



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 01:51 AM BST

PDB ID : 3PGH
Title : CYCLOOXYGENASE-2 (PROSTAGLANDIN SYNTHASE-2) COM-
PLEXED WITH A NON-SELECTIVE INHIBITOR, FLURBIPROFEN
Authors : Kurumbail, R.; Stallings, W.
Deposited on : 1996-12-18
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

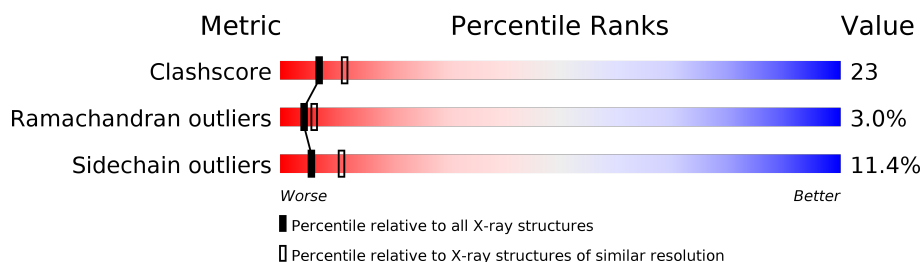
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 on 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	587	
1	B	587	
1	C	587	
1	D	587	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18304 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 CYCLOOXYGENASE-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			
1	B	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			
1	C	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			
1	D	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			

There are 8 discrepancies between the modelled and reference sequences:

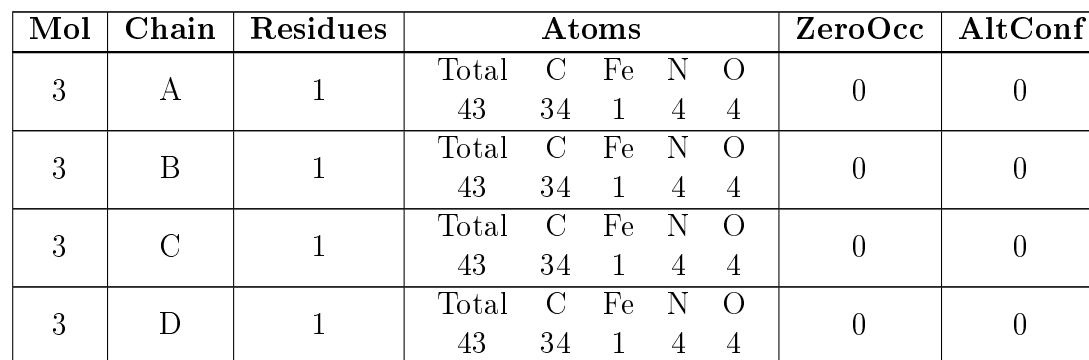
Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLN	ASN	conflict	UNP Q05769
A	333	LYS	ARG	conflict	UNP Q05769
B	310	GLN	ASN	conflict	UNP Q05769
B	333	LYS	ARG	conflict	UNP Q05769
C	310	GLN	ASN	conflict	UNP Q05769
C	333	LYS	ARG	conflict	UNP Q05769
D	310	GLN	ASN	conflict	UNP Q05769
D	333	LYS	ARG	conflict	UNP Q05769

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



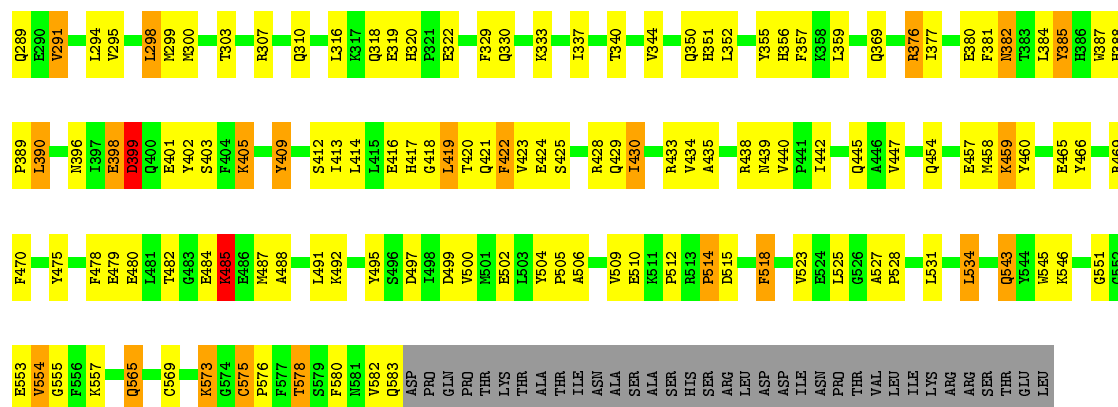
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



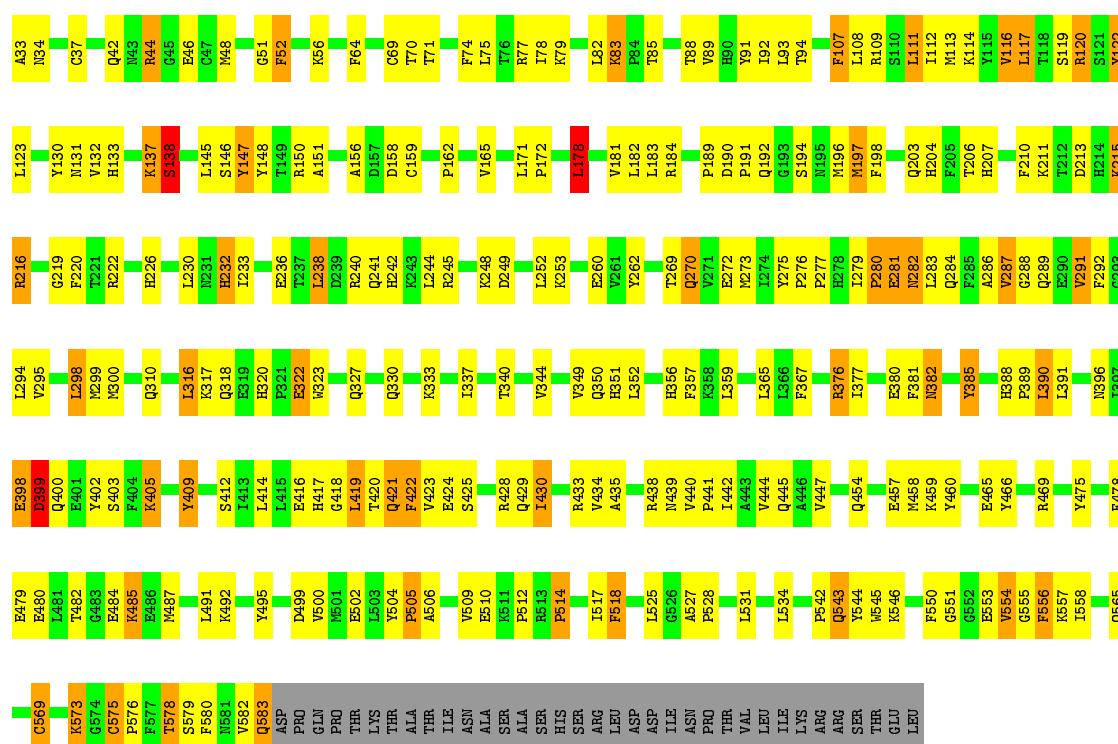
- FLP
-
- The chemical structure shows a central carbon atom (C12(S)) bonded to a hydroxyl group (OH, O1), a methyl group (C13), and two phenyl rings. One phenyl ring is substituted with two fluorine atoms (F) at the 2 and 4 positions. The atoms are labeled with green text: C1 through C14, O, O1, and F. The stereochemistry at C12 is (S), indicated by the label C12(S) and a wedge bond to the methyl group C13.
- CC(O)(c1ccccc1)c2cc(F)cc(F)c2

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	O	0	0
			18	15	1	2		
4	B	1	Total	C	F	O	0	0
			18	15	1	2		
4	C	1	Total	C	F	O	0	0
			18	15	1	2		
4	D	1	Total	C	F	O	0	0
			18	15	1	2		



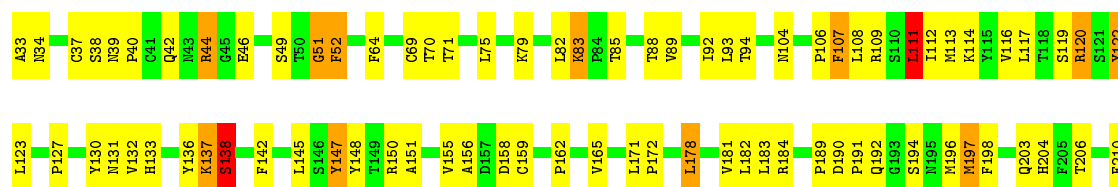
• Molecule 1: CYCLOOXYGENASE-2

Chain C: 51% 34% 8% 6%



• Molecule 1: CYCLOOXYGENASE-2

Chain D: 52% 34% 7% 6%



C575	P576	F577	T578	S579	F580	N581	V582	Q583	ASP	PRO	GLN	PRO	THR	LYS	THR	ALA	THR	ILE	ASN	ALA	SER	ALA	SER	HIS	SER	ARG	LEU	ASP	ASP	ILE	ASN	PRO	THR	THR	VAL	LEU	LEU	ILE	LYS	ARG	ARG	SER	THR	THR	GLU	LEU														
L481	T482	G483	E484	K485	E486	M487	A488		L491	K492	Y495		D499	V500	M501	E502	I503	Y504	P505	A506		V509	E510	K511	P512	R513	P514		I517	F518		L525	G526	A527	P528		L531		L534		Q543	K546	G551	G552	E553	V554	G555	F556	K557		Q565		C569	K573	G574					
E398	D399	Q400	E401	Y402	S403	F404	K405		Y409		S412	I413	L414	L415	E416	H417	G418	I419	T420	F422	V423	E424	S425		R428	Q429	I430		R433	V434		R438	N439	V440	P441	I442		Q445	A446	V447		Q454		E457	M458	K459	Y460		E465	Y466		R469		Y475		F478	E479	E480		
V291	F292	G293	L294	V295		L298	M299	M300		T303		R307		Q310		L316	K317	Q318	E319	H320	P321	E322		F329		K333		I337		V344		Q350	H351	L352		Y355	H356	F357	K358	L359		Q369		R376	I377		E380	F381	N382		Y385		P389	L390	I391	P392		N396	I397	
K211	I212	D213	H214	K215	R216		G219		R222		L230	N231	H232	I233		E236	T237	L238		H242	K243	L244	R245		K248		L252	K253		G258	G259	E260	V261	Y262		K267	D268	T269	Q270	V271	E272	M273	I274	Y275	P276	P277		H278	I279	P280	E281	N282	L283	Q284	P285	A286	V287	G288	Q289	E290

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	179.50Å 133.80Å 117.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	63.1 (8.00-2.50)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.236 , 0.316	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18304	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: FLP, 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	0.67	1/4600 (0.0%)	0.85	5/6237 (0.1%)
1	B	0.68	1/4600 (0.0%)	0.86	6/6237 (0.1%)
1	C	0.65	0/4600	0.86	5/6237 (0.1%)
1	D	0.67	1/4600 (0.0%)	0.85	6/6237 (0.1%)
All	All	0.67	3/18400 (0.0%)	0.86	22/24948 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	CYS	CB-SG	-5.72	1.72	1.81
1	B	236	GLU	CG-CD	5.45	1.60	1.51
1	D	479	GLU	CG-CD	5.12	1.59	1.51

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	390	LEU	CA-CB-CG	6.90	131.17	115.30
1	B	287	VAL	N-CA-C	6.78	129.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	287	VAL	N-CA-C	6.43	128.35	111.00
1	A	390	LEU	CA-CB-CG	6.42	130.08	115.30
1	A	287	VAL	N-CA-C	6.42	128.32	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	TYR	Sidechain
1	B	147	TYR	Sidechain
1	C	147	TYR	Sidechain
1	C	91	TYR	Sidechain
1	D	147	TYR	Sidechain

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	4473	0	4374	207	0
1	B	4473	0	4374	217	0
1	C	4473	0	4375	215	0
1	D	4473	0	4375	201	0
2	A	42	0	39	4	0
2	B	42	0	39	3	0
2	C	42	0	39	0	0
2	D	42	0	39	0	0
3	A	43	0	30	6	0
3	B	43	0	30	9	0
3	C	43	0	30	6	0
3	D	43	0	30	9	0
4	A	18	0	12	1	0
4	B	18	0	12	6	0
4	C	18	0	12	3	0
4	D	18	0	12	3	0
All	All	18304	0	17822	829	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 23.

The worst 5 of 829 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:C:424:GLU:HA	1:C:428:ARG:HH21	1.27	0.97
1:A:458:MET:HE2	1:A:460:TYR:HE1	1.27	0.96
1:A:424:GLU:HA	1:A:428:ARG:HH21	1.31	0.96
1:D:424:GLU:HA	1:D:428:ARG:HH21	1.30	0.95
1:B:479:GLU:HG2	1:B:485:LYS:NZ	1.82	0.95

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	550/587 (94%)	473 (86%)	62 (11%)	15 (3%)	5	7
1	B	550/587 (94%)	484 (88%)	49 (9%)	17 (3%)	4	5
1	C	550/587 (94%)	479 (87%)	54 (10%)	17 (3%)	4	5
1	D	550/587 (94%)	477 (87%)	57 (10%)	16 (3%)	4	6
All	All	2200/2348 (94%)	1913 (87%)	222 (10%)	65 (3%)	4	6

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	PHE
1	A	82	LEU
1	A	130	TYR
1	A	138	SER
1	A	282	ASN

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	493/525 (94%)	436 (88%)	57 (12%)	5	10
1	B	493/525 (94%)	437 (89%)	56 (11%)	5	11
1	C	493/525 (94%)	437 (89%)	56 (11%)	5	11
1	D	493/525 (94%)	437 (89%)	56 (11%)	5	11
All	All	1972/2100 (94%)	1747 (89%)	225 (11%)	5	11

5 of 225 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	484	GLU
1	C	165	VAL
1	D	422	PHE
1	B	518	PHE
1	C	52	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	417	HIS
1	C	232	HIS
1	D	396	ASN
1	B	454	GLN
1	C	95	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 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	$\# Z > 2$
2	NAG	A	681	1	14,14,15	0.78	0	17,19,21	0.77	0
4	FLP	A	701	-	16,19,19	1.45	3 (18%)	22,26,26	1.05	2 (9%)
3	HEM	D	682	1	27,50,50	1.91	6 (22%)	17,82,82	0.99	1 (5%)
4	FLP	C	701	-	16,19,19	1.07	1 (6%)	22,26,26	1.11	2 (9%)
3	HEM	B	682	1	27,50,50	1.95	6 (22%)	17,82,82	1.21	2 (11%)
2	NAG	A	671	1	14,14,15	0.74	0	17,19,21	1.58	5 (29%)
2	NAG	C	661	1	14,14,15	0.27	0	17,19,21	0.88	1 (5%)
2	NAG	C	671	1	14,14,15	0.81	1 (7%)	17,19,21	1.60	4 (23%)
2	NAG	A	661	1	14,14,15	0.57	0	17,19,21	0.90	1 (5%)
2	NAG	D	671	1	14,14,15	0.64	0	17,19,21	1.48	3 (17%)
2	NAG	B	661	1	14,14,15	0.52	0	17,19,21	1.02	1 (5%)
2	NAG	B	681	1	14,14,15	0.75	0	17,19,21	0.90	0
4	FLP	D	701	-	16,19,19	1.47	1 (6%)	22,26,26	0.98	1 (4%)
2	NAG	D	681	1	14,14,15	0.79	0	17,19,21	0.87	0
2	NAG	B	671	1	14,14,15	0.78	0	17,19,21	1.41	3 (17%)
2	NAG	D	661	1	14,14,15	0.67	0	17,19,21	0.94	1 (5%)
2	NAG	C	681	1	14,14,15	0.62	0	17,19,21	0.83	0
3	HEM	A	682	1	27,50,50	1.92	6 (22%)	17,82,82	1.15	0
3	HEM	C	682	1	27,50,50	1.86	6 (22%)	17,82,82	1.28	1 (5%)
4	FLP	B	701	-	16,19,19	1.77	5 (31%)	22,26,26	1.11	1 (4%)

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	A	681	1	-	2/6/23/26	0/1/1/1
4	FLP	A	701	-	-	0/8/12/12	0/2/2/2
3	HEM	D	682	1	-	0/6/54/54	-
4	FLP	C	701	-	-	0/8/12/12	0/2/2/2
3	HEM	B	682	1	-	0/6/54/54	-
2	NAG	A	671	1	-	2/6/23/26	0/1/1/1
2	NAG	C	661	1	-	0/6/23/26	0/1/1/1
2	NAG	C	671	1	-	2/6/23/26	0/1/1/1
2	NAG	A	661	1	-	0/6/23/26	0/1/1/1
2	NAG	D	671	1	-	2/6/23/26	0/1/1/1
2	NAG	B	661	1	-	0/6/23/26	0/1/1/1
2	NAG	B	681	1	-	2/6/23/26	0/1/1/1
4	FLP	D	701	-	-	0/8/12/12	0/2/2/2
2	NAG	D	681	1	-	2/6/23/26	0/1/1/1
2	NAG	B	671	1	-	2/6/23/26	0/1/1/1
2	NAG	D	661	1	-	0/6/23/26	0/1/1/1
2	NAG	C	681	1	-	2/6/23/26	0/1/1/1
3	HEM	A	682	1	-	0/6/54/54	-
3	HEM	C	682	1	-	0/6/54/54	-
4	FLP	B	701	-	-	0/8/12/12	0/2/2/2

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	682	HEM	C3C-CAC	-5.16	1.37	1.47
3	B	682	HEM	C3B-CAB	-5.00	1.37	1.47
3	A	682	HEM	C3C-CAC	-4.78	1.38	1.47
3	A	682	HEM	C3C-C2C	-4.75	1.33	1.40
3	C	682	HEM	C3C-CAC	-4.70	1.38	1.47

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	671	NAG	C1-C2-N2	3.48	116.43	110.49
2	A	671	NAG	C4-C3-C2	-3.31	106.17	111.02
2	B	671	NAG	C4-C3-C2	-3.29	106.19	111.02
2	C	671	NAG	C1-O5-C5	3.07	116.35	112.19
2	D	671	NAG	C4-C3-C2	-3.05	106.55	111.02

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

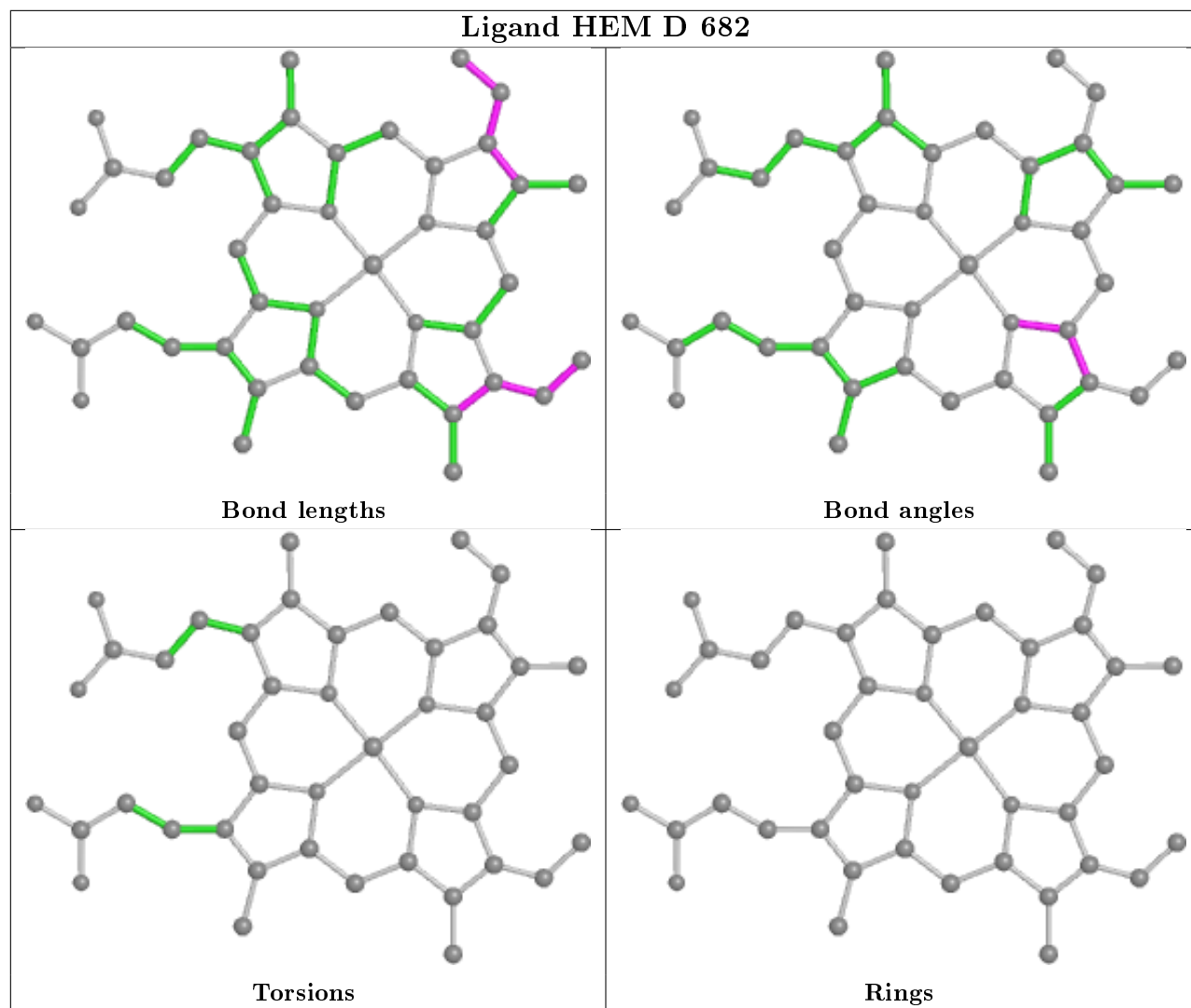
Mol	Chain	Res	Type	Atoms
2	B	671	NAG	O5-C5-C6-O6
2	A	671	NAG	O5-C5-C6-O6
2	C	671	NAG	O5-C5-C6-O6
2	D	671	NAG	O5-C5-C6-O6
2	C	671	NAG	C4-C5-C6-O6

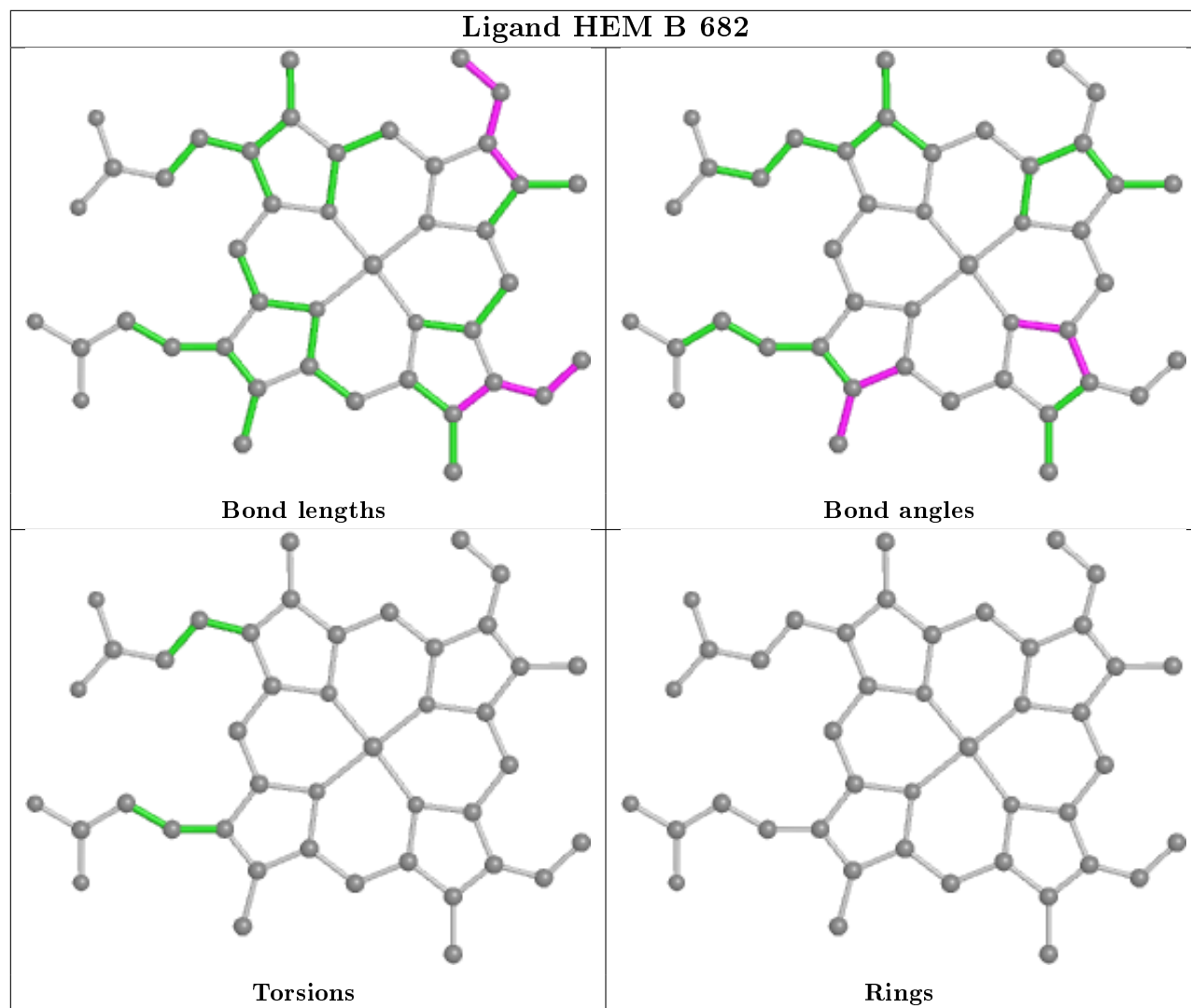
There are no ring outliers.

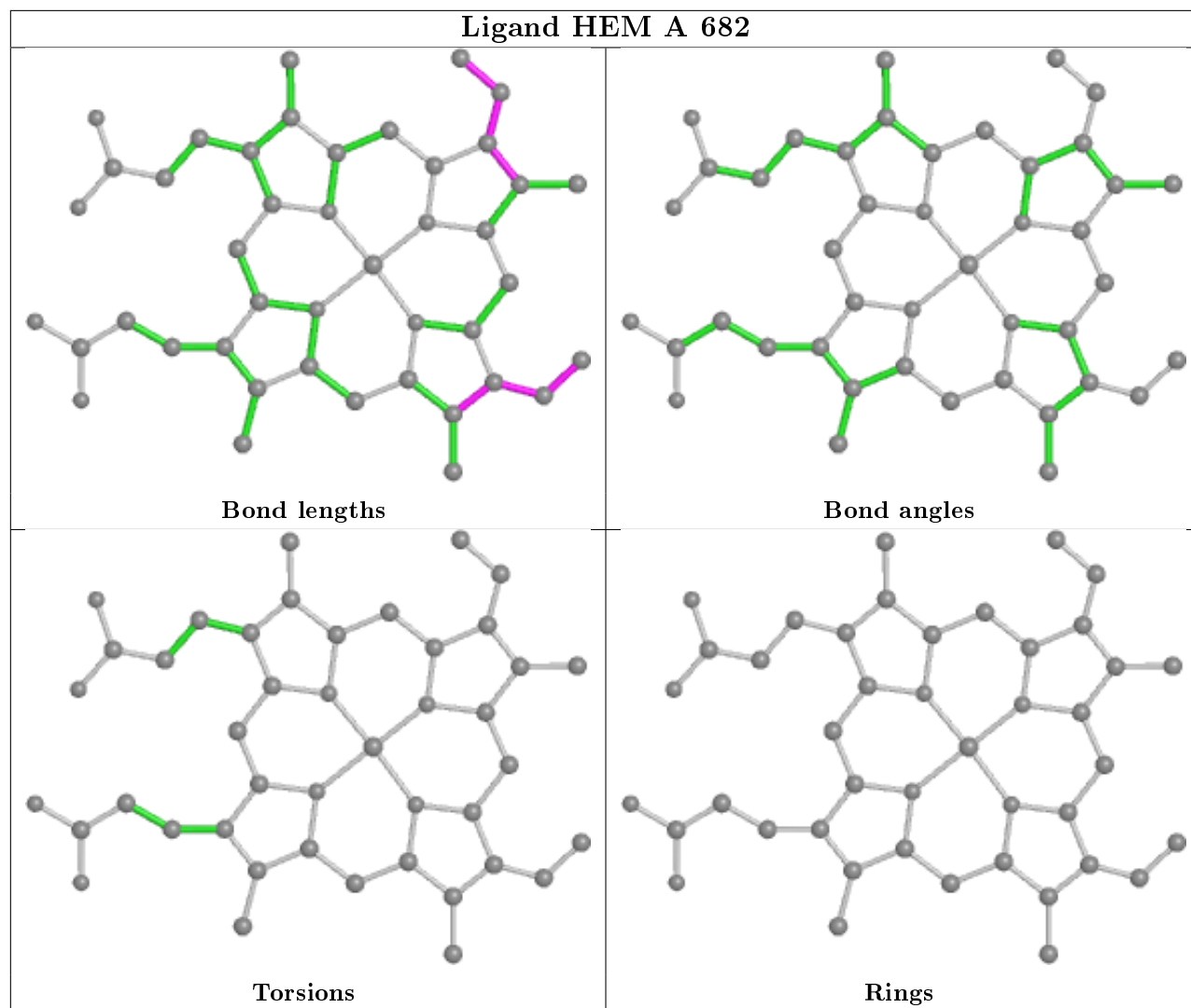
12 monomers are involved in 50 short contacts:

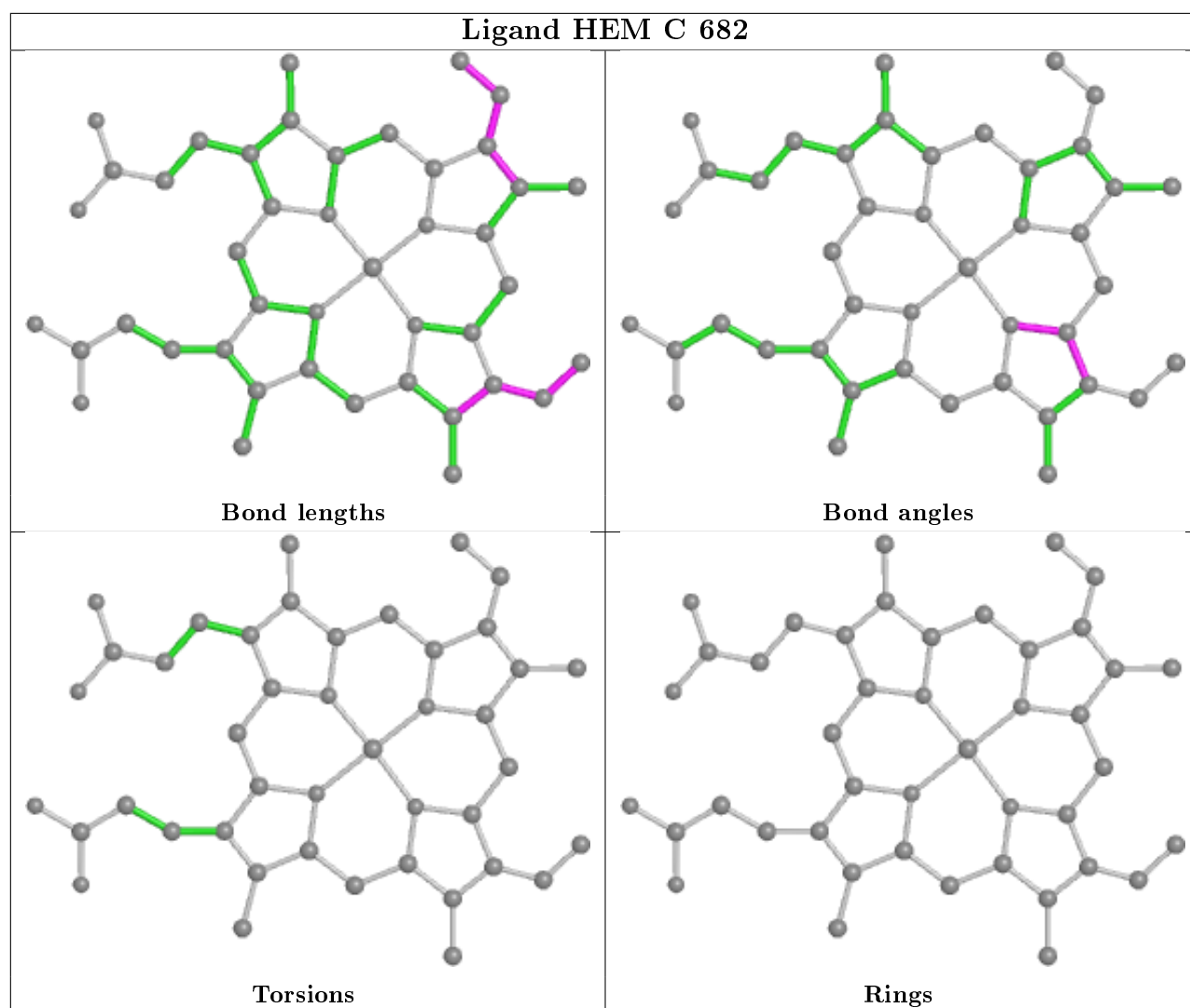
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	FLP	1	0
3	D	682	HEM	9	0
4	C	701	FLP	3	0
3	B	682	HEM	9	0
2	A	671	NAG	4	0
2	B	661	NAG	1	0
2	B	681	NAG	1	0
4	D	701	FLP	3	0
2	B	671	NAG	1	0
3	A	682	HEM	6	0
3	C	682	HEM	6	0
4	B	701	FLP	6	0

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.