



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:31 AM UTC

PDB ID : 3EBD / pdb_00003ebd
Title : Structure of inhibited murine iNOS oxygenase domain
Authors : Garcin, E.D.; Arvai, A.S.; Rosenfeld, R.J.; Kroeger, M.D.; Crane, B.R.; Anderson, G.; Andrews, G.; Hamley, P.J.; Mallinder, P.R.; Nicholls, D.J.; St-Gallay, S.A.; Tinker, A.C.; Gensmantel, N.P.; Mete, A.; Cheshire, D.R.; Connolly, S.; Stuehr, D.J.; Aberg, A.; Wallace, A.V.; Tainer, J.A.; Getzoff, E.D.
Deposited on : 2008-08-27
Resolution : 2.40 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](#) ①) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

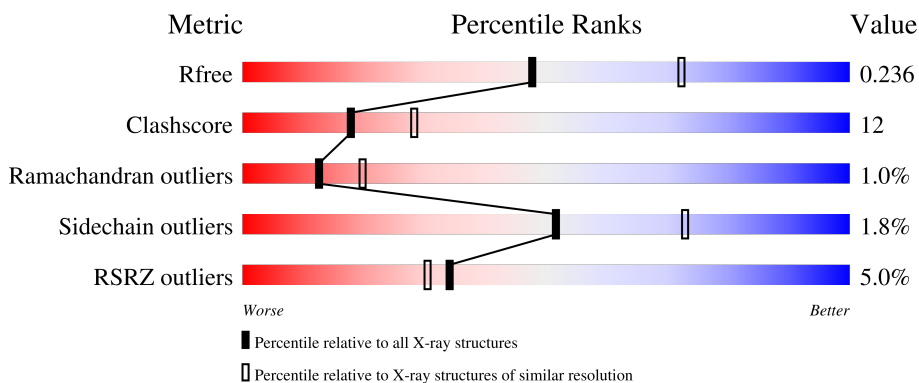
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.



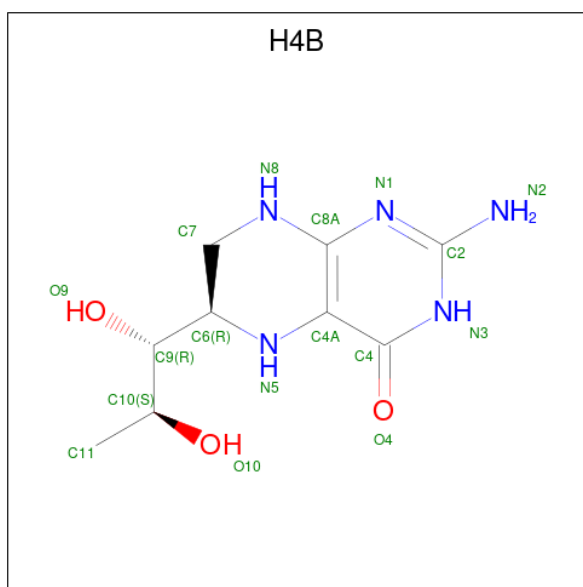
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	
1	B	433	

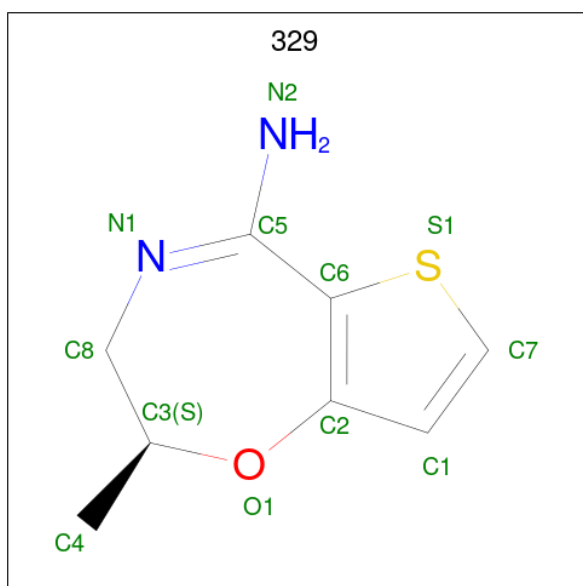
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	H4B	A	902	X	-	-	-
3	H4B	B	2902	X	-	-	-



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

- Molecule 4 is (2S)-2-methyl-2,3-dihydrothieno[2,3-f][1,4]oxazepin-5-amine (CCD ID: 329) (formula: C₈H₁₀N₂OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	12	8	2	1	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	12	8	2	1	1	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	A	1	5	4	1	0	0
5	A	1	5	4	1	0	0
5	B	1	5	4	1	0	0
5	B	1	5	4	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	395	395	395	0	0
6	B	401	401	401	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	213.44Å 213.44Å 116.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.65 – 2.40 44.65 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.9 (44.65-2.40) 90.0 (44.65-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.39Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.215 , 0.248 0.205 , 0.236	Depositor DCC
R_{free} test set	2801 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtrriage
Anisotropy	0.352	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 70.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7806	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: H4B, HEM, 329, SO4

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	0.38	0/3525	0.92	15/4792 (0.3%)
1	B	0.41	0/3521	0.92	14/4787 (0.3%)
All	All	0.39	0/7046	0.92	29/9579 (0.3%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	ASN	N-CA-C	6.86	121.31	112.26
1	B	367	TYR	N-CA-C	6.71	119.61	110.55
1	B	253	LEU	N-CA-C	-6.64	98.39	109.07
1	B	348	ASN	N-CA-C	6.59	120.97	112.41
1	A	386	LEU	N-CA-C	6.26	117.77	111.07
1	B	368	MET	N-CA-C	-6.01	98.61	108.41
1	A	153	ILE	N-CA-C	5.97	116.63	110.36
1	B	325	MET	N-CA-C	5.86	118.22	109.25
1	A	106	SER	N-CA-C	-5.82	106.72	113.88
1	B	197	ARG	N-CA-C	5.67	119.68	112.87
1	A	368	MET	N-CA-C	-5.60	99.39	108.52
1	A	365	GLY	N-CA-C	-5.55	100.03	113.18
1	A	234	ILE	N-CA-C	5.50	117.38	109.51
1	B	393	MET	N-CA-C	-5.50	106.58	113.28
1	B	365	GLY	N-CA-C	-5.47	100.22	113.18
1	A	188	TRP	N-CA-C	-5.41	105.29	111.14
1	B	176	THR	N-CA-C	-5.40	103.56	110.53
1	B	386	LEU	N-CA-C	5.32	116.76	111.07
1	B	485	TYR	N-CA-C	-5.24	102.99	110.59
1	A	343	LEU	N-CA-C	5.23	118.10	108.69
1	A	251	PHE	N-CA-C	-5.21	100.75	109.24
1	A	478	VAL	N-CA-C	5.21	115.27	107.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	MET	N-CA-C	-5.21	106.93	113.28
1	B	303	LEU	N-CA-C	5.19	117.43	109.07
1	A	367	TYR	N-CA-C	5.16	118.11	110.48
1	A	485	TYR	N-CA-C	-5.12	102.42	110.36
1	B	251	PHE	N-CA-C	-5.08	101.43	109.76
1	A	176	THR	N-CA-C	-5.04	103.75	110.55
1	B	378	CYS	N-CA-C	5.03	119.56	113.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3425	0	3318	85	0
1	B	3421	0	3312	82	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
3	A	17	0	14	0	0
3	B	17	0	14	1	0
4	A	12	0	10	1	0
4	B	12	0	10	1	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
6	A	395	0	0	7	3
6	B	401	0	0	10	0
All	All	7806	0	6738	169	3

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 12.

All (169) 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:81:ILE:HD11	1:B:475:LEU:HD13	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LYS:O	1:B:108:SER:HB3	1.77	0.82
1:B:388:GLU:HG2	6:B:4779:HOH:O	1.84	0.77
1:A:442:GLN:HE21	1:A:446:ARG:NH1	1.84	0.75
1:A:104:CYS:HA	1:A:110:LEU:HD13	1.70	0.72
1:A:81:ILE:HD11	1:A:475:LEU:HD13	1.71	0.71
1:A:83:ASN:HD22	1:A:86:SER:H	1.40	0.70
1:A:83:ASN:ND2	1:A:86:SER:H	1.89	0.69
1:B:441:MET:HE1	1:B:472:GLN:CG	2.23	0.67
1:B:98:ALA:O	1:B:100:SER:N	2.23	0.67
1:B:249:HIS:HB3	1:B:306:ASP:OD2	1.95	0.67
2:A:901:HEM:HMC2	2:A:901:HEM:HBC2	1.76	0.66
1:A:105:LYS:HD2	1:A:108:SER:HB3	1.78	0.65
1:A:442:GLN:HE21	1:A:446:ARG:HH12	1.40	0.65
1:A:266:MET:HE2	1:A:272:ARG:CZ	2.28	0.64
1:A:176:THR:OG1	1:A:179:GLU:HG3	1.97	0.64
1:A:441:MET:HE1	1:A:472:GLN:HG2	1.80	0.64
1:B:263:GLY:O	1:B:278:LEU:HD23	1.97	0.64
1:A:134:LEU:O	1:A:138:ILE:HG12	1.99	0.63
1:B:77:GLN:O	1:B:96:HIS:HE1	1.81	0.63
1:A:82:LYS:O	1:A:473:GLU:HG3	1.99	0.62
1:A:125:ASP:OD1	1:A:126:LYS:HG3	1.98	0.62
1:B:441:MET:HE1	1:B:472:GLN:CD	2.25	0.61
1:B:153:ILE:O	1:B:157:LEU:HG	2.00	0.61
1:A:153:ILE:HG22	1:A:157:LEU:HD23	1.83	0.61
1:A:215:GLN:HG3	1:A:219:GLN:NE2	2.16	0.61
1:B:398:HIS:HB2	6:B:4580:HOH:O	2.01	0.61
1:B:441:MET:HE1	1:B:472:GLN:HG2	1.82	0.60
1:A:215:GLN:HG3	1:A:219:GLN:HE21	1.66	0.60
1:B:107:LYS:O	1:B:108:SER:CB	2.49	0.60
1:B:304:GLN:HG3	1:B:308:GLN:O	2.03	0.59
1:B:385:ILE:O	1:B:389:VAL:HG23	2.02	0.59
1:A:138:ILE:HG22	1:A:142:ASN:HD21	1.68	0.58
1:A:137:ALA:O	1:A:141:ILE:HG12	2.03	0.57
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.40	0.57
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.39	0.57
1:B:327:HIS:ND1	1:B:328:PRO:HD2	2.20	0.56
1:A:407:ARG:HD2	6:A:4140:HOH:O	2.04	0.56
1:B:78:TYR:C	1:B:78:TYR:CD1	2.83	0.56
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.36	0.56
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.41	0.56
1:B:446:ARG:HG2	1:B:446:ARG:HH21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:PRO:HB2	1:A:132:GLU:HG3	1.87	0.56
1:A:110:LEU:O	1:A:112:SER:N	2.31	0.55
1:A:86:SER:OG	1:A:88:GLU:HG2	2.06	0.55
1:A:110:LEU:N	1:A:110:LEU:HD12	2.21	0.55
1:A:331:GLU:O	1:A:334:GLN:HG2	2.07	0.55
1:B:213:THR:OG1	1:B:216:GLU:HG3	2.08	0.54
1:A:465:SER:O	1:A:471:HIS:HE1	1.91	0.54
1:A:223:ARG:HD2	6:A:4190:HOH:O	2.07	0.53
1:A:239:THR:O	1:A:361:CYS:HA	2.07	0.53
1:A:241:PHE:HB3	1:A:242:PRO:HD2	1.91	0.53
1:B:375:ARG:O	1:B:379:ASP:HB2	2.07	0.53
1:A:138:ILE:HG22	1:A:142:ASN:ND2	2.23	0.53
1:A:132:GLU:O	1:A:135:PRO:HD2	2.08	0.53
1:B:132:GLU:O	1:B:135:PRO:HD2	2.08	0.53
1:A:254:TRP:CZ3	1:A:490:TRP:HB3	2.43	0.53
1:A:165:LYS:N	1:A:165:LYS:HD2	2.24	0.52
1:A:441:MET:CE	1:A:472:GLN:HG2	2.39	0.52
1:B:145:TYR:HA	1:B:148:PHE:CE1	2.45	0.52
1:A:480:SER:HA	1:A:481:PRO:C	2.35	0.52
1:A:132:GLU:C	1:A:135:PRO:HD2	2.35	0.52
1:B:81:ILE:HD11	1:B:475:LEU:CD1	2.32	0.51
1:A:263:GLY:O	1:A:278:LEU:HD23	2.10	0.51
1:B:241:PHE:HB3	1:B:242:PRO:HD2	1.92	0.50
1:B:137:ALA:O	1:B:141:ILE:HG12	2.12	0.50
1:A:264:TYR:CE1	1:A:293:TYR:HA	2.47	0.49
1:B:130:LEU:HD21	1:B:167:ILE:HG22	1.95	0.49
1:B:285:ILE:HD11	1:B:291:PRO:HB3	1.94	0.49
1:A:249:HIS:HB3	1:A:306:ASP:OD1	2.13	0.49
1:A:83:ASN:HD22	1:A:83:ASN:C	2.20	0.49
1:A:164:THR:O	1:A:168:GLU:HG3	2.13	0.49
1:A:188:TRP:CZ3	1:A:200:TRP:HA	2.48	0.49
1:A:246:ASP:OD1	1:A:248:LYS:HB2	2.13	0.49
1:A:283:LEU:O	1:A:287:LEU:HG	2.13	0.49
1:A:330:TYR:HB3	1:A:332:TRP:CE2	2.47	0.48
1:B:110:LEU:HD12	1:B:110:LEU:N	2.28	0.48
1:B:445:TYR:HA	1:B:450:GLY:H	1.77	0.48
1:B:266:MET:HE2	1:B:272:ARG:CZ	2.43	0.48
1:A:294:GLY:N	1:A:297:ASP:OD2	2.33	0.48
1:A:83:ASN:ND2	1:A:85:GLY:H	2.12	0.48
1:A:131:GLU:O	1:A:135:PRO:HG2	2.14	0.48
1:A:295:ARG:HG3	6:A:4299:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ARG:O	1:A:163:VAL:HG23	2.14	0.48
1:B:254:TRP:CE3	1:B:283:LEU:HD21	2.49	0.47
1:B:334:GLN:OE1	1:B:335:GLU:HG3	2.13	0.47
1:A:398:HIS:HB2	6:A:4216:HOH:O	2.15	0.47
1:B:257:GLN:HA	1:B:345:ALA:O	2.15	0.47
1:A:172:THR:HG23	1:A:173:TYR:N	2.30	0.46
1:B:80:ARG:NH1	6:B:4605:HOH:O	2.48	0.46
1:B:254:TRP:CZ3	1:B:490:TRP:HB3	2.49	0.46
1:B:294:GLY:N	1:B:297:ASP:OD2	2.43	0.46
1:A:325:MET:HB3	1:A:333:PHE:HE2	1.81	0.46
1:B:103:THR:HA	6:B:4501:HOH:O	2.15	0.46
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.45	0.46
1:A:130:LEU:HD12	1:A:130:LEU:N	2.30	0.46
1:B:283:LEU:O	1:B:287:LEU:HG	2.15	0.46
1:A:213:THR:OG1	1:A:216:GLU:HG3	2.16	0.46
1:B:104:CYS:HA	1:B:110:LEU:HD13	1.97	0.46
1:A:190:ASN:O	1:A:192:PRO:HD3	2.16	0.46
1:B:239:THR:O	1:B:361:CYS:HA	2.16	0.46
1:B:445:TYR:CE2	1:B:450:GLY:HA2	2.51	0.46
1:B:125:ASP:OD2	1:B:126:LYS:HG2	2.16	0.46
1:A:371:GLU:OE1	4:A:903:329:N1	2.48	0.46
1:B:98:ALA:C	1:B:100:SER:H	2.18	0.45
1:B:102:PHE:HZ	1:B:476:ASN:ND2	2.14	0.45
1:B:105:LYS:HB2	6:B:4719:HOH:O	2.16	0.45
1:B:107:LYS:HB2	6:B:4570:HOH:O	2.16	0.45
1:A:334:GLN:HG3	1:A:335:GLU:N	2.31	0.45
1:A:244:ARG:HA	6:A:4079:HOH:O	2.16	0.45
1:A:470:PHE:C	1:A:470:PHE:CD1	2.95	0.45
1:A:83:ASN:ND2	1:A:83:ASN:C	2.75	0.45
1:A:349:MET:HE3	1:A:485:TYR:CD1	2.52	0.45
1:A:410:THR:O	1:A:414:VAL:HG23	2.16	0.45
1:B:295:ARG:HD2	6:B:4564:HOH:O	2.16	0.45
1:A:350:LEU:C	1:A:350:LEU:HD23	2.42	0.45
1:B:264:TYR:CE1	1:B:293:TYR:HA	2.51	0.44
1:B:466:ILE:HG22	1:B:466:ILE:O	2.16	0.44
1:B:121:ARG:HA	1:B:121:ARG:HD3	1.76	0.44
1:A:99:THR:HG23	1:A:478:VAL:O	2.18	0.44
1:A:303:LEU:O	1:A:310:PRO:HA	2.17	0.44
1:B:190:ASN:O	1:B:192:PRO:HD3	2.18	0.44
1:B:86:SER:OG	1:B:88:GLU:HB2	2.18	0.43
1:B:327:HIS:ND1	1:B:328:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:N	1:A:110:LEU:CD1	2.81	0.43
1:B:82:LYS:O	1:B:473:GLU:HG3	2.18	0.43
1:A:257:GLN:HA	1:A:345:ALA:O	2.19	0.43
1:B:125:ASP:O	1:B:248:LYS:HE3	2.19	0.43
1:B:334:GLN:OE1	1:B:335:GLU:N	2.52	0.43
2:B:2901:HEM:HHC	2:B:2901:HEM:HBB2	2.00	0.43
1:A:193:ARG:HD3	1:A:457:TRP:CD2	2.53	0.43
1:A:333:PHE:HB3	6:A:4056:HOH:O	2.18	0.43
1:B:152:LYS:HE2	1:B:155:GLU:CD	2.44	0.43
1:B:249:HIS:O	1:B:306:ASP:HA	2.19	0.43
1:A:78:TYR:CD1	1:A:78:TYR:C	2.97	0.43
1:A:439:LYS:HG2	6:A:4316:HOH:O	2.18	0.43
1:B:465:SER:HA	1:B:470:PHE:CG	2.53	0.43
1:A:330:TYR:CD1	1:A:332:TRP:CZ2	3.06	0.43
1:B:286:ASP:C	1:B:288:GLY:H	2.27	0.43
1:B:98:ALA:C	1:B:100:SER:N	2.75	0.42
1:A:153:ILE:O	1:A:157:LEU:HD23	2.19	0.42
1:A:215:GLN:HE21	1:A:219:GLN:HE21	1.66	0.42
1:A:488:GLU:OE1	1:A:488:GLU:HA	2.19	0.42
1:B:407:ARG:HD2	6:B:4483:HOH:O	2.20	0.42
1:A:304:GLN:HG3	1:A:308:GLN:O	2.19	0.42
1:B:410:THR:O	1:B:414:VAL:HG23	2.19	0.42
1:A:195:ILE:O	1:A:195:ILE:HG12	2.19	0.42
1:B:368:MET:HA	1:B:428:MET:O	2.20	0.42
1:B:145:TYR:HA	1:B:148:PHE:CD1	2.54	0.41
1:A:442:GLN:HG2	1:A:446:ARG:NH1	2.34	0.41
1:A:77:GLN:O	1:A:96:HIS:HE1	2.03	0.41
1:B:480:SER:HA	1:B:481:PRO:C	2.44	0.41
1:B:487:ILE:O	1:B:488:GLU:C	2.64	0.41
1:B:130:LEU:CD2	1:B:167:ILE:HG22	2.51	0.41
1:B:445:TYR:O	1:B:449:GLY:HA2	2.20	0.41
1:B:188:TRP:CD2	1:B:200:TRP:HA	2.56	0.41
1:B:371:GLU:OE1	4:B:2903:329:N1	2.53	0.41
1:B:457:TRP:HA	3:B:2902:H4B:N1	2.35	0.41
1:A:145:TYR:HA	1:A:148:PHE:CE2	2.56	0.41
1:B:348:ASN:H	1:B:348:ASN:ND2	2.19	0.41
1:A:134:LEU:HB3	1:A:135:PRO:HD3	2.03	0.41
1:B:123:PRO:HD3	6:B:4456:HOH:O	2.20	0.40
1:B:134:LEU:HB3	1:B:135:PRO:HD3	2.03	0.40
1:A:125:ASP:OD1	1:A:125:ASP:C	2.65	0.40
1:B:204:GLN:HG2	1:B:227:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:TYR:CE1	1:B:356:LEU:HD21	2.56	0.40
1:B:445:TYR:CZ	1:B:450:GLY:HA2	2.56	0.40
1:A:185:LYS:HD3	1:A:201:SER:HA	2.03	0.40
1:B:422:LYS:HG2	6:B:4766:HOH:O	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:4177:HOH:O	6:A:4227:HOH:O[11_655]	1.97	0.23
6:A:4145:HOH:O	6:A:4177:HOH:O[11_655]	2.19	0.01
6:A:4261:HOH:O	6:A:4261:HOH:O[11_655]	2.19	0.01

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	419/433 (97%)	378 (90%)	36 (9%)	5 (1%)	10	16
1	B	419/433 (97%)	385 (92%)	31 (7%)	3 (1%)	18	28
All	All	838/866 (97%)	763 (91%)	67 (8%)	8 (1%)	12	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	99	THR
1	A	99	THR
1	A	111	GLY
1	A	464	GLY
1	A	105	LYS
1	B	108	SER
1	B	307	GLY

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Mol	Chain	Res	Type
1	A	269	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	367/381 (96%)	361 (98%)	6 (2%)	55 76
1	B	366/381 (96%)	359 (98%)	7 (2%)	50 71
All	All	733/762 (96%)	720 (98%)	13 (2%)	51 73

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	107	LYS
1	A	118	SER
1	A	223	ARG
1	A	422	LYS
1	A	475	LEU
1	B	88	GLU
1	B	105	LYS
1	B	130	LEU
1	B	334	GLN
1	B	348	ASN
1	B	475	LEU
1	B	494	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	96	HIS
1	A	136	HIS
1	A	142	ASN

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Mol	Chain	Res	Type
1	A	219	GLN
1	A	384	ASN
1	A	421	GLN
1	A	442	GLN
1	A	471	HIS
1	A	486	GLN
1	A	496	GLN
1	B	96	HIS
1	B	115	ASN
1	B	143	GLN
1	B	202	ASN
1	B	215	GLN
1	B	348	ASN
1	B	418	HIS
1	B	421	GLN
1	B	476	ASN
1	B	486	GLN

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](#)

10 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
4	329	B	2903	-	8,13,13	1.45	2 (25%)	5,18,18	2.02	2 (40%)
5	SO4	A	3004	-	4,4,4	0.39	0	6,6,6	0.10	0
2	HEM	B	2901	1	50,50,50	1.40	10 (20%)	67,82,82	1.21	8 (11%)
5	SO4	A	3003	-	4,4,4	0.39	0	6,6,6	0.09	0
2	HEM	A	901	1	50,50,50	1.34	7 (14%)	67,82,82	1.12	7 (10%)
3	H4B	A	902	-	17,18,18	2.55	4 (23%)	14,26,26	9.43	10 (71%)
4	329	A	903	-	8,13,13	1.42	2 (25%)	5,18,18	1.47	1 (20%)
5	SO4	B	3003	-	4,4,4	0.38	0	6,6,6	0.10	0
5	SO4	B	3004	-	4,4,4	0.40	0	6,6,6	0.07	0
3	H4B	B	2902	-	17,18,18	2.69	3 (17%)	14,26,26	6.58	11 (78%)

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	329	B	2903	-	-	-	0/1/2/2
2	HEM	B	2901	1	-	3/14/54/54	-
2	HEM	A	901	1	-	1/14/54/54	-
3	H4B	A	902	-	1/1/3/5	3/8/17/17	0/2/2/2
4	329	A	903	-	-	-	0/1/2/2
3	H4B	B	2902	-	1/1/3/5	2/8/17/17	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2902	H4B	C7-N8	-8.44	1.38	1.46
3	A	902	H4B	C7-N8	-7.90	1.38	1.46
3	B	2902	H4B	C7-C6	-5.26	1.47	1.52
3	A	902	H4B	C7-C6	-5.03	1.47	1.52
2	A	901	HEM	FE-NA	3.56	2.06	1.95
2	B	2901	HEM	FE-NB	3.38	2.05	1.94
2	B	2901	HEM	FE-NA	3.22	2.05	1.95
2	B	2901	HEM	FE-ND	3.21	2.04	1.94
2	A	901	HEM	FE-NB	3.18	2.04	1.94
3	B	2902	H4B	C4-N3	-3.01	1.33	1.38
3	A	902	H4B	C4-N3	-2.88	1.33	1.38
2	A	901	HEM	FE-NC	2.77	2.04	1.95
2	B	2901	HEM	CAC-C3C	-2.67	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2901	HEM	CAB-C3B	-2.51	1.40	1.47
4	A	903	329	C1-C2	2.35	1.46	1.42
2	A	901	HEM	CAB-C3B	-2.34	1.41	1.47
2	A	901	HEM	FE-ND	2.34	2.02	1.94
4	B	2903	329	C7-S1	2.24	1.80	1.70
2	B	2901	HEM	CBB-CAB	2.22	1.41	1.30
2	A	901	HEM	CBC-CAC	2.19	1.40	1.30
2	B	2901	HEM	CBC-CAC	2.16	1.40	1.30
4	A	903	329	C7-S1	2.16	1.80	1.70
2	B	2901	HEM	FE-NC	2.15	2.02	1.95
4	B	2903	329	C1-C2	2.10	1.46	1.42
2	B	2901	HEM	C2A-C3A	-2.07	1.33	1.38
3	A	902	H4B	C4A-C8A	2.05	1.42	1.38
2	B	2901	HEM	C1B-NB	-2.04	1.36	1.40
2	A	901	HEM	CAC-C3C	-2.00	1.42	1.47

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	H4B	O9-C9-C10	-16.04	78.60	109.14
3	A	902	H4B	C11-C10-C9	15.55	131.16	112.11
3	A	902	H4B	C4A-C4-N3	14.03	150.66	112.13
3	A	902	H4B	C2-N3-C4	-12.78	101.93	125.11
3	A	902	H4B	C4-C4A-N5	12.19	149.51	116.27
3	B	2902	H4B	O4-C4-C4A	-11.55	99.42	127.26
3	B	2902	H4B	C2-N3-C4	-11.00	105.15	125.11
3	B	2902	H4B	C4A-C4-N3	10.39	140.67	112.13
3	A	902	H4B	O4-C4-C4A	-9.77	103.70	127.26
3	B	2902	H4B	C4-C4A-N5	9.48	142.13	116.27
3	B	2902	H4B	O9-C9-C10	-9.38	91.28	109.14
3	A	902	H4B	O4-C4-N3	-7.70	105.63	120.11
3	A	902	H4B	O10-C10-C11	-5.69	92.68	109.68
3	A	902	H4B	N2-C2-N1	-5.56	108.82	119.67
3	B	2902	H4B	N3-C2-N1	4.52	131.59	123.32
3	B	2902	H4B	O9-C9-C6	4.00	118.86	109.28
4	B	2903	329	C2-C6-S1	3.56	112.60	109.84
3	A	902	H4B	N2-C2-N3	3.55	124.25	116.76
3	B	2902	H4B	C11-C10-C9	3.30	116.16	112.11
2	B	2901	HEM	CHC-C4B-NB	-3.04	121.16	124.42
2	B	2901	HEM	C3B-C4B-NB	2.97	111.60	109.47
2	B	2901	HEM	C4B-C3B-C2B	-2.94	104.57	107.28
2	B	2901	HEM	CAD-C3D-C4D	2.94	129.82	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2901	HEM	CAD-C3D-C2D	-2.75	122.72	127.87
4	A	903	329	C2-C6-S1	2.69	111.92	109.84
2	B	2901	HEM	CAA-C2A-C1A	2.67	130.16	124.94
2	A	901	HEM	CAD-C3D-C4D	2.64	129.30	124.70
4	B	2903	329	C7-S1-C6	-2.61	88.71	91.38
3	B	2902	H4B	N2-C2-N1	-2.61	114.58	119.67
2	A	901	HEM	C4C-C3C-C2C	-2.61	104.55	106.81
2	A	901	HEM	CAA-C2A-C1A	2.54	129.89	124.94
2	A	901	HEM	CMD-C2D-C1D	2.41	128.79	125.03
3	B	2902	H4B	O10-C10-C11	-2.40	102.49	109.68
2	A	901	HEM	CAD-C3D-C2D	-2.30	123.56	127.87
2	B	2901	HEM	CAA-C2A-C3A	-2.18	122.17	127.07
3	B	2902	H4B	C2-N1-C8A	-2.18	109.51	113.36
2	B	2901	HEM	C4C-C3C-C2C	-2.15	104.95	106.81
2	A	901	HEM	C4B-C3B-C2B	-2.14	105.31	107.28
2	A	901	HEM	CAB-C3B-C2B	-2.11	121.58	128.43

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	902	H4B	C6
3	B	2902	H4B	C6

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	H4B	N5-C6-C9-O9
3	A	902	H4B	C7-C6-C9-C10
3	A	902	H4B	O10-C10-C9-C6
3	B	2902	H4B	N5-C6-C9-O9
2	B	2901	HEM	C4B-C3B-CAB-CBB
3	B	2902	H4B	C7-C6-C9-C10
2	B	2901	HEM	CAD-CBD-CGD-O2D
2	A	901	HEM	CAA-CBA-CGA-O2A
2	B	2901	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

5 monomers are involved in 5 short contacts:

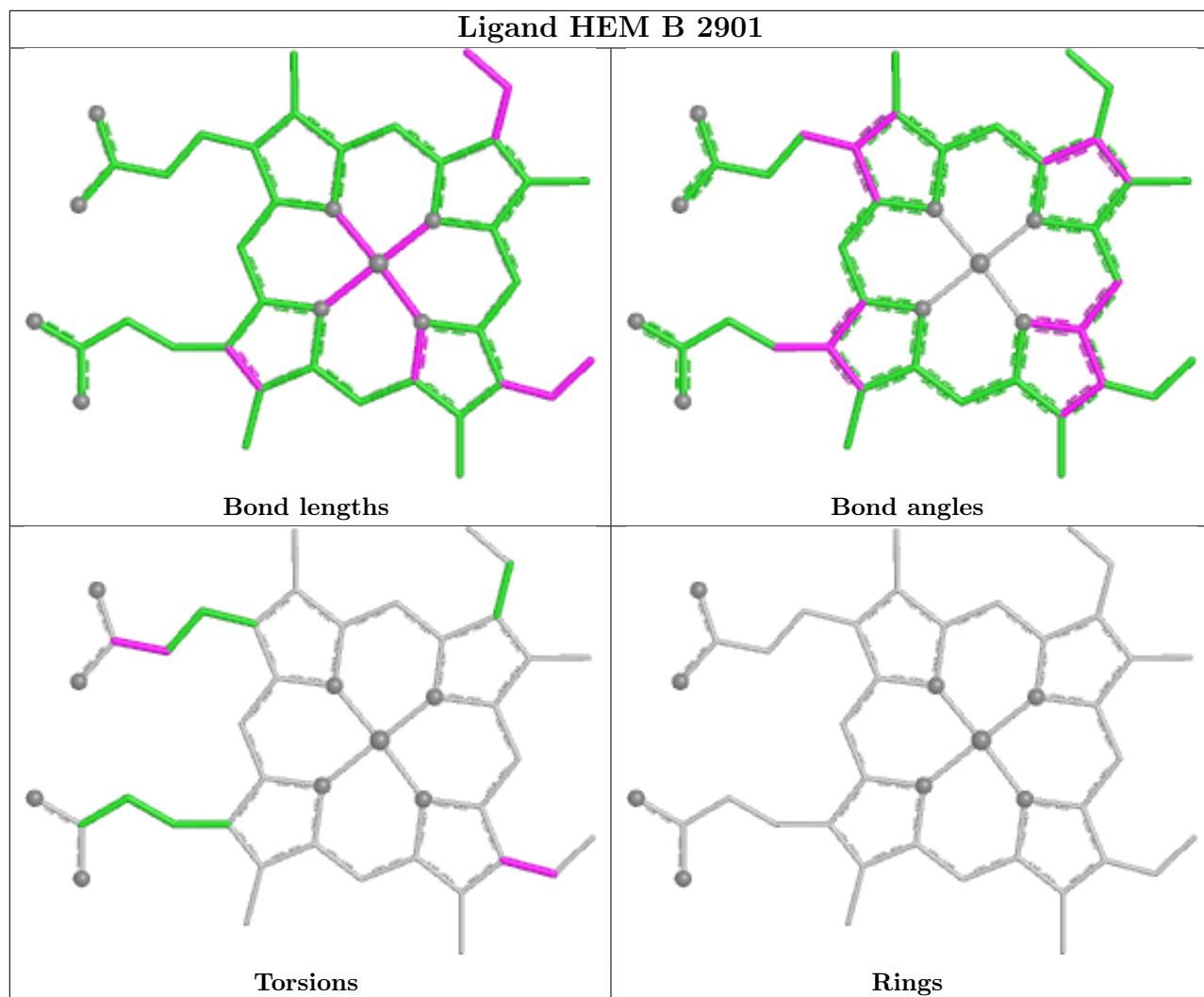
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2903	329	1	0

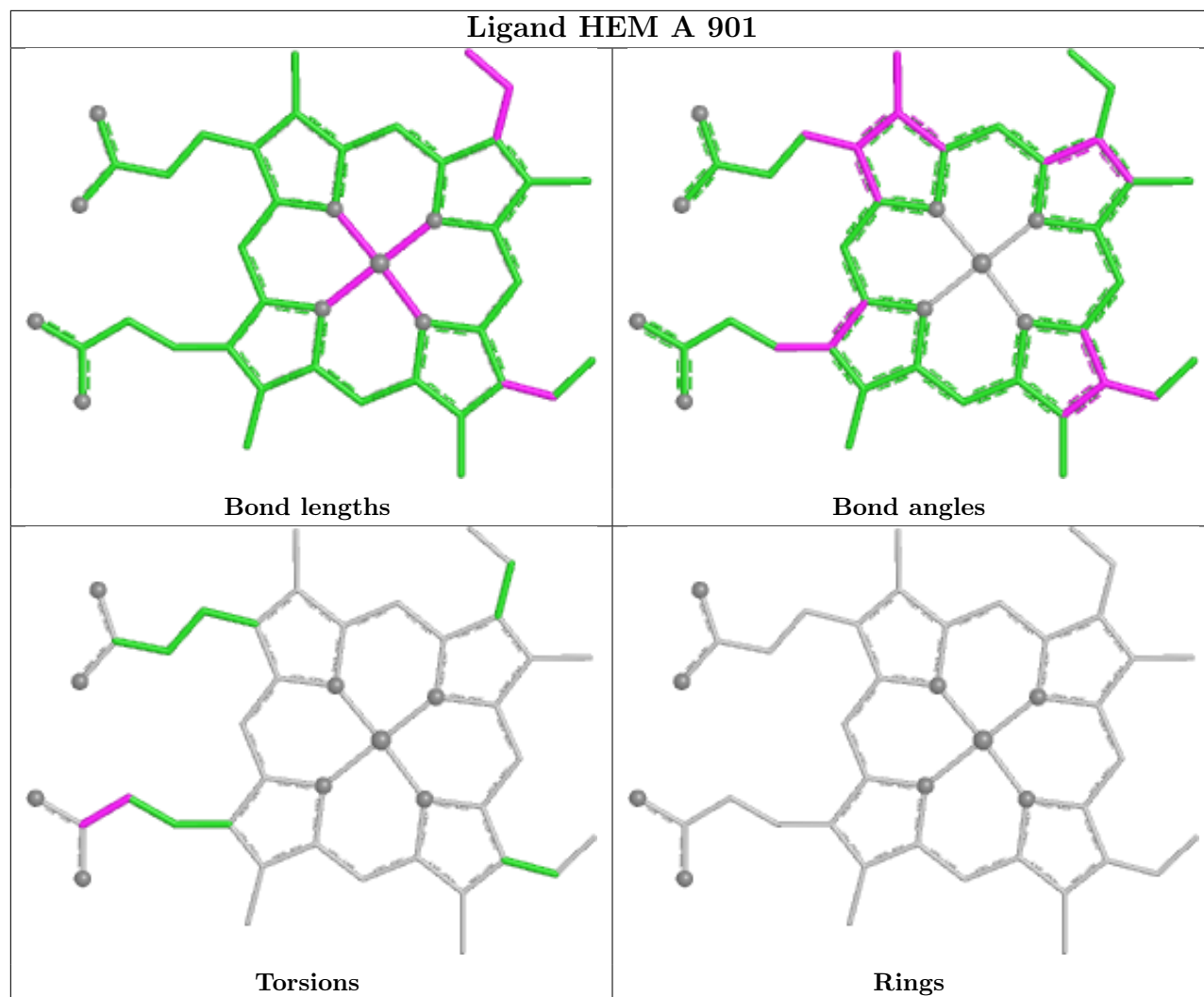
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2901	HEM	1	0
2	A	901	HEM	1	0
4	A	903	329	1	0
3	B	2902	H4B	1	0

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	421/433 (97%)	0.19	18 (4%) 40 36	23, 44, 74, 98	0
1	B	421/433 (97%)	0.19	24 (5%) 29 25	24, 41, 72, 100	0
All	All	842/866 (97%)	0.19	42 (4%) 34 30	23, 43, 73, 100	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	497	ASN	5.1
1	B	103	THR	5.0
1	A	77	GLN	5.0
1	B	99	THR	4.9
1	B	108	SER	4.4
1	A	110	LEU	4.2
1	B	106	SER	3.7
1	A	103	THR	3.7
1	B	102	PHE	3.6
1	A	497	ASN	3.6
1	B	98	ALA	3.4
1	B	100	SER	3.3
1	A	102	PHE	3.3
1	B	105	LYS	3.3
1	B	110	LEU	3.3
1	B	130	LEU	3.3
1	A	105	LYS	3.2
1	A	269	GLY	3.2
1	B	269	GLY	3.2
1	A	308	GLN	2.8
1	A	99	THR	2.8
1	B	334	GLN	2.8
1	B	267	PRO	2.7
1	B	496	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	106	SER	2.7
1	A	334	GLN	2.6
1	B	77	GLN	2.5
1	B	109	CYS	2.4
1	B	107	LYS	2.4
1	A	111	GLY	2.4
1	A	153	ILE	2.3
1	B	81	ILE	2.3
1	A	108	SER	2.2
1	A	150	GLU	2.2
1	B	171	GLY	2.1
1	B	131	GLU	2.1
1	B	292	ARG	2.1
1	B	265	GLN	2.1
1	A	104	CYS	2.1
1	A	266	MET	2.1
1	A	292	ARG	2.1
1	B	330	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

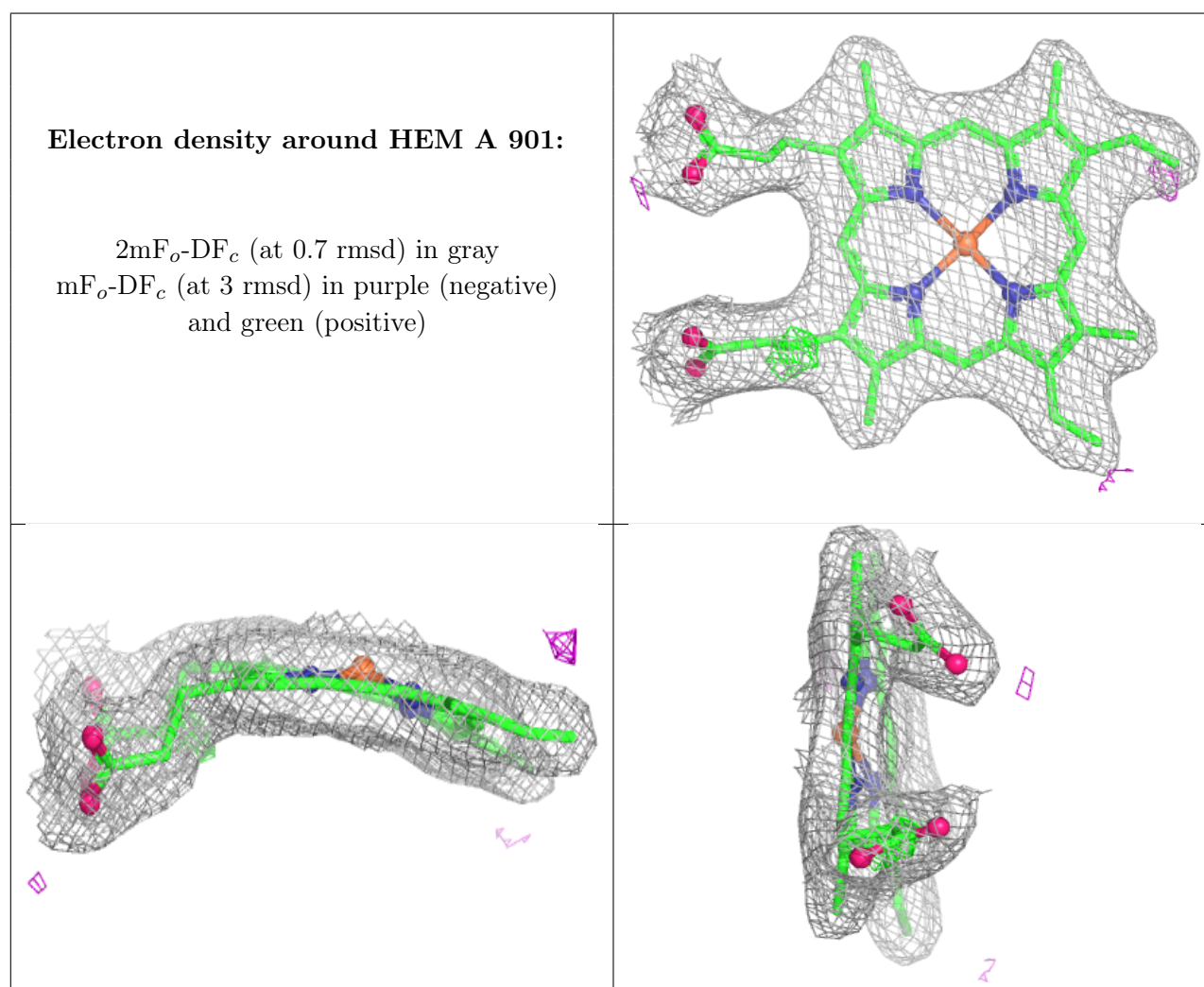
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	B	3004	5/5	0.76	0.13	103,103,104,104	0
5	SO4	A	3004	5/5	0.80	0.12	95,95,96,96	0
5	SO4	B	3003	5/5	0.81	0.13	112,113,113,114	0
5	SO4	A	3003	5/5	0.83	0.11	115,116,116,116	0
2	HEM	A	901	43/43	0.98	0.06	19,23,26,31	0

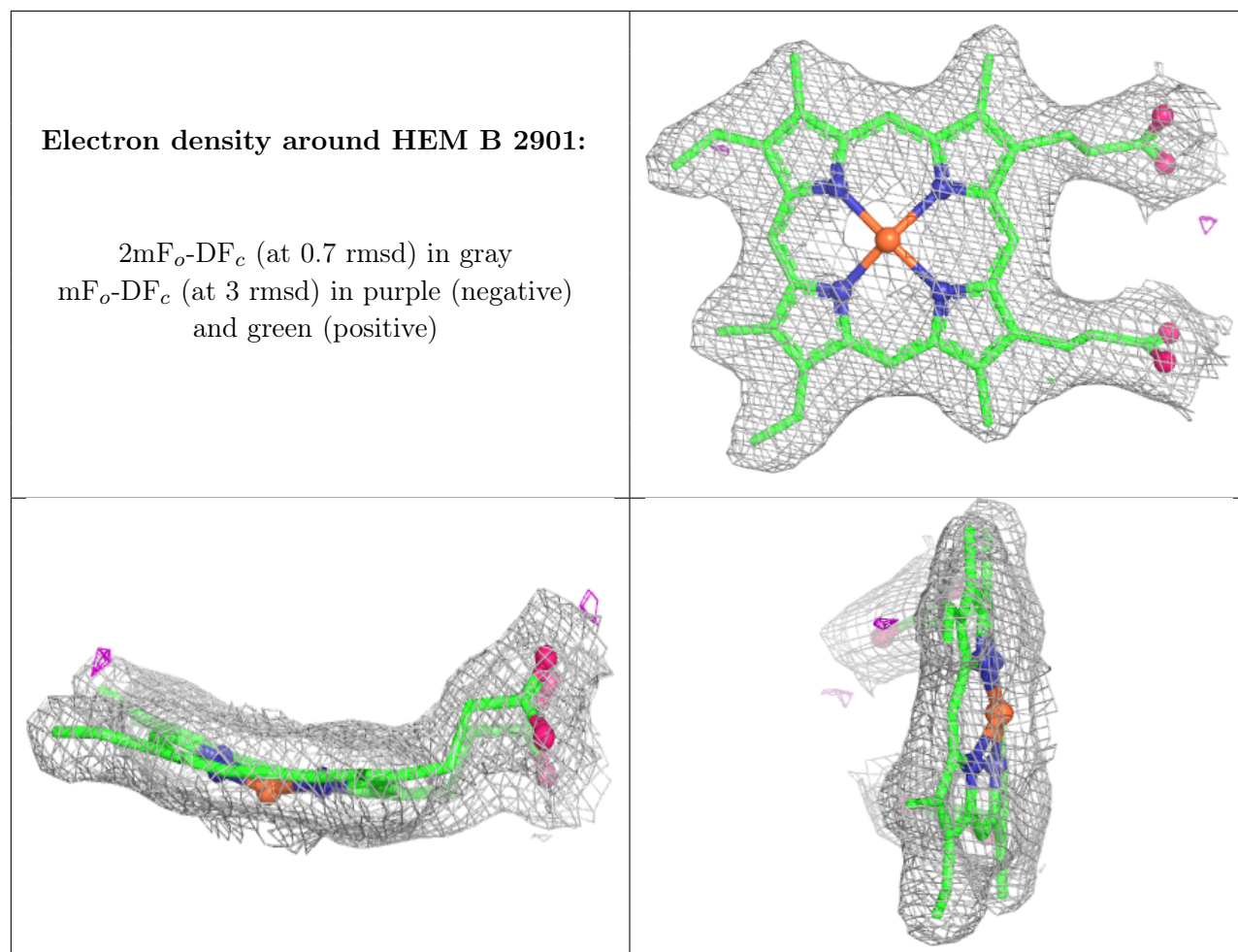
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	H4B	A	902	17/17	0.98	0.04	17,25,30,33	0
4	329	A	903	12/12	0.98	0.06	26,27,30,30	0
4	329	B	2903	12/12	0.98	0.07	25,27,30,31	0
2	HEM	B	2901	43/43	0.99	0.05	18,23,27,29	0
3	H4B	B	2902	17/17	0.99	0.04	16,24,26,28	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.