



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:26 am BST

PDB ID : 1BU7
Title : CRYOGENIC STRUCTURE OF CYTOCHROME P450BM-3 HEME DO-MAIN
Authors : Li, H.; Poulos, T.L.
Deposited on : 1998-09-14
Resolution : 1.65 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 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)
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) : 2.11

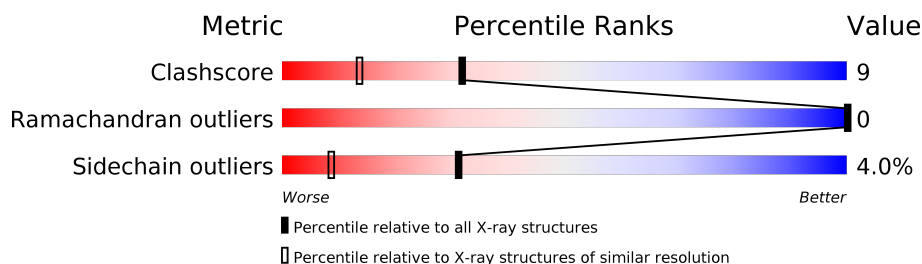
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)

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 on 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	455	
1	B	455	

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
3	EDO	A	1008	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8482 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 PROTEIN (CYTOCHROME P450).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3671	2345	623	686	17			
1	B	455	Total	C	N	O	S	0	0	0
			3671	2345	623	686	17			

- 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
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is water.

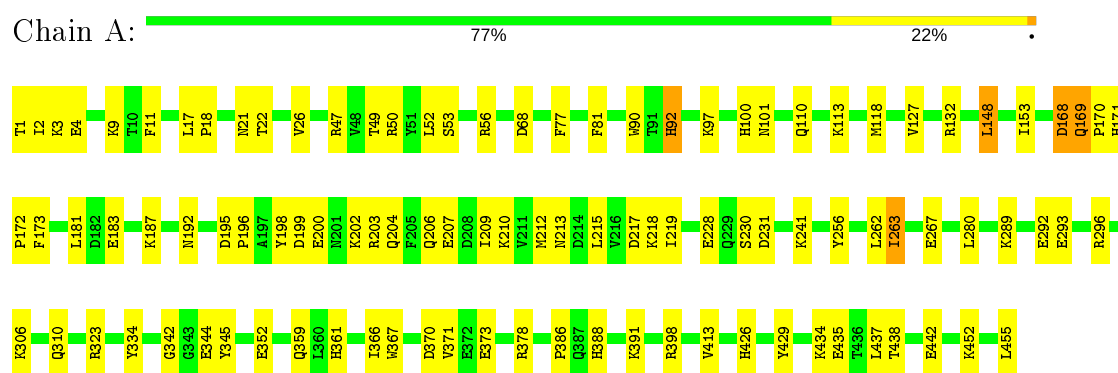
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	475	Total 475	O 475	0	0
4	B	523	Total 523	O 523	0	0

3 Residue-property plots

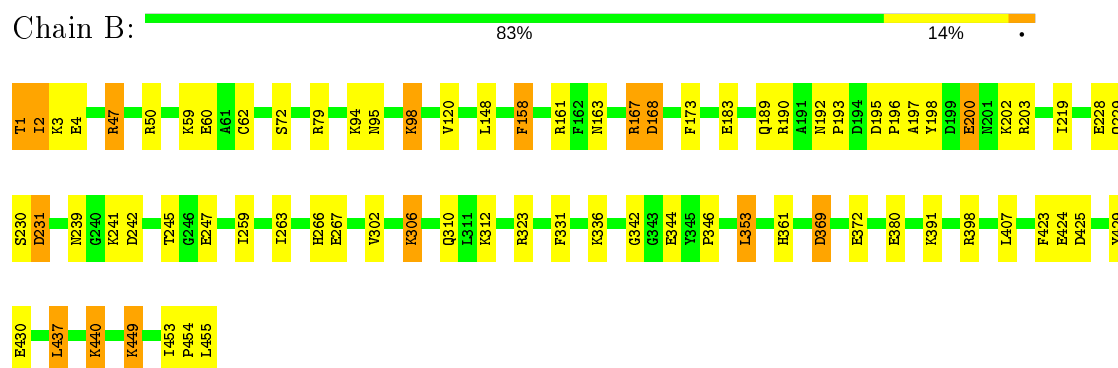
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: PROTEIN (CYTOCHROME P450)



• Molecule 1: PROTEIN (CYTOCHROME P450)



4 Data and refinement statistics

Xtriage (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, α , β , γ	59.38 Å 151.90 Å 62.77 Å 90.00° 96.02° 90.00°	Depositor
Resolution (Å)	10.00 – 1.65	Depositor
% Data completeness (in resolution range)	98.0 (10.00-1.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	3.80	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.197 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8482	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: HEM, EDO

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	0.44	0/3756	1.08	7/5077 (0.1%)
1	B	0.47	0/3756	1.11	14/5077 (0.3%)
All	All	0.45	0/7512	1.10	21/10154 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	425	ASP	CB-CG-OD1	10.58	127.82	118.30
1	B	167	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	A	50	ARG	NE-CZ-NH2	-8.31	116.15	120.30
1	A	378	ARG	NE-CZ-NH1	-8.03	116.28	120.30
1	B	167	ARG	CD-NE-CZ	7.87	134.62	123.60
1	A	148	LEU	CA-CB-CG	7.52	132.61	115.30
1	A	398	ARG	CD-NE-CZ	7.40	133.96	123.60
1	B	167	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	B	398	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	B	398	ARG	CD-NE-CZ	6.02	132.03	123.60
1	A	429	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	A	132	ARG	NE-CZ-NH1	-5.85	117.37	120.30
1	B	331	PHE	CB-CG-CD1	5.57	124.70	120.80
1	B	79	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	B	161	ARG	CD-NE-CZ	5.42	131.19	123.60
1	B	173	PHE	CB-CG-CD2	5.25	124.47	120.80
1	B	423	PHE	CB-CG-CD1	-5.20	117.16	120.80
1	A	256	TYR	CB-CG-CD1	5.16	124.09	121.00
1	B	398	ARG	NH1-CZ-NH2	-5.08	113.81	119.40
1	B	429	TYR	CB-CG-CD1	5.06	124.04	121.00
1	B	369	ASP	CB-CG-OD1	5.03	122.83	118.30

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	3671	0	3645	80	0
1	B	3671	0	3645	54	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	24	0	36	12	0
3	B	32	0	48	2	0
4	A	475	0	0	14	0
4	B	523	0	0	13	0
All	All	8482	0	7434	132	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 9.

All (132) 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:296:ARG:HH12	3:A:1008:EDO:H11	1.33	0.92
1:B:361:HIS:HE1	1:B:391:LYS:H	1.25	0.84
1:A:181:LEU:HD22	1:A:437:LEU:HD13	1.60	0.82
1:B:449:LYS:HD3	4:B:1414:HOH:O	1.84	0.76
1:A:361:HIS:HE1	1:A:391:LYS:H	1.31	0.76
1:A:118:MET:HG2	4:A:1138:HOH:O	1.88	0.72
1:B:3:LYS:HD3	1:B:4:GLU:O	1.89	0.71
1:B:424:GLU:HB2	1:B:449:LYS:HE3	1.72	0.70
1:B:94:LYS:NZ	1:B:245:THR:HG21	2.08	0.69
1:A:435:GLU:HB3	3:A:1013:EDO:H21	1.75	0.67
1:B:168:ASP:HB3	4:B:1130:HOH:O	1.96	0.66
1:B:310:GLN:HG3	4:B:1521:HOH:O	1.98	0.63
1:B:190:ARG:HG2	1:B:198:TYR:CZ	2.32	0.63
1:A:293:GLU:HB2	3:A:1008:EDO:H21	1.83	0.60
1:A:206:GLN:O	1:A:210:LYS:HD3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:HIS:HD2	4:A:1093:HOH:O	1.85	0.59
1:B:198:TYR:O	1:B:202:LYS:HG3	2.03	0.58
1:A:9:LYS:HE2	1:A:11:PHE:CE2	2.38	0.58
1:A:3:LYS:HE2	1:A:345:TYR:HE1	1.69	0.58
1:B:72:SER:HA	3:B:1009:EDO:H22	1.86	0.58
1:A:267:GLU:HG3	4:A:1370:HOH:O	2.03	0.58
1:A:171:HIS:HD2	1:A:173:PHE:H	1.53	0.57
1:A:110:GLN:HE22	1:A:113:LYS:NZ	2.03	0.57
1:A:388:HIS:HE1	4:A:1100:HOH:O	1.89	0.55
1:A:215:LEU:HD12	4:A:1403:HOH:O	2.07	0.54
1:B:195:ASP:OD1	1:B:196:PRO:HD2	2.08	0.54
1:A:196:PRO:O	1:A:199:ASP:HB2	2.08	0.54
1:B:306:LYS:HE2	4:B:1431:HOH:O	2.07	0.53
1:A:173:PHE:CE2	1:A:262:LEU:HD13	2.44	0.53
1:A:3:LYS:HE3	1:A:4:GLU:O	2.08	0.53
1:B:195:ASP:OD2	1:B:197:ALA:HB3	2.08	0.53
1:A:3:LYS:HD3	1:A:345:TYR:OH	2.10	0.52
1:A:181:LEU:CD2	1:A:437:LEU:HD13	2.36	0.52
1:B:59:LYS:HE3	4:B:1378:HOH:O	2.10	0.52
1:A:388:HIS:HD2	1:A:391:LYS:HZ3	1.58	0.52
1:B:424:GLU:CB	1:B:449:LYS:HE3	2.40	0.52
1:A:215:LEU:O	1:A:219:ILE:HG13	2.10	0.52
1:A:267:GLU:HG2	1:A:438:THR:OG1	2.10	0.52
1:A:426:HIS:HE1	4:A:1132:HOH:O	1.93	0.51
1:A:148:LEU:HD11	1:A:413:VAL:HG21	1.93	0.51
1:A:310:GLN:HG2	4:A:1397:HOH:O	2.10	0.51
1:B:1:THR:O	1:B:344:GLU:HG2	2.09	0.51
1:A:296:ARG:HH12	3:A:1008:EDO:C1	2.13	0.51
1:A:53:SER:HB3	1:A:359:GLN:HB3	1.92	0.50
1:A:200:GLU:O	1:A:200:GLU:HG3	2.11	0.50
1:A:1:THR:O	1:A:344:GLU:HA	2.11	0.50
1:A:168:ASP:OD1	1:B:168:ASP:OD1	2.29	0.50
1:A:17:LEU:HB3	1:A:18:PRO:HD3	1.94	0.50
1:A:388:HIS:HD2	1:A:391:LYS:NZ	2.10	0.49
1:A:289:LYS:CG	3:A:1008:EDO:H22	2.42	0.49
1:B:193:PRO:HB3	4:B:1393:HOH:O	2.12	0.49
1:A:289:LYS:O	3:A:1008:EDO:H12	2.13	0.48
1:B:47:ARG:HG3	1:B:47:ARG:HH11	1.77	0.48
1:B:336:LYS:HG2	4:B:1485:HOH:O	2.13	0.48
1:B:231:ASP:OD1	1:B:231:ASP:N	2.47	0.48
1:B:323:ARG:HA	1:B:361:HIS:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:GLU:HA	4:B:1420:HOH:O	2.13	0.48
1:A:81:PHE:HB3	1:A:209:ILE:HG12	1.95	0.47
1:B:202:LYS:NZ	4:B:1168:HOH:O	2.46	0.47
1:A:3:LYS:HE2	1:A:345:TYR:CE1	2.48	0.47
1:A:97:LYS:HE3	1:A:101:ASN:OD1	2.15	0.47
1:B:259:ILE:HG22	1:B:263:ILE:HD12	1.97	0.47
1:A:153:ILE:HG13	4:A:1384:HOH:O	2.14	0.47
1:B:306:LYS:HD3	1:B:306:LYS:N	2.29	0.47
1:B:60:GLU:OE2	1:B:342:GLY:HA2	2.15	0.47
1:B:2:ILE:HD12	1:B:346:PRO:CG	2.45	0.47
1:B:312:LYS:HE2	4:B:1412:HOH:O	2.15	0.47
1:A:171:HIS:CD2	1:A:172:PRO:HD2	2.50	0.46
1:B:361:HIS:CE1	1:B:391:LYS:H	2.17	0.46
1:A:173:PHE:CD1	1:A:212:MET:HA	2.50	0.46
1:A:26:VAL:HG23	3:A:1013:EDO:H22	1.97	0.46
1:A:192:ASN:O	1:A:198:TYR:HE2	1.98	0.46
1:A:169:GLN:HG3	1:B:168:ASP:CG	2.36	0.46
1:A:192:ASN:OD1	1:A:195:ASP:HB2	2.15	0.46
1:B:120:VAL:HG11	1:B:302:VAL:HG13	1.98	0.45
1:A:56:ARG:NH2	1:A:342:GLY:O	2.50	0.45
1:B:440:LYS:HB3	4:B:1158:HOH:O	2.15	0.45
1:B:98:LYS:HG2	1:B:242:ASP:HB2	1.99	0.45
1:B:229:GLN:NE2	1:B:239:ASN:OD1	2.49	0.45
1:A:388:HIS:CD2	1:A:391:LYS:HZ3	2.35	0.45
1:A:292:GLU:HB2	3:A:1008:EDO:H12	1.98	0.45
1:A:127:VAL:HG11	1:A:455:LEU:HD11	1.98	0.45
1:B:449:LYS:N	1:B:449:LYS:HD2	2.32	0.45
1:B:192:ASN:OD1	1:B:192:ASN:N	2.50	0.45
1:B:50:ARG:HB2	1:B:353:LEU:HD12	1.97	0.45
1:B:200:GLU:OE1	1:B:203:ARG:NE	2.50	0.45
1:B:200:GLU:OE1	1:B:203:ARG:NH2	2.50	0.45
1:A:241:LYS:NZ	4:A:1412:HOH:O	2.50	0.44
1:B:372:GLU:HB2	4:B:1161:HOH:O	2.17	0.44
1:A:183:GLU:OE2	1:A:187:LYS:NZ	2.50	0.44
1:A:204:GLN:NE2	1:A:207:GLU:OE2	2.49	0.44
1:A:306:LYS:HG2	4:A:1354:HOH:O	2.16	0.44
1:A:426:HIS:CD2	1:A:426:HIS:H	2.36	0.44
1:A:169:GLN:HA	1:A:170:PRO:HD2	1.79	0.44
1:A:203:ARG:NH2	1:A:204:GLN:OE1	2.50	0.44
1:A:370:ASP:HB2	1:A:373:GLU:HG3	2.00	0.44
1:A:49:THR:OG1	1:A:352:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ASN:O	1:B:167:ARG:HD2	2.17	0.44
1:B:189:GLN:NE2	4:B:1020:HOH:O	2.50	0.43
1:A:435:GLU:OE1	3:A:1013:EDO:H22	2.18	0.43
1:A:213:ASN:O	1:A:217:ASP:HB2	2.18	0.43
1:A:323:ARG:HA	1:A:361:HIS:CD2	2.53	0.43
1:A:21:ASN:HB2	4:A:1335:HOH:O	2.19	0.43
1:B:183:GLU:OE2	1:B:190:ARG:NH2	2.50	0.43
1:A:296:ARG:NH1	3:A:1008:EDO:H11	2.14	0.43
1:A:68:ASP:HB3	1:A:334:TYR:CE1	2.54	0.42
1:A:289:LYS:HG3	3:A:1008:EDO:H22	2.00	0.42
1:B:2:ILE:HD12	1:B:346:PRO:HG3	2.00	0.42
1:A:198:TYR:O	1:A:202:LYS:HG3	2.19	0.42
1:B:62:CYS:SG	1:B:391:LYS:HE2	2.60	0.42
1:B:95:ASN:HA	1:B:95:ASN:HD22	1.68	0.42
1:A:183:GLU:HG3	1:A:187:LYS:NZ	2.34	0.42
1:B:245:THR:HB	1:B:247:GLU:HG3	2.02	0.42
1:A:173:PHE:CE1	1:A:212:MET:HA	2.55	0.42
1:A:289:LYS:HG2	3:A:1008:EDO:H22	2.02	0.41
1:B:455:LEU:HA	1:B:455:LEU:HD23	1.87	0.41
1:A:200:GLU:O	1:A:203:ARG:HB3	2.20	0.41
1:B:453:ILE:HA	1:B:454:PRO:HD3	1.80	0.41
1:A:118:MET:HG3	4:A:1308:HOH:O	2.21	0.41
1:A:263:ILE:HG21	1:A:263:ILE:HD13	1.69	0.41
1:B:94:LYS:HZ3	1:B:245:THR:HG21	1.82	0.41
1:A:241:LYS:HE3	4:A:1316:HOH:O	2.21	0.41
1:B:266:HIS:CD2	1:B:267:GLU:HG2	2.56	0.41
1:A:77:PHE:CE2	1:A:187:LYS:HB3	2.56	0.41
1:A:90:TRP:HB3	1:A:92:HIS:CE1	2.55	0.40
1:A:366:ILE:HD12	1:A:386:PRO:HG2	2.03	0.40
1:A:452:LYS:HE3	4:A:1434:HOH:O	2.21	0.40
1:A:367:TRP:HB2	1:A:371:VAL:HG12	2.04	0.40
1:B:158:PHE:HD2	1:B:219:ILE:HD13	1.86	0.40
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.96	0.40
1:A:434:LYS:HB2	1:A:442:GLU:HB2	2.04	0.40
1:B:437:LEU:HB3	3:B:1012:EDO:H11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	453/455 (100%)	440 (97%)	13 (3%)	0	100	100
1	B	453/455 (100%)	446 (98%)	7 (2%)	0	100	100
All	All	906/910 (100%)	886 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	399/399 (100%)	387 (97%)	12 (3%)	41	15
1	B	399/399 (100%)	379 (95%)	20 (5%)	24	5
All	All	798/798 (100%)	766 (96%)	32 (4%)	31	9

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	22	THR
1	A	47	ARG
1	A	52	LEU
1	A	92	HIS
1	A	168	ASP
1	A	169	GLN
1	A	218	LYS

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Mol	Chain	Res	Type
1	A	228	GLU
1	A	230	SER
1	A	231	ASP
1	A	263	ILE
1	B	1	THR
1	B	2	ILE
1	B	47	ARG
1	B	98	LYS
1	B	148	LEU
1	B	158	PHE
1	B	168	ASP
1	B	200	GLU
1	B	230	SER
1	B	231	ASP
1	B	241	LYS
1	B	306	LYS
1	B	353	LEU
1	B	369	ASP
1	B	380	GLU
1	B	407	LEU
1	B	430	GLU
1	B	437	LEU
1	B	440	LYS
1	B	449	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	100	HIS
1	A	110	GLN
1	A	159	ASN
1	A	171	HIS
1	A	361	HIS
1	A	388	HIS
1	A	395	ASN
1	A	403	GLN
1	A	426	HIS
1	B	92	HIS
1	B	95	ASN
1	B	189	GLN
1	B	213	ASN

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Mol	Chain	Res	Type
1	B	229	GLN
1	B	239	ASN
1	B	359	GLN
1	B	361	HIS
1	B	387	GLN
1	B	395	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

16 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	EDO	A	1003	-	3,3,3	0.60	0	2,2,2	0.09	0
3	EDO	B	1004	-	3,3,3	0.81	0	2,2,2	0.90	0
3	EDO	B	1010	-	3,3,3	0.56	0	2,2,2	0.44	0
3	EDO	A	1014	-	3,3,3	0.55	0	2,2,2	0.20	0
3	EDO	A	1002	-	3,3,3	0.58	0	2,2,2	0.36	0
3	EDO	B	1009	-	3,3,3	0.53	0	2,2,2	0.15	0
3	EDO	B	1005	-	3,3,3	0.49	0	2,2,2	0.27	0
3	EDO	A	1001	-	3,3,3	0.58	0	2,2,2	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	1012	-	3,3,3	0.50	0	2,2,2	0.25	0
2	HEM	B	1000	1,4	27,50,50	1.53	4 (14%)	17,82,82	1.52	3 (17%)
3	EDO	A	1013	-	3,3,3	0.41	0	2,2,2	0.25	0
3	EDO	B	1006	-	3,3,3	0.54	0	2,2,2	0.31	0
3	EDO	B	1007	-	3,3,3	0.56	0	2,2,2	0.49	0
3	EDO	B	1011	-	3,3,3	0.51	0	2,2,2	0.07	0
2	HEM	A	999	1,4	27,50,50	1.60	4 (14%)	17,82,82	2.03	8 (47%)
3	EDO	A	1008	-	3,3,3	0.47	0	2,2,2	0.25	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	EDO	A	1003	-	-	0/1/1/1	-
3	EDO	B	1004	-	-	0/1/1/1	-
3	EDO	B	1010	-	-	1/1/1/1	-
3	EDO	A	1014	-	-	1/1/1/1	-
3	EDO	A	1002	-	-	0/1/1/1	-
3	EDO	B	1009	-	-	1/1/1/1	-
3	EDO	B	1005	-	-	0/1/1/1	-
3	EDO	A	1001	-	-	0/1/1/1	-
3	EDO	B	1012	-	-	0/1/1/1	-
2	HEM	B	1000	1,4	-	0/6/54/54	-
3	EDO	A	1013	-	-	1/1/1/1	-
3	EDO	B	1006	-	-	0/1/1/1	-
3	EDO	B	1007	-	-	1/1/1/1	-
3	EDO	B	1011	-	-	1/1/1/1	-
2	HEM	A	999	1,4	-	0/6/54/54	-
3	EDO	A	1008	-	-	1/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	999	HEM	C3C-CAC	-3.79	1.40	1.47
2	B	1000	HEM	C3C-CAC	-3.76	1.40	1.47
2	B	1000	HEM	C3B-CAB	-3.67	1.40	1.47
2	A	999	HEM	C3B-C2B	-3.58	1.35	1.40
2	A	999	HEM	C3C-C2C	-3.50	1.35	1.40
2	A	999	HEM	C3B-CAB	-3.31	1.41	1.47
2	B	1000	HEM	C3C-C2C	-2.98	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	HEM	C3B-C2B	-2.86	1.36	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	HEM	CMA-C3A-C4A	-3.74	122.71	128.46
2	A	999	HEM	CMA-C3A-C4A	-3.35	123.32	128.46
2	A	999	HEM	CMD-C2D-C1D	-3.26	123.45	128.46
2	B	1000	HEM	CMC-C2C-C3C	2.92	130.13	124.68
2	A	999	HEM	CMB-C2B-C3B	2.86	130.02	124.68
2	A	999	HEM	CAA-CBA-CGA	2.83	117.42	112.67
2	B	1000	HEM	CMA-C3A-C2A	2.73	130.08	124.94
2	A	999	HEM	CBA-CAA-C2A	2.65	117.37	112.49
2	A	999	HEM	CMA-C3A-C2A	2.45	129.56	124.94
2	A	999	HEM	CMD-C2D-C3D	2.41	129.48	124.94
2	A	999	HEM	CMC-C2C-C3C	2.41	129.18	124.68

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1013	EDO	O1-C1-C2-O2
3	B	1009	EDO	O1-C1-C2-O2
3	B	1011	EDO	O1-C1-C2-O2
3	A	1014	EDO	O1-C1-C2-O2
3	B	1007	EDO	O1-C1-C2-O2
3	A	1008	EDO	O1-C1-C2-O2
3	B	1010	EDO	O1-C1-C2-O2

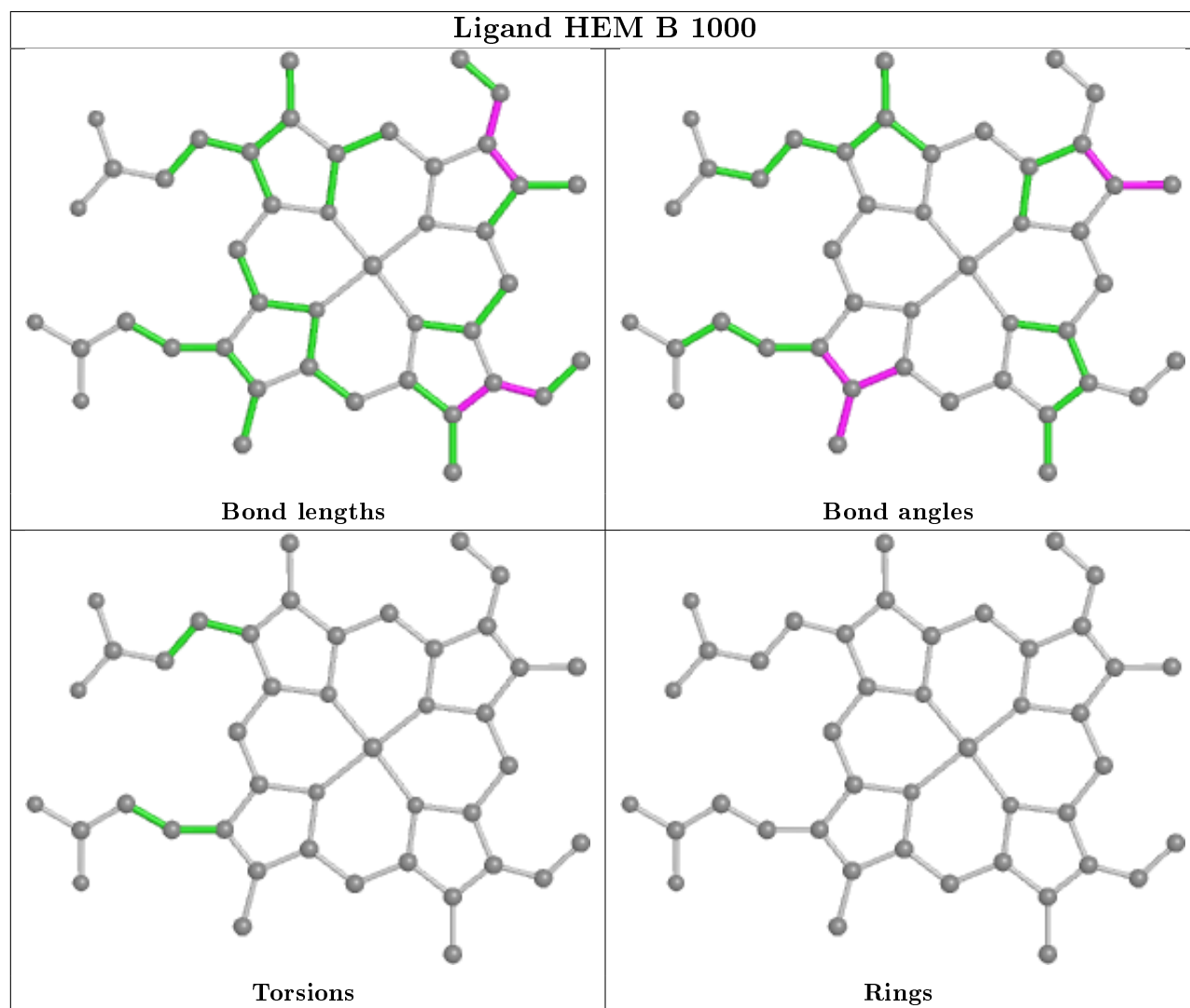
There are no ring outliers.

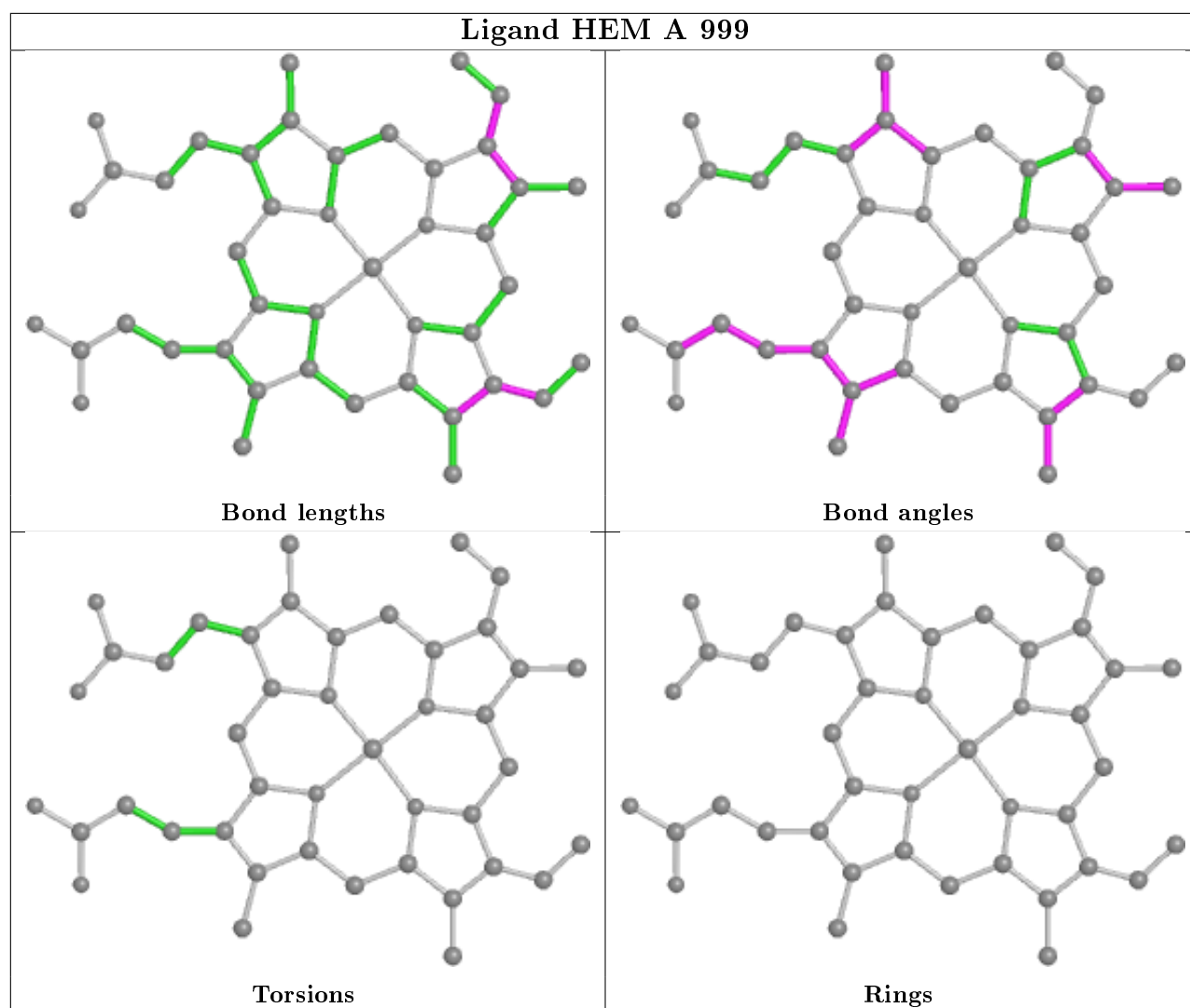
4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1009	EDO	1	0
3	B	1012	EDO	1	0
3	A	1013	EDO	3	0
3	A	1008	EDO	9	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.