



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:20 AM UTC

PDB ID : 1BU7 / pdb_00001bu7
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 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

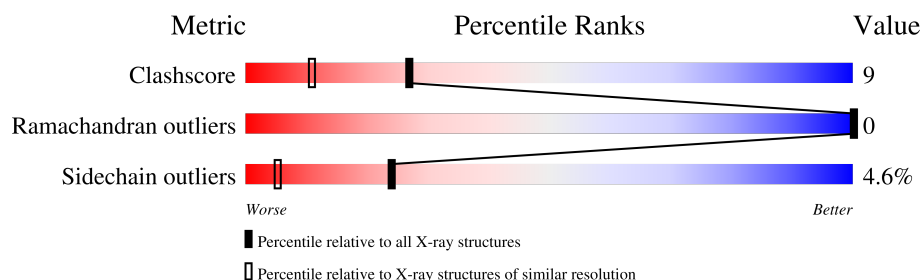
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (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 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	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 (CCD ID: 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 (CCD ID: 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.

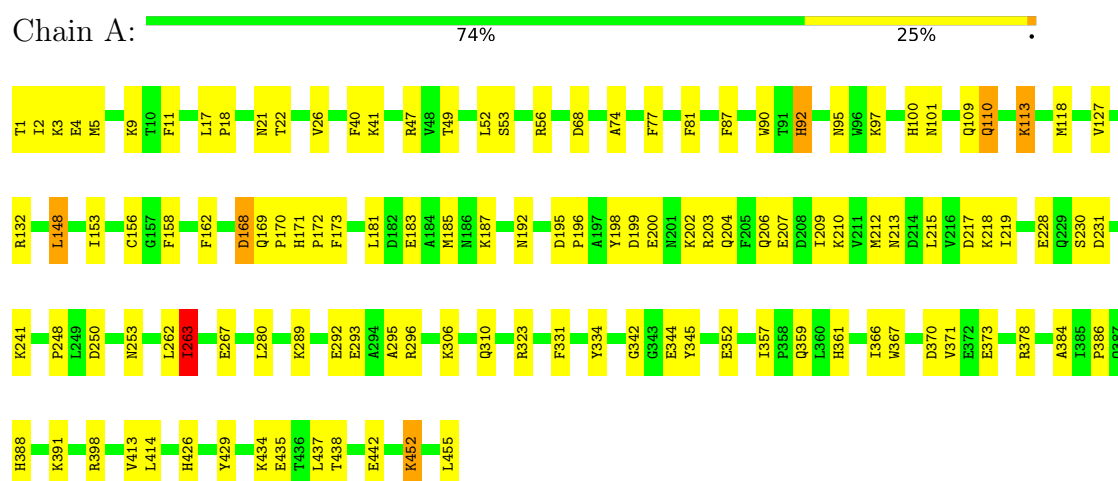
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	475	Total 475	O 475	0	0
4	B	523	Total 523	O 523	0	0

3 Residue-property plots

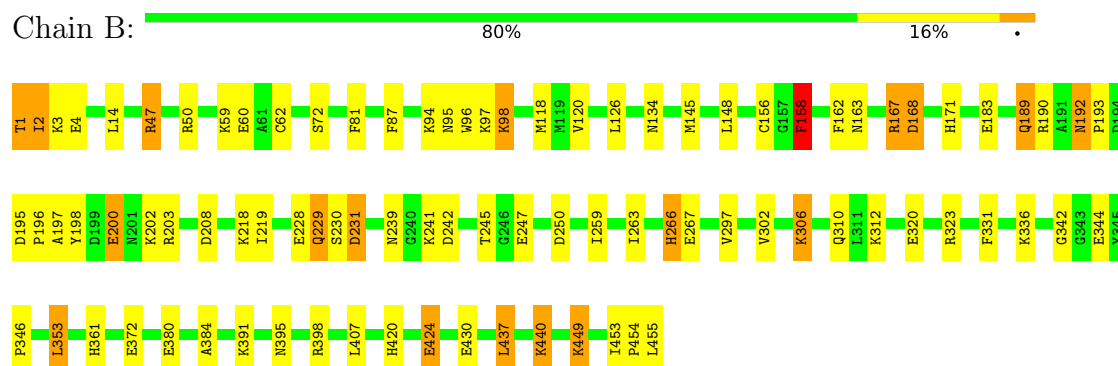
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: 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	0.57	0/3756	1.43	30/5077 (0.6%)
1	B	0.60	0/3756	1.41	27/5077 (0.5%)
All	All	0.58	0/7512	1.42	57/10154 (0.6%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ASN	OD1-CG-ND2	9.25	131.85	122.60
1	B	266	HIS	CA-CB-CG	7.52	121.32	113.80
1	A	156	CYS	CA-C-N	7.40	128.16	119.94
1	A	156	CYS	C-N-CA	7.40	128.16	119.94
1	B	167	ARG	CD-NE-CZ	7.30	134.62	124.40
1	A	87	PHE	CA-CB-CG	7.18	120.98	113.80
1	A	158	PHE	CA-CB-CG	7.01	120.81	113.80
1	A	398	ARG	CD-NE-CZ	6.83	133.96	124.40
1	A	248	PRO	O-C-N	-6.67	115.82	123.23
1	B	420	HIS	CA-CB-CG	-6.64	107.16	113.80
1	B	98	LYS	O-C-N	6.61	128.88	122.07
1	B	171	HIS	CA-CB-CG	6.59	120.39	113.80
1	B	134	ASN	OD1-CG-ND2	6.49	129.09	122.60
1	A	132	ARG	O-C-N	-6.25	114.85	122.34
1	B	189	GLN	CA-C-N	-6.23	113.89	122.30
1	B	189	GLN	C-N-CA	-6.23	113.89	122.30
1	A	384	ALA	CA-C-N	-6.18	118.14	122.59
1	A	384	ALA	C-N-CA	-6.18	118.14	122.59
1	B	158	PHE	CA-CB-CG	6.17	119.97	113.80
1	B	331	PHE	CA-CB-CG	6.16	119.96	113.80
1	B	320	GLU	O-C-N	-6.06	114.81	122.27
1	A	113	LYS	CA-C-N	5.99	126.59	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	LYS	C-N-CA	5.99	126.59	120.00
1	A	429	TYR	O-C-N	5.97	130.21	122.87
1	A	109	GLN	O-C-N	-5.89	115.88	122.12
1	B	162	PHE	O-C-N	5.85	130.53	122.46
1	B	250	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	331	PHE	CA-CB-CG	5.67	119.47	113.80
1	B	208	ASP	CA-C-O	5.55	126.30	120.42
1	B	384	ALA	CA-C-N	-5.53	116.55	122.85
1	B	384	ALA	C-N-CA	-5.53	116.55	122.85
1	B	266	HIS	CA-C-O	-5.53	115.01	120.70
1	A	5	MET	CA-C-O	5.45	125.51	120.60
1	B	398	ARG	CD-NE-CZ	5.45	132.03	124.40
1	B	87	PHE	CA-CB-CG	5.44	119.24	113.80
1	B	395	ASN	N-CA-C	5.40	118.23	109.06
1	A	40	PHE	CA-CB-CG	5.36	119.16	113.80
1	A	95	ASN	CA-CB-CG	5.35	117.95	112.60
1	B	424	GLU	CA-C-O	5.35	126.02	120.30
1	A	162	PHE	O-C-N	5.25	129.47	122.43
1	A	250	ASP	CA-CB-CG	5.25	117.85	112.60
1	B	156	CYS	CA-C-N	5.23	131.66	121.41
1	B	156	CYS	C-N-CA	5.23	131.66	121.41
1	A	378	ARG	NE-CZ-NH1	-5.21	116.28	121.50
1	B	96	TRP	CA-C-O	5.21	126.26	120.90
1	A	263	ILE	CA-C-N	5.13	127.67	120.28
1	A	263	ILE	C-N-CA	5.13	127.67	120.28
1	B	395	ASN	O-C-N	5.12	129.52	123.33
1	B	297	VAL	N-CA-C	5.11	115.78	110.82
1	B	81	PHE	CA-CB-CG	5.11	118.91	113.80
1	A	295	ALA	CA-C-N	5.08	127.51	120.29
1	A	295	ALA	C-N-CA	5.08	127.51	120.29
1	A	263	ILE	CA-C-O	-5.04	115.89	121.29
1	A	357	ILE	CB-CA-C	-5.03	109.02	114.35
1	A	414	LEU	CA-C-N	5.03	125.52	119.94
1	A	414	LEU	C-N-CA	5.03	125.52	119.94
1	A	110	GLN	O-C-N	5.01	127.43	122.12

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	81	0
1	B	3671	0	3645	58	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	137	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 (137) 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:126:LEU:HD21	1:B:145:MET:HE1	1.74	0.69
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:206:GLN:O	1:A:210:LYS:HD3	2.01	0.60
1:A:293:GLU:HB2	3:A:1008:EDO:H21	1.83	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:B:306:LYS:HZ3	1.56	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:B:94:LYS:HZ1	1:B:245:THR:HG21	1.74	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:169:GLN:HG3	1:B:168:ASP:CG	2.36	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:17:LEU:HB3	1:A:18:PRO:HD3	1.94	0.50
1:A:168:ASP:OD1	1:B:168:ASP:OD1	2.29	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:323:ARG:HA	1:B:361:HIS:CD2	2.49	0.48
1:B:231:ASP:OD1	1:B:231:ASP:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LEU:CD2	1:B:145:MET:HE1	2.44	0.48
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:60:GLU:OE2	1:B:342:GLY:HA2	2.15	0.47
1:B:306:LYS:N	1:B:306:LYS:HD3	2.29	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: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:98:LYS:HG2	1:B:242:ASP:HB2	1.99	0.45
1:B:440:LYS:HB3	4:B:1158:HOH:O	2.15	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:127:VAL:HG11	1:A:455:LEU:HD11	1.98	0.45
1:A:292:GLU:HB2	3:A:1008:EDO:H12	1.98	0.45
1:B:449:LYS:N	1:B:449:LYS:HD2	2.32	0.45
1:B:192:ASN:N	1:B:192:ASN:OD1	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:B:118:MET:HE2	1:B:118:MET:HA	1.98	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: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:A:370:ASP:HB2	1:A:373:GLU:HG3	2.00	0.44
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: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:435:GLU:OE1	3:A:1013:EDO:H22	2.18	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:A:74:ALA:HB1	1:A:185:MET:HE1	2.02	0.42
1:B:62:CYS:SG	1:B:391:LYS:HE2	2.60	0.42
1:B:95:ASN:HD22	1:B:95:ASN:HA	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:HD13	1:A:263:ILE:HG21	1.69	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%)	385 (96%)	14 (4%)	32	10
1	B	399/399 (100%)	376 (94%)	23 (6%)	18	3
All	All	798/798 (100%)	761 (95%)	37 (5%)	24	5

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	22	THR
1	A	41	LYS
1	A	47	ARG
1	A	52	LEU
1	A	92	HIS
1	A	148	LEU
1	A	168	ASP

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Mol	Chain	Res	Type
1	A	218	LYS
1	A	228	GLU
1	A	230	SER
1	A	231	ASP
1	A	263	ILE
1	A	452	LYS
1	B	1	THR
1	B	2	ILE
1	B	14	LEU
1	B	47	ARG
1	B	97	LYS
1	B	148	LEU
1	B	158	PHE
1	B	168	ASP
1	B	192	ASN
1	B	200	GLU
1	B	218	LYS
1	B	229	GLN
1	B	230	SER
1	B	231	ASP
1	B	241	LYS
1	B	306	LYS
1	B	353	LEU
1	B	380	GLU
1	B	407	LEU
1	B	430	GLU
1	B	437	LEU
1	B	440	LYS
1	B	449	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	70	ASN
1	A	95	ASN
1	A	100	HIS
1	A	110	GLN
1	A	159	ASN
1	A	171	HIS
1	A	186	ASN
1	A	189	GLN

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Mol	Chain	Res	Type
1	A	266	HIS
1	A	359	GLN
1	A	361	HIS
1	A	388	HIS
1	A	395	ASN
1	A	403	GLN
1	A	426	HIS
1	B	70	ASN
1	B	73	GLN
1	B	92	HIS
1	B	95	ASN
1	B	186	ASN
1	B	189	GLN
1	B	204	GLN
1	B	213	ASN
1	B	229	GLN
1	B	239	ASN
1	B	361	HIS
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 oligosaccharides 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	1002	-	3,3,3	0.54	0	2,2,2	0.40	0
3	EDO	A	1003	-	3,3,3	0.57	0	2,2,2	0.13	0
2	HEM	A	999	4,1	50,50,50	1.02	3 (6%)	67,82,82	1.01	1 (1%)
3	EDO	A	1013	-	3,3,3	0.38	0	2,2,2	0.23	0
3	EDO	B	1011	-	3,3,3	0.48	0	2,2,2	0.13	0
3	EDO	B	1010	-	3,3,3	0.53	0	2,2,2	0.48	0
3	EDO	A	1008	-	3,3,3	0.44	0	2,2,2	0.30	0
3	EDO	B	1006	-	3,3,3	0.50	0	2,2,2	0.35	0
3	EDO	A	1014	-	3,3,3	0.51	0	2,2,2	0.25	0
3	EDO	B	1004	-	3,3,3	0.77	0	2,2,2	0.91	0
3	EDO	B	1009	-	3,3,3	0.50	0	2,2,2	0.20	0
3	EDO	B	1005	-	3,3,3	0.45	0	2,2,2	0.22	0
3	EDO	B	1007	-	3,3,3	0.52	0	2,2,2	0.52	0
3	EDO	B	1012	-	3,3,3	0.45	0	2,2,2	0.30	0
2	HEM	B	1000	4,1	50,50,50	0.95	2 (4%)	67,82,82	1.08	4 (5%)
3	EDO	A	1001	-	3,3,3	0.54	0	2,2,2	0.62	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	1002	-	-	0/1/1/1	-
3	EDO	A	1003	-	-	0/1/1/1	-
2	HEM	A	999	4,1	-	2/14/54/54	-
3	EDO	A	1013	-	-	1/1/1/1	-
3	EDO	B	1011	-	-	1/1/1/1	-
3	EDO	B	1010	-	-	1/1/1/1	-
3	EDO	A	1008	-	-	1/1/1/1	-
3	EDO	B	1006	-	-	0/1/1/1	-
3	EDO	A	1014	-	-	1/1/1/1	-
3	EDO	B	1004	-	-	0/1/1/1	-
3	EDO	B	1009	-	-	1/1/1/1	-
3	EDO	B	1005	-	-	0/1/1/1	-
3	EDO	B	1007	-	-	1/1/1/1	-
3	EDO	B	1012	-	-	0/1/1/1	-
2	HEM	B	1000	4,1	-	3/14/54/54	-
3	EDO	A	1001	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	999	HEM	CAC-C3C	-2.76	1.40	1.47
2	B	1000	HEM	CAC-C3C	-2.73	1.40	1.47
2	B	1000	HEM	CAB-C3B	-2.60	1.40	1.47
2	A	999	HEM	CAB-C3B	-2.32	1.41	1.47
2	A	999	HEM	O2D-CGD	-2.17	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	HEM	C3B-C4B-NB	2.20	111.05	109.47
2	A	999	HEM	O2D-CGD-CBD	2.20	120.94	114.00
2	B	1000	HEM	CHC-C1C-C2C	-2.12	121.08	125.49
2	B	1000	HEM	CMA-C3A-C2A	2.10	130.08	125.62
2	B	1000	HEM	CHC-C1C-NC	2.07	126.71	124.45

There are no chirality outliers.

All (12) torsion outliers are listed below:

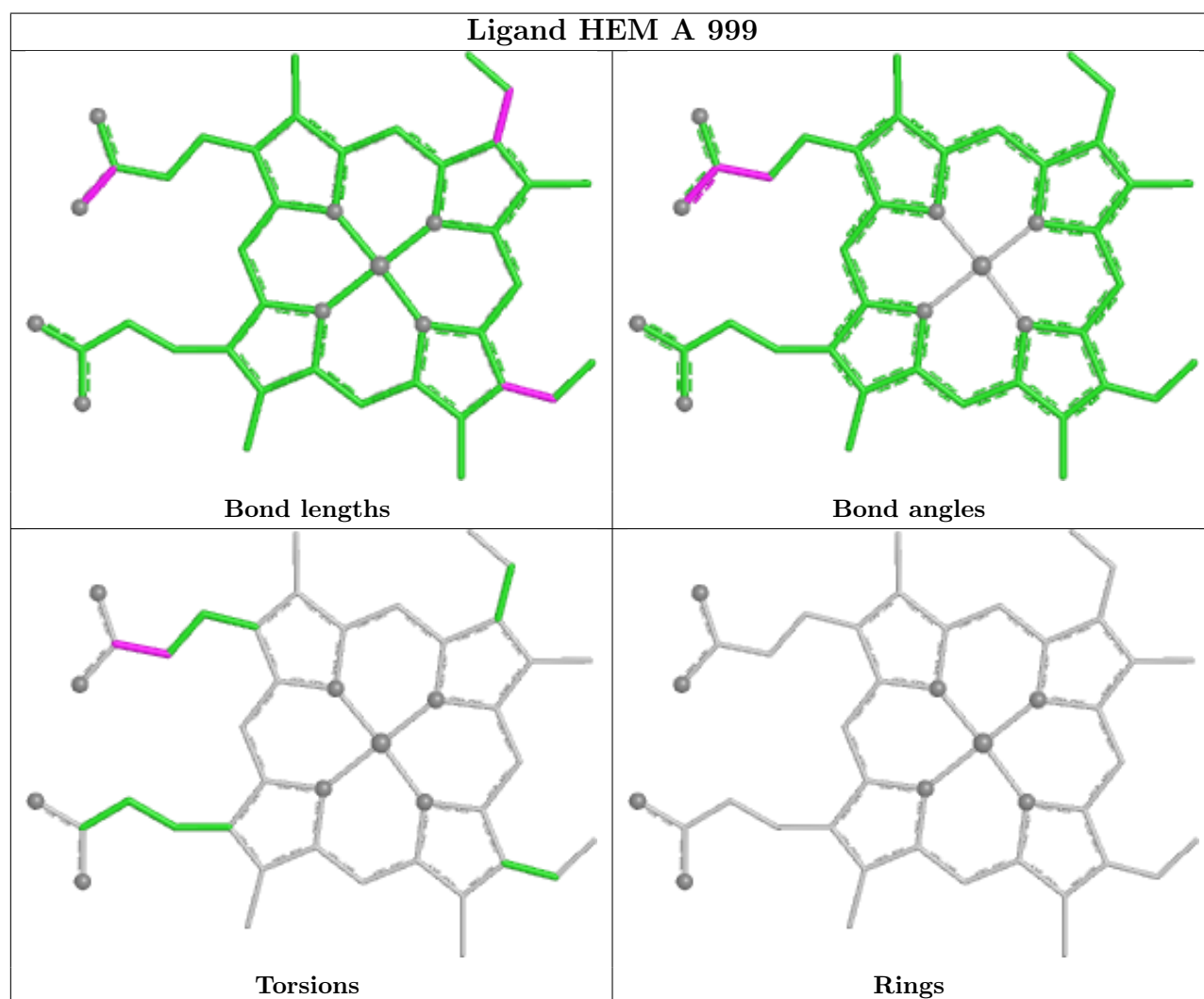
Mol	Chain	Res	Type	Atoms
2	B	1000	HEM	C2B-C3B-CAB-CBB
3	A	1013	EDO	O1-C1-C2-O2
3	B	1009	EDO	O1-C1-C2-O2
3	B	1011	EDO	O1-C1-C2-O2
3	A	1014	EDO	O1-C1-C2-O2
2	A	999	HEM	CAD-CBD-CGD-O1D
2	A	999	HEM	CAD-CBD-CGD-O2D
3	B	1007	EDO	O1-C1-C2-O2
2	B	1000	HEM	CAD-CBD-CGD-O2D
2	B	1000	HEM	CAD-CBD-CGD-O1D
3	A	1008	EDO	O1-C1-C2-O2
3	B	1010	EDO	O1-C1-C2-O2

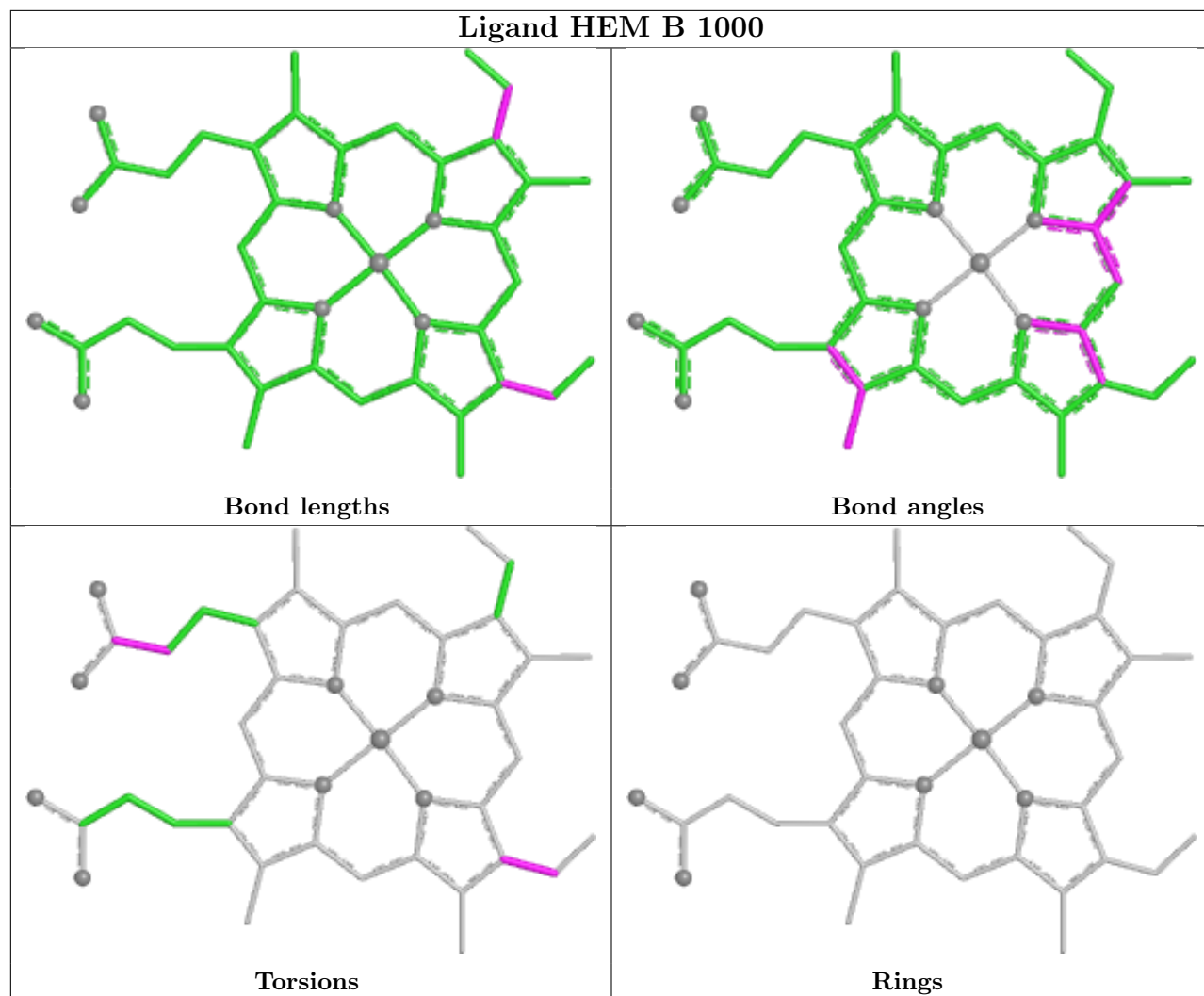
There are no ring outliers.

4 monomers are involved in 14 short contacts:

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