



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 06:10 AM EDT

PDB ID : 1GZA / pdb_00001gza
Title : PEROXIDASE
Authors : Fukuyama, K.; Itakura, H.
Deposited on : 1996-11-13
Resolution : 2.06 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

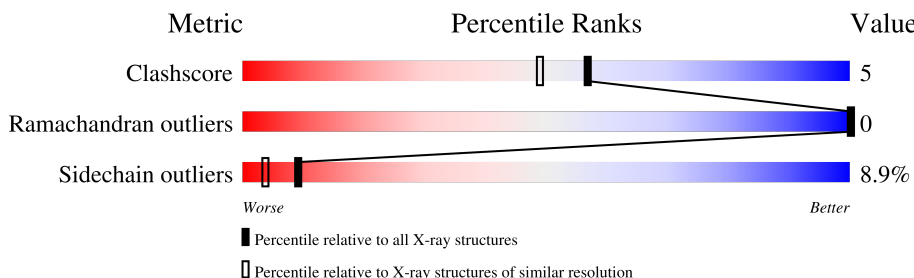
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)

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	344	
2	B	2	

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
4	IOD	A	702	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2786 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 PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2465	1537	421	492	15			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

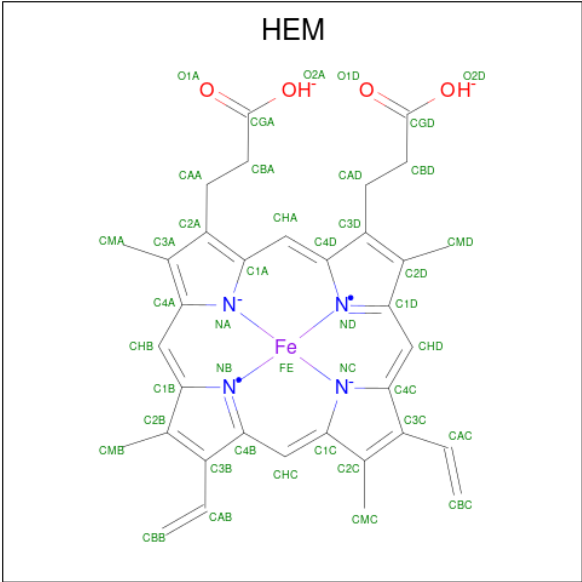
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	I	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

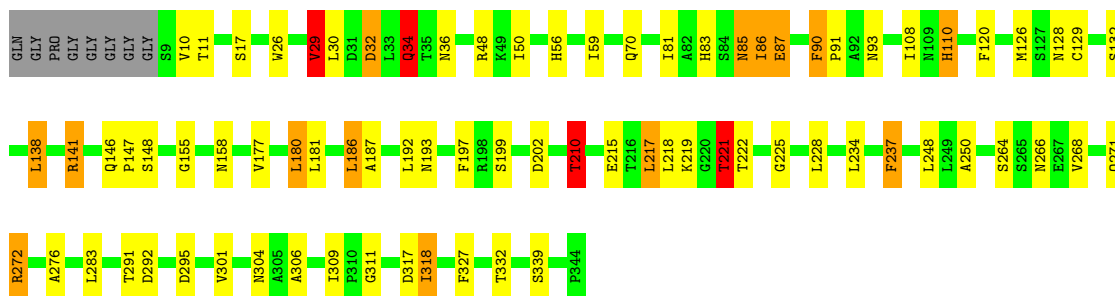
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	247	Total	O	0	0
			247	247		

i

Note EDS was not executed.

Chain A: 75% 18% . . .



Chain B:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	74.57Å 74.57Å 117.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.06	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.06)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2786	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

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: IOD, CA, NAG, HEM

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	0.96	3/2521 (0.1%)	1.85	66/3436 (1.9%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	318	ILE	CA-CB	7.19	1.63	1.54
1	A	36	ASN	CA-C	-6.92	1.48	1.52
1	A	29	VAL	CA-CB	6.05	1.63	1.54

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	ASP	CA-CB-CG	13.76	126.36	112.60
1	A	309	ILE	N-CA-C	-12.57	95.06	107.76
1	A	48	ARG	NE-CZ-NH2	-10.92	109.37	119.20
1	A	83	HIS	CA-CB-CG	-10.41	103.39	113.80
1	A	187	ALA	N-CA-C	9.00	123.12	108.99
1	A	210	THR	N-CA-CB	-8.98	95.32	110.41
1	A	141	ARG	NE-CZ-NH2	-8.54	111.52	119.20
1	A	34	GLN	OE1-CD-NE2	-8.24	114.36	122.60
1	A	237	PHE	CA-CB-CG	7.93	121.73	113.80
1	A	193	ASN	OD1-CG-ND2	-7.80	114.80	122.60
1	A	221	THR	N-CA-CB	-7.66	99.47	110.81
1	A	141	ARG	NE-CZ-NH1	7.00	128.50	121.50
1	A	339	SER	N-CA-C	-6.89	97.04	108.34
1	A	126	MET	CA-CB-CG	-6.83	100.45	114.10
1	A	146	GLN	N-CA-C	-6.79	100.18	110.50
1	A	83	HIS	CB-CG-CD2	-6.75	122.42	131.20
1	A	311	GLY	N-CA-C	6.68	123.23	113.48
1	A	304	ASN	OD1-CG-ND2	-6.63	115.97	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	ASN	OD1-CG-ND2	-6.59	116.00	122.60
1	A	158	ASN	OD1-CG-ND2	-6.56	116.04	122.60
1	A	271	GLN	CB-CG-CD	6.51	123.66	112.60
1	A	272	ARG	CB-CG-CD	6.33	125.87	111.30
1	A	70	GLN	OE1-CD-NE2	-6.29	116.31	122.60
1	A	177	VAL	N-CA-C	-6.21	104.29	110.62
1	A	141	ARG	CG-CD-NE	-6.21	98.35	112.00
1	A	48	ARG	NE-CZ-NH1	6.17	127.67	121.50
1	A	110	HIS	CB-CG-CD2	-6.12	123.25	131.20
1	A	11	THR	N-CA-C	-6.11	99.23	109.07
1	A	197	PHE	CA-CB-CG	5.92	119.72	113.80
1	A	48	ARG	CB-CG-CD	-5.88	97.77	111.30
1	A	271	GLN	OE1-CD-NE2	-5.80	116.80	122.60
1	A	225	GLY	CA-C-N	5.80	125.49	119.05
1	A	225	GLY	C-N-CA	5.80	125.49	119.05
1	A	110	HIS	CG-CD2-NE2	-5.79	101.41	107.20
1	A	83	HIS	CG-CD2-NE2	-5.75	101.45	107.20
1	A	93	ASN	OD1-CG-ND2	-5.74	116.86	122.60
1	A	264	SER	N-CA-C	5.71	121.14	113.72
1	A	210	THR	OG1-CB-CG2	5.70	120.69	109.30
1	A	132	SER	N-CA-C	5.57	117.77	110.08
1	A	83	HIS	ND1-CG-CD2	5.55	111.66	106.10
1	A	186	LEU	N-CA-CB	-5.50	102.81	111.23
1	A	215	GLU	N-CA-C	5.48	118.18	111.82
1	A	128	ASN	OD1-CG-ND2	-5.47	117.13	122.60
1	A	155	GLY	CA-C-N	5.47	125.09	119.56
1	A	155	GLY	C-N-CA	5.47	125.09	119.56
1	A	158	ASN	CB-CG-ND2	5.44	124.56	116.40
1	A	129	CYS	CA-C-N	5.39	125.40	119.90
1	A	129	CYS	C-N-CA	5.39	125.40	119.90
1	A	81	ILE	N-CA-C	-5.33	106.61	111.67
1	A	110	HIS	ND1-CG-CD2	5.31	111.41	106.10
1	A	306	ALA	CA-C-N	5.28	125.29	119.90
1	A	306	ALA	C-N-CA	5.28	125.29	119.90
1	A	148	SER	CA-C-N	5.24	123.49	119.66
1	A	148	SER	C-N-CA	5.24	123.49	119.66
1	A	34	GLN	CG-CD-NE2	5.23	124.25	116.40
1	A	327	PHE	CA-CB-CG	-5.16	108.64	113.80
1	A	56	HIS	CG-CD2-NE2	-5.15	102.05	107.20
1	A	199	SER	CA-C-N	5.14	125.08	119.78
1	A	199	SER	C-N-CA	5.14	125.08	119.78
1	A	90	PHE	CA-C-N	5.10	125.13	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	PHE	C-N-CA	5.10	125.13	119.32
1	A	32	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	291	THR	CA-CB-OG1	-5.05	102.02	109.60
1	A	87	GLU	N-CA-C	5.03	117.66	111.82
1	A	266	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	A	295	ASP	CA-CB-CG	5.00	117.60	112.60

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	2465	0	2373	23	0
2	B	28	0	25	1	0
3	A	2	0	0	0	0
4	A	1	0	0	2	0
5	A	43	0	30	0	0
6	A	247	0	0	4	0
All	All	2786	0	2428	23	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 5.

All (23) 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:219:LYS:HE2	1:A:317:ASP:HA	1.75	0.69
1:A:34:GLN:HE21	1:A:34:GLN:HA	1.58	0.68
1:A:86:ILE:HG12	1:A:147:PRO:HB3	1.84	0.58
1:A:210:THR:HG22	6:A:530:HOH:O	2.07	0.53
1:A:86:ILE:HG13	1:A:87:GLU:N	2.22	0.53
1:A:301:VAL:HG12	6:A:482:HOH:O	2.09	0.52
1:A:26:TRP:HA	1:A:29:VAL:HG13	1.91	0.52
1:A:217:LEU:HD13	1:A:250:ALA:HB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LYS:HE3	6:A:611:HOH:O	2.10	0.51
1:A:180:LEU:HD13	1:A:276:ALA:HB1	1.92	0.51
1:A:221:THR:HG21	6:A:538:HOH:O	2.11	0.51
1:A:90:PHE:HB3	4:A:702:IOD:I	2.82	0.49
1:A:268:VAL:O	1:A:272:ARG:HG3	2.13	0.49
1:A:32:ASP:OD2	1:A:110:HIS:HE1	1.97	0.47
1:A:138:LEU:HD12	1:A:292:ASP:HA	1.95	0.47
1:A:108:ILE:HD11	2:B:2:NAG:H2	1.97	0.47
1:A:219:LYS:HG3	1:A:317:ASP:O	2.15	0.46
1:A:34:GLN:HA	1:A:34:GLN:NE2	2.29	0.46
1:A:91:PRO:HD2	4:A:702:IOD:I	2.86	0.46
1:A:138:LEU:O	1:A:141:ARG:NH2	2.49	0.45
1:A:29:VAL:HG22	1:A:120:PHE:CE2	2.51	0.45
1:A:221:THR:HG22	1:A:222:THR:OG1	2.18	0.43
1:A:59:ILE:HD12	1:A:59:ILE:HA	1.92	0.42

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	334/344 (97%)	325 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	271/273 (99%)	247 (91%)	24 (9%)	9 4

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	17	SER
1	A	29	VAL
1	A	30	LEU
1	A	34	GLN
1	A	50	ILE
1	A	85	ASN
1	A	86	ILE
1	A	138	LEU
1	A	180	LEU
1	A	181	LEU
1	A	186	LEU
1	A	192	LEU
1	A	210	THR
1	A	217	LEU
1	A	218	LEU
1	A	221	THR
1	A	228	LEU
1	A	234	LEU
1	A	237	PHE
1	A	248	LEU
1	A	283	LEU
1	A	318	ILE
1	A	332	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	110	HIS
1	A	128	ASN
1	A	193	ASN
1	A	206	GLN
1	A	223	GLN

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 ⓘ

2 monosaccharides 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$
2	NAG	B	1	2,1	14,14,15	0.71	0	17,19,21	1.29	3 (17%)
2	NAG	B	2	2	14,14,15	0.59	0	17,19,21	1.40	4 (23%)

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
2	NAG	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C6-C5-C4	3.07	120.57	113.02
2	B	1	NAG	O5-C1-C2	-2.60	107.27	111.29
2	B	2	NAG	O5-C5-C4	-2.44	104.88	110.83
2	B	1	NAG	C3-C4-C5	2.30	114.41	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	2.26	115.22	112.19
2	B	2	NAG	C3-C4-C5	-2.22	106.20	110.23
2	B	2	NAG	O4-C4-C5	2.13	114.57	109.32

There are no chirality outliers.

All (2) torsion outliers are listed below:

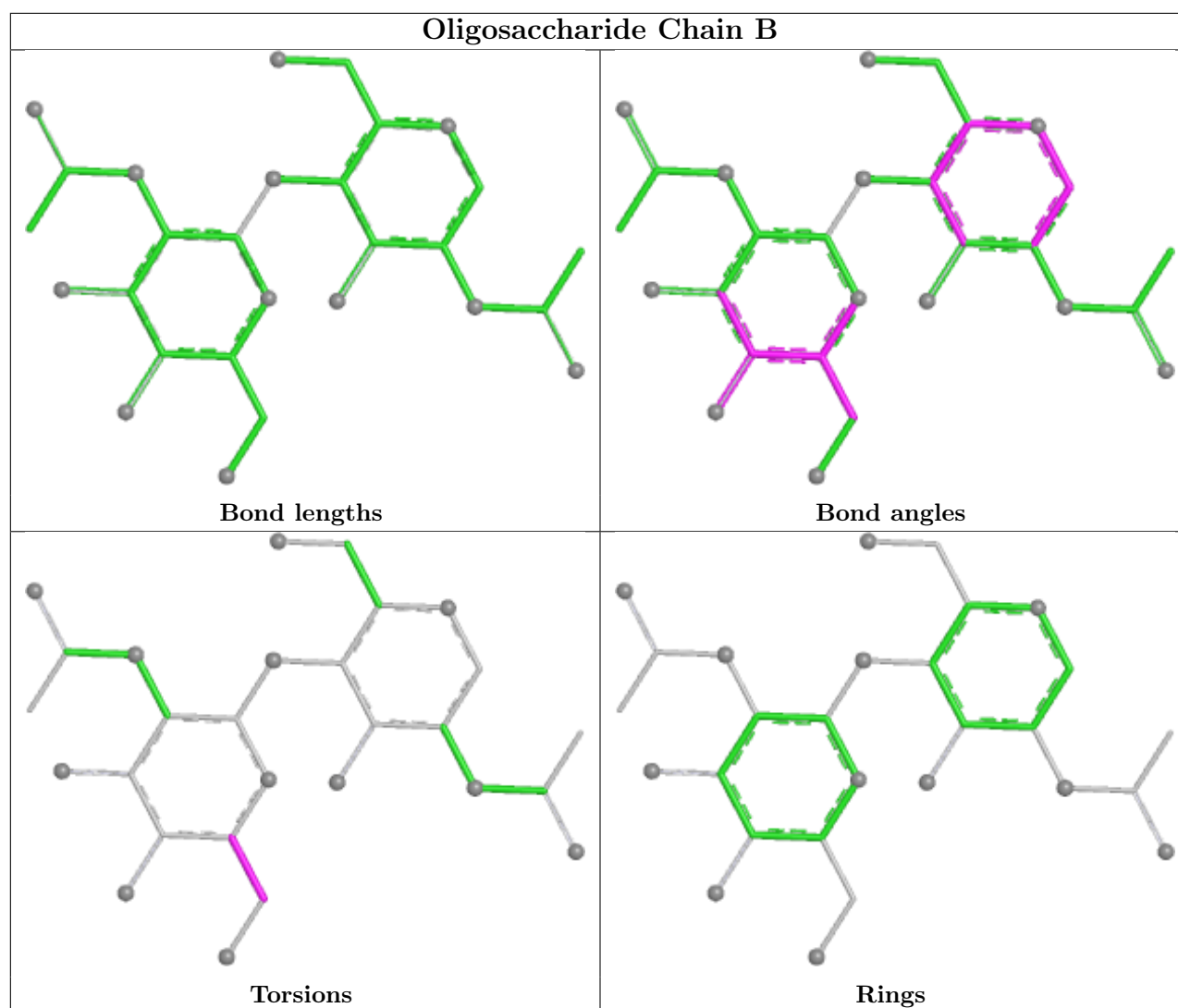
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	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 oligosaccharide.



5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z > 2$
5	HEM	A	345	1	50,50,50	1.22	6 (12%)	67,82,82	0.89	2 (2%)

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
5	HEM	A	345	1	-	6/14/54/54	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	345	HEM	CBB-CAB	3.31	1.46	1.30
5	A	345	HEM	CBC-CAC	3.15	1.45	1.30
5	A	345	HEM	CAC-C3C	-2.97	1.39	1.47
5	A	345	HEM	O2A-CGA	-2.71	1.21	1.30
5	A	345	HEM	O2D-CGD	-2.60	1.22	1.30
5	A	345	HEM	CAB-C3B	-2.50	1.40	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	345	HEM	C3B-C4B-NB	3.54	112.01	109.47
5	A	345	HEM	O2A-CGA-CBA	2.30	121.27	114.00

There are no chirality outliers.

All (6) torsion outliers are listed below:

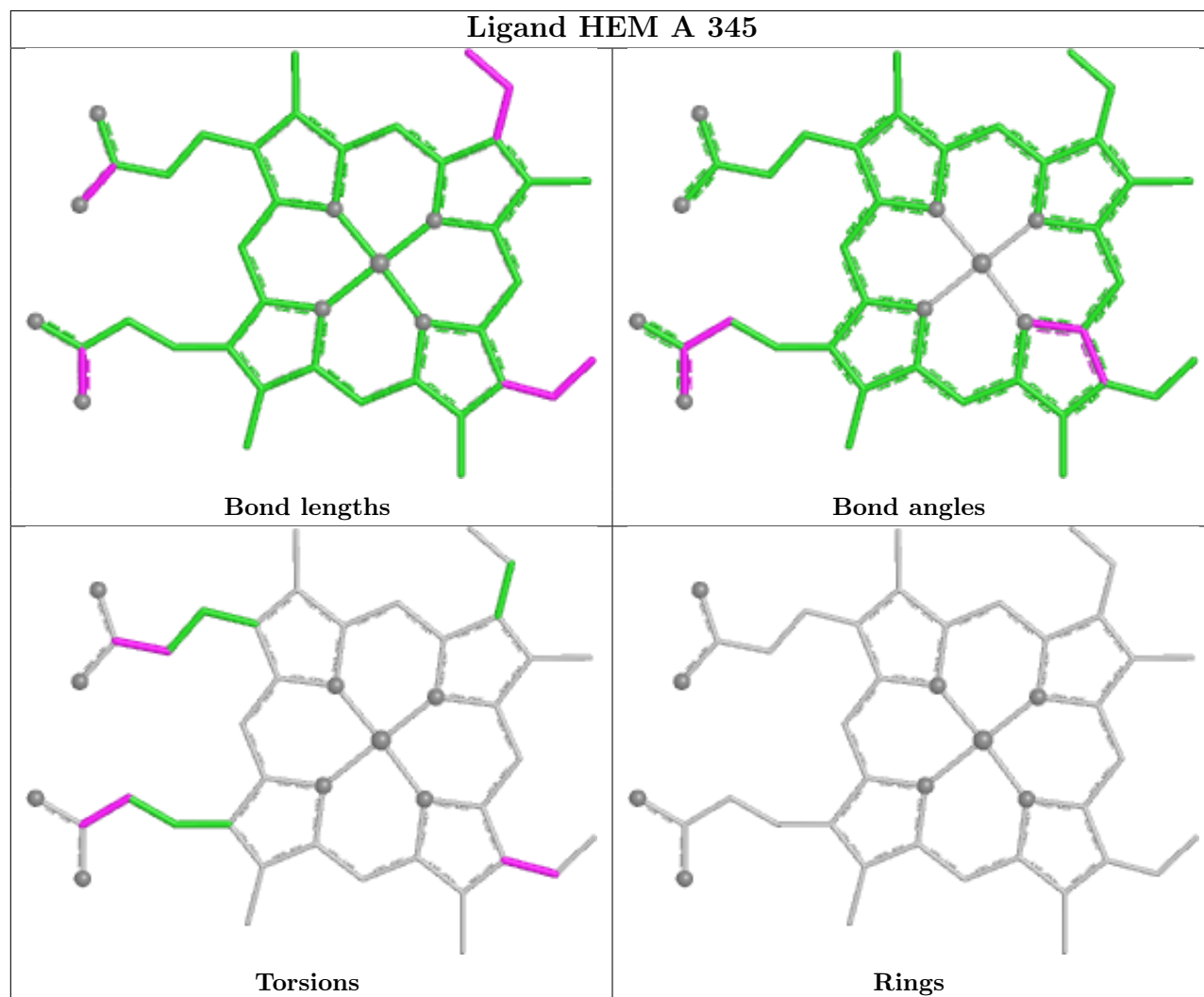
Mol	Chain	Res	Type	Atoms
5	A	345	HEM	C2B-C3B-CAB-CBB
5	A	345	HEM	C4B-C3B-CAB-CBB
5	A	345	HEM	CAA-CBA-CGA-O2A
5	A	345	HEM	CAA-CBA-CGA-O1A
5	A	345	HEM	CAD-CBD-CGD-O2D
5	A	345	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

No monomer is involved in short contacts.

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.