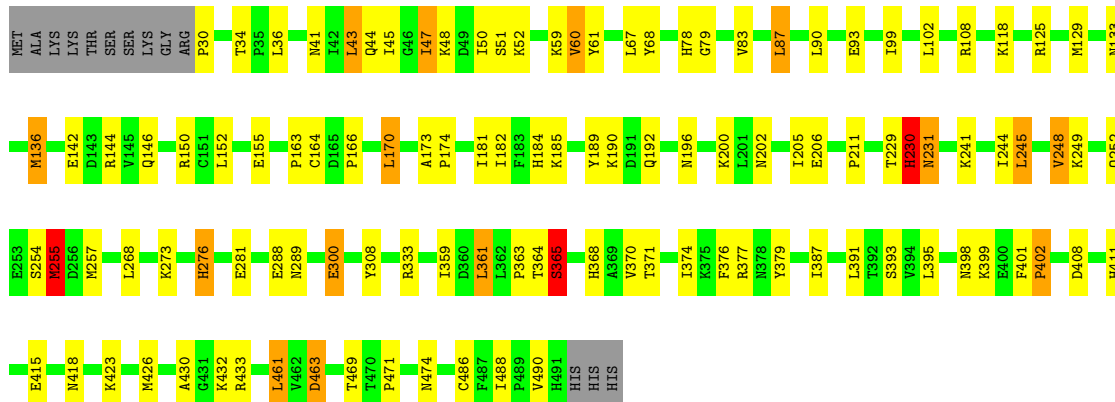
• Molecule 1: CYTOCHROME P450 2C9

Chain A: 



• Molecule 1: CYTOCHROME P450 2C9

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.87Å 164.87Å 111.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	55.90 – 2.60	Depositor
% Data completeness (in resolution range)	96.4 (55.90-2.60)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.208 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7619	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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: HEC

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	0.84	4/3784 (0.1%)	1.02	6/5121 (0.1%)
1	B	0.83	2/3784 (0.1%)	1.02	5/5121 (0.1%)
All	All	0.84	6/7568 (0.1%)	1.02	11/10242 (0.1%)

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	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	406	MET	SD-CE	6.94	1.96	1.79
1	B	129	MET	SD-CE	6.68	1.96	1.79
1	A	198	MET	SD-CE	5.90	1.94	1.79
1	B	490	VAL	C-N	-5.85	1.25	1.33
1	A	255	MET	SD-CE	5.84	1.94	1.79
1	A	129	MET	SD-CE	5.48	1.93	1.79

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	398	ASN	CB-CA-C	-6.28	100.36	110.79
1	A	47	ILE	N-CA-CB	-6.27	104.87	112.33
1	B	136	MET	N-CA-C	5.88	117.20	107.20
1	B	231	ASN	N-CA-C	-5.57	104.84	111.69
1	A	212	TRP	CB-CA-C	5.47	119.54	111.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	LYS	N-CA-C	-5.45	103.30	110.33
1	A	331	ILE	CA-C-N	-5.33	114.36	122.04
1	A	331	ILE	C-N-CA	-5.33	114.36	122.04
1	B	423	LYS	N-CA-C	-5.15	106.94	113.18
1	A	280	SER	N-CA-C	5.05	121.56	110.80
1	A	416	GLY	O-C-N	-5.05	118.77	122.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	278	GLN	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	3693	0	3720	57	0
1	B	3693	0	3720	64	0
2	A	43	0	32	6	0
2	B	43	0	32	2	0
3	A	84	0	0	5	0
3	B	63	0	0	3	0
All	All	7619	0	7504	124	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 8.

All (124) 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:41:ASN:HD22	1:A:68:TYR:H	1.18	0.87
1:B:211:PRO:HG3	1:B:474:ASN:HD22	1.48	0.78
1:B:41:ASN:HD22	1:B:68:TYR:H	1.39	0.70
1:A:365:SER:HB2	2:A:501:HEC:HBA1	1.71	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HD11	1:A:215:VAL:HG23	1.74	0.69
1:B:133:ASN:HD21	1:B:142:GLU:H	1.41	0.68
1:B:144:ARG:HH12	1:B:184:HIS:HD2	1.39	0.68
1:A:60:VAL:HG22	1:A:61:TYR:CD2	2.28	0.67
1:B:401:PHE:HB3	1:B:411:HIS:CE1	2.29	0.67
1:B:408:ASP:HB3	1:B:411:HIS:HD2	1.60	0.66
1:B:276:HIS:N	1:B:276:HIS:ND1	2.44	0.66
1:B:166:PRO:HB2	1:B:170:LEU:HD22	1.77	0.65
1:B:364:THR:C	1:B:365:SER:O	2.34	0.65
2:A:501:HEC:HHD	2:A:501:HEC:HBC2	1.79	0.64
1:B:359:ILE:HD12	1:B:361:LEU:HD13	1.79	0.63
1:B:155:GLU:HG3	1:B:189:TYR:CD1	2.34	0.62
1:A:155:GLU:HG3	1:A:189:TYR:CD1	2.35	0.62
1:B:41:ASN:HD22	1:B:68:TYR:N	1.98	0.61
1:A:155:GLU:HG3	1:A:189:TYR:HD1	1.66	0.60
1:A:41:ASN:HD22	1:A:68:TYR:N	1.96	0.60
1:B:93:GLU:HA	1:B:371:THR:HG22	1.84	0.60
1:A:133:ASN:HD21	1:A:142:GLU:H	1.49	0.60
1:B:60:VAL:HG22	1:B:61:TYR:CD2	2.39	0.58
1:B:45:ILE:HG21	1:B:67:LEU:HD21	1.86	0.57
1:B:229:THR:O	1:B:230:HIS:HB3	2.02	0.57
1:B:401:PHE:HB3	1:B:411:HIS:ND1	2.20	0.56
2:B:501:HEC:HBB2	2:B:501:HEC:HMB3	1.87	0.56
1:B:173:ALA:HB3	1:B:174:PRO:HD3	1.87	0.56
1:B:163:PRO:HB3	1:B:461:LEU:HD11	1.88	0.56
1:B:205:ILE:CD1	1:B:300:GLU:HG2	2.35	0.56
1:A:136:MET:HE1	1:A:181:ILE:HG23	1.87	0.56
1:A:192:GLN:HE21	1:A:196:ASN:ND2	2.03	0.56
1:B:136:MET:HE1	1:B:181:ILE:HG23	1.87	0.56
1:A:45:ILE:HG21	1:A:67:LEU:HD21	1.88	0.55
1:B:401:PHE:O	1:B:402:PRO:C	2.49	0.54
1:B:241:LYS:HE2	1:B:289:ASN:ND2	2.22	0.54
1:A:327:ILE:O	1:A:331:ILE:O	2.25	0.54
1:B:230:HIS:C	1:B:230:HIS:CD2	2.85	0.54
1:B:93:GLU:HG2	1:B:374:ILE:HD13	1.89	0.54
1:A:326:GLU:OE1	1:A:346:PRO:HD2	2.08	0.53
1:B:364:THR:O	1:B:365:SER:C	2.51	0.53
1:A:192:GLN:HE21	1:A:196:ASN:HD21	1.56	0.52
1:A:47:ILE:HD11	1:A:215:VAL:CG2	2.38	0.52
1:B:408:ASP:HB3	1:B:411:HIS:CD2	2.41	0.52
1:A:237:VAL:HG12	1:A:241:LYS:HD2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:HIS:O	1:A:255:MET:HB2	2.11	0.51
1:A:268:LEU:HD12	1:A:271:MET:HE2	1.91	0.51
1:B:30:PRO:N	3:B:2001:HOH:O	2.42	0.51
1:B:184:HIS:O	1:B:184:HIS:CD2	2.63	0.51
1:B:426:MET:HE3	1:B:430:ALA:HB2	1.93	0.51
1:B:229:THR:O	1:B:230:HIS:CB	2.59	0.51
1:B:255:MET:HE1	1:B:257:MET:HE2	1.91	0.51
1:B:144:ARG:HH12	1:B:184:HIS:CD2	2.24	0.51
1:B:83:VAL:HG13	1:B:87:LEU:HD22	1.93	0.50
1:A:184:HIS:CE1	1:A:261:GLN:HB3	2.47	0.50
1:A:365:SER:HB2	2:A:501:HEC:CBA	2.39	0.50
1:A:119:LYS:HA	1:A:281:GLU:CG	2.42	0.49
1:A:126:PHE:O	1:A:130:THR:HG23	2.12	0.49
1:B:211:PRO:HG3	1:B:474:ASN:ND2	2.22	0.49
1:B:241:LYS:HE2	1:B:289:ASN:HD22	1.77	0.49
1:B:146:GLN:NE2	3:B:2016:HOH:O	2.45	0.48
2:B:501:HEC:HBC2	2:B:501:HEC:HHD	1.95	0.48
1:B:254:SER:O	1:B:255:MET:C	2.56	0.48
1:A:322:LYS:NZ	3:A:2042:HOH:O	2.47	0.48
1:A:244:ILE:O	1:A:248:VAL:HG13	2.12	0.48
1:B:359:ILE:CD1	1:B:361:LEU:HD13	2.41	0.48
1:A:119:LYS:HA	1:A:281:GLU:HG3	1.96	0.48
1:A:318:GLU:HB2	3:A:2039:HOH:O	2.13	0.47
1:B:36:LEU:HD12	1:B:43:LEU:HD22	1.96	0.47
1:A:241:LYS:HE2	1:A:289:ASN:ND2	2.30	0.47
1:A:364:THR:O	1:A:365:SER:C	2.58	0.47
1:B:205:ILE:HG12	1:B:300:GLU:HG2	1.95	0.47
1:A:364:THR:HA	1:A:389:ILE:O	2.14	0.47
1:A:133:ASN:HD22	1:A:141:ILE:HB	1.79	0.46
1:A:267:PHE:CE2	1:A:287:LEU:HB2	2.51	0.46
1:B:205:ILE:HD13	1:B:300:GLU:HG2	1.97	0.45
1:A:60:VAL:HG22	1:A:61:TYR:CE2	2.51	0.45
1:B:202:ASN:HA	1:B:205:ILE:HD12	1.98	0.45
1:A:278:GLN:O	1:A:278:GLN:HG3	2.16	0.45
1:B:230:HIS:HD2	1:B:231:ASN:N	2.14	0.45
1:A:426:MET:HA	3:A:2070:HOH:O	2.17	0.45
1:A:54:LEU:HD22	1:A:76:VAL:HG21	1.99	0.45
1:B:364:THR:O	1:B:365:SER:O	2.35	0.45
1:A:166:PRO:HB2	1:A:170:LEU:HD22	1.98	0.45
1:A:365:SER:HB3	1:A:391:LEU:HD11	1.99	0.44
1:A:434:ILE:O	1:A:435:CYS:C	2.59	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:GLN:HE21	1:B:196:ASN:HD21	1.64	0.44
1:B:376:PHE:O	1:B:379:TYR:HB2	2.17	0.44
1:B:469:THR:O	1:B:471:PRO:HD3	2.18	0.44
1:B:78:HIS:CD2	1:B:393:SER:HB3	2.53	0.44
1:B:245:LEU:HG	1:B:288:GLU:OE2	2.19	0.43
1:B:152:LEU:HD23	1:B:152:LEU:O	2.19	0.43
1:A:31:PRO:HD3	1:A:379:TYR:CE2	2.53	0.43
1:A:97:ARG:HG2	1:A:114:PHE:HA	2.01	0.43
1:B:41:ASN:ND2	1:B:68:TYR:HB2	2.34	0.43
1:B:244:ILE:O	1:B:248:VAL:HG13	2.18	0.43
1:A:298:GLY:HA2	2:A:501:HEC:C2C	2.48	0.43
1:B:368:HIS:HE1	1:B:433:ARG:HB2	1.84	0.43
1:A:332:GLY:HA3	3:A:2046:HOH:O	2.18	0.42
1:B:370:VAL:HG13	1:B:387:ILE:HD11	2.00	0.42
1:A:36:LEU:HD12	1:A:39:ILE:HD11	2.01	0.42
1:A:313:LEU:HD13	1:A:453:LEU:HD11	2.02	0.42
1:A:207:ILE:CG2	1:A:229:THR:HG23	2.48	0.42
1:B:486:CYS:HB2	1:B:488:ILE:CD1	2.49	0.42
1:A:60:VAL:CG2	1:A:61:TYR:CE2	3.03	0.42
1:A:229:THR:O	1:A:230:HIS:CB	2.68	0.42
1:B:249:LYS:HA	1:B:252:GLN:HE21	1.85	0.42
1:B:365:SER:HB2	1:B:391:LEU:HD11	2.02	0.42
1:A:301:THR:HG22	2:A:501:HEC:HBB3	2.02	0.42
1:B:190:LYS:HB2	1:B:190:LYS:NZ	2.34	0.41
1:A:78:HIS:ND1	3:A:2002:HOH:O	2.36	0.41
1:A:214:GLN:NE2	1:A:217:ASN:HD22	2.17	0.41
1:B:133:ASN:ND2	1:B:142:GLU:H	2.13	0.41
1:B:361:LEU:C	1:B:363:PRO:HD3	2.46	0.41
1:A:301:THR:HG21	2:A:501:HEC:C2B	2.51	0.41
1:B:426:MET:HA	3:B:2057:HOH:O	2.20	0.41
1:A:133:ASN:ND2	1:A:142:GLU:H	2.15	0.41
1:B:205:ILE:CG1	1:B:300:GLU:HG2	2.50	0.41
1:A:55:THR:HA	1:A:78:HIS:NE2	2.37	0.40
1:A:155:GLU:OE1	1:A:158:LYS:HE3	2.22	0.40
1:A:239:PHE:CD1	1:A:239:PHE:C	2.99	0.40
1:A:278:GLN:N	1:A:279:PRO:CD	2.85	0.40
1:A:462:VAL:O	1:A:462:VAL:HG13	2.21	0.40
1:B:79:GLY:O	1:B:83:VAL:HG23	2.21	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	460/475 (97%)	426 (93%)	26 (6%)	8 (2%)	7	15
1	B	460/475 (97%)	416 (90%)	36 (8%)	8 (2%)	7	15
All	All	920/950 (97%)	842 (92%)	62 (7%)	16 (2%)	7	15

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	SER
1	B	255	MET
1	A	230	HIS
1	A	380	LEU
1	B	48	LYS
1	B	230	HIS
1	B	365	SER
1	B	418	ASN
1	A	48	LYS
1	A	334	ASN
1	B	402	PRO
1	A	279	PRO
1	A	463	ASP
1	B	47	ILE
1	A	280	SER
1	B	463	ASP

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	416/428 (97%)	374 (90%)	42 (10%)	7	15
1	B	416/428 (97%)	374 (90%)	42 (10%)	7	15
All	All	832/856 (97%)	748 (90%)	84 (10%)	7	15

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	THR
1	A	43	LEU
1	A	45	ILE
1	A	48	LYS
1	A	50	ILE
1	A	59	LYS
1	A	60	VAL
1	A	84	LYS
1	A	87	LEU
1	A	99	ILE
1	A	108	ARG
1	A	118	LYS
1	A	121	LYS
1	A	139	ARG
1	A	152	LEU
1	A	164	CYS
1	A	170	LEU
1	A	185	LYS
1	A	190	LYS
1	A	203	GLU
1	A	212	TRP
1	A	224	ASP
1	A	230	HIS
1	A	232	LYS
1	A	245	LEU
1	A	247	LYS
1	A	248	VAL
1	A	255	MET
1	A	268	LEU
1	A	272	GLU
1	A	281	GLU
1	A	318	GLU
1	A	333	ARG
1	A	361	LEU
1	A	366	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	377	ARG
1	A	398	ASN
1	A	461	LEU
1	A	462	VAL
1	A	465	LYS
1	A	467	LEU
1	A	468	ASP
1	B	34	THR
1	B	43	LEU
1	B	44	GLN
1	B	47	ILE
1	B	50	ILE
1	B	51	SER
1	B	52	LYS
1	B	59	LYS
1	B	60	VAL
1	B	87	LEU
1	B	90	LEU
1	B	99	ILE
1	B	102	LEU
1	B	108	ARG
1	B	118	LYS
1	B	125	ARG
1	B	150	ARG
1	B	164	CYS
1	B	170	LEU
1	B	182	ILE
1	B	185	LYS
1	B	200	LYS
1	B	206	GLU
1	B	230	HIS
1	B	245	LEU
1	B	248	VAL
1	B	255	MET
1	B	268	LEU
1	B	276	HIS
1	B	281	GLU
1	B	300	GLU
1	B	308	TYR
1	B	333	ARG
1	B	361	LEU
1	B	365	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	377	ARG
1	B	395	LEU
1	B	399	LYS
1	B	415	GLU
1	B	432	LYS
1	B	461	LEU
1	B	463	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	44	GLN
1	A	107	ASN
1	A	133	ASN
1	A	192	GLN
1	A	196	ASN
1	A	202	ASN
1	A	204	ASN
1	A	214	GLN
1	A	230	HIS
1	A	236	ASN
1	A	252	GLN
1	A	289	ASN
1	A	316	HIS
1	A	353	HIS
1	A	378	ASN
1	A	411	HIS
1	A	454	GLN
1	A	474	ASN
1	B	41	ASN
1	B	133	ASN
1	B	184	HIS
1	B	196	ASN
1	B	202	ASN
1	B	204	ASN
1	B	217	ASN
1	B	230	HIS
1	B	236	ASN
1	B	252	GLN
1	B	259	ASN
1	B	289	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	324	GLN
1	B	334	ASN
1	B	396	HIS
1	B	410	HIS
1	B	418	ASN
1	B	454	GLN
1	B	466	ASN
1	B	474	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	HEC	A	501	1	50,50,50	2.96	26 (52%)	68,82,82	2.90	33 (48%)
2	HEC	B	501	1	50,50,50	2.86	24 (48%)	68,82,82	2.71	33 (48%)

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	HEC	A	501	1	1/1/3/7	7/14/54/54	-
2	HEC	B	501	1	1/1/3/7	9/14/54/54	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEC	FE-NA	7.45	2.20	1.95
2	A	501	HEC	FE-NC	7.33	2.20	1.95
2	B	501	HEC	FE-NC	7.20	2.19	1.95
2	B	501	HEC	FE-NA	7.00	2.18	1.95
2	A	501	HEC	CBD-CGD	-6.23	1.36	1.50
2	B	501	HEC	CBD-CGD	-6.09	1.36	1.50
2	A	501	HEC	C2A-C3A	5.48	1.48	1.36
2	B	501	HEC	C2A-C3A	5.19	1.47	1.36
2	A	501	HEC	CHC-C4B	4.99	1.48	1.38
2	B	501	HEC	C3B-C2B	4.58	1.46	1.36
2	A	501	HEC	C3B-C2B	4.58	1.46	1.36
2	B	501	HEC	CHB-C4A	4.54	1.47	1.38
2	B	501	HEC	C3D-C2D	4.39	1.46	1.36
2	B	501	HEC	CHC-C4B	4.20	1.47	1.38
2	A	501	HEC	CHB-C4A	4.07	1.46	1.38
2	A	501	HEC	C4A-NA	-3.94	1.32	1.39
2	A	501	HEC	CHD-C1D	3.83	1.46	1.38
2	A	501	HEC	CHC-C1C	3.75	1.47	1.39
2	B	501	HEC	CHB-C1B	3.72	1.47	1.39
2	B	501	HEC	CHD-C1D	3.62	1.45	1.38
2	A	501	HEC	CHB-C1B	3.43	1.47	1.39
2	B	501	HEC	C4B-NB	-3.34	1.34	1.40
2	A	501	HEC	C1B-C2B	3.33	1.51	1.44
2	A	501	HEC	C3D-C2D	3.27	1.43	1.36
2	A	501	HEC	C1C-NC	-3.24	1.33	1.39
2	A	501	HEC	C3C-C2C	3.21	1.47	1.38
2	B	501	HEC	CHA-C1A	3.20	1.44	1.38
2	B	501	HEC	C1C-NC	-3.16	1.33	1.39
2	B	501	HEC	C1C-C2C	3.09	1.50	1.43
2	A	501	HEC	C4C-NC	-3.07	1.33	1.39
2	B	501	HEC	C3C-C2C	3.04	1.46	1.38
2	B	501	HEC	CHA-C4D	2.95	1.46	1.39
2	B	501	HEC	CHC-C1C	2.92	1.46	1.39
2	A	501	HEC	C1C-C2C	2.89	1.50	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEC	C1D-C2D	2.83	1.50	1.44
2	A	501	HEC	CHA-C1A	2.81	1.43	1.38
2	A	501	HEC	CHD-C4C	2.78	1.45	1.39
2	A	501	HEC	C4D-C3D	2.75	1.49	1.45
2	A	501	HEC	CHA-C4D	2.75	1.45	1.39
2	A	501	HEC	O2A-CGA	-2.74	1.21	1.30
2	B	501	HEC	C4D-C3D	2.73	1.49	1.45
2	B	501	HEC	C1B-C2B	2.66	1.49	1.44
2	B	501	HEC	C1D-C2D	2.63	1.49	1.44
2	A	501	HEC	O2D-CGD	-2.58	1.22	1.30
2	B	501	HEC	C1A-NA	-2.50	1.34	1.39
2	A	501	HEC	C4A-C3A	2.43	1.50	1.45
2	B	501	HEC	O2A-CGA	-2.35	1.22	1.30
2	B	501	HEC	O2D-CGD	-2.35	1.22	1.30
2	A	501	HEC	C1A-NA	-2.22	1.35	1.39
2	B	501	HEC	C4A-NA	-2.14	1.35	1.39

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEC	C3D-C4D-ND	8.08	118.18	110.36
2	B	501	HEC	C1B-C2B-C3B	-7.09	99.50	106.96
2	A	501	HEC	CHA-C4D-C3D	-6.53	115.24	124.84
2	A	501	HEC	CMD-C2D-C1D	5.81	133.89	125.04
2	A	501	HEC	C2D-C1D-ND	5.77	116.67	109.84
2	B	501	HEC	C2B-C1B-NB	5.75	116.77	109.88
2	A	501	HEC	C1D-ND-C4D	-5.75	99.13	105.07
2	A	501	HEC	C2A-C1A-NA	5.20	115.38	110.32
2	B	501	HEC	CHA-C4D-C3D	-5.09	117.36	124.84
2	A	501	HEC	C1C-C2C-C3C	-5.05	100.92	106.83
2	B	501	HEC	C3D-C4D-ND	5.03	115.23	110.36
2	A	501	HEC	C1B-C2B-C3B	-4.61	102.11	106.96
2	B	501	HEC	C1C-C2C-C3C	-4.56	101.49	106.83
2	B	501	HEC	C2D-C1D-ND	4.44	115.10	109.84
2	A	501	HEC	C2B-C1B-NB	4.43	115.19	109.88
2	B	501	HEC	CAD-C3D-C4D	4.42	132.38	124.66
2	B	501	HEC	CAC-C3C-C4C	4.26	130.83	124.92
2	B	501	HEC	CMB-C2B-C1B	4.25	131.51	125.04
2	B	501	HEC	C3C-C4C-NC	4.19	114.83	110.15
2	A	501	HEC	CHB-C4A-NA	-4.03	120.08	124.44
2	A	501	HEC	CAD-C3D-C4D	3.99	131.63	124.66
2	B	501	HEC	C2C-C1C-NC	3.96	116.11	110.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEC	CHB-C1B-C2B	-3.92	118.86	124.98
2	A	501	HEC	CAA-C2A-C3A	3.87	135.09	127.88
2	B	501	HEC	CHD-C1D-C2D	-3.78	116.22	126.73
2	A	501	HEC	CHD-C1D-C2D	-3.68	116.50	126.73
2	A	501	HEC	CBB-CAB-C3B	3.61	122.38	112.43
2	B	501	HEC	CHD-C1D-ND	3.46	128.64	124.37
2	A	501	HEC	C3B-C4B-NB	3.42	113.98	110.17
2	A	501	HEC	CMB-C2B-C1B	3.40	130.22	125.04
2	B	501	HEC	C4A-C3A-C2A	-3.36	102.04	106.94
2	A	501	HEC	C4D-C3D-C2D	-3.33	102.04	106.90
2	A	501	HEC	C3C-C4C-NC	3.28	113.82	110.15
2	A	501	HEC	C4A-C3A-C2A	-3.23	102.22	106.94
2	A	501	HEC	CHC-C4B-C3B	-3.22	119.28	125.33
2	B	501	HEC	C3B-C4B-NB	3.20	113.72	110.17
2	A	501	HEC	C1A-C2A-C3A	-3.20	102.96	107.13
2	B	501	HEC	CMC-C2C-C1C	3.10	130.08	125.37
2	B	501	HEC	C2A-C1A-NA	3.08	113.32	110.32
2	B	501	HEC	CHC-C4B-C3B	-3.02	119.67	125.33
2	B	501	HEC	CMA-C3A-C4A	2.99	129.99	124.71
2	A	501	HEC	C1D-C2D-C3D	-2.89	103.92	106.96
2	A	501	HEC	C2C-C1C-NC	2.86	114.44	110.08
2	B	501	HEC	C1D-ND-C4D	-2.79	102.19	105.07
2	B	501	HEC	CAA-C2A-C1A	2.78	130.13	124.89
2	A	501	HEC	CHA-C1A-C2A	-2.72	120.52	124.94
2	B	501	HEC	CHA-C4D-ND	2.66	127.31	124.42
2	A	501	HEC	O2D-CGD-O1D	-2.65	116.69	123.30
2	B	501	HEC	CHA-C1A-NA	-2.60	121.63	124.44
2	B	501	HEC	C4D-C3D-C2D	-2.59	103.12	106.90
2	B	501	HEC	CMD-C2D-C1D	2.57	128.96	125.04
2	B	501	HEC	CBB-CAB-C3B	2.57	119.52	112.43
2	B	501	HEC	C1D-C2D-C3D	-2.54	104.29	106.96
2	A	501	HEC	CHB-C1B-C2B	-2.53	121.02	124.98
2	B	501	HEC	CBC-CAC-C3C	2.52	119.37	112.43
2	A	501	HEC	CMC-C2C-C1C	2.44	129.08	125.37
2	B	501	HEC	C3A-C4A-NA	2.41	114.13	109.69
2	A	501	HEC	CBA-CAA-C2A	2.39	119.28	112.63
2	A	501	HEC	C3A-C4A-NA	2.38	114.08	109.69
2	B	501	HEC	O2A-CGA-CBA	2.35	121.59	114.03
2	A	501	HEC	CAD-CBD-CGD	2.31	118.58	113.60
2	A	501	HEC	O2D-CGD-CBD	2.23	121.20	114.03
2	B	501	HEC	CHC-C1C-NC	-2.16	119.88	123.85
2	A	501	HEC	CBD-CAD-C3D	2.10	118.45	112.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEC	O2A-CGA-O1A	-2.03	118.25	123.30
2	A	501	HEC	CMC-C2C-C3C	2.02	129.98	125.61

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	HEC	NA
2	B	501	HEC	NA

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEC	C2B-C3B-CAB-CBB
2	B	501	HEC	C2B-C3B-CAB-CBB
2	A	501	HEC	C4B-C3B-CAB-CBB
2	B	501	HEC	C4B-C3B-CAB-CBB
2	A	501	HEC	C3A-C2A-CAA-CBA
2	A	501	HEC	C1A-C2A-CAA-CBA
2	B	501	HEC	C2C-C3C-CAC-CBC
2	A	501	HEC	C2C-C3C-CAC-CBC
2	B	501	HEC	C4C-C3C-CAC-CBC
2	A	501	HEC	C4C-C3C-CAC-CBC
2	B	501	HEC	C1A-C2A-CAA-CBA
2	B	501	HEC	CAA-CBA-CGA-O2A
2	A	501	HEC	C2A-CAA-CBA-CGA
2	B	501	HEC	C3A-C2A-CAA-CBA
2	B	501	HEC	CAA-CBA-CGA-O1A
2	B	501	HEC	CAD-CBD-CGD-O2D

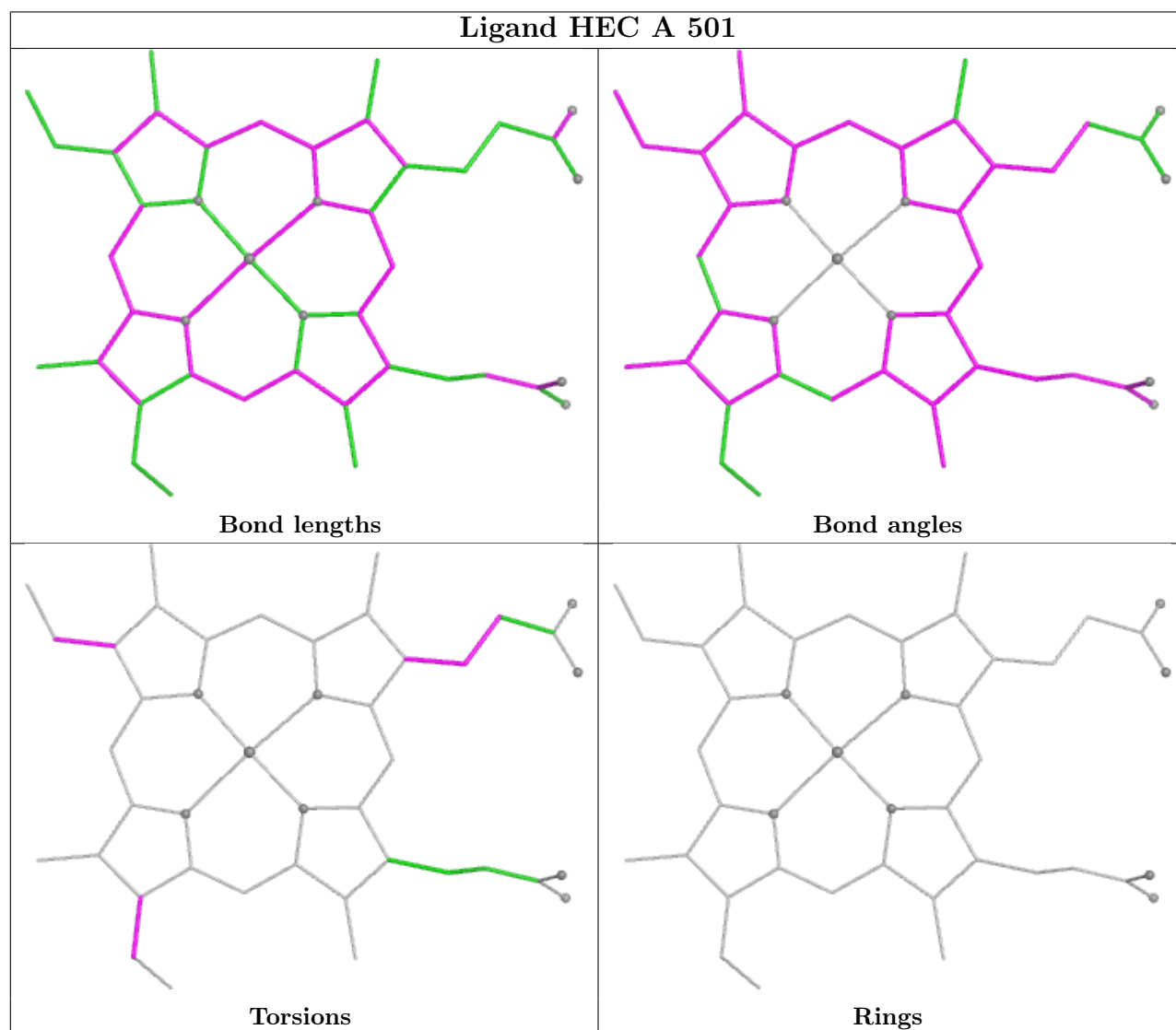
There are no ring outliers.

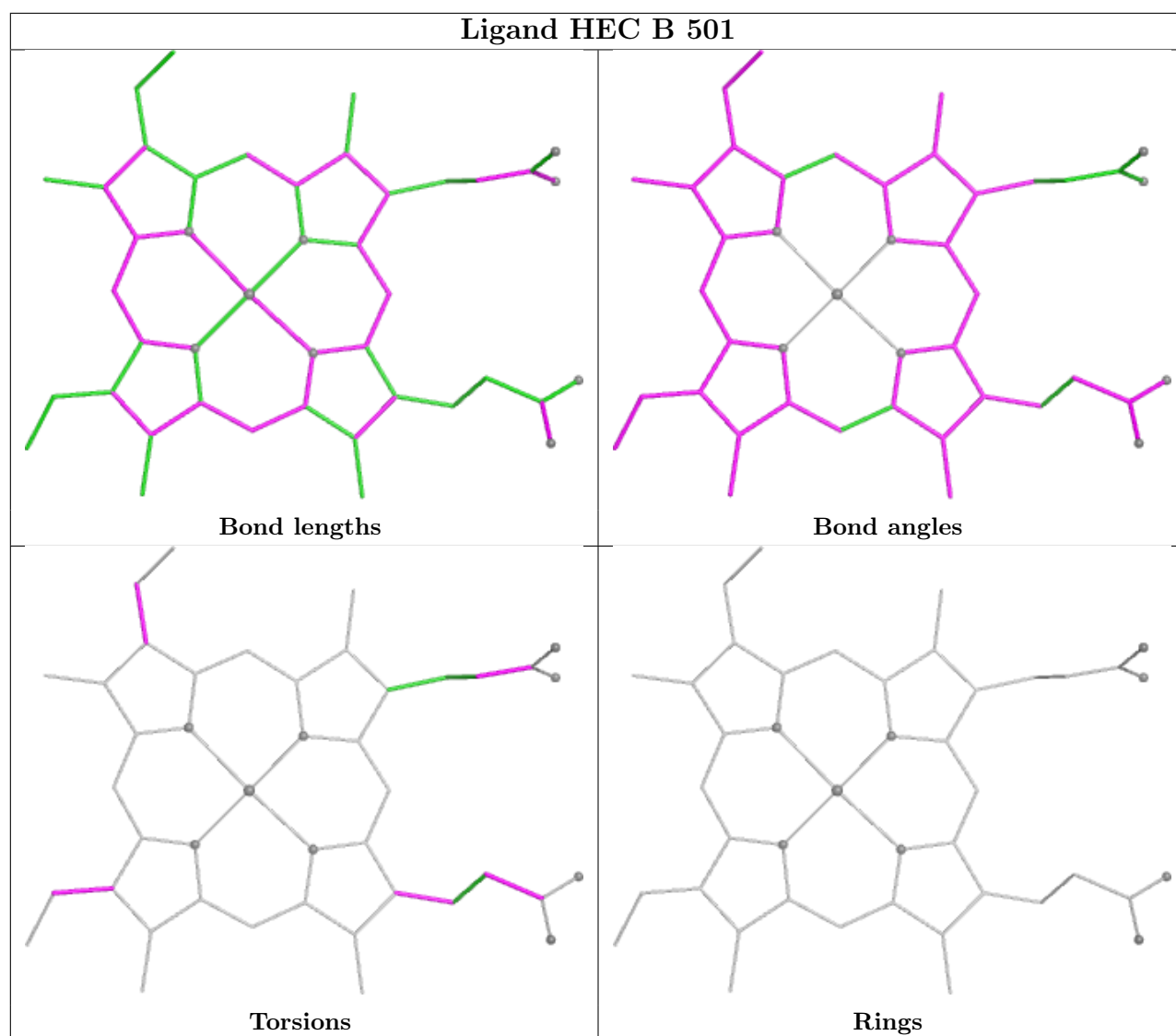
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEC	6	0
2	B	501	HEC	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.