



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 03:01 PM EDT

PDB ID : 2FC2 / pdb_00002fc2
Title : NO-HEME complex in a bacterial nitric oxide synthase. An Fe(III)-NO may cause nitrosation.
Authors : Pant, K.; Crane, B.R.
Deposited on : 2005-12-10
Resolution : 2.20 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)	:	2.50

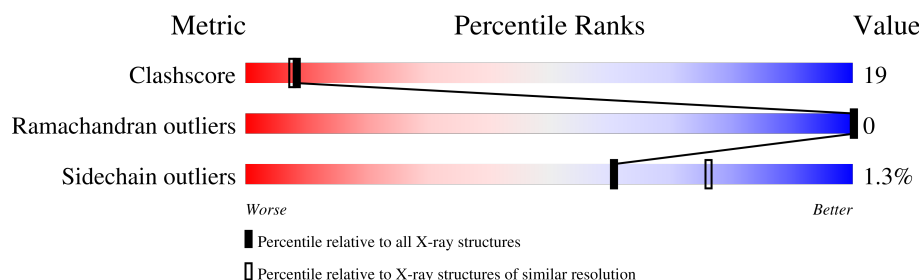
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	363	76% 22% .
1	B	363	73% 25% .

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	NO	B	2903	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6707 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.

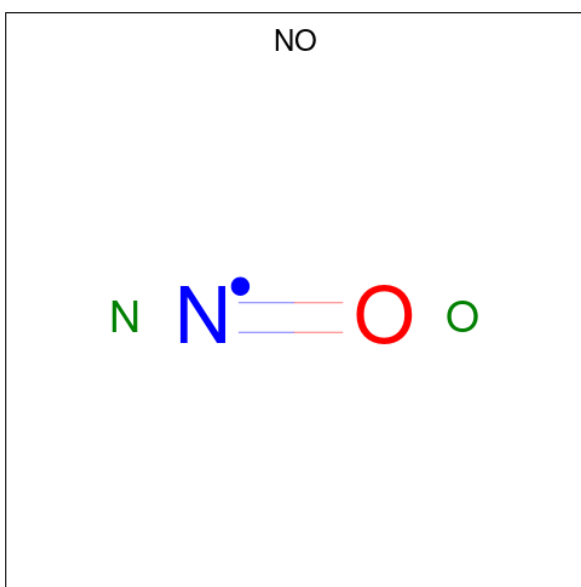
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2928	1866	503	551	8			
1	B	362	Total	C	N	O	S	0	0	0
			2928	1866	503	551	8			

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



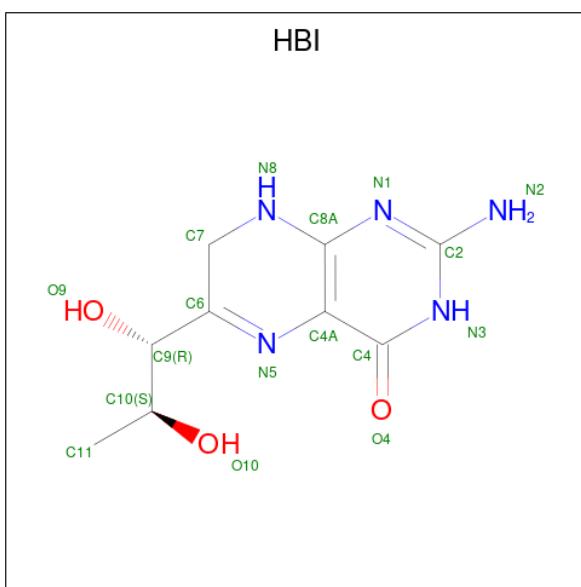
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is NITRIC OXIDE (CCD ID: NO) (formula: NO).



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

- Molecule 4 is 7,8-DIHYDROBIOPTERIN (CCD ID: HBI) (formula: $C_9H_{13}N_5O_3$).



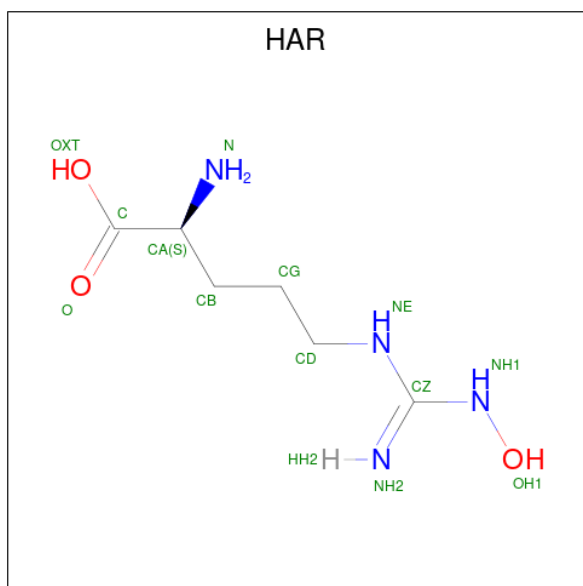
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	9	5	3		

Continued on next page...

Continued from previous page...

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

- Molecule 5 is N-OMEGA-HYDROXY-L-ARGININE (CCD ID: HAR) (formula: $C_6H_{14}N_4O_3$).



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

- Molecule 6 is water.

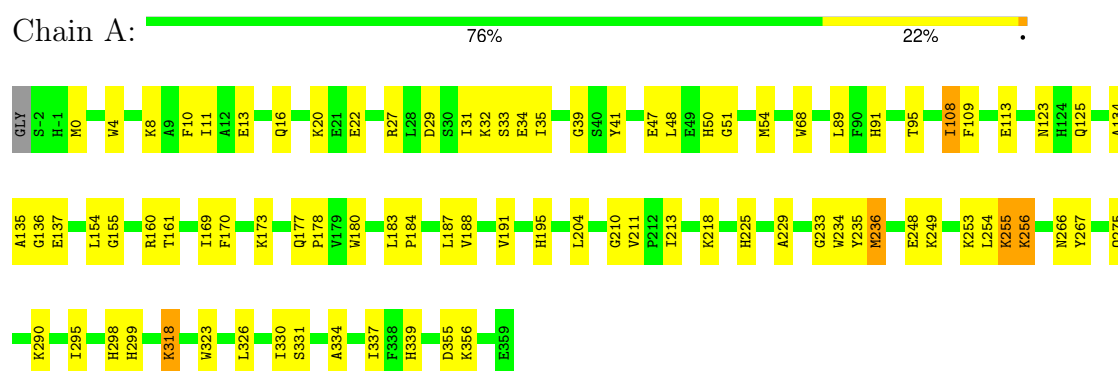
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	370	Total	O	0	0
			370	370		
6	B	329	Total	O	0	0
			329	329		

3 Residue-property plots

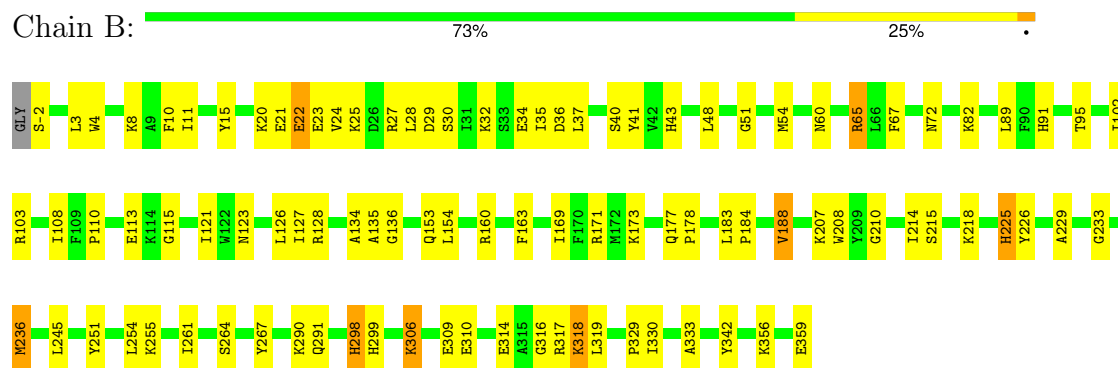
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: Nitric Oxide Synthase



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.74Å 96.17Å 129.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.02 – 2.20	Depositor
% Data completeness (in resolution range)	100.0 (27.02-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.273 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6707	wwPDB-VP
Average B, all atoms (Å ²)	54.0	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, NO, HBI, HAR

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	0.65	0/3005	0.98	20/4077 (0.5%)
1	B	0.66	0/3005	1.00	18/4077 (0.4%)
All	All	0.65	0/6010	0.99	38/8154 (0.5%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	VAL	N-CA-C	6.93	117.83	107.51
1	B	229	ALA	CA-C-N	6.79	126.75	119.76
1	B	229	ALA	C-N-CA	6.79	126.75	119.76
1	B	188	VAL	N-CA-C	6.76	117.86	107.99
1	A	210	GLY	N-CA-C	6.30	123.31	113.86
1	B	210	GLY	N-CA-C	6.20	123.16	113.86
1	B	254	LEU	N-CA-C	6.11	117.94	111.28
1	A	229	ALA	CA-C-N	5.97	125.91	119.76
1	A	229	ALA	C-N-CA	5.97	125.91	119.76
1	A	253	LYS	N-CA-C	5.90	120.61	113.17
1	B	110	PRO	CA-C-N	5.83	126.29	120.52
1	B	110	PRO	C-N-CA	5.83	126.29	120.52
1	A	254	LEU	N-CA-C	5.80	118.34	111.33
1	A	298	HIS	N-CA-C	5.77	118.52	111.82
1	A	68	TRP	N-CA-C	5.63	118.14	111.33
1	B	215	SER	N-CA-C	5.61	119.70	112.41
1	B	298	HIS	N-CA-C	5.60	118.15	111.71
1	B	233	GLY	N-CA-C	-5.57	101.92	110.77
1	A	339	HIS	N-CA-C	5.55	119.15	112.93
1	A	108	ILE	N-CA-C	5.50	115.70	107.51
1	A	233	GLY	N-CA-C	-5.37	102.23	110.77
1	B	65	ARG	N-CA-C	5.36	119.30	112.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	ASN	N-CA-C	5.35	117.80	111.33
1	A	211	VAL	N-CA-C	5.29	116.07	107.71
1	B	267	TYR	N-CA-C	5.24	117.62	108.76
1	B	115	GLY	N-CA-C	-5.22	108.42	115.21
1	A	236	MET	N-CA-C	-5.20	100.25	108.73
1	A	161	THR	N-CA-C	-5.19	102.33	110.17
1	B	225	HIS	N-CA-C	5.17	117.37	107.75
1	A	267	TYR	N-CA-C	5.11	117.23	108.90
1	A	235	TYR	N-CA-C	5.09	117.68	110.50
1	B	102	ILE	N-CA-C	5.08	116.94	109.63
1	B	236	MET	N-CA-C	-5.07	100.46	108.73
1	B	163	PHE	N-CA-C	5.05	117.29	110.06
1	A	266	ASN	N-CA-C	5.03	117.88	111.69
1	A	195	HIS	CA-C-N	5.01	124.79	119.28
1	A	195	HIS	C-N-CA	5.01	124.79	119.28
1	A	191	VAL	N-CA-C	5.00	115.62	107.71

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	2928	0	2821	97	0
1	B	2928	0	2821	122	0
2	A	43	0	30	1	0
2	B	43	0	30	3	0
3	A	2	0	0	0	0
3	B	4	0	0	3	0
4	A	17	0	13	0	0
4	B	17	0	13	0	0
5	A	26	0	22	1	0
6	A	370	0	0	77	0
6	B	329	0	0	89	0
All	All	6707	0	5750	224	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 19.

All (224) 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:B:34:GLU:HB3	6:B:1953:HOH:O	1.45	1.14
1:B:236:MET:HE3	1:B:298:HIS:CB	1.77	1.13
1:B:25:LYS:O	1:B:28:LEU:CD1	1.99	1.10
1:B:24:VAL:O	1:B:28:LEU:HG	1.48	1.10
1:B:236:MET:HE3	1:B:298:HIS:HB3	1.13	1.08
1:B:27:ARG:HA	6:B:2263:HOH:O	1.54	1.06
1:B:35:ILE:HG12	6:B:2103:HOH:O	1.55	1.05
1:B:23:GLU:HB2	6:B:2469:HOH:O	1.58	1.03
1:B:329:PRO:HG2	6:B:2240:HOH:O	1.60	1.00
1:A:48:LEU:HD21	1:A:108:ILE:HG21	1.42	0.99
1:B:48:LEU:HD21	1:B:108:ILE:HG21	1.45	0.98
5:A:910:HAR:NH1	3:B:1902:NO:N	2.12	0.98
1:B:177:GLN:HG2	6:B:2320:HOH:O	1.63	0.97
1:B:236:MET:CE	1:B:298:HIS:HB3	1.95	0.96
1:B:25:LYS:O	1:B:28:LEU:HD12	1.64	0.96
1:B:126:LEU:HD21	6:B:2237:HOH:O	1.64	0.96
1:B:20:LYS:HB3	6:B:2469:HOH:O	1.63	0.95
1:B:154:LEU:HG	6:B:2414:HOH:O	1.68	0.94
1:A:326:LEU:HB3	6:A:2274:HOH:O	1.68	0.93
1:B:30:SER:HB2	6:B:2263:HOH:O	1.67	0.93
1:A:8:LYS:HG2	6:A:2389:HOH:O	1.67	0.91
1:B:214:ILE:HG13	3:B:2903:NO:O	1.73	0.89
1:B:25:LYS:O	1:B:28:LEU:HD11	1.72	0.88
1:A:136:GLY:HA2	6:A:2325:HOH:O	1.72	0.88
1:B:113:GLU:HG3	6:B:2076:HOH:O	1.74	0.88
1:A:13:GLU:HG3	6:A:2329:HOH:O	1.72	0.88
1:A:113:GLU:HG3	6:A:2261:HOH:O	1.73	0.88
1:B:22:GLU:HB3	6:B:2018:HOH:O	1.74	0.88
1:B:67:PHE:HB2	6:B:2249:HOH:O	1.74	0.86
1:B:32:LYS:HE3	6:B:1996:HOH:O	1.76	0.86
1:A:170:PHE:HE2	6:A:2433:HOH:O	1.60	0.84
1:B:121:ILE:HB	6:B:2499:HOH:O	1.78	0.83
1:A:154:LEU:HG	6:A:2210:HOH:O	1.77	0.83
1:A:109:PHE:HZ	6:A:1976:HOH:O	1.60	0.83
1:A:39:GLY:HA2	6:A:2262:HOH:O	1.78	0.83
1:B:207:LYS:HB2	6:B:2333:HOH:O	1.79	0.82
1:A:295:ILE:HA	6:A:2366:HOH:O	1.80	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ASP:HB2	6:B:2014:HOH:O	1.79	0.81
1:B:261:ILE:HA	6:B:2245:HOH:O	1.82	0.80
1:B:37:LEU:HD11	6:B:2300:HOH:O	1.81	0.79
1:A:234:TRP:HB2	6:A:2366:HOH:O	1.81	0.78
1:A:123:ASN:HD21	1:A:169:ILE:H	1.32	0.78
1:B:89:LEU:HD22	6:B:2237:HOH:O	1.82	0.78
1:B:134:ALA:HB1	6:B:2178:HOH:O	1.84	0.78
1:B:35:ILE:HG22	6:B:2501:HOH:O	1.83	0.78
1:B:236:MET:CE	1:B:298:HIS:CB	2.58	0.78
1:A:11:ILE:HD11	6:A:2425:HOH:O	1.84	0.76
1:A:31:ILE:HG12	6:A:1914:HOH:O	1.85	0.76
1:B:264:SER:HB3	6:B:2120:HOH:O	1.86	0.76
1:A:255:LYS:HB3	1:A:255:LYS:NZ	2.01	0.75
1:A:331:SER:HB3	6:A:2230:HOH:O	1.84	0.75
1:B:306:LYS:HE2	1:B:310:GLU:OE2	1.85	0.75
1:B:123:ASN:HD21	1:B:169:ILE:H	1.32	0.74
1:B:330:ILE:HG12	6:B:2240:HOH:O	1.87	0.74
1:A:290:LYS:HD2	6:A:2128:HOH:O	1.86	0.74
1:B:127:ILE:HG23	6:B:2465:HOH:O	1.87	0.74
1:A:134:ALA:HB3	6:A:2334:HOH:O	1.87	0.73
1:A:4:TRP:NE1	6:A:2144:HOH:O	2.24	0.71
1:B:103:ARG:NH1	6:B:1970:HOH:O	2.20	0.70
1:A:11:ILE:CD1	6:A:2425:HOH:O	2.38	0.70
1:B:359:GLU:C	6:B:2321:HOH:O	2.35	0.69
1:B:153:GLN:HB3	6:B:2485:HOH:O	1.92	0.69
1:B:3:LEU:HD21	6:B:2103:HOH:O	1.93	0.69
1:A:337:ILE:HD13	6:A:2274:HOH:O	1.92	0.68
1:B:41:TYR:HB3	6:B:1953:HOH:O	1.93	0.68
1:A:154:LEU:HD13	6:A:2379:HOH:O	1.94	0.67
1:A:47:GLU:CD	6:A:2425:HOH:O	2.37	0.67
1:B:218:LYS:HD3	1:B:225:HIS:HD2	1.60	0.67
1:B:188:VAL:CG2	6:B:2465:HOH:O	2.43	0.66
1:B:8:LYS:HD2	6:B:2348:HOH:O	1.96	0.66
1:B:154:LEU:HD21	1:B:178:PRO:HG2	1.77	0.66
1:A:204:LEU:HD21	1:A:256:LYS:HD2	1.79	0.65
1:B:236:MET:HE3	1:B:298:HIS:CA	2.28	0.62
1:A:323:TRP:HA	6:A:2193:HOH:O	1.99	0.62
1:A:136:GLY:N	6:A:2334:HOH:O	2.32	0.62
1:A:326:LEU:HB2	6:A:2193:HOH:O	2.00	0.61
1:B:330:ILE:N	6:B:2240:HOH:O	2.33	0.61
1:A:173:LYS:NZ	6:A:2261:HOH:O	2.23	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ILE:HG13	6:B:2091:HOH:O	2.02	0.60
1:A:255:LYS:HB3	1:A:255:LYS:HZ3	1.67	0.59
1:B:40:SER:HA	6:B:2103:HOH:O	2.03	0.59
1:A:32:LYS:CE	6:A:2114:HOH:O	2.51	0.59
1:A:51:GLY:HA2	1:A:54:MET:HE3	1.84	0.58
1:A:154:LEU:HD21	1:A:178:PRO:HG2	1.85	0.58
1:B:30:SER:HA	6:B:2296:HOH:O	2.03	0.58
1:B:127:ILE:HG12	6:B:2465:HOH:O	2.03	0.58
1:B:290:LYS:HD2	6:B:2453:HOH:O	2.04	0.58
1:B:36:ASP:O	6:B:2057:HOH:O	2.17	0.58
1:B:127:ILE:CG2	6:B:2465:HOH:O	2.50	0.57
1:B:65:ARG:HB2	6:B:1980:HOH:O	2.04	0.57
1:A:0:MET:HA	6:A:1972:HOH:O	2.05	0.57
1:A:35:ILE:CG2	6:A:1972:HOH:O	2.52	0.57
1:A:218:LYS:HD3	1:A:225:HIS:HD2	1.70	0.56
1:A:236:MET:HB2	6:A:1986:HOH:O	2.05	0.56
1:B:316:GLY:C	6:B:2479:HOH:O	2.48	0.56
1:A:33:SER:C	6:A:2372:HOH:O	2.47	0.56
1:B:23:GLU:HG3	6:B:2018:HOH:O	2.05	0.56
1:B:28:LEU:HD12	1:B:29:ASP:N	2.20	0.56
1:A:41:TYR:HB2	6:A:2584:HOH:O	2.04	0.55
1:A:177:GLN:CB	6:A:1994:HOH:O	2.54	0.55
1:B:4:TRP:CH2	1:B:32:LYS:HB2	2.42	0.55
1:A:248:GLU:HG2	6:A:2486:HOH:O	2.07	0.55
1:A:255:LYS:NZ	1:A:255:LYS:CB	2.69	0.55
1:B:188:VAL:HG21	6:B:2465:HOH:O	2.06	0.55
1:B:10:PHE:CE1	1:B:54:MET:HE1	2.41	0.54
1:A:27:ARG:NH1	6:A:1914:HOH:O	2.41	0.54
1:B:40:SER:CA	6:B:2103:HOH:O	2.56	0.54
1:B:136:GLY:C	6:B:2301:HOH:O	2.51	0.54
1:A:155:GLY:HA3	6:A:2236:HOH:O	2.07	0.53
1:B:37:LEU:CD1	6:B:2300:HOH:O	2.49	0.53
1:A:20:LYS:HD3	6:A:2392:HOH:O	2.08	0.53
1:A:135:ALA:C	6:A:2416:HOH:O	2.50	0.53
1:A:249:LYS:HB2	6:A:2184:HOH:O	2.08	0.53
1:B:160:ARG:HH11	1:B:160:ARG:HG3	1.73	0.52
2:A:901:HEM:HHB	6:A:1986:HOH:O	2.07	0.52
1:B:10:PHE:HE1	1:B:54:MET:HE1	1.75	0.52
1:B:43:HIS:HD2	1:B:226:TYR:OH	1.91	0.52
1:A:32:LYS:HE3	6:A:2114:HOH:O	2.09	0.52
1:B:91:HIS:O	1:B:95:THR:HG22	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ALA:C	6:A:2334:HOH:O	2.52	0.52
1:B:20:LYS:HE3	6:B:2361:HOH:O	2.10	0.52
2:B:902:HEM:HAC	6:B:2303:HOH:O	2.11	0.51
1:A:180:TRP:NE1	6:A:2236:HOH:O	2.33	0.51
1:B:188:VAL:HG22	6:B:2465:HOH:O	2.07	0.51
1:A:50:HIS:CD2	1:A:54:MET:HE2	2.45	0.51
1:A:334:ALA:HB2	6:A:2230:HOH:O	2.11	0.51
1:B:208:TRP:N	6:B:2333:HOH:O	2.36	0.51
1:B:314:GLU:HB3	6:B:2594:HOH:O	2.10	0.51
1:B:11:ILE:HG21	6:B:2091:HOH:O	2.11	0.50
1:B:82:LYS:HE2	6:B:2269:HOH:O	2.11	0.50
1:A:29:ASP:CG	6:A:2457:HOH:O	2.54	0.50
1:A:154:LEU:CD1	6:A:2379:HOH:O	2.55	0.50
1:A:137:GLU:N	6:A:2416:HOH:O	2.43	0.50
1:B:264:SER:CB	6:B:2120:HOH:O	2.52	0.50
1:A:91:HIS:O	1:A:95:THR:HG22	2.12	0.49
1:A:355:ASP:O	6:A:2232:HOH:O	2.20	0.49
1:B:20:LYS:CE	6:B:2361:HOH:O	2.60	0.49
1:A:236:MET:CB	6:A:1986:HOH:O	2.61	0.49
1:B:23:GLU:CD	6:B:2242:HOH:O	2.55	0.49
1:B:40:SER:C	6:B:2151:HOH:O	2.55	0.49
1:B:317:ARG:HA	6:B:2595:HOH:O	2.12	0.48
1:A:31:ILE:HA	6:A:1914:HOH:O	2.13	0.48
1:B:28:LEU:HA	6:B:2091:HOH:O	2.13	0.48
2:B:902:HEM:HMC2	2:B:902:HEM:HBC2	1.95	0.48
1:B:255:LYS:CE	6:B:2070:HOH:O	2.61	0.48
1:B:22:GLU:C	6:B:2018:HOH:O	2.57	0.48
1:A:20:LYS:NZ	6:A:2392:HOH:O	2.28	0.47
1:A:39:GLY:CA	6:A:2262:HOH:O	2.48	0.47
1:B:171:ARG:NH2	6:B:2538:HOH:O	2.47	0.47
1:A:34:GLU:CD	6:A:2584:HOH:O	2.57	0.47
1:B:218:LYS:HD3	1:B:225:HIS:CD2	2.46	0.47
1:A:29:ASP:HB2	6:A:2001:HOH:O	2.13	0.47
1:B:40:SER:O	6:B:1953:HOH:O	2.21	0.47
1:B:333:ALA:N	6:B:2099:HOH:O	2.47	0.47
1:A:0:MET:CB	6:A:2213:HOH:O	2.62	0.47
1:A:330:ILE:HG13	6:A:2396:HOH:O	2.15	0.47
1:B:20:LYS:O	6:B:2469:HOH:O	2.21	0.46
1:A:318:LYS:HB2	1:A:318:LYS:HZ3	1.80	0.46
1:B:171:ARG:NH1	6:B:2538:HOH:O	2.47	0.46
1:A:177:GLN:C	6:A:1994:HOH:O	2.58	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LYS:CG	6:A:2020:HOH:O	2.64	0.46
1:B:135:ALA:C	6:B:2301:HOH:O	2.58	0.46
1:A:89:LEU:N	6:A:1976:HOH:O	2.49	0.46
1:B:-2:SER:N	6:B:2418:HOH:O	2.46	0.46
1:A:160:ARG:HH11	1:A:160:ARG:HG3	1.81	0.46
1:A:318:LYS:HZ2	1:A:318:LYS:H	1.64	0.46
1:B:173:LYS:NZ	6:B:2076:HOH:O	2.39	0.45
1:A:31:ILE:O	1:A:35:ILE:HG13	2.16	0.45
1:A:255:LYS:CB	1:A:255:LYS:HZ2	2.29	0.45
1:A:8:LYS:HD3	6:A:2144:HOH:O	2.15	0.45
1:A:177:GLN:HB2	6:A:1994:HOH:O	2.16	0.45
1:A:334:ALA:CB	6:A:2230:HOH:O	2.65	0.45
1:B:40:SER:C	6:B:1953:HOH:O	2.60	0.45
1:B:309:GLU:OE2	1:B:342:TYR:OH	2.31	0.45
1:B:291:GLN:HB2	6:B:2253:HOH:O	2.17	0.45
1:A:29:ASP:CB	6:A:2001:HOH:O	2.65	0.44
1:A:275:GLN:NE2	6:A:2125:HOH:O	2.34	0.44
1:A:330:ILE:HG21	6:A:2396:HOH:O	2.16	0.44
1:A:109:PHE:CZ	6:A:1976:HOH:O	2.48	0.44
1:A:31:ILE:CG1	6:A:1914:HOH:O	2.54	0.44
1:B:160:ARG:HG3	1:B:160:ARG:NH1	2.32	0.44
1:B:154:LEU:CD2	1:B:178:PRO:HG2	2.45	0.44
1:A:50:HIS:HD2	1:A:54:MET:HE2	1.82	0.43
1:B:15:TYR:HD2	6:B:2469:HOH:O	2.01	0.43
1:B:128:ARG:NE	6:B:2313:HOH:O	2.29	0.43
1:B:183:LEU:HA	1:B:184:PRO:HD3	1.92	0.43
2:B:902:HEM:HHD	6:B:2303:HOH:O	2.18	0.43
1:A:204:LEU:CD2	1:A:256:LYS:HD2	2.46	0.43
1:B:29:ASP:C	6:B:2446:HOH:O	2.60	0.43
1:B:40:SER:N	6:B:2103:HOH:O	2.51	0.43
1:B:28:LEU:CA	6:B:2091:HOH:O	2.67	0.43
1:A:125:GLN:HA	1:A:213:ILE:O	2.19	0.43
1:A:183:LEU:HA	1:A:184:PRO:HD3	1.91	0.43
1:B:23:GLU:N	6:B:2018:HOH:O	2.52	0.43
1:B:30:SER:N	6:B:2446:HOH:O	2.51	0.43
1:B:318:LYS:HG3	1:B:319:LEU:N	2.33	0.43
1:B:72:ASN:ND2	6:B:2318:HOH:O	2.35	0.42
1:A:356:LYS:CE	6:A:2020:HOH:O	2.66	0.42
1:B:299:HIS:HD2	6:B:1969:HOH:O	2.02	0.42
1:B:-2:SER:CA	6:B:2418:HOH:O	2.67	0.42
1:A:0:MET:CB	6:A:1972:HOH:O	2.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:LEU:HD13	6:B:2485:HOH:O	2.18	0.42
1:A:331:SER:C	6:A:1981:HOH:O	2.62	0.42
1:B:10:PHE:HE1	1:B:54:MET:CE	2.32	0.42
1:A:10:PHE:CE1	1:A:54:MET:HE1	2.55	0.42
1:A:0:MET:CA	6:A:1972:HOH:O	2.64	0.41
1:A:27:ARG:NH1	6:A:2006:HOH:O	2.53	0.41
1:A:136:GLY:C	6:A:2416:HOH:O	2.62	0.41
1:A:249:LYS:HD3	6:A:2287:HOH:O	2.19	0.41
1:B:25:LYS:HA	1:B:28:LEU:HD11	2.02	0.41
1:B:214:ILE:HG13	3:B:2903:NO:N	2.33	0.41
1:B:29:ASP:CB	6:B:2456:HOH:O	2.69	0.41
1:A:16:GLN:CB	6:A:2086:HOH:O	2.69	0.41
1:B:21:GLU:CB	6:B:1991:HOH:O	2.68	0.41
1:B:236:MET:HE3	1:B:298:HIS:HA	2.02	0.41
1:A:4:TRP:CH2	6:A:2389:HOH:O	2.73	0.41
1:A:299:HIS:HD2	6:A:1924:HOH:O	2.03	0.41
1:B:25:LYS:C	1:B:28:LEU:HD11	2.45	0.41
1:A:136:GLY:CA	6:A:2334:HOH:O	2.67	0.41
1:B:51:GLY:HA2	1:B:54:MET:HE3	2.03	0.41
1:B:30:SER:CA	6:B:2296:HOH:O	2.64	0.40
1:B:245:LEU:HA	1:B:251:TYR:HB2	2.03	0.40
1:B:40:SER:CB	6:B:2151:HOH:O	2.68	0.40
1:B:356:LYS:CG	6:B:1949:HOH:O	2.69	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	360/363 (99%)	340 (94%)	20 (6%)	0	100	100
1	B	360/363 (99%)	340 (94%)	20 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	720/726 (99%)	680 (94%)	40 (6%)	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	308/314 (98%)	303 (98%)	5 (2%)	55	71
1	B	308/314 (98%)	305 (99%)	3 (1%)	68	81
All	All	616/628 (98%)	608 (99%)	8 (1%)	61	76

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	187	LEU
1	A	255	LYS
1	A	256	LYS
1	A	318	LYS
1	B	22	GLU
1	B	306	LYS
1	B	318	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	50	HIS
1	A	72	ASN
1	A	92	HIS
1	A	123	ASN
1	A	225	HIS
1	A	281	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	291	GLN
1	A	311	GLN
1	A	339	HIS
1	B	43	HIS
1	B	123	ASN
1	B	125	GLN
1	B	225	HIS
1	B	291	GLN
1	B	299	HIS
1	B	311	GLN
1	B	339	HIS

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](#)

9 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	NO	B	2903	-	0,1,1	-	-	-		
4	HBI	A	903	-	15,18,18	3.18	4 (26%)	14,26,26	1.84	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HBI	B	904	-	15,18,18	3.14	4 (26%)	14,26,26	1.71	3 (21%)
5	HAR	A	909	-	9,12,12	1.19	1 (11%)	10,14,14	7.55	6 (60%)
3	NO	A	1901	2	0,1,1	-	-	-	-	-
2	HEM	B	902	1,3	50,50,50	2.00	21 (42%)	67,82,82	1.49	10 (14%)
2	HEM	A	901	1,3	50,50,50	1.55	10 (20%)	67,82,82	1.52	13 (19%)
3	NO	B	1902	2	0,1,1	-	-	-	-	-
5	HAR	A	910	-	9,12,12	1.20	1 (11%)	10,14,14	9.10	5 (50%)

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
4	HBI	A	903	-	-	4/4/17/17	0/2/2/2
4	HBI	B	904	-	-	0/4/17/17	0/2/2/2
5	HAR	A	909	-	-	1/11/13/13	-
2	HEM	B	902	1,3	-	4/14/54/54	-
2	HEM	A	901	1,3	-	1/14/54/54	-
5	HAR	A	910	-	-	0/11/13/13	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	904	HBI	C6-N5	10.32	1.45	1.28
4	A	903	HBI	C6-N5	10.12	1.44	1.28
4	A	903	HBI	C7-N8	-4.45	1.38	1.45
2	B	902	HEM	CMB-C2B	4.33	1.59	1.50
4	B	904	HBI	C7-N8	-4.27	1.39	1.45
2	B	902	HEM	FE-ND	3.87	2.06	1.94
2	B	902	HEM	C4B-NB	3.73	1.46	1.38
4	A	903	HBI	C7-C6	-3.32	1.46	1.49
2	A	901	HEM	CAA-C2A	3.23	1.59	1.51
2	A	901	HEM	CMB-C2B	3.21	1.57	1.50
2	B	902	HEM	CMA-C3A	3.16	1.57	1.50
2	A	901	HEM	CHD-C4C	3.13	1.44	1.38
2	B	902	HEM	C1A-NA	-3.05	1.33	1.39
2	B	902	HEM	C3C-C2C	2.96	1.43	1.37
2	B	902	HEM	CMC-C2C	2.95	1.56	1.50
5	A	910	HAR	OH1-NH1	-2.87	1.33	1.40
4	B	904	HBI	C4-N3	-2.84	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	HEM	CAD-C3D	2.81	1.58	1.51
2	B	902	HEM	C4D-C3D	2.80	1.49	1.45
4	A	903	HBI	C4-N3	-2.78	1.33	1.38
5	A	909	HAR	OH1-NH1	-2.77	1.33	1.40
2	A	901	HEM	C1C-C2C	-2.65	1.40	1.45
2	A	901	HEM	CMD-C2D	2.64	1.56	1.50
2	B	902	HEM	CAD-C3D	2.53	1.57	1.51
2	B	902	HEM	FE-NA	2.48	2.03	1.95
2	B	902	HEM	C3B-C4B	2.47	1.49	1.44
2	B	902	HEM	CBB-CAB	2.47	1.42	1.30
2	B	902	HEM	CHC-C1C	-2.47	1.33	1.38
2	B	902	HEM	FE-NC	2.44	2.03	1.95
2	B	902	HEM	CHD-C4C	2.43	1.43	1.38
2	A	901	HEM	C1D-C2D	2.39	1.49	1.44
2	A	901	HEM	CBB-CAB	2.37	1.41	1.30
2	B	902	HEM	C1B-NB	2.35	1.44	1.40
2	B	902	HEM	CBC-CAC	2.35	1.41	1.30
2	B	902	HEM	CMD-C2D	2.34	1.55	1.50
2	A	901	HEM	CAB-C3B	-2.23	1.41	1.47
2	B	902	HEM	CHA-C4D	2.22	1.42	1.38
2	A	901	HEM	CMA-C3A	2.20	1.55	1.50
4	B	904	HBI	C7-C6	-2.19	1.47	1.49
2	B	902	HEM	O2A-CGA	-2.14	1.23	1.30
2	B	902	HEM	FE-NB	2.09	2.01	1.94

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	910	HAR	CD-NE-CZ	22.18	164.13	123.46
5	A	909	HAR	CD-NE-CZ	17.22	155.03	123.46
5	A	910	HAR	CG-CD-NE	12.60	147.53	112.20
5	A	909	HAR	NE-CZ-NH1	-10.72	92.26	116.80
5	A	909	HAR	NH1-CZ-NH2	9.30	141.38	120.15
5	A	910	HAR	NH1-CZ-NH2	8.89	140.45	120.15
5	A	910	HAR	NE-CZ-NH1	-8.73	96.81	116.80
5	A	909	HAR	CG-CD-NE	7.08	132.05	112.20
2	B	902	HEM	C4A-C3A-C2A	-5.05	101.04	106.82
2	A	901	HEM	CMD-C2D-C1D	4.05	131.36	125.03
4	A	903	HBI	C2-N1-C8A	3.71	119.90	113.36
2	A	901	HEM	CMB-C2B-C1B	3.60	130.66	125.03
5	A	910	HAR	CB-CG-CD	-3.55	101.83	112.07
2	B	902	HEM	C1A-C2A-C3A	3.50	112.28	106.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	903	HBI	O4-C4-C4A	-3.44	117.45	126.53
4	B	904	HBI	O4-C4-C4A	-3.41	117.53	126.53
5	A	909	HAR	NE-CZ-NH2	3.31	126.36	120.26
2	A	901	HEM	CMB-C2B-C3B	-3.20	120.68	128.43
2	B	902	HEM	CAD-C3D-C4D	3.09	130.08	124.70
5	A	909	HAR	CG-CB-CA	3.03	123.02	113.22
2	B	902	HEM	CAB-C3B-C2B	-3.01	118.65	128.43
4	B	904	HBI	C2-N1-C8A	2.97	118.61	113.36
2	A	901	HEM	CHC-C1C-NC	-2.72	121.49	124.45
2	A	901	HEM	CAB-C3B-C2B	-2.72	119.59	128.43
2	A	901	HEM	CHA-C4D-C3D	-2.68	120.28	125.23
2	A	901	HEM	CAA-C2A-C1A	2.53	129.89	124.94
2	B	902	HEM	CHB-C4A-C3A	-2.52	120.12	127.43
2	A	901	HEM	C3B-C2B-C1B	2.46	108.26	106.41
4	A	903	HBI	C4A-C4-N3	2.38	119.32	113.25
2	A	901	HEM	C3D-C4D-ND	2.30	112.69	110.17
2	B	902	HEM	CHA-C4D-ND	-2.25	121.58	124.37
4	B	904	HBI	C4A-C4-N3	2.25	118.98	113.25
2	A	901	HEM	CAB-C3B-C4B	2.24	134.29	124.39
4	A	903	HBI	C2-N3-C4	-2.21	121.10	125.11
2	A	901	HEM	O2A-CGA-CBA	2.18	120.89	114.00
2	B	902	HEM	CMA-C3A-C4A	2.18	128.73	125.42
2	B	902	HEM	CAB-C3B-C4B	2.13	133.78	124.39
2	B	902	HEM	CHD-C1D-ND	-2.12	122.14	124.42
2	A	901	HEM	O2D-CGD-CBD	2.09	120.60	114.00
2	A	901	HEM	CHA-C4D-ND	2.09	126.95	124.37
2	B	902	HEM	CMB-C2B-C3B	-2.02	123.55	128.43

There are no chirality outliers.

All (10) torsion outliers are listed below:

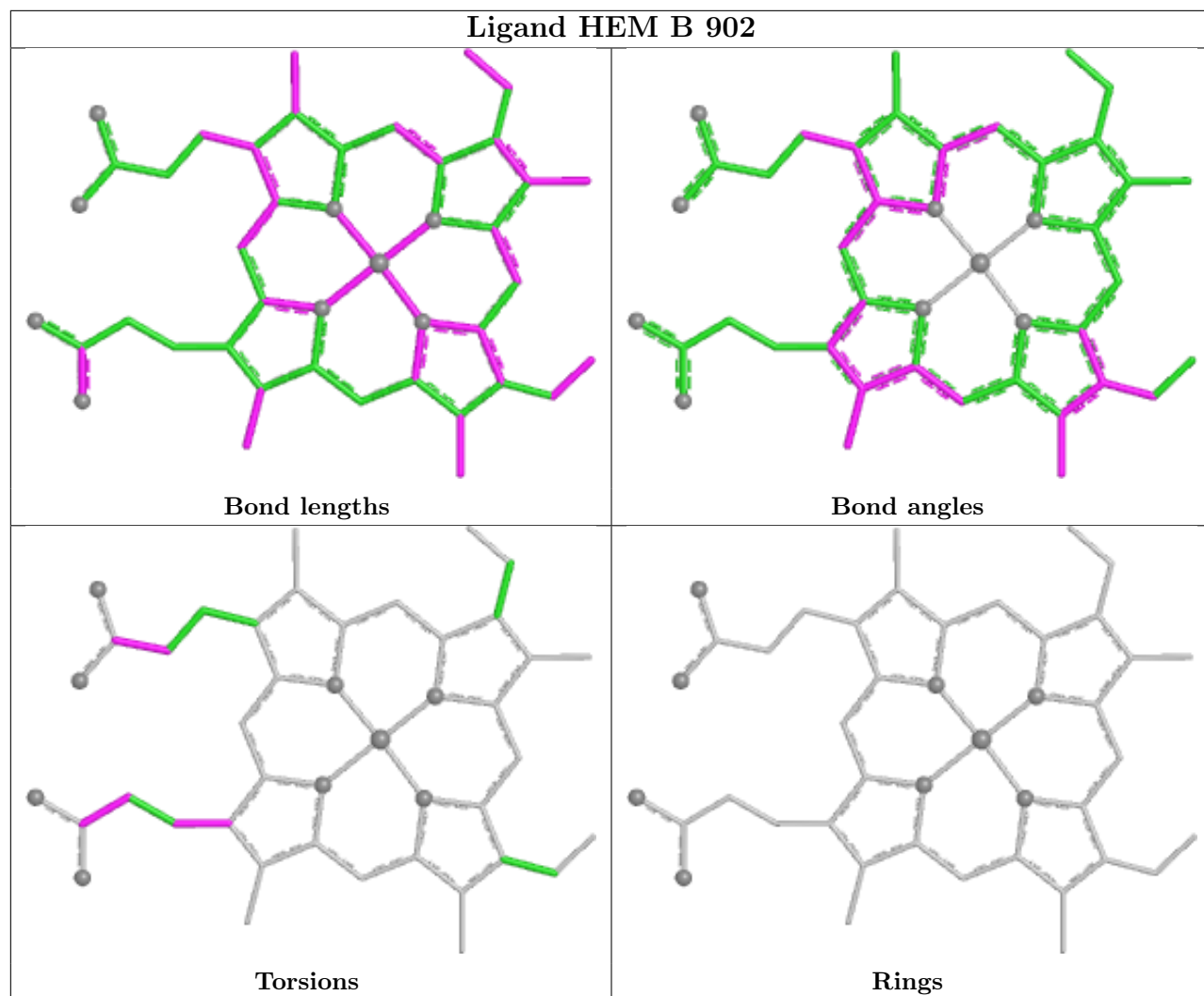
Mol	Chain	Res	Type	Atoms
4	A	903	HBI	O10-C10-C9-C6
4	A	903	HBI	C11-C10-C9-C6
4	A	903	HBI	O10-C10-C9-O9
4	A	903	HBI	C11-C10-C9-O9
5	A	909	HAR	O-C-CA-N
2	B	902	HEM	C1A-C2A-CAA-CBA
2	B	902	HEM	CAA-CBA-CGA-O1A
2	B	902	HEM	CAA-CBA-CGA-O2A
2	A	901	HEM	CAD-CBD-CGD-O2D
2	B	902	HEM	CAD-CBD-CGD-O2D

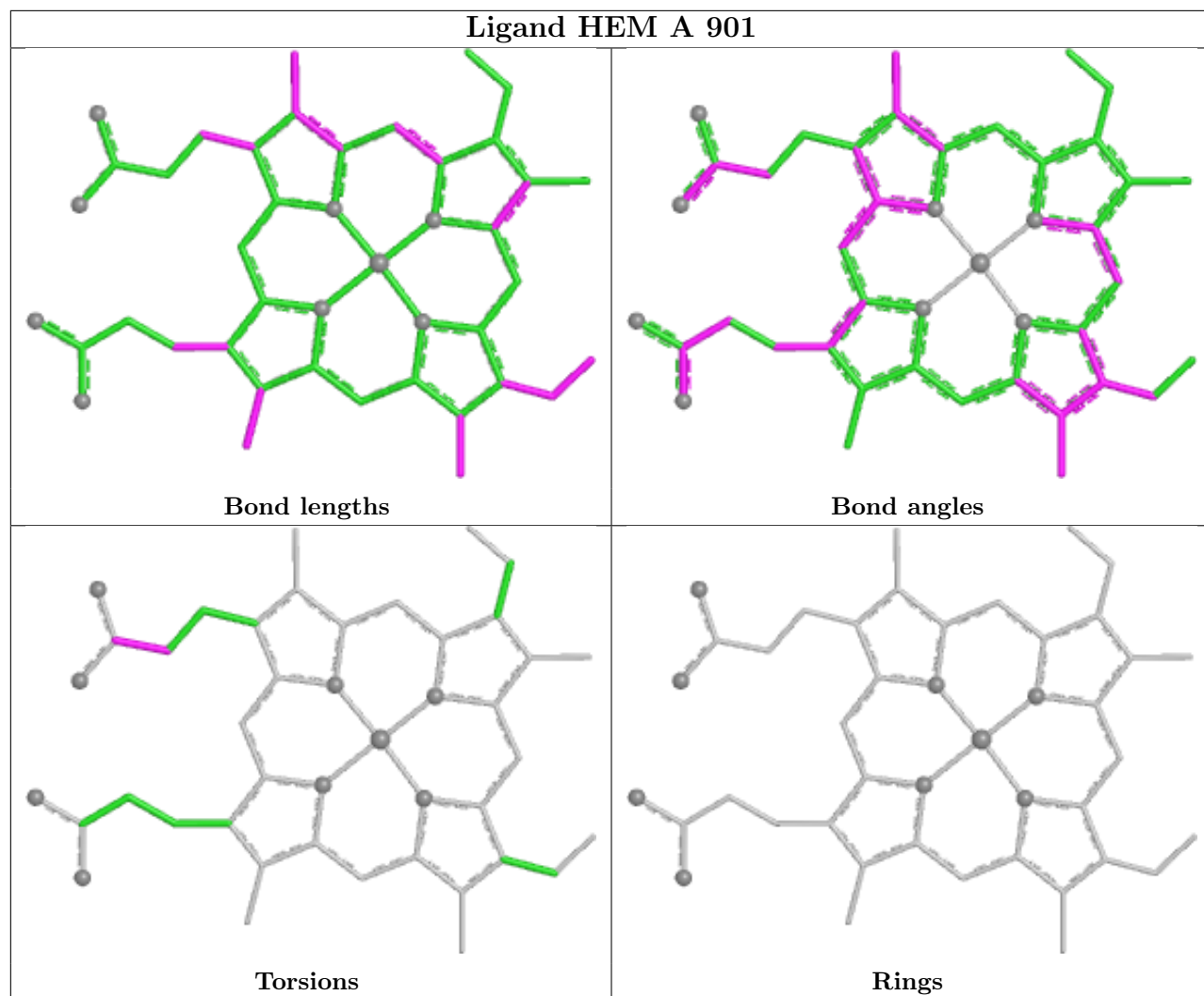
There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2903	NO	2	0
2	B	902	HEM	3	0
2	A	901	HEM	1	0
3	B	1902	NO	1	0
5	A	910	HAR	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.