



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 05:12 AM BST

PDB ID : 5COX
Title : UNINHIBITED MOUSE CYCLOOXYGENASE-2 (PROSTAGLANDIN SYNTHASE-2)
Authors : Kurumbail, R.; Stallings, W.
Deposited on : 1996-12-18
Resolution : 3.00 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) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

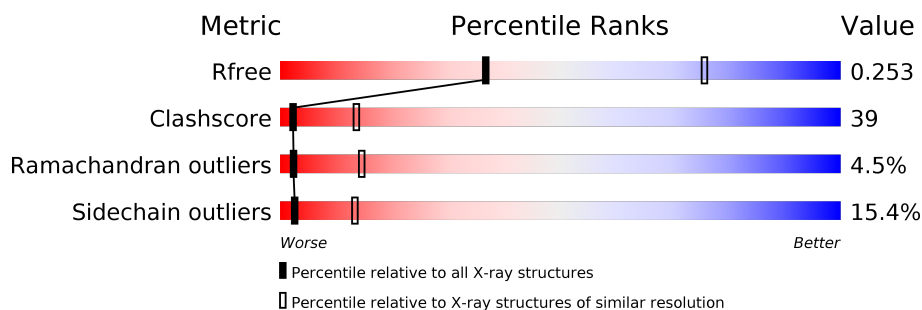
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	587	<div> <div>35%</div> <div>45%</div> <div>13%</div> <div>6%</div> </div>
1	B	587	<div> <div>35%</div> <div>47%</div> <div>11%</div> <div>6%</div> </div>
1	C	587	<div> <div>33%</div> <div>47%</div> <div>13%</div> <div>6%</div> </div>
1	D	587	<div> <div>33%</div> <div>49%</div> <div>12%</div> <div>6%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18232 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:

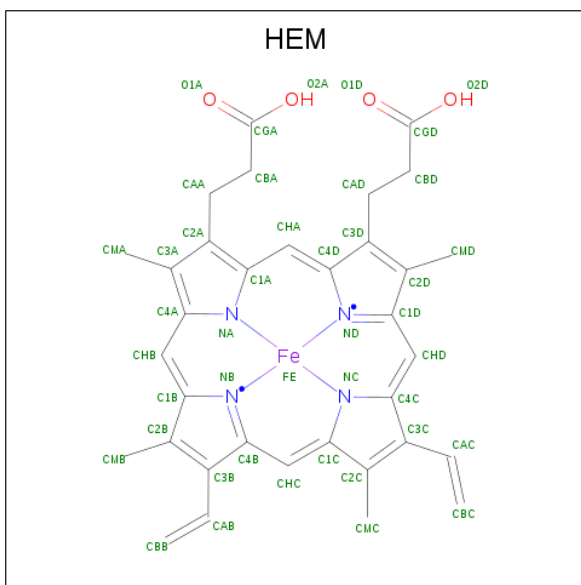
Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLN	ASN	conflict	UNP Q05769
A	333	LYS	ARG	conflict	UNP Q05769
B	310	GLN	ASN	conflict	UNP Q05769
B	333	LYS	ARG	conflict	UNP Q05769
C	310	GLN	ASN	conflict	UNP Q05769
C	333	LYS	ARG	conflict	UNP Q05769
D	310	GLN	ASN	conflict	UNP Q05769
D	333	LYS	ARG	conflict	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: $C_{34}H_{32}FeN_4O_4$).

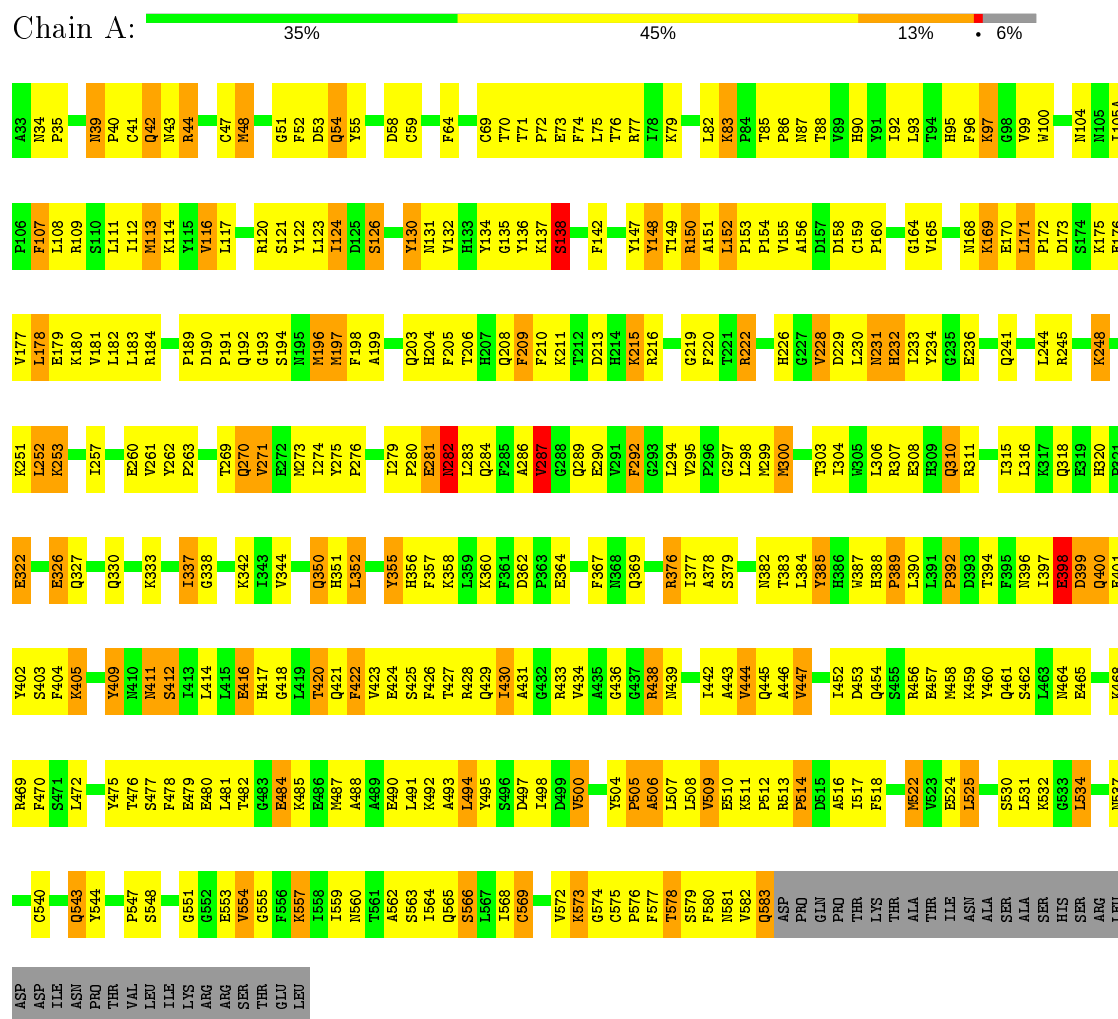


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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.

• Molecule 1: CYCLOOXYGENASE-2

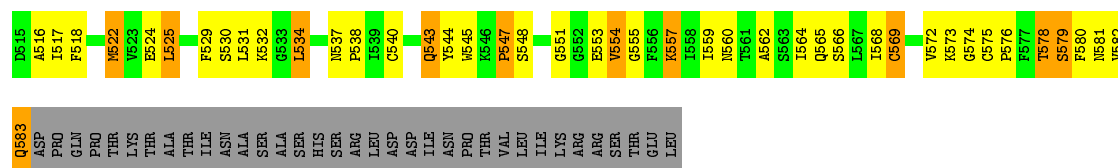


SER	ALA	HIS	SER	ARG	LEU	ASP	ASP	ILE	ASN	PRO	THR	VAL	LEU	ILE	LYS	ARG	SER	THR	GLU	LEU																																								
M522	V523	E524	L525	F529	S530	L531	K532	G533	L534	M535	Q543	S548	G551	G552	S553	V554	F555	F556	K557	M560	T561	E562	S563	L564	S565	C566	S567	T568	G569	F570	S571	T572	K573	G574	C575	P576	F577	S578	S579	F580	N581	V582	Q583	ASP	PRO	GLN	THR	ILE	ASN	ALA	T521									
R456	E457	M458	K459	Y460	Q461	S462	L463	L464	Y465	Y466	K467	K468	R469	F470	S471	L472	Y475	T476	F477	F478	Y479	E480	H481	T482	G483	E484	K485	A486	L487	A488	L489	E490	L491	K492	A493	L494	Y495	T498	D499	V500	Y504	P505	A506	L507	L508	V509	E510	K511	P512	THR	P514	D515	A516	I517	F518	T521				
T394	F395	N396	I397	E398	D399	Q400	E401	Y402	S403	F404	K405	Q406	F407	L408	Y409	N410	N411	S412	L413	L414	Y348	Q350	E480	H417	G418	L419	T420	E421	F422	V423	E424	S425	F426	T427	K428	Q429	L430	A431	G432	R433	V434	A435	G436	Q437	R438	N439	I442	F381	N382	T383	V444	Q445	A446	V447	A448	K449	I452	D453	Q454	S455
E319	H320	E321	E322	D325	E326	Q327	Q330	K333	I337	G338	E339	K342	L343	V344	Y348	Q350	E480	H417	G418	L419	T420	E421	F422	V423	E424	S425	F426	T427	K428	Q429	L430	A431	G432	R433	V434	A435	G436	Q437	R438	N439	I442	F381	N382	T383	V444	Q445	A446	V447	A448	K449	I452	D453	Q454	S455						
L244	E245	K248	K251	L252	K253	Y254	I257	V261	Y262	P263	T269	Q270	V271	E272	M273	I274	Y275	P276	I279	P280	E281	R282	F283	Q284	V287	G288	Q289	E290	P291	F292	G293	V295	L298	M299	K300	Y301	T303	L306	K307	E308	H309	Q310	R311	I315	L316	K317	Q318													
L178	E179	K180	V181	L182	L183	R184	R185	P189	D190	P191	Q192	G193	S194	N195	M196	M197	F198	A199	F200	F201	A202	Q203	H204	P205	T206	H207	Q208	Q209	F210	K211	T212	D213	T149	R215	K216	G217	P218	G219	F220	T221	R222	H226	V228	D229	L230	J0231	H232	L233	Y234	G235	E236	R240	Q241	H242	K243					
P106	F107	L108	R109	S110	L111	I112	M113	V116	D117	R120	S121	Y122	L123	I124	D125	S126	F127	N131	V132	H133	Y134	G135	Y136	K137	S138	F142	Y147	Y148	R150	A151	L152	P153	V154	A156	D157	C159	P160	G164	V165	M168	K169	E170	L171	P172	D173	S174	K175	E176	V177											

• Molecule 1: CYCLOOXYGENASE-2

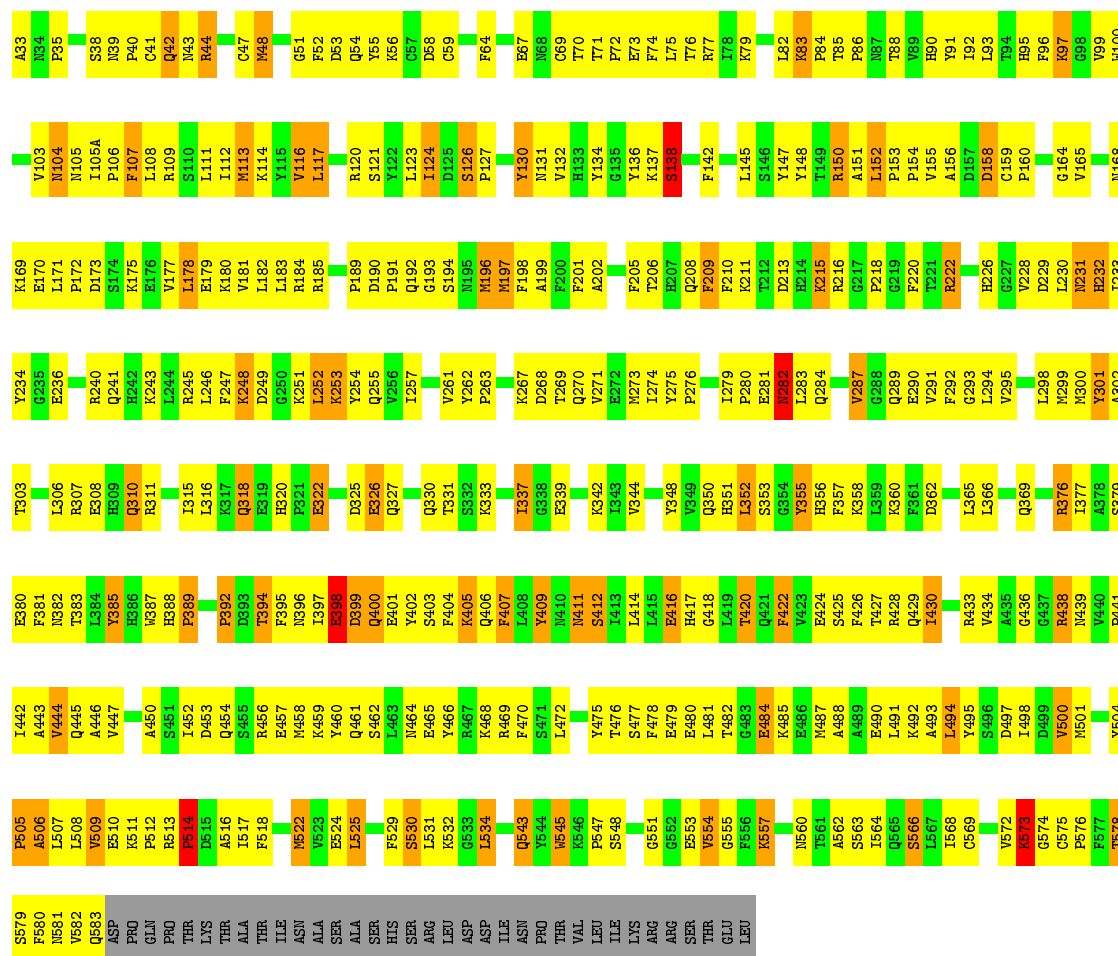
Chain C:  33% 47% 13% 6%

V447	Y385	E308	Q241	K169	V99	A33
A448	H386	H309		E170	W100	N34
K449	R387	Q310	L244	L171		P35
	H388	R311	R245	P172		
I452	P389	T315	L246	D173	M104	S38
D453	L390	F247		S174	I105A	N39
Q454	D453	L316	K248	K175	P106	P40
S455	P392	K317	D249	E176	F107	C41
R456	D393	Q318	G250	V177	L108	Q42
E457	T394	E319	K251	L178	R109	N43
M458	P395	R320	L252	E179	S110	R44
K459	N396	F321	K253	K180	L111	
Y460	L397	E322	Y254	V181	L112	C47
Q461	E398		Q255	M113		M48
S462	D399	D325	V256	L182	M113	G51
	Q400	E326	L257	L183	K114	F52
E465	E401	Q327		R184		D53
R469	Y402		E260	P189	L117	Q54
F470	S403	Q330	V261	D190		K56
S471	F404	K333	Y262	P191	R120	
L472	K405		P263	Q192	S121	
				G193	Y122	G57
Y475	Y409	I337	T269		L123	D58
T476	N410	G338	Q270	M196	I124	C59
S477	M411		V271	M197	D125	
F478	S412	K342	E272	F198	T60	T60
E479	I413	L343	M273	A199	S126	R61
L480	L414	V344	L274	F200	P127	G63
	L415		Y275	F201		F64
L481	E416	Y348	P276	A202	Y130	
T482	H417	V349		Q203	N131	
G483	G418	Q350	L279	H204	V132	E67
E484	L419	R351	P280	F205	H133	N68
K495	T420	L352	E281	T206	C69	
E486	Q421	S353	N282	Q207	G135	T70
M487	F422	G354	L283	Q208	V136	T71
A488	V423	Y355	Q284	Q209	K137	P72
E489	E424	H356	F285	F210	S138	E73
E490	S425	F357	A286	K211	F142	F74
L491	L491	K358	V287	T212	L75	T76
K492	T427	L359	G288	D213		
A493	R428	K360	Q289	R214	S146	K79
L494	Q429	F361	E290	R215	Y147	
Y495	I430	D362	V291	K216	T149	L82
S496	A431	P363	F292	R216	R150	K83
D497	G432	E364	G293	G219	A151	P84
	R433		L294	F220	L152	T85
V500	V434	F367	V295	T221	P153	P86
	A435	N368	P296	R222	P154	N87
Y504	G436	Q369	L298	V228	V155	T88
P505	G437		G297	D229	A156	V89
A506	R438	R376	M299	L230	D157	H90
L507	N439	L377	K300	L230	D158	Y91
L508	V440	A378	Y301	N231	C159	I92
V509	P441	S379	A302	R232	P160	L93
E510	F503	E380	T303	L233	T94	
K511	A443	F381	I304	G234	G164	H95
P512	V444	N382	N305	V235	V165	F96
R513	Q445	T383	L306	E236		K97
E514	A446	L284	P307		V168	G98



• Molecule 1: CYCLOOXYGENASE-2

Chain D: 33% 49% 12% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	180.46 Å 134.42 Å 119.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	74.3 (8.00-3.00) 86.0 (20.00-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.98 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.321 , 0.308 0.254 , 0.253	Depositor DCC
R_{free} test set	5077 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.932	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	18232	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1137e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: HEM, NAG

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	0.73	0/4600	0.87	4/6237 (0.1%)
1	B	0.73	0/4600	0.88	4/6237 (0.1%)
1	C	0.71	0/4600	0.87	3/6237 (0.0%)
1	D	0.72	0/4600	0.88	4/6237 (0.1%)
All	All	0.72	0/18400	0.87	15/24948 (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	B	0	2
1	D	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	355	TYR	N-CA-C	6.18	127.69	111.00
1	A	355	TYR	N-CA-C	5.84	126.78	111.00
1	B	355	TYR	N-CA-C	5.79	126.65	111.00
1	D	355	TYR	N-CA-C	5.77	126.58	111.00
1	A	281	GLU	N-CA-C	-5.64	95.78	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	262	TYR	Sidechain
1	B	301	TYR	Sidechain
1	D	301	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	353	0
1	B	4473	0	4375	341	0
1	C	4473	0	4374	343	0
1	D	4473	0	4374	386	0
2	A	42	0	39	0	0
2	B	42	0	39	1	0
2	C	42	0	39	3	0
2	D	42	0	39	5	0
3	A	43	0	30	1	0
3	B	43	0	30	2	0
3	C	43	0	30	2	0
3	D	43	0	30	2	0
All	All	18232	0	17773	1388	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 39.

The worst 5 of 1388 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:322:GLU:HG2	1:B:52:PHE:H	1.23	1.00
1:C:322:GLU:HG2	1:D:52:PHE:H	1.29	0.94
1:C:52:PHE:H	1:D:322:GLU:HG2	1.32	0.91
1:A:52:PHE:H	1:B:322:GLU:HG2	1.35	0.90
1:D:189:PRO:HB2	1:D:430:ILE:HD13	1.54	0.90

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	550/587 (94%)	446 (81%)	78 (14%)	26 (5%)	2	14
1	B	550/587 (94%)	442 (80%)	87 (16%)	21 (4%)	3	18
1	C	550/587 (94%)	443 (80%)	80 (14%)	27 (5%)	2	13
1	D	550/587 (94%)	440 (80%)	85 (16%)	25 (4%)	2	14
All	All	2200/2348 (94%)	1771 (80%)	330 (15%)	99 (4%)	2	14

5 of 99 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	SER
1	A	429	GLN
1	A	438	ARG
1	A	514	PRO
1	A	573	LYS

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	493/525 (94%)	417 (85%)	76 (15%)	2	13
1	B	493/525 (94%)	418 (85%)	75 (15%)	3	14
1	C	493/525 (94%)	416 (84%)	77 (16%)	2	13
1	D	493/525 (94%)	417 (85%)	76 (15%)	2	13
All	All	1972/2100 (94%)	1668 (85%)	304 (15%)	2	13

5 of 304 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	484	GLU
1	C	152	LEU
1	D	405	LYS
1	B	522	MET
1	C	54	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	417	HIS
1	C	203	GLN
1	D	411	ASN
1	B	454	GLN
1	C	39	ASN

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 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	C	661	1	14,14,15	0.57	0	17,19,21	0.95	1 (5%)
2	NAG	D	661	1	14,14,15	0.62	0	17,19,21	0.84	1 (5%)
3	HEM	D	682	1	27,50,50	1.91	5 (18%)	17,82,82	1.02	1 (5%)
2	NAG	B	661	1	14,14,15	0.67	1 (7%)	17,19,21	0.91	0
3	HEM	B	682	1	27,50,50	1.75	5 (18%)	17,82,82	0.95	0
2	NAG	D	681	1	14,14,15	0.62	0	17,19,21	0.75	1 (5%)
3	HEM	A	682	1	27,50,50	1.99	6 (22%)	17,82,82	0.83	0
2	NAG	B	671	1	14,14,15	0.83	0	17,19,21	1.49	3 (17%)
2	NAG	A	671	1	14,14,15	0.86	0	17,19,21	1.57	3 (17%)
2	NAG	D	671	1	14,14,15	0.65	0	17,19,21	1.40	1 (5%)
2	NAG	B	681	1	14,14,15	0.57	0	17,19,21	0.87	2 (11%)
2	NAG	A	681	1	14,14,15	0.38	0	17,19,21	0.80	1 (5%)
2	NAG	C	681	1	14,14,15	0.61	0	17,19,21	0.99	2 (11%)
2	NAG	C	671	1	14,14,15	0.83	0	17,19,21	1.60	3 (17%)
2	NAG	A	661	1	14,14,15	0.64	0	17,19,21	0.74	0
3	HEM	C	682	1	27,50,50	1.99	6 (22%)	17,82,82	0.78	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	C	661	1	-	0/6/23/26	0/1/1/1
2	NAG	D	661	1	-	0/6/23/26	0/1/1/1
3	HEM	D	682	1	-	0/6/54/54	-
2	NAG	B	661	1	-	0/6/23/26	0/1/1/1
3	HEM	B	682	1	-	0/6/54/54	-
2	NAG	D	681	1	-	2/6/23/26	0/1/1/1
3	HEM	A	682	1	-	0/6/54/54	-
2	NAG	B	671	1	-	2/6/23/26	0/1/1/1
2	NAG	A	671	1	-	2/6/23/26	0/1/1/1
2	NAG	D	671	1	-	2/6/23/26	0/1/1/1
2	NAG	B	681	1	-	2/6/23/26	0/1/1/1
2	NAG	A	681	1	-	2/6/23/26	0/1/1/1
2	NAG	C	681	1	-	2/6/23/26	0/1/1/1
2	NAG	C	671	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	661	1	-	0/6/23/26	0/1/1/1
3	HEM	C	682	1	-	0/6/54/54	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	682	HEM	C3C-C2C	-5.12	1.33	1.40
3	D	682	HEM	C3C-CAC	-4.79	1.38	1.47
3	A	682	HEM	C3B-C2B	-4.69	1.33	1.40
3	C	682	HEM	C3C-C2C	-4.44	1.34	1.40
3	C	682	HEM	C3B-C2B	-4.43	1.34	1.40

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	671	NAG	C4-C3-C2	-5.09	103.55	111.02
2	C	671	NAG	C4-C3-C2	-4.72	104.10	111.02
2	D	671	NAG	C4-C3-C2	-4.60	104.28	111.02
2	B	671	NAG	C4-C3-C2	-4.53	104.38	111.02
2	C	671	NAG	C2-N2-C7	-3.19	118.36	122.90

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	D	671	NAG	O5-C5-C6-O6
2	A	671	NAG	O5-C5-C6-O6
2	D	671	NAG	C4-C5-C6-O6
2	B	681	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 16 short contacts:

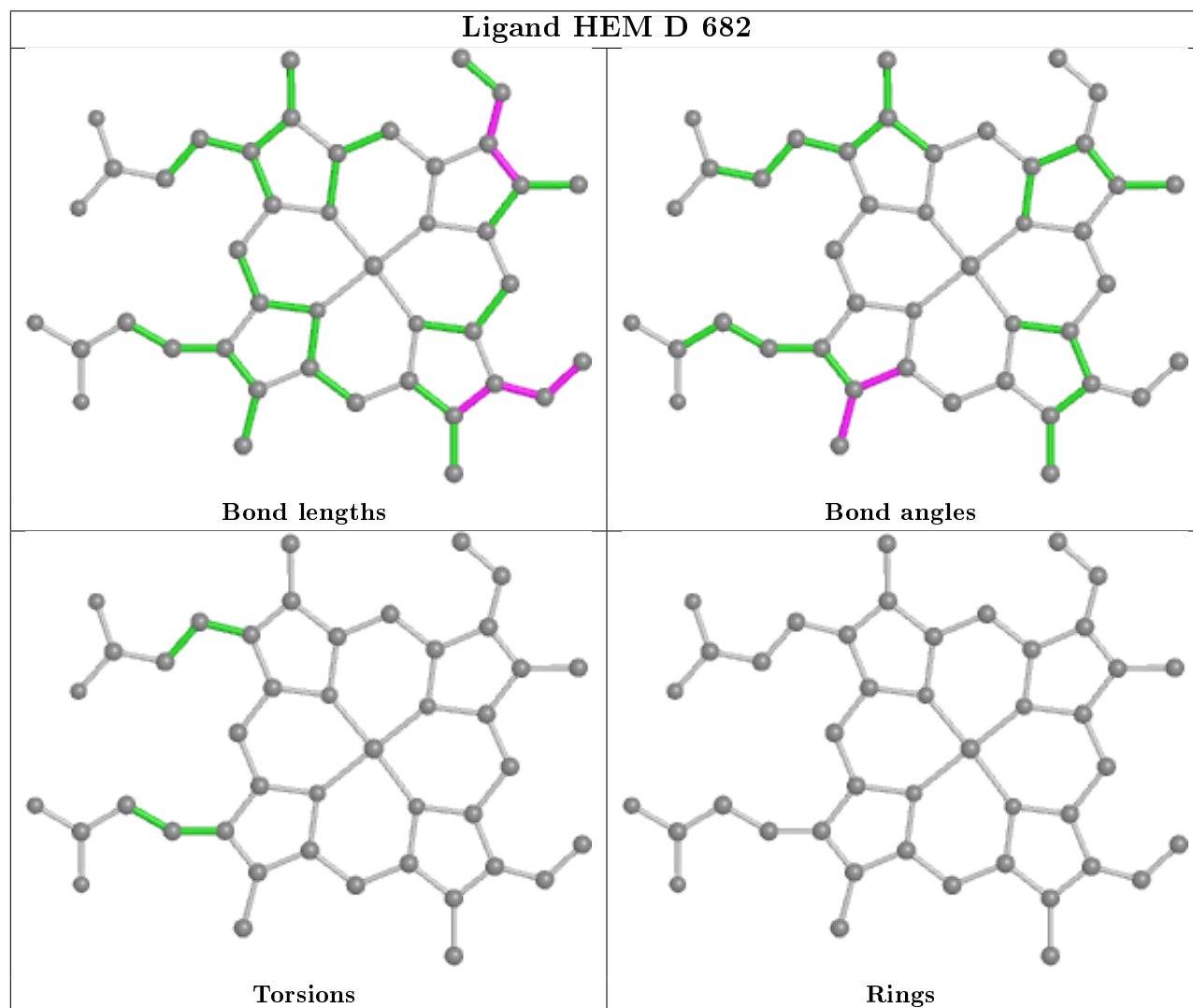
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	661	NAG	2	0
2	D	661	NAG	1	0
3	D	682	HEM	2	0
3	B	682	HEM	2	0
2	D	681	NAG	4	0
3	A	682	HEM	1	0

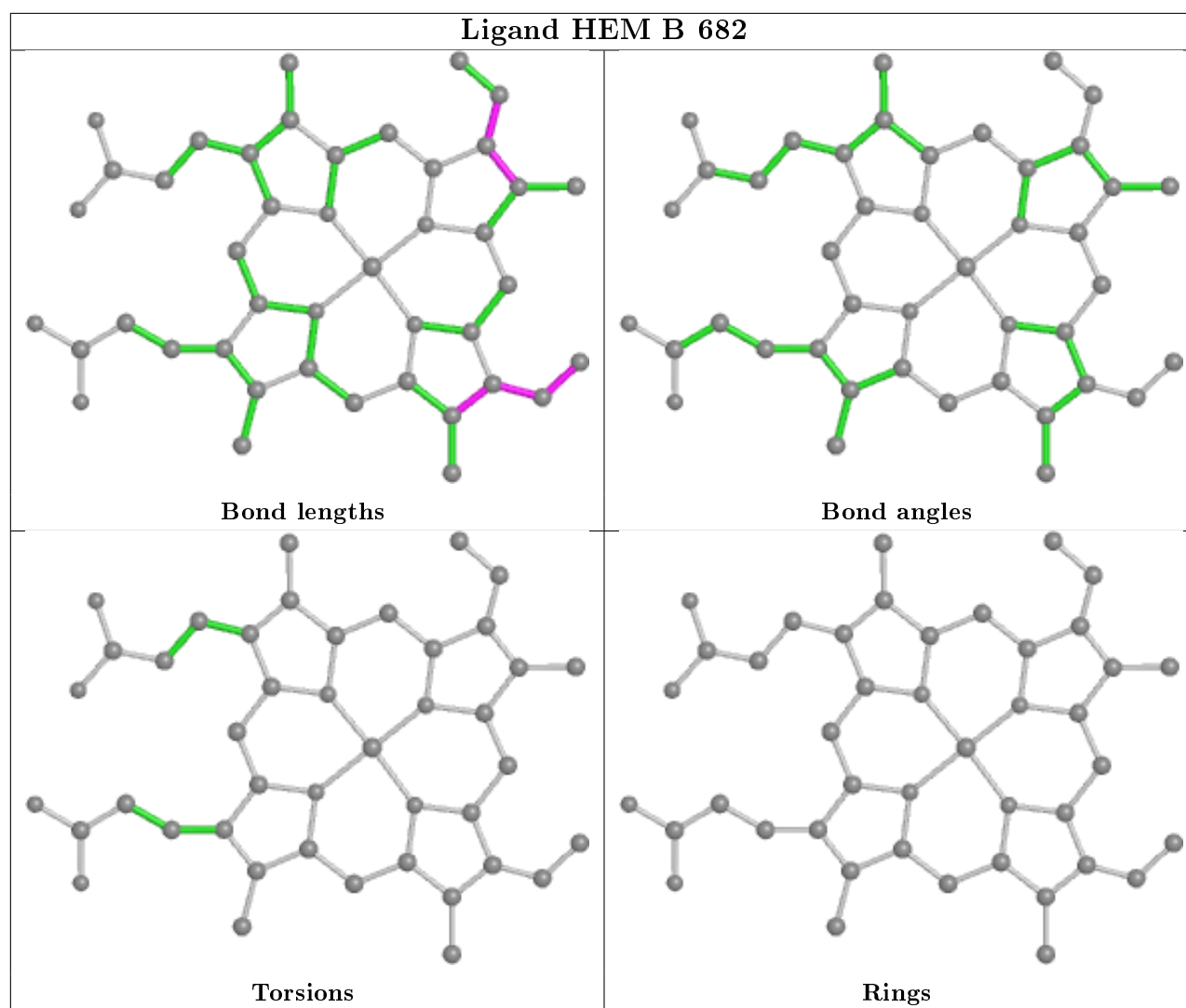
Continued on next page...

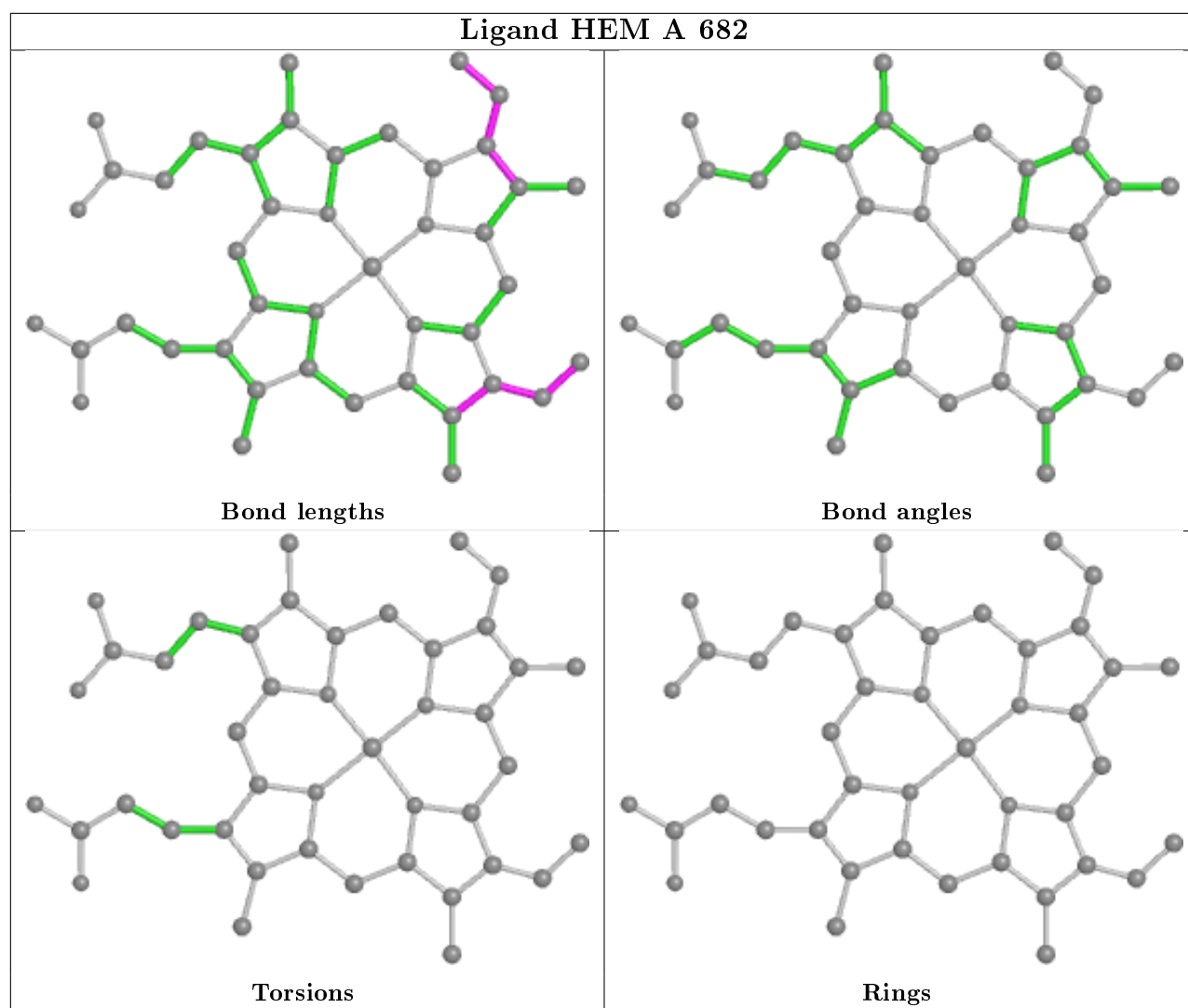
Continued from previous page...

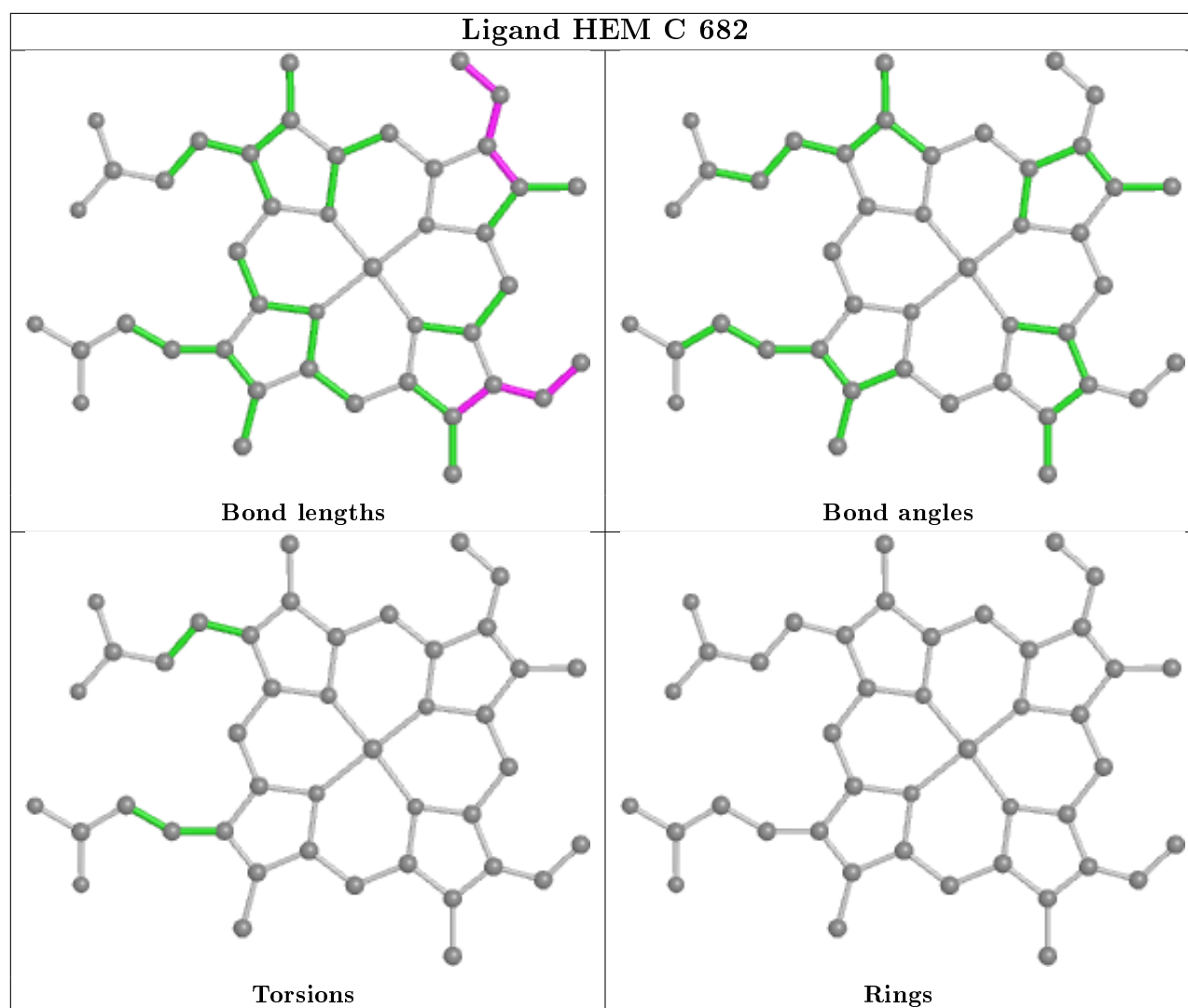
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	681	NAG	1	0
2	C	671	NAG	1	0
3	C	682	HEM	2	0

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 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

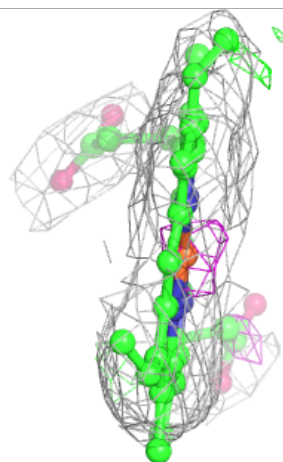
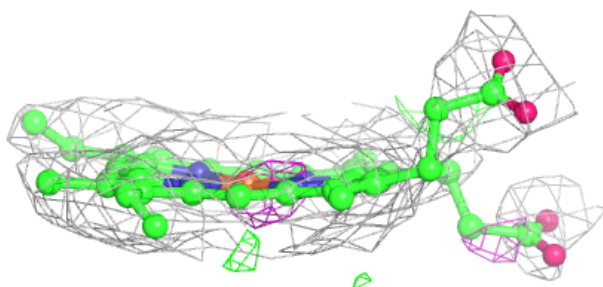
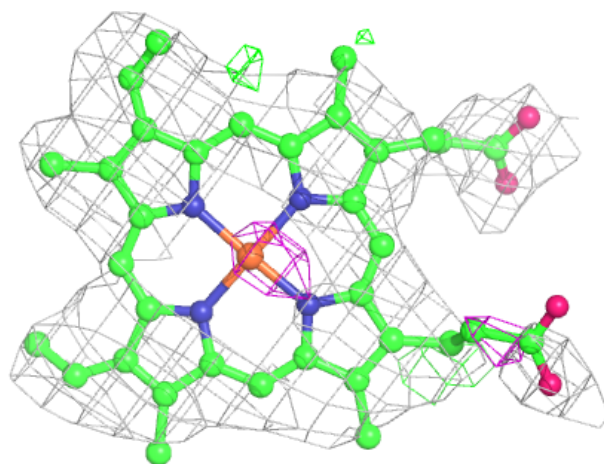
6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

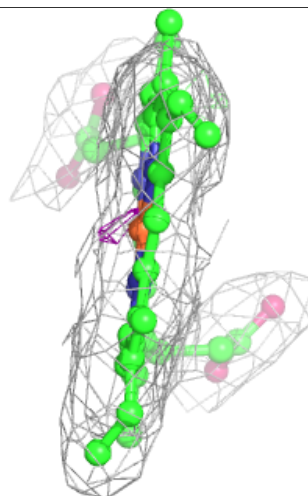
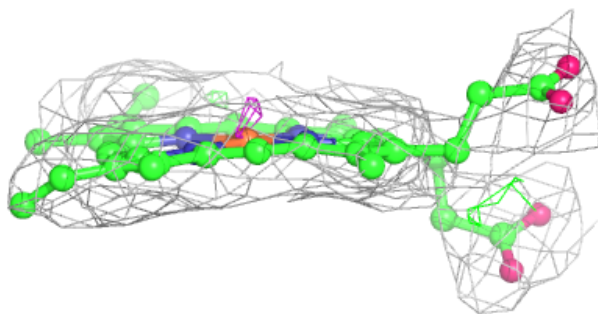
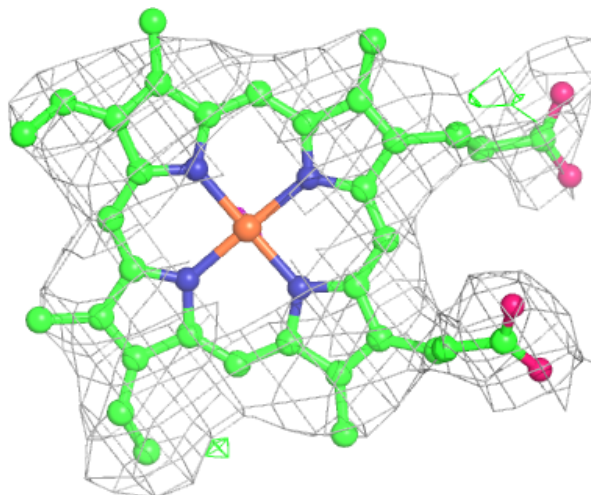
Electron density around HEM D 682:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



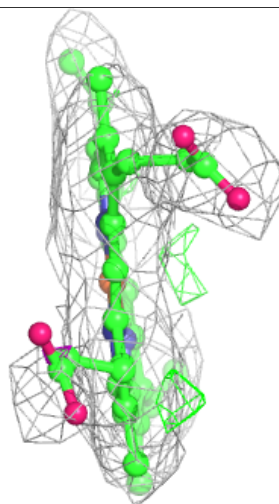
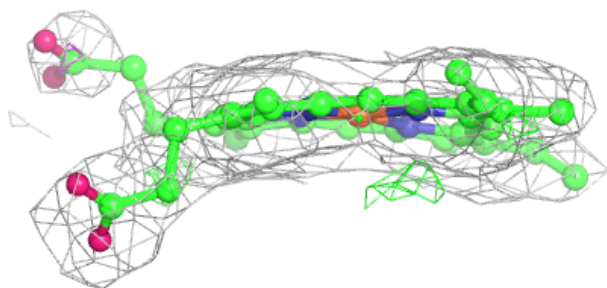
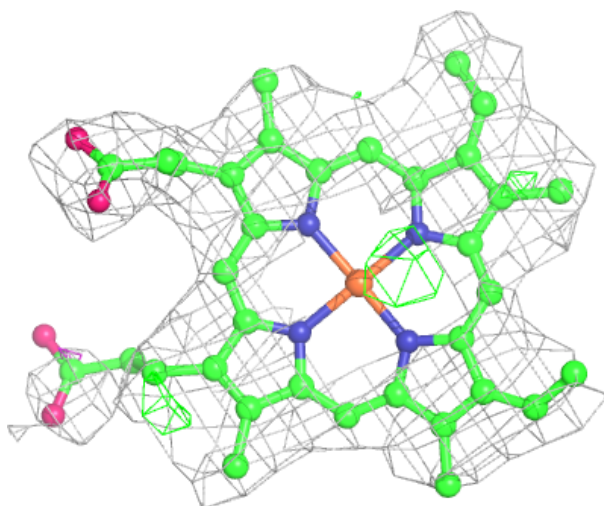
Electron density around HEM B 682:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



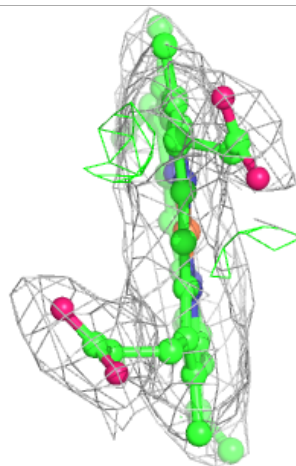
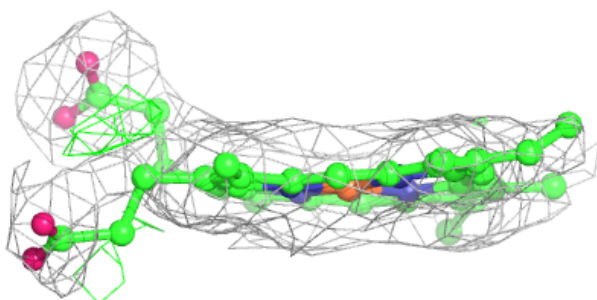
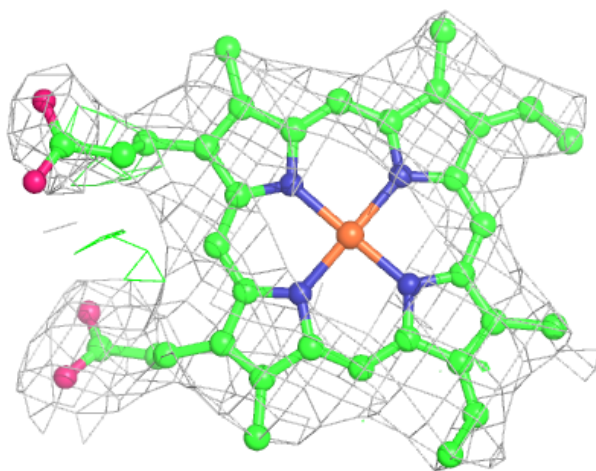
Electron density around HEM A 682:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 682:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.