wwPDB X-ray Structure Validation Summary Report (i)

Jul 31, 2023 – 10:06 PM EDT

PDB ID	:	6COX
Title	:	CYCLOOXYGENASE-2 (PROSTAGLANDIN SYNTHASE-2) COMPLEXED WITH A SELECTIVE INHIBITOR, SC-558 IN I222 SPACE GROUP
Authors	:	Kurumbail, R.; Stallings, W.
Deposited on	:	1996-12-18
Resolution	:	2.80 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 (i) 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:

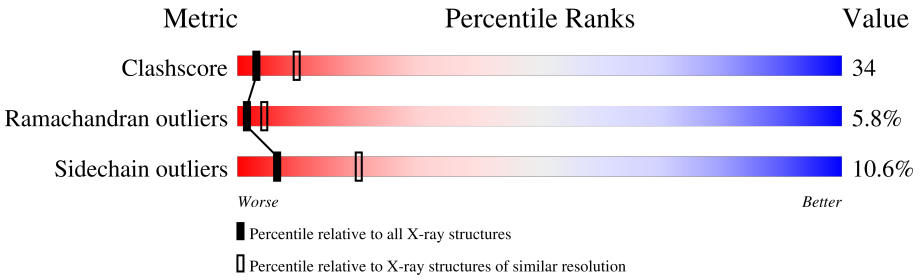
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	587	39% 45% 9% • 6%
1	B	587	40% 45% 9% • 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9168 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.

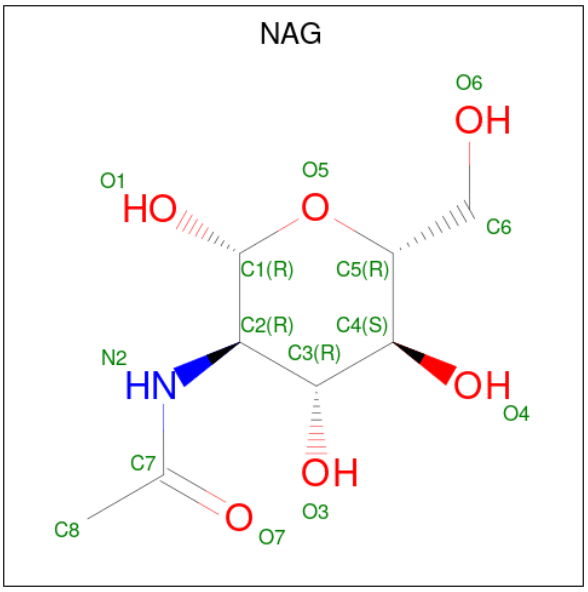
- Molecule 1 is a protein called CYCLOOXYGENASE-2.

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			

There are 4 discrepancies between the modelled and reference sequences:

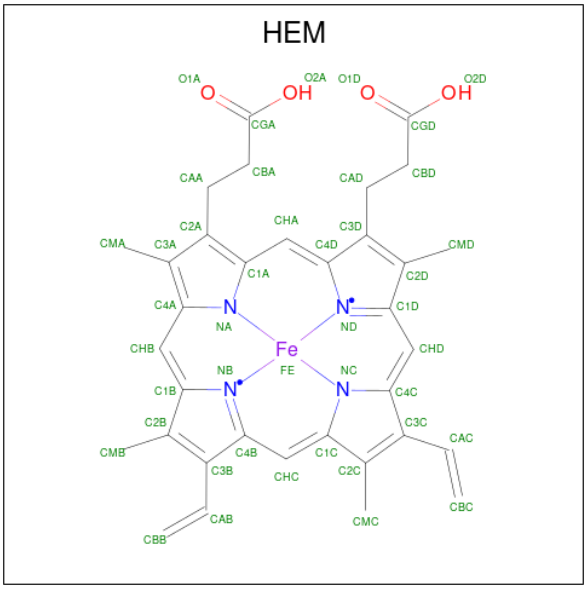
Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLN	ASN	conflict	UNP Q05769
A	333	LYS	ARG	conflict	UNP Q05769
B	310	GLN	ASN	conflict	UNP Q05769
B	333	LYS	ARG	conflict	UNP Q05769

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



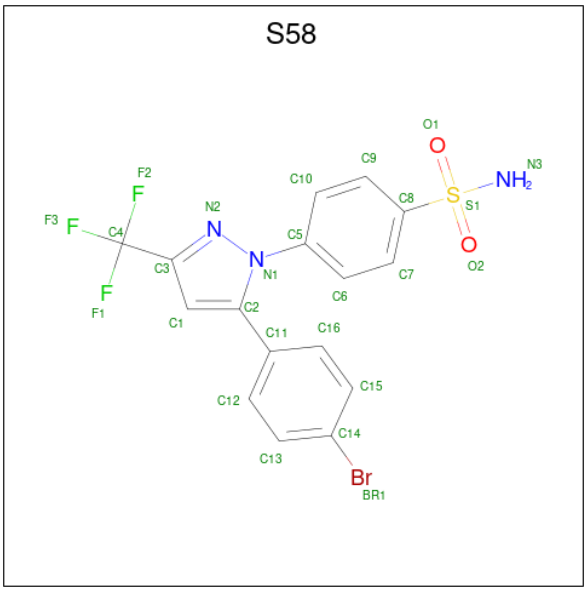
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

- Molecule 4 is 1-PHENYLSULFONAMIDE-3-TRIFLUOROMETHYL-5-PARABROMOPHENYLPYRAZOLE (three-letter code: S58) (formula: $C_{16}H_{11}BrF_3N_3O_2S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total	Br	C	F	N	O	S	0	0
			26	1	16	3	3	2	1		
4	B	1	Total	Br	C	F	N	O	S	0	0
			26	1	16	3	3	2	1		

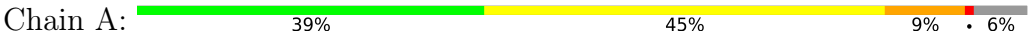
3 Residue-property plots (i)

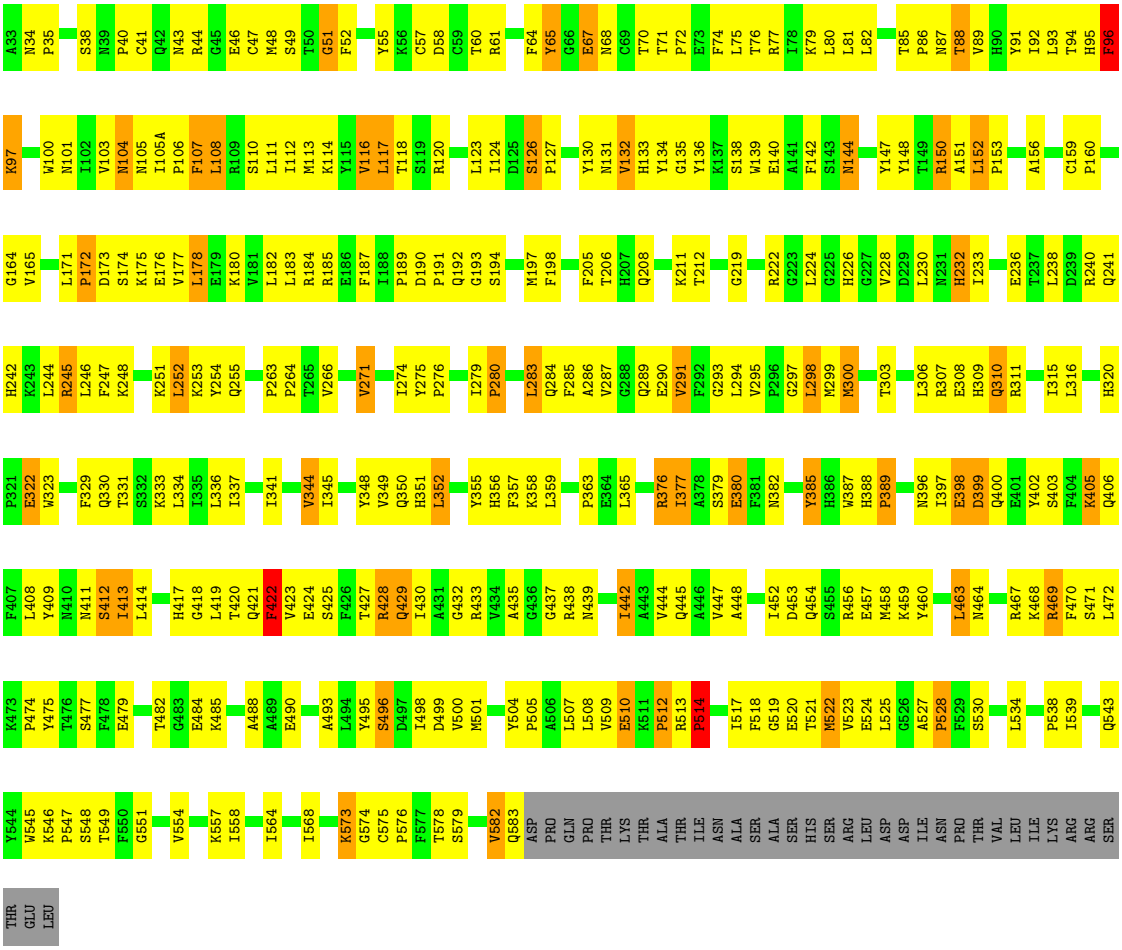
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: CYCLOOXYGENASE-2

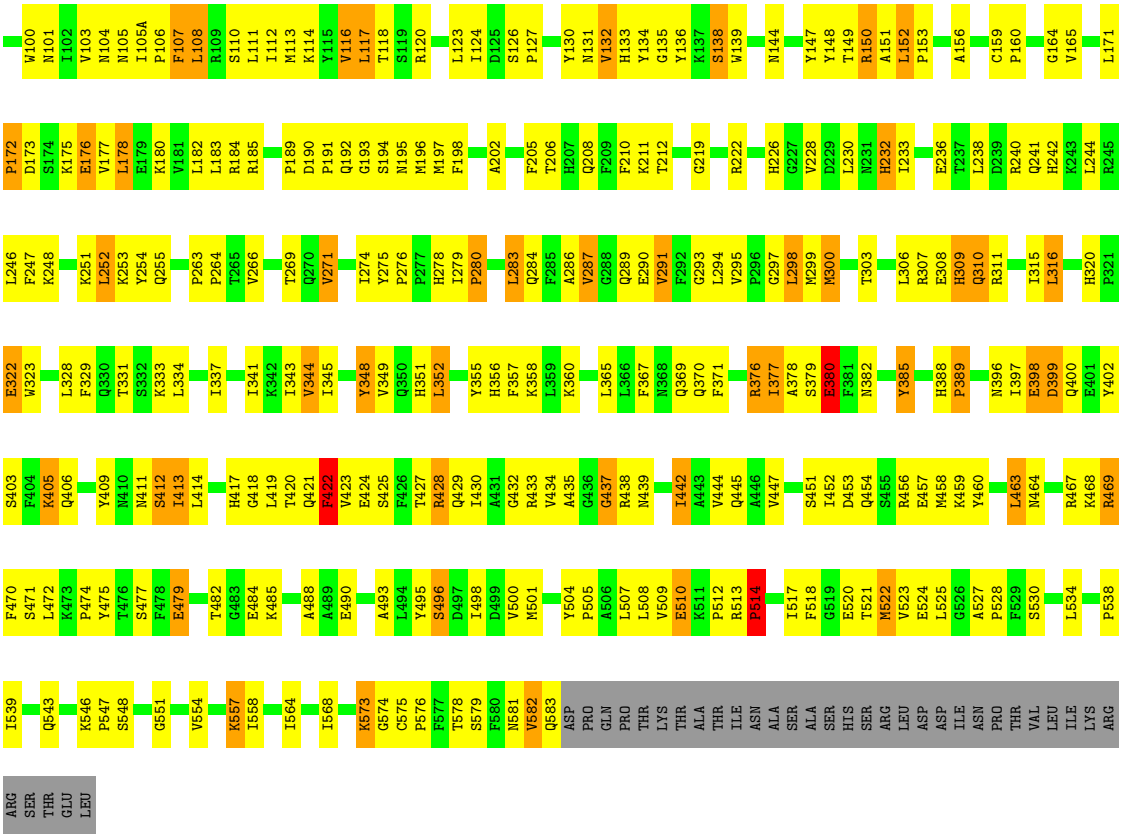
Chain A:





• Molecule 1: CYCLOOXYGENASE-2

Chain B:


W100 N101 I102 V103 N104 N105 I105A P106 F107 L108 R109 S110 L111 I112 M113 K114 Y115 V116 L117 T118 S119 R120 L123 I124 D125 S126 P127 Y130 N131 V132 H133 Y134 G135 Y136 K137 S138 W139 N144 Y147 Y148 T149 R150 A151 L152 P153 A156 C159 P160 G164 V165 L171
P172 D173 S174 K175 E176 V177 L178 E179 K180 V181 L182 L183 R184 R185 P189 D190 P191 Q192 G193 S194 N195 M196 M197 F198 A202 F205 T206 H207 Q208 F209 F210 K211 T212 G219 R222 H226 G227 V228 D229 L230 N231 H232 I233 E236 T237 L238 D239 R240 Q241 H242 K243 L244 R245
L246 F247 K248 K251 L252 K253 Y254 Q255 P263 P264 T265 V266 T269 Q270 V271 I274 Y275 P276 P277 H278 I279 P280 L283 Q284 F285 A286 V287 C288 Q289 E290 V291 F292 G293 L294 V295 P296 G297 L298 M299 M300 T303 L306 R307 E308 H309 Q310 R311 I315 L316 H320 P321
E322 W323 L328 F329 Q330 T331 S332 K333 L334 I337 I341 K342 I343 V344 I345 Y348 V349 Q350 H351 L352 Y355 H356 F357 K358 L359 K360 L365 L366 F367 N368 Q369 Q370 F371 R376 I377 A378 S379 E380 F381 N382 Y385 H388 P389 N396 I397 E398 D399 Q400 E401 Y402
S403 F404 K405 Q406 Y409 N410 N411 S412 I413 L414 H417 G418 L419 T420 Q421 F422 V423 E424 S425 F426 T427 R428 Q429 I430 A431 G432 R433 V434 A435 G436 G437 R438 N439 T442 A443 V444 Q445 A446 V447 S451 I452 D453 Q454 S455 R456 E457 M458 K459 Y460 L463 N464 R467 K468 R469
F470 S471 L472 K473 P474 Y475 T476 S477 F478 E479 T482 G483 E484 K485 A488 A489 E490 A493 L494 Y495 S496 D497 I498 D499 V500 M501 Y504 P505 A506 L507 L508 V509 E510 K511 P512 R513 P514 I517 F518 G519 E520 T521 M522 V523 E524 L525 G526 A527 P528 F529 S530 L534 P538
I539 Q543 K546 P547 S548 G551 V554 K557 I558 I564 I568 K573 G574 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 VAL LEU ILE LYS ARG
ARG SER THR GLU LEU

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	181.17Å 132.81Å 122.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	88.5 (8.00-2.80)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.220 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9168	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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, NAG, S58

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.65	0/4600	0.84	1/6237 (0.0%)
1	B	0.65	1/4600 (0.0%)	0.85	2/6237 (0.0%)
All	All	0.65	1/9200 (0.0%)	0.85	3/12474 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	479	GLU	CB-CG	5.55	1.62	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	287	VAL	N-CA-C	5.54	125.97	111.00
1	B	287	VAL	N-CA-C	5.29	125.28	111.00
1	B	437	GLY	N-CA-C	-5.17	100.17	113.10

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	4473	0	4375	324	0
1	B	4473	0	4375	301	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	42	0	39	1	0
2	B	42	0	39	0	0
3	A	43	0	30	2	0
3	B	43	0	30	1	0
4	A	26	0	11	3	0
4	B	26	0	11	2	0
All	All	9168	0	8910	607	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 34.

The worst 5 of 607 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:283:LEU:HD22	1:A:411:ASN:HB2	1.32	1.11
1:B:280:PRO:HD2	1:B:283:LEU:HD23	1.35	1.09
1:A:279:ILE:HG23	1:A:283:LEU:HG	1.32	1.08
1:B:279:ILE:HG23	1:B:283:LEU:HG	1.37	1.07
1:A:280:PRO:HD2	1:A:283:LEU:HD23	1.41	1.02

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%)	435 (79%)	84 (15%)	31 (6%)	2 5
1	B	550/587 (94%)	431 (78%)	86 (16%)	33 (6%)	1 4
All	All	1100/1174 (94%)	866 (79%)	170 (16%)	64 (6%)	1 4

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	SER
1	A	348	TYR
1	A	398	GLU
1	A	510	GLU
1	A	514	PRO

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%)	439 (89%)	54 (11%)	6	19
1	B	493/525 (94%)	442 (90%)	51 (10%)	7	21
All	All	986/1050 (94%)	881 (89%)	105 (11%)	6	20

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	96	PHE
1	B	238	LEU
1	B	464	ASN
1	B	107	PHE
1	B	150	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	350	GLN
1	B	454	GLN
1	B	565	GLN
1	B	543	GLN
1	A	351	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)

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	$\#\|Z\| > 2$
2	NAG	A	661	1	14,14,15	0.64	0	17,19,21	0.52	0
4	S58	B	701	-	25,28,28	2.56	7 (28%)	31,43,43	1.95	8 (25%)
3	HEM	B	682	1	41,50,50	1.50	5 (12%)	45,82,82	1.01	2 (4%)
2	NAG	B	661	1	14,14,15	0.57	0	17,19,21	0.59	0
2	NAG	A	681	1	14,14,15	0.32	0	17,19,21	0.97	1 (5%)
2	NAG	B	681	1	14,14,15	0.68	0	17,19,21	0.84	0
2	NAG	A	671	1	14,14,15	0.42	0	17,19,21	0.81	1 (5%)
4	S58	A	701	-	25,28,28	2.66	8 (32%)	31,43,43	2.20	10 (32%)
2	NAG	B	671	1	14,14,15	0.55	0	17,19,21	0.91	1 (5%)
3	HEM	A	682	1	41,50,50	1.47	5 (12%)	45,82,82	0.93	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
2	NAG	A	661	1	-	2/6/23/26	0/1/1/1
4	S58	B	701	-	-	0/12/20/20	0/3/3/3
3	HEM	B	682	1	-	5/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	661	1	-	2/6/23/26	0/1/1/1
2	NAG	A	681	1	-	0/6/23/26	0/1/1/1
2	NAG	B	681	1	-	0/6/23/26	0/1/1/1
2	NAG	A	671	1	-	2/6/23/26	0/1/1/1
4	S58	A	701	-	-	0/12/20/20	0/3/3/3
2	NAG	B	671	1	-	2/6/23/26	0/1/1/1
3	HEM	A	682	1	-	5/12/54/54	-

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	S58	S1-N3	8.09	1.76	1.60
4	B	701	S58	S1-N3	7.31	1.74	1.60
4	B	701	S58	C1-C3	6.12	1.47	1.39
4	A	701	S58	C1-C3	5.83	1.47	1.39
3	A	682	HEM	C3C-CAC	-4.57	1.38	1.47

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	701	S58	C4-C3-N2	5.59	126.29	119.72
4	A	701	S58	C4-C3-N2	5.39	126.05	119.72
4	A	701	S58	O2-S1-O1	-5.26	110.11	118.76
4	B	701	S58	O2-S1-O1	-4.51	111.34	118.76
4	A	701	S58	O1-S1-N3	4.35	113.81	107.36

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	682	HEM	C2A-CAA-CBA-CGA
3	A	682	HEM	C2B-C3B-CAB-CBB
3	B	682	HEM	C2A-CAA-CBA-CGA
3	B	682	HEM	C2B-C3B-CAB-CBB
2	A	671	NAG	O5-C5-C6-O6

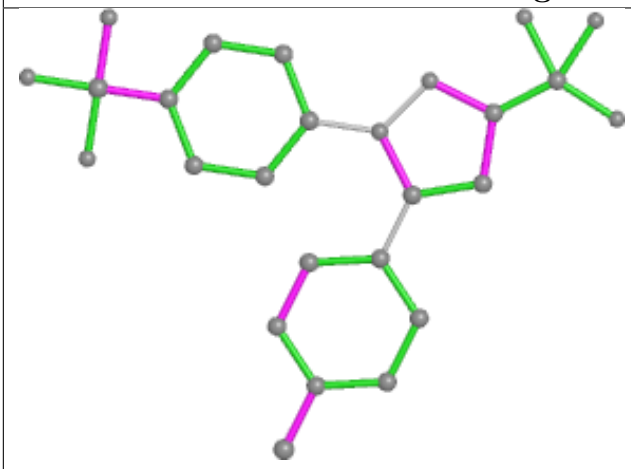
There are no ring outliers.

5 monomers are involved in 9 short contacts:

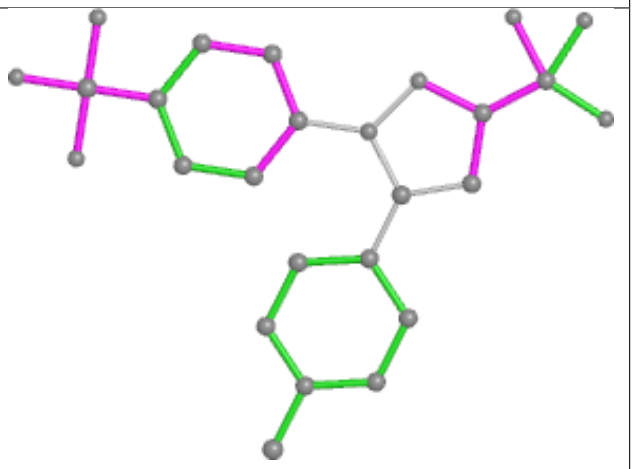
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	661	NAG	1	0
4	B	701	S58	2	0
3	B	682	HEM	1	0
4	A	701	S58	3	0
3	A	682	HEM	2	0

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 then 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.

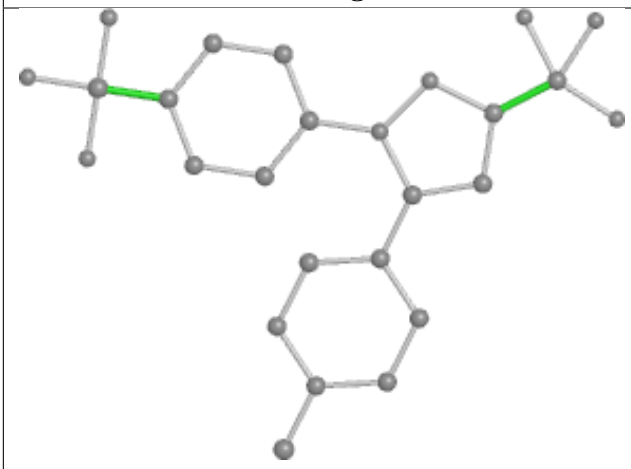
Ligand S58 B 701



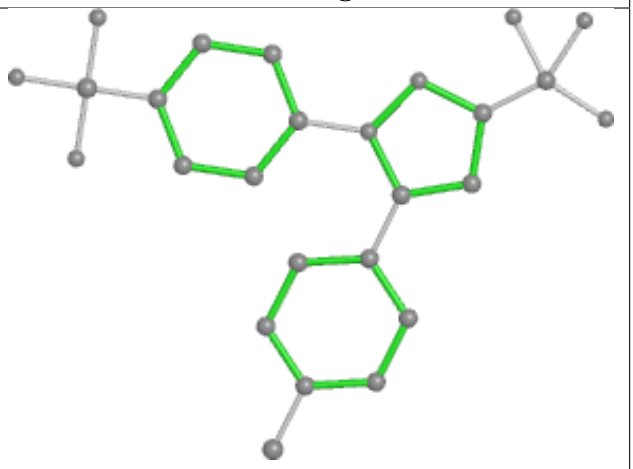
Bond lengths



Bond angles

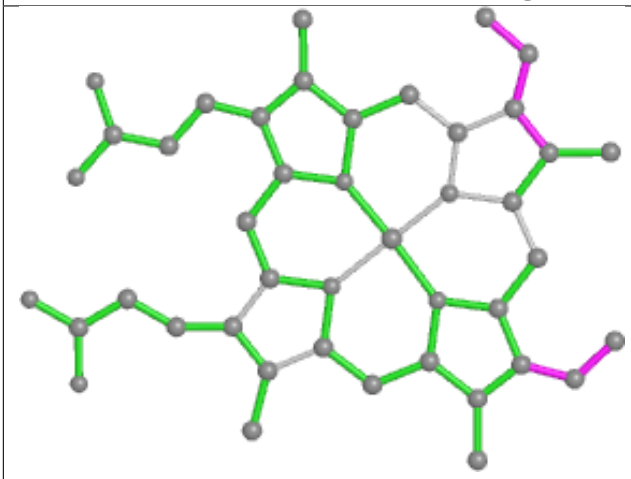


Torsions

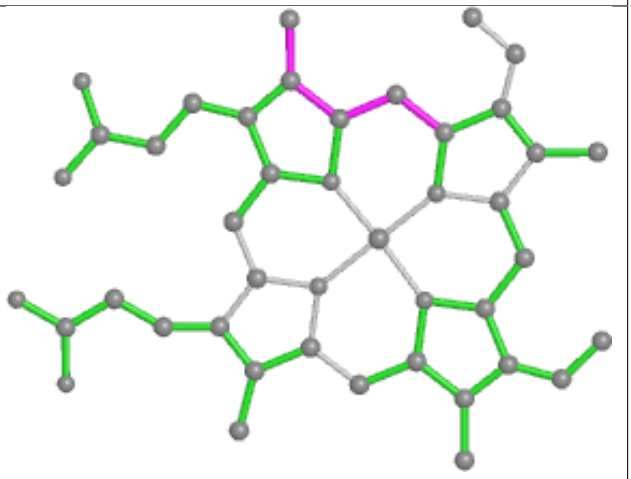


Rings

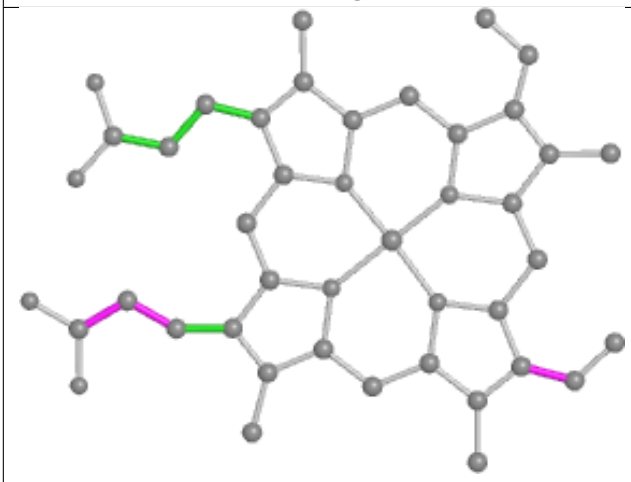
Ligand HEM B 682



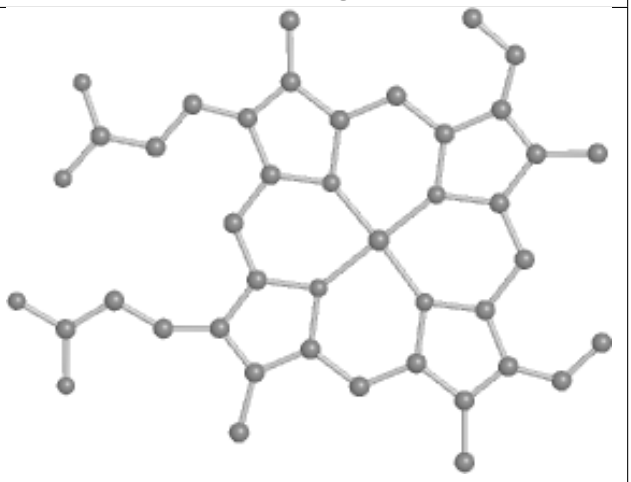
Bond lengths



Bond angles

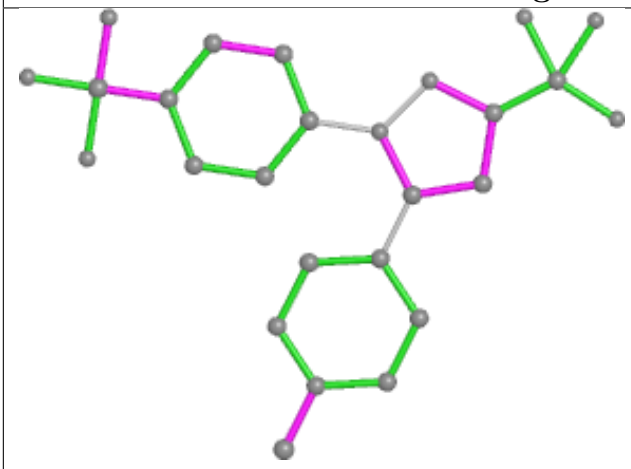


Torsions

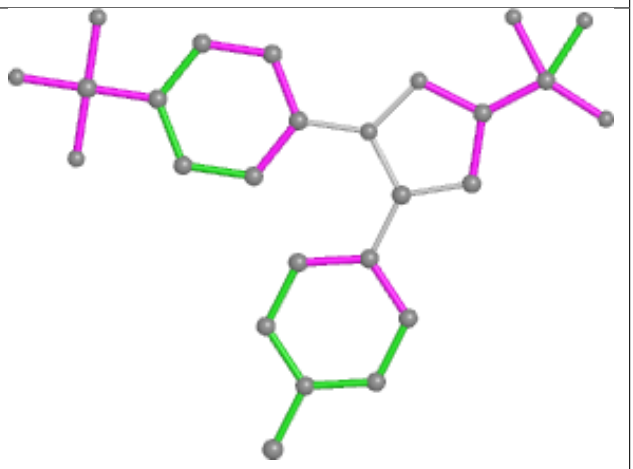


Rings

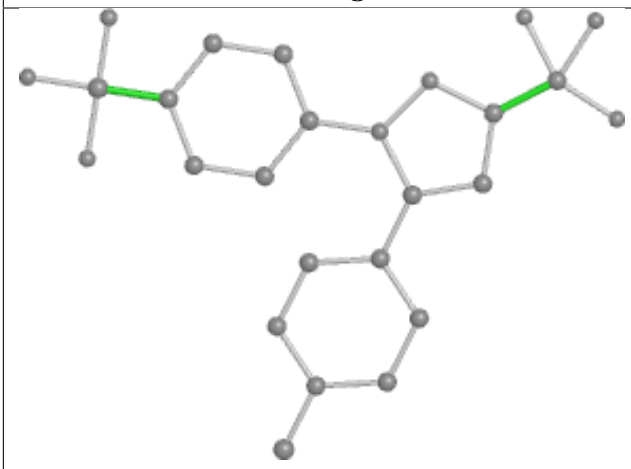
Ligand S58 A 701



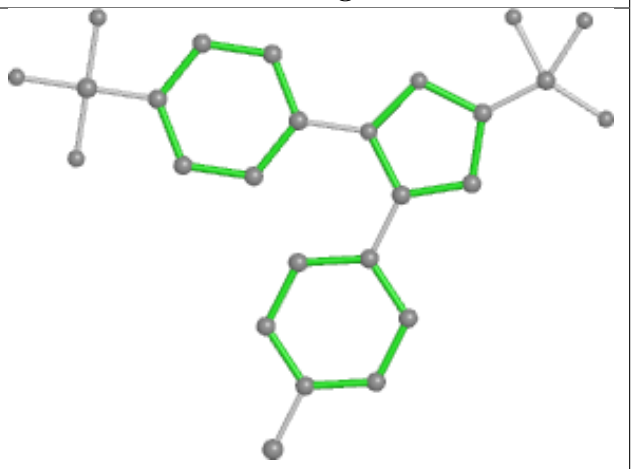
Bond lengths



Bond angles

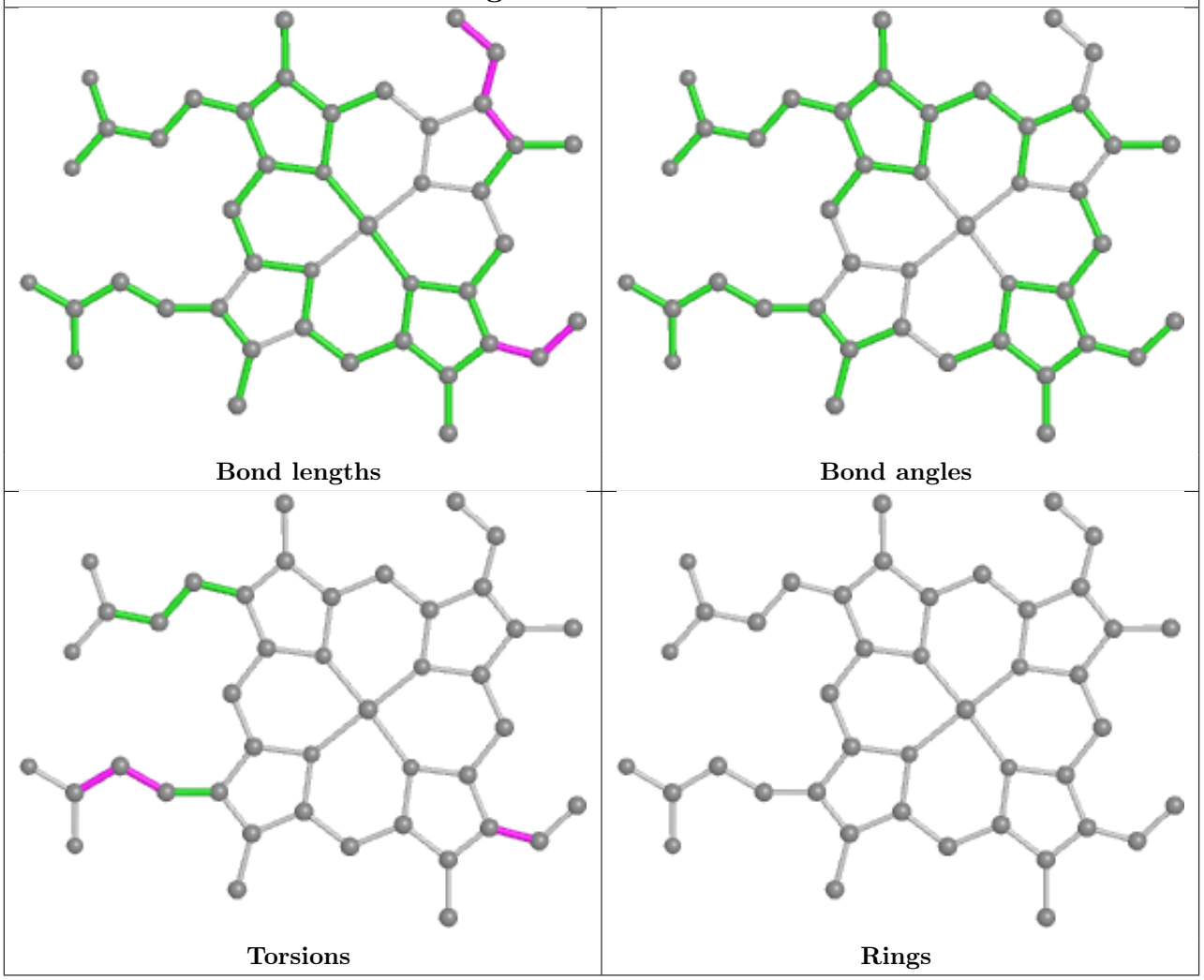


Torsions



Rings

Ligand HEM A 682



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.