



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:08 AM UTC

PDB ID : 2NSE / pdb_00002nse
Title : BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE SUBSTRATE COMPLEX
Authors : Raman, C.S.; Li, H.; Martasek, P.; Kral, V.; Masters, B.S.S.; Poulos, T.L.
Deposited on : 1998-08-13
Resolution : 2.34 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

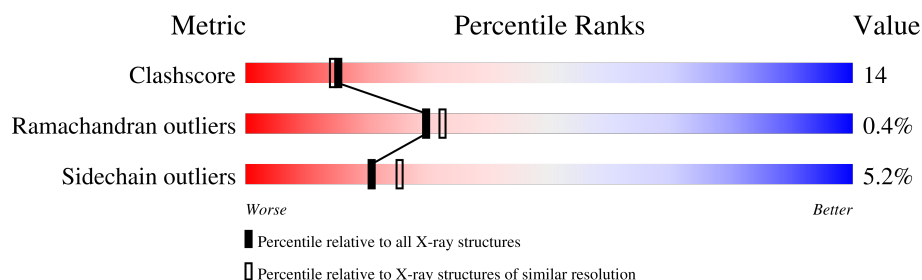
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)

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	444	 62% 28% • 6%
1	B	444	 67% 23% • 7%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7007 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.

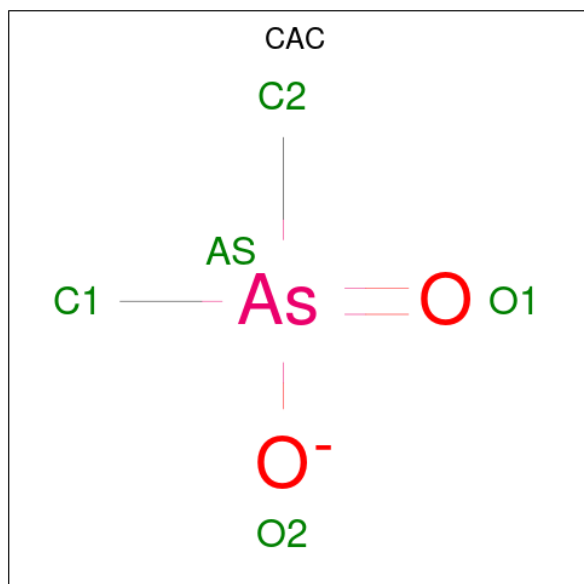
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3302	2099	584	603	16			
1	B	414	Total	C	N	O	S	0	0	0
			3291	2092	582	601	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	conflict	UNP P29473
B	100	ARG	CYS	conflict	UNP P29473

- Molecule 2 is CACODYLATE ION (CCD ID: CAC) (formula: $\text{C}_2\text{H}_6\text{AsO}_2$).



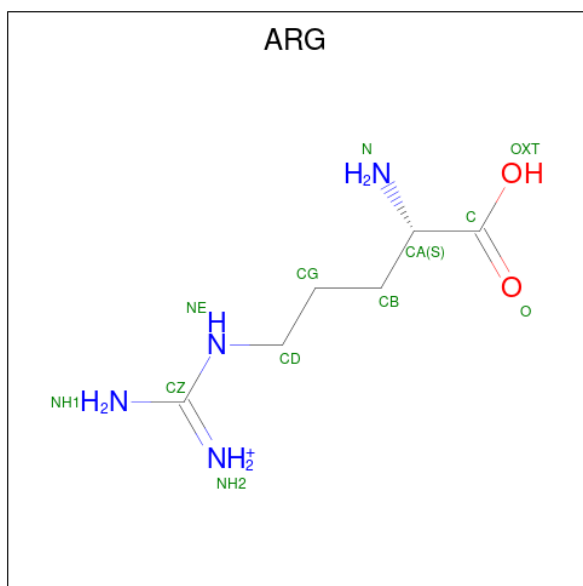
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	As	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	As	0	0
			1	1		

- Molecule 3 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



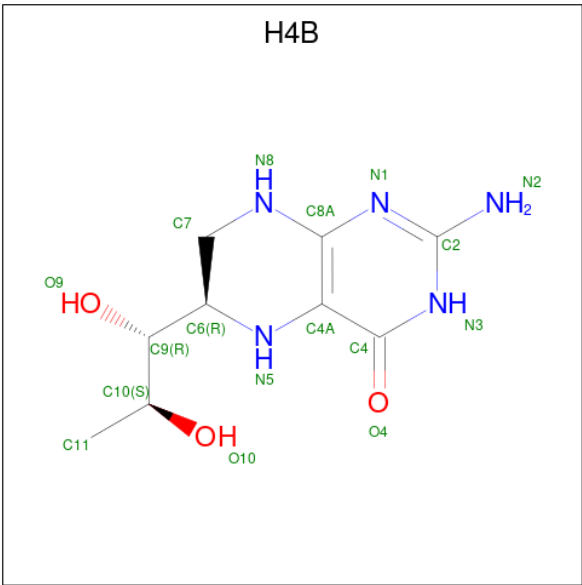
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	6	4	2		
3	B	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 5 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $C_9H_{15}N_5O_3$).

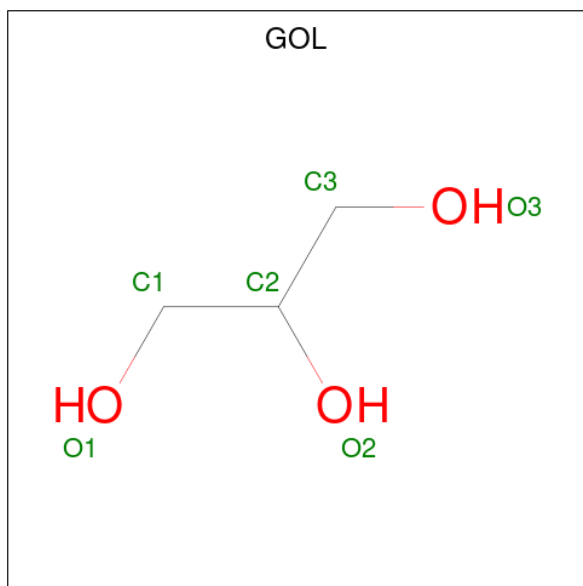


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			17	9	5	3		
5	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Zn	0	0
			1	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is water.

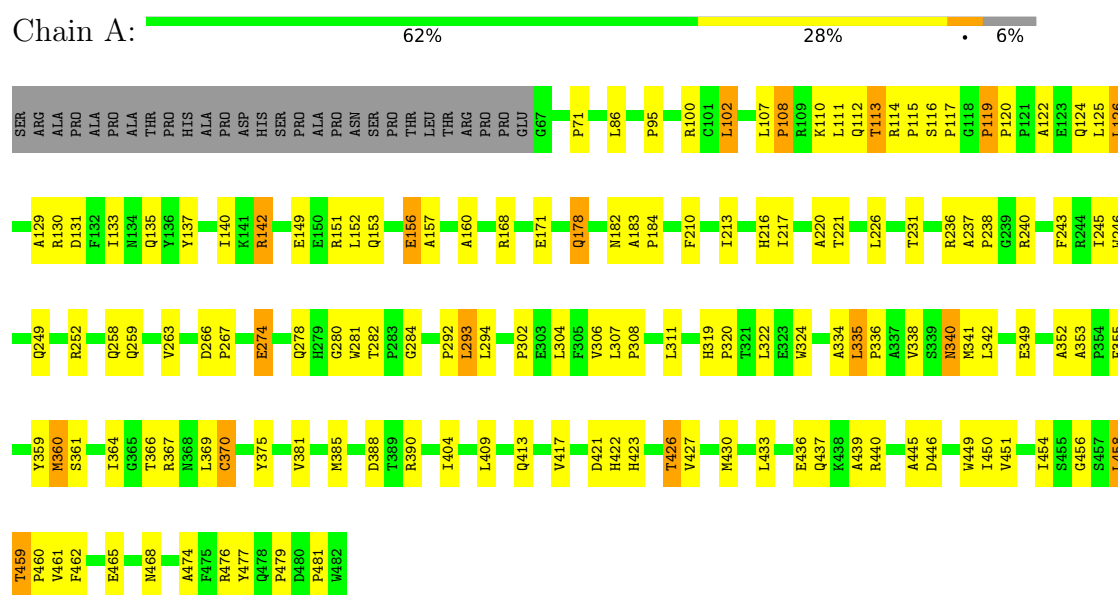
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	149	Total	O	0	0
			149	149		
8	B	112	Total	O	0	0
			112	112		

3 Residue-property plots

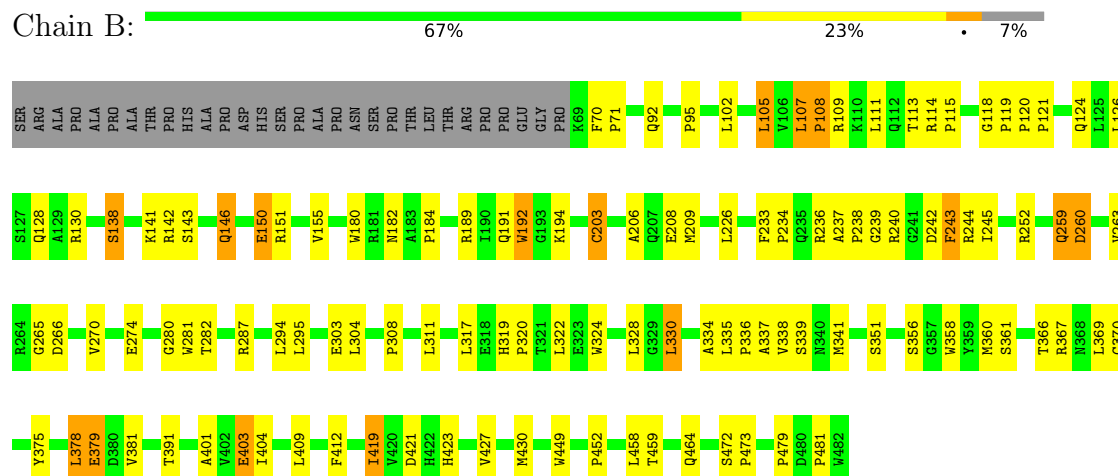
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 21	Depositor
Cell constants a, b, c, α , β , γ	58.06Å 106.38Å 156.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.34	Depositor
% Data completeness (in resolution range)	96.2 (30.00-2.34)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.216 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7007	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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, H4B, GOL, ZN, CAC

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	0.54	1/3397 (0.0%)	1.05	21/4631 (0.5%)
1	B	0.50	0/3385	1.03	22/4614 (0.5%)
All	All	0.52	1/6782 (0.0%)	1.04	43/9245 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	PRO	CA-C	6.28	1.55	1.51

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	PRO	N-CA-C	-7.89	98.59	111.77
1	B	452	PRO	CA-C-N	7.30	126.97	119.82
1	B	452	PRO	C-N-CA	7.30	126.97	119.82
1	A	360	MET	N-CA-C	-7.05	97.72	109.07
1	A	258	GLN	N-CA-C	6.94	119.28	110.33
1	B	280	GLY	N-CA-C	6.84	125.44	114.90
1	B	360	MET	N-CA-C	-6.79	98.62	109.76
1	B	118	GLY	CA-C-N	6.76	124.60	119.66
1	B	118	GLY	C-N-CA	6.76	124.60	119.66
1	A	284	GLY	N-CA-C	-6.71	102.88	112.55
1	A	439	ALA	N-CA-C	6.59	119.44	111.40
1	B	243	PHE	N-CA-C	-6.37	99.50	109.25
1	A	370	CYS	N-CA-C	6.29	121.02	113.23
1	A	183	ALA	CA-C-N	6.22	125.95	119.05
1	A	183	ALA	C-N-CA	6.22	125.95	119.05
1	A	266	ASP	CA-C-N	6.20	126.10	119.28
1	A	266	ASP	C-N-CA	6.20	126.10	119.28
1	A	280	GLY	N-CA-C	6.11	124.04	115.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	LEU	N-CA-C	5.90	119.31	108.69
1	A	282	THR	CA-C-N	5.89	125.80	119.85
1	A	282	THR	C-N-CA	5.89	125.80	119.85
1	A	474	ALA	N-CA-C	5.73	117.22	108.52
1	B	282	THR	CA-C-N	5.65	125.55	119.85
1	B	282	THR	C-N-CA	5.65	125.55	119.85
1	B	459	THR	CA-C-N	5.63	126.00	119.47
1	B	459	THR	C-N-CA	5.63	126.00	119.47
1	B	245	ILE	N-CA-C	-5.61	99.67	107.80
1	A	458	LEU	N-CA-C	-5.53	106.49	113.18
1	A	437	GLN	N-CA-C	-5.51	104.91	111.03
1	B	150	GLU	N-CA-C	-5.49	104.94	111.69
1	B	237	ALA	CA-C-N	5.47	125.18	119.82
1	B	237	ALA	C-N-CA	5.47	125.18	119.82
1	B	339	SER	N-CA-C	5.42	119.45	112.41
1	B	192	TRP	N-CA-C	5.34	117.85	111.71
1	B	108	PRO	N-CA-C	-5.31	103.50	111.57
1	B	107	LEU	N-CA-C	5.29	121.51	109.81
1	A	308	PRO	CA-C-N	5.29	125.60	119.47
1	A	308	PRO	C-N-CA	5.29	125.60	119.47
1	B	266	ASP	CA-C-N	5.28	124.94	119.56
1	B	266	ASP	C-N-CA	5.28	124.94	119.56
1	B	335	LEU	N-CA-C	5.18	117.81	109.15
1	A	245	ILE	N-CA-C	-5.14	99.76	107.37
1	A	117	PRO	N-CA-C	-5.06	108.90	114.92

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	3302	0	3215	107	0
1	B	3291	0	3205	78	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	12	1	0
3	B	12	0	12	0	0
4	A	43	0	30	1	0
4	B	43	0	30	2	0
5	A	17	0	15	2	0
5	B	17	0	15	2	0
6	B	1	0	0	0	0
7	B	6	0	8	0	0
8	A	149	0	0	0	0
8	B	112	0	0	3	0
All	All	7007	0	6542	181	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 14.

All (181) 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:114:ARG:HG3	1:A:115:PRO:HD2	1.43	0.97
1:A:120:PRO:HG2	1:A:125:LEU:HD12	1.42	0.97
1:B:114:ARG:HD3	1:B:479:PRO:HG3	1.47	0.93
1:A:115:PRO:HD3	1:A:479:PRO:HG2	1.49	0.92
1:A:430:MET:HE3	1:A:461:VAL:HG12	1.51	0.91
1:A:113:THR:HG21	1:A:476:ARG:HH11	1.35	0.89
1:B:114:ARG:HD3	1:B:479:PRO:CG	2.05	0.85
1:B:209:MET:HE3	1:B:295:LEU:HB3	1.57	0.85
1:A:113:THR:CG2	1:A:476:ARG:HH11	1.91	0.83
1:B:409:LEU:HD23	1:B:419:ILE:HD12	1.61	0.82
1:B:111:LEU:HD23	8:B:1051:HOH:O	1.82	0.79
1:A:116:SER:H	1:A:236:ARG:HH22	1.31	0.78
1:B:115:PRO:HD3	1:B:479:PRO:HG2	1.69	0.74
1:A:422:HIS:O	1:A:426:THR:HB	1.88	0.73
1:A:237:ALA:HB3	1:A:240:ARG:HD3	1.71	0.72
1:A:459:THR:CG2	1:A:461:VAL:HG22	2.22	0.70
1:A:95:PRO:HA	1:A:110:LYS:HG3	1.74	0.69
1:A:116:SER:H	1:A:236:ARG:NH2	1.91	0.68
1:A:114:ARG:HG3	1:A:115:PRO:CD	2.22	0.67
1:A:426:THR:HG21	1:A:459:THR:HG23	1.77	0.67
1:B:265:GLY:H	1:B:287:ARG:HG2	1.61	0.66
1:A:111:LEU:O	1:A:111:LEU:HG	1.96	0.66
1:B:361:SER:OG	1:B:421:ASP:HA	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLN:HE21	1:A:178:GLN:HA	1.62	0.65
1:A:340:ASN:H	1:A:340:ASN:HD22	1.45	0.64
1:B:308:PRO:HD2	1:B:311:LEU:HD12	1.79	0.63
1:A:116:SER:N	1:A:236:ARG:HH22	1.98	0.62
1:A:126:LEU:HB3	1:A:130:ARG:HH21	1.63	0.62
1:B:341:MET:HE1	4:B:500:HEM:HBD2	1.80	0.62
1:A:113:THR:OG1	1:A:476:ARG:HD3	2.00	0.61
1:B:95:PRO:HB3	1:B:108:PRO:HG2	1.83	0.61
1:B:111:LEU:HD21	8:B:1006:HOH:O	2.01	0.60
1:B:366:THR:O	1:B:370:CYS:HB2	2.02	0.60
1:A:430:MET:HE2	1:A:433:LEU:HD12	1.82	0.60
1:A:342:LEU:HD11	1:A:349:GLU:HB3	1.83	0.59
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.84	0.59
3:A:700:ARG:HG3	4:A:500:HEM:HBA1	1.84	0.58
1:A:102:LEU:HD21	1:B:71:PRO:HB3	1.85	0.58
1:A:409:LEU:O	1:A:413:GLN:HG3	2.04	0.57
1:A:178:GLN:HA	1:A:178:GLN:NE2	2.19	0.57
1:B:124:GLN:HG2	1:B:128:GLN:HE21	1.69	0.57
1:B:114:ARG:HD3	1:B:479:PRO:HG2	1.88	0.56
1:B:119:PRO:HG3	1:B:238:PRO:HB2	1.88	0.56
1:B:191:GLN:HE22	1:B:194:LYS:HD3	1.71	0.56
1:A:231:THR:O	1:A:353:ALA:HA	2.05	0.56
1:B:412:PHE:HB2	1:B:419:ILE:HD13	1.87	0.55
1:B:124:GLN:HG2	1:B:128:GLN:NE2	2.22	0.55
1:B:367:ARG:HH12	5:B:600:H4B:C4	2.19	0.55
1:A:274:GLU:HG2	1:A:278:GLN:HE21	1.72	0.55
1:B:449:TRP:HA	5:B:600:H4B:N1	2.22	0.54
1:A:111:LEU:HD23	1:A:477:TYR:CE2	2.43	0.54
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.43	0.54
1:B:378:LEU:HB2	8:B:1047:HOH:O	2.08	0.54
1:A:126:LEU:HB3	1:A:130:ARG:NH2	2.23	0.54
1:A:249:GLN:HB2	1:A:252:ARG:HG2	1.90	0.54
1:B:244:ARG:NH2	1:B:481:PRO:HD3	2.22	0.54
1:A:426:THR:CG2	1:A:459:THR:HG23	2.39	0.53
1:B:182:ASN:O	1:B:184:PRO:HD3	2.10	0.52
1:A:126:LEU:O	1:A:130:ARG:HG3	2.09	0.52
1:A:86:LEU:HD22	1:A:440:ARG:HB2	1.91	0.52
1:A:249:GLN:HB2	1:A:252:ARG:HD3	1.92	0.51
1:A:178:GLN:HE21	1:A:178:GLN:CA	2.24	0.51
1:B:379:GLU:H	1:B:379:GLU:CD	2.17	0.51
1:A:100:ARG:HH11	1:A:100:ARG:HG3	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:THR:CG2	1:A:476:ARG:HD3	2.41	0.51
1:A:436:GLU:OE1	1:A:440:ARG:HD2	2.11	0.51
1:B:209:MET:CE	1:B:295:LEU:HB3	2.37	0.50
1:B:423:HIS:O	1:B:427:VAL:HG23	2.11	0.50
1:A:341:MET:HE3	1:A:355:PHE:HZ	1.77	0.50
1:B:236:ARG:HD2	1:B:242:ASP:CG	2.36	0.50
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.52	0.50
1:B:259:GLN:HG3	1:B:260:ASP:H	1.75	0.50
1:A:221:THR:HA	1:A:226:LEU:HD13	1.93	0.50
1:B:206:ALA:HB3	1:B:303:GLU:OE2	2.11	0.49
1:B:430:MET:HE1	1:B:464:GLN:OE1	2.12	0.49
1:A:220:ALA:O	1:A:226:LEU:HA	2.13	0.49
1:A:71:PRO:HB3	1:B:102:LEU:HD21	1.94	0.49
1:A:423:HIS:O	1:A:427:VAL:HG23	2.12	0.49
1:A:445:ALA:O	1:A:468:ASN:HB2	2.11	0.49
1:B:126:LEU:O	1:B:130:ARG:HG3	2.13	0.49
1:A:129:ALA:O	1:A:133:ILE:HG12	2.12	0.49
1:A:292:PRO:HB3	1:A:306:VAL:HG22	1.95	0.48
1:A:182:ASN:O	1:A:184:PRO:HD3	2.13	0.48
1:A:459:THR:HG22	1:A:461:VAL:HG22	1.95	0.48
1:A:359:TYR:CD2	1:A:364:ILE:HD11	2.48	0.48
1:A:151:ARG:HD3	1:A:168:ARG:NH2	2.28	0.48
1:A:430:MET:CE	1:A:433:LEU:HD12	2.44	0.48
1:A:113:THR:OG1	1:A:476:ARG:CD	2.62	0.48
1:A:168:ARG:HB2	1:A:171:GLU:HG3	1.94	0.48
1:A:149:GLU:O	1:A:153:GLN:HG3	2.14	0.48
1:A:381:VAL:O	1:A:385:MET:HG3	2.13	0.48
1:A:446:ASP:O	1:A:450:ILE:HG12	2.13	0.48
1:A:108:PRO:C	1:A:110:LYS:H	2.22	0.48
1:A:213:ILE:O	1:A:217:ILE:HG13	2.13	0.48
1:B:234:PRO:HB2	1:B:243:PHE:CE2	2.49	0.47
1:B:236:ARG:HD2	1:B:242:ASP:OD1	2.14	0.47
1:A:334:ALA:HB1	1:A:417:VAL:HG11	1.96	0.47
1:B:412:PHE:CD2	1:B:419:ILE:HG23	2.49	0.47
1:A:112:GLN:OE1	1:A:114:ARG:NH2	2.47	0.47
1:A:114:ARG:CG	1:A:115:PRO:HD2	2.31	0.47
1:A:131:ASP:O	1:A:135:GLN:HG3	2.15	0.47
1:A:451:VAL:HG22	1:A:461:VAL:HG23	1.97	0.47
1:B:281:TRP:HB2	1:B:304:LEU:HD11	1.96	0.47
1:B:287:ARG:HH12	1:B:375:TYR:HA	1.80	0.47
1:B:381:VAL:HG21	1:B:404:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ALA:H	1:A:240:ARG:NH1	2.12	0.46
1:B:206:ALA:HA	1:B:209:MET:HE2	1.97	0.46
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.50	0.46
1:B:226:LEU:HD21	1:B:334:ALA:O	2.15	0.46
1:B:191:GLN:NE2	1:B:194:LYS:HD3	2.31	0.46
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.45	0.46
1:A:369:LEU:HA	1:A:375:TYR:HB2	1.98	0.46
1:B:138:SER:HA	1:B:143:SER:HB2	1.98	0.46
1:A:334:ALA:CB	1:A:417:VAL:HG11	2.46	0.45
1:B:319:HIS:NE2	1:B:403:GLU:HG3	2.31	0.45
1:B:412:PHE:HB2	1:B:419:ILE:CD1	2.45	0.45
1:A:120:PRO:CG	1:A:125:LEU:HD12	2.31	0.45
1:A:281:TRP:HB2	1:A:304:LEU:HD11	1.99	0.45
1:B:180:TRP:O	1:B:189:ARG:HD3	2.17	0.45
1:A:449:TRP:HA	5:A:600:H4B:N1	2.32	0.45
1:A:113:THR:CG2	1:A:476:ARG:NH1	2.72	0.45
1:B:338:VAL:HG11	1:B:341:MET:HE3	1.99	0.45
1:A:388:ASP:OD1	1:A:390:ARG:HB2	2.17	0.45
1:B:234:PRO:HB2	1:B:243:PHE:CD2	2.51	0.45
1:A:137:TYR:HA	1:A:140:ILE:HG12	1.98	0.45
1:A:338:VAL:HG11	1:A:341:MET:HE3	1.98	0.45
1:B:203:CYS:SG	1:B:208:GLU:HB3	2.57	0.45
1:A:122:ALA:O	1:A:126:LEU:HB2	2.17	0.44
1:B:265:GLY:HA2	1:B:287:ARG:HA	1.98	0.44
1:B:369:LEU:HA	1:B:375:TYR:HB2	2.00	0.44
1:A:361:SER:OG	1:A:421:ASP:HA	2.16	0.44
1:A:456:GLY:O	1:A:462:PHE:HB2	2.17	0.44
1:B:146:GLN:O	1:B:150:GLU:HB2	2.17	0.44
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.53	0.44
1:A:246:TRP:CE2	1:A:481:PRO:HB2	2.53	0.44
1:A:210:PHE:HE1	1:A:307:LEU:HD23	1.83	0.43
1:A:226:LEU:H	1:A:226:LEU:CD2	2.31	0.43
1:A:366:THR:HG21	1:A:454:ILE:HG23	2.00	0.43
1:B:239:GLY:O	1:B:240:ARG:HB3	2.17	0.43
1:A:100:ARG:HG3	1:A:100:ARG:NH1	2.34	0.43
1:A:458:LEU:HG	1:B:378:LEU:HD21	2.00	0.43
1:A:249:GLN:HB2	1:A:252:ARG:CG	2.49	0.43
1:B:95:PRO:CB	1:B:108:PRO:HG2	2.47	0.43
1:B:328:LEU:HB3	1:B:330:LEU:HD13	2.01	0.43
1:A:367:ARG:HH12	5:A:600:H4B:C4	2.31	0.43
1:B:472:SER:HA	1:B:473:PRO:C	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:PRO:O	1:B:311:LEU:HB2	2.19	0.42
1:A:152:LEU:O	1:A:156:GLU:HG2	2.19	0.42
1:A:226:LEU:HD12	1:A:335:LEU:HD12	2.00	0.42
1:B:120:PRO:HA	1:B:121:PRO:HD3	1.93	0.42
1:B:70:PHE:HA	1:B:71:PRO:HD2	1.81	0.42
1:A:458:LEU:HD21	1:B:401:ALA:HB2	2.01	0.42
1:A:423:HIS:O	1:A:426:THR:HG22	2.19	0.42
1:A:126:LEU:HD11	1:A:156:GLU:HA	2.02	0.42
1:A:246:TRP:HB2	1:A:294:LEU:HB3	2.00	0.42
1:A:125:LEU:HD23	1:A:125:LEU:O	2.20	0.41
1:A:263:VAL:HG11	1:A:267:PRO:HA	2.02	0.41
1:B:265:GLY:N	1:B:287:ARG:HG2	2.31	0.41
1:B:378:LEU:HD12	1:B:378:LEU:HA	1.80	0.41
1:A:426:THR:CG2	1:A:460:PRO:HD2	2.50	0.41
1:B:259:GLN:HG3	1:B:260:ASP:OD1	2.19	0.41
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.55	0.41
1:B:358:TRP:H	4:B:500:HEM:HAB	1.85	0.41
1:A:137:TYR:HD1	1:A:142:ARG:HB2	1.86	0.41
1:A:465:GLU:OE1	1:B:105:LEU:HD13	2.20	0.41
1:B:194:LYS:O	1:B:194:LYS:HG2	2.20	0.41
1:A:119:PRO:HB3	1:A:238:PRO:HG3	2.03	0.41
1:A:293:LEU:CD2	1:A:307:LEU:HD21	2.51	0.41
1:A:335:LEU:HA	1:A:336:PRO:HD2	1.93	0.41
1:A:338:VAL:HG11	1:A:341:MET:CE	2.51	0.41
1:B:151:ARG:O	1:B:155:VAL:HG23	2.21	0.41
1:B:270:VAL:O	1:B:274:GLU:HG3	2.21	0.41
1:B:319:HIS:CG	1:B:320:PRO:HD2	2.55	0.41
1:A:243:PHE:O	1:A:352:ALA:HB2	2.20	0.41
1:B:191:GLN:HE21	1:B:358:TRP:HH2	1.67	0.41
1:A:157:ALA:O	1:A:160:ALA:HB3	2.21	0.40
1:A:294:LEU:HG	1:A:302:PRO:HB2	2.03	0.40
1:A:95:PRO:CA	1:A:110:LYS:HG3	2.48	0.40
1:A:370:CYS:SG	1:A:404:ILE:HD12	2.61	0.40
1:B:337:ALA:HA	1:B:356:SER:HB3	2.03	0.40
1:A:216:HIS:CD2	1:A:216:HIS:C	3.00	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	414/444 (93%)	382 (92%)	32 (8%)	0	100	100
1	B	412/444 (93%)	377 (92%)	32 (8%)	3 (1%)	18	18
All	All	826/888 (93%)	759 (92%)	64 (8%)	3 (0%)	30	32

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	GLN
1	B	260	ASP
1	B	336	PRO

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	354/377 (94%)	338 (96%)	16 (4%)	24	32
1	B	353/377 (94%)	332 (94%)	21 (6%)	18	21
All	All	707/754 (94%)	670 (95%)	37 (5%)	21	25

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

Mol	Chain	Res	Type
1	A	102	LEU
1	A	107	LEU
1	A	113	THR

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Mol	Chain	Res	Type
1	A	124	GLN
1	A	126	LEU
1	A	142	ARG
1	A	156	GLU
1	A	178	GLN
1	A	259	GLN
1	A	274	GLU
1	A	293	LEU
1	A	311	LEU
1	A	340	ASN
1	A	360	MET
1	A	426	THR
1	A	459	THR
1	B	92	GLN
1	B	105	LEU
1	B	107	LEU
1	B	109	ARG
1	B	113	THR
1	B	138	SER
1	B	141	LYS
1	B	142	ARG
1	B	146	GLN
1	B	203	CYS
1	B	252	ARG
1	B	263	VAL
1	B	294	LEU
1	B	317	LEU
1	B	330	LEU
1	B	378	LEU
1	B	379	GLU
1	B	391	THR
1	B	403	GLU
1	B	419	ILE
1	B	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	191	GLN
1	A	278	GLN
1	A	285	ASN

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Mol	Chain	Res	Type
1	A	296	GLN
1	A	340	ASN
1	A	405	ASN
1	A	468	ASN
1	B	92	GLN
1	B	124	GLN
1	B	128	GLN
1	B	178	GLN
1	B	191	GLN
1	B	196	GLN
1	B	222	ASN
1	B	405	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](#)

Of 10 ligands modelled in this entry, 2 are modelled with single atom and 1 is monoatomic - leaving 7 for Mogul analysis.

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	ARG	A	700	-	10,11,11	0.72	0	9,13,13	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEM	B	500	1	50,50,50	1.08	3 (6%)	67,82,82	1.14	5 (7%)
7	GOL	B	880	-	5,5,5	0.18	0	5,5,5	0.16	0
4	HEM	A	500	1	50,50,50	1.07	3 (6%)	67,82,82	1.35	7 (10%)
5	H4B	B	600	-	17,18,18	1.56	4 (23%)	14,26,26	1.66	3 (21%)
5	H4B	A	600	-	17,18,18	1.41	2 (11%)	14,26,26	1.74	2 (14%)
3	ARG	B	700	-	10,11,11	0.73	0	9,13,13	0.38	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	ARG	A	700	-	-	0/11/11/11	-
4	HEM	B	500	1	-	2/14/54/54	-
7	GOL	B	880	-	-	0/4/4/4	-
4	HEM	A	500	1	-	3/14/54/54	-
5	H4B	B	600	-	-	0/8/17/17	0/2/2/2
5	H4B	A	600	-	-	0/8/17/17	0/2/2/2
3	ARG	B	700	-	-	1/11/11/11	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	600	H4B	C7-C6	-4.11	1.48	1.52
5	A	600	H4B	C7-C6	-3.81	1.48	1.52
4	A	500	HEM	CAC-C3C	-3.05	1.39	1.47
4	B	500	HEM	CAB-C3B	-2.89	1.39	1.47
4	A	500	HEM	CHB-C4A	-2.62	1.33	1.39
4	B	500	HEM	CAC-C3C	-2.54	1.40	1.47
5	B	600	H4B	C4A-N5	2.40	1.43	1.37
5	A	600	H4B	C6-N5	2.36	1.51	1.47
4	A	500	HEM	CAB-C3B	-2.25	1.41	1.47
4	B	500	HEM	FE-NC	2.24	2.02	1.95
5	B	600	H4B	C6-N5	2.12	1.51	1.47
5	B	600	H4B	C7-N8	-2.10	1.44	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	600	H4B	C2-N1-C8A	4.83	121.88	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	600	H4B	C2-N1-C8A	4.60	121.47	113.36
4	A	500	HEM	CAD-C3D-C4D	3.26	130.37	124.70
4	A	500	HEM	C3B-C4B-NB	3.24	111.80	109.47
4	A	500	HEM	C2B-C1B-NB	3.24	113.57	109.84
4	A	500	HEM	CAD-C3D-C2D	-2.88	122.48	127.87
5	A	600	H4B	N3-C2-N1	-2.86	118.08	123.32
4	A	500	HEM	CHB-C1B-C2B	-2.73	119.20	126.95
4	B	500	HEM	C4C-C3C-C2C	-2.67	104.50	106.81
5	B	600	H4B	N3-C2-N1	-2.49	118.76	123.32
5	B	600	H4B	O9-C9-C6	2.44	115.13	109.28
4	B	500	HEM	CMD-C2D-C1D	2.34	128.68	125.03
4	B	500	HEM	C3B-C4B-NB	2.30	111.12	109.47
4	B	500	HEM	C2D-C1D-ND	2.22	112.47	109.90
4	B	500	HEM	CAD-C3D-C2D	-2.21	123.72	127.87
4	A	500	HEM	CHD-C4C-NC	-2.19	122.06	124.45
4	A	500	HEM	CMD-C2D-C1D	2.12	128.34	125.03

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	500	HEM	C4D-C3D-CAD-CBD
4	A	500	HEM	C1A-C2A-CAA-CBA
4	A	500	HEM	C2D-C3D-CAD-CBD
4	B	500	HEM	CAA-CBA-CGA-O2A
4	B	500	HEM	CAA-CBA-CGA-O1A
3	B	700	ARG	O-C-CA-CB

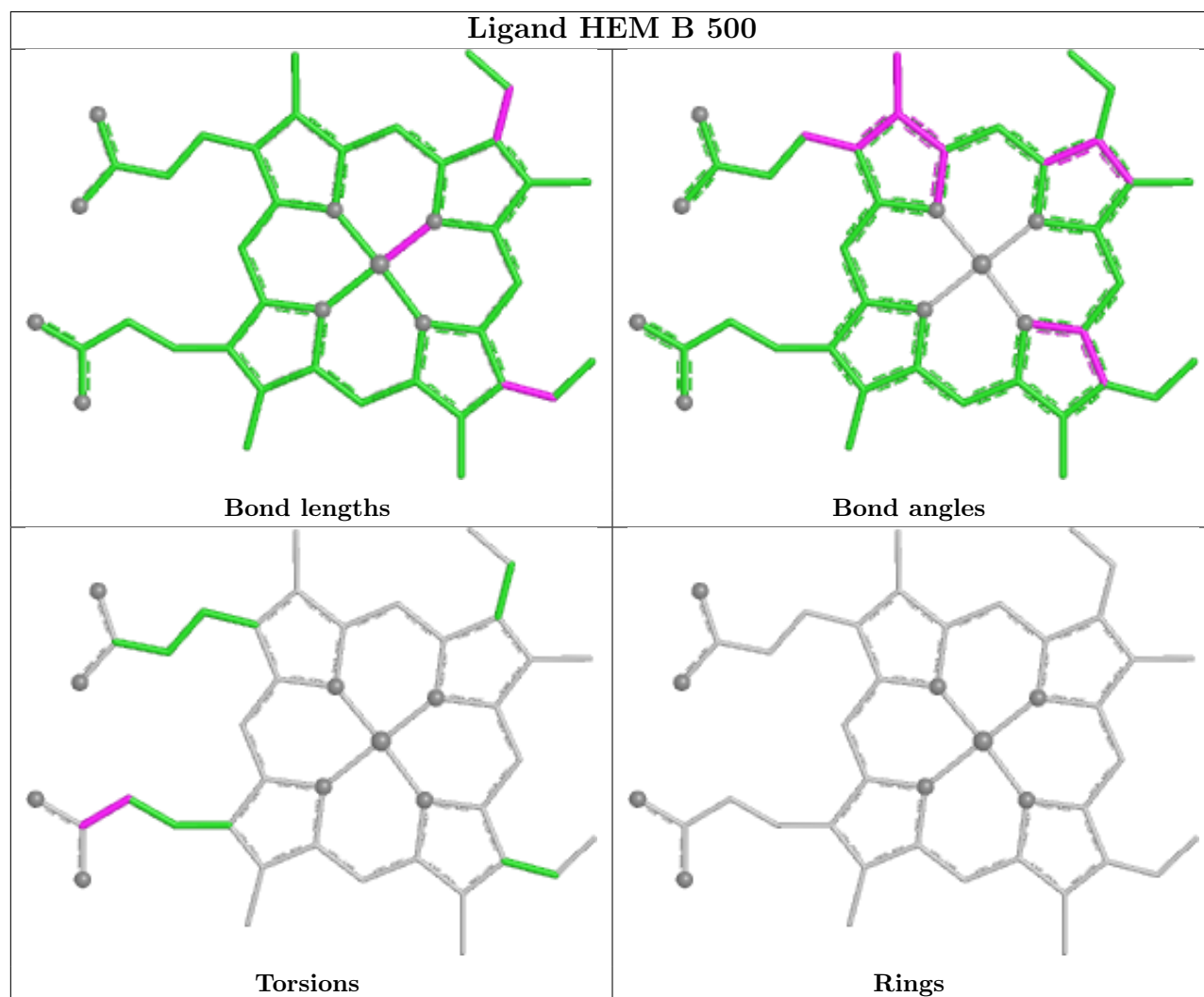
There are no ring outliers.

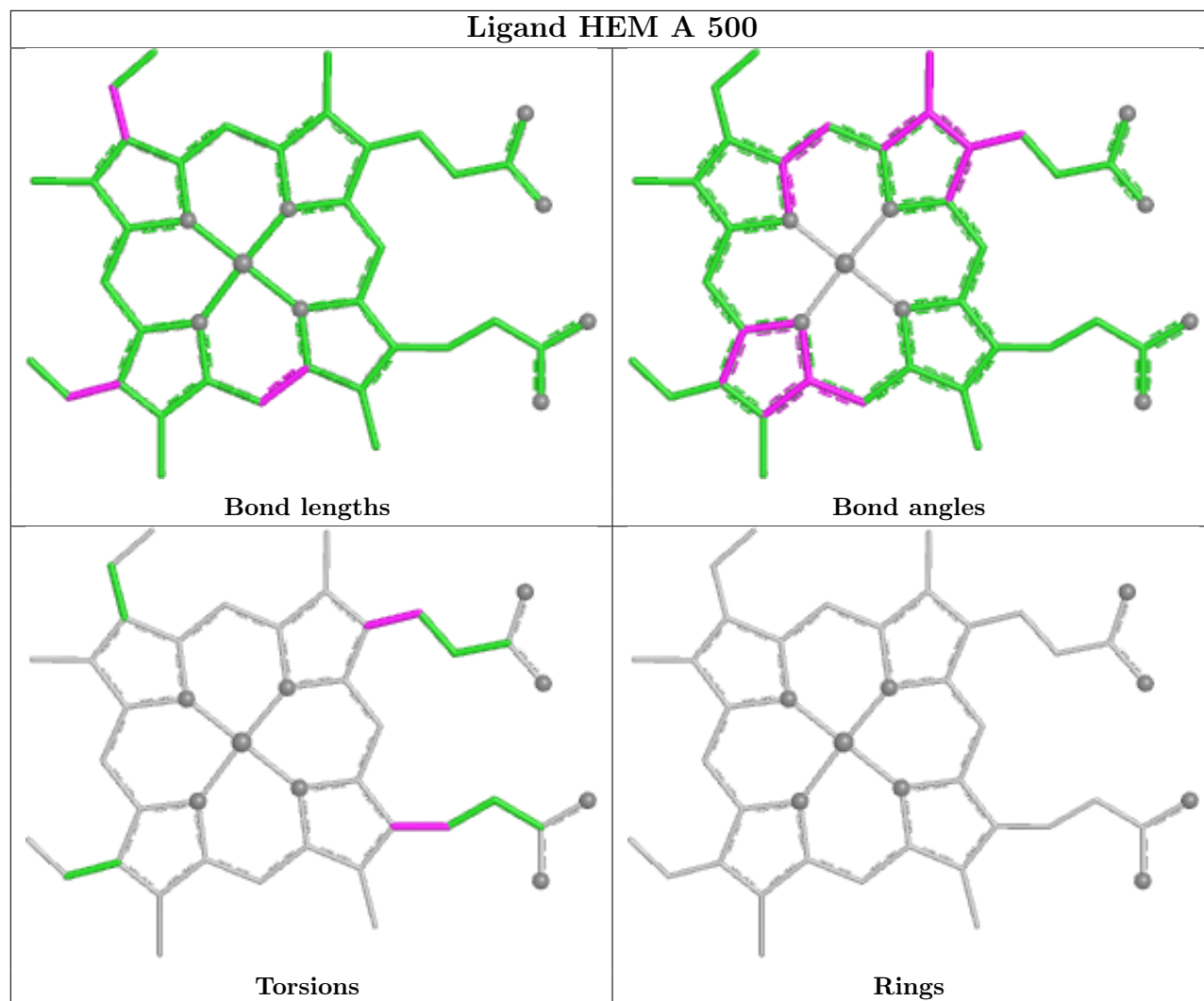
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	700	ARG	1	0
4	B	500	HEM	2	0
4	A	500	HEM	1	0
5	B	600	H4B	2	0
5	A	600	H4B	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.