



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 11:46 PM UTC

PDB ID : 4BLC / pdb_00004blc
Title : THE STRUCTURE OF ORTHORHOMBIC CRYSTALS OF BEEF LIVER CATALASE
Authors : Ko, T.P.; Day, J.; Malkin, A.; McPherson, A.
Deposited on : 1998-09-27
Resolution : 2.30 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 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)
Xtrriage (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) : 2.49

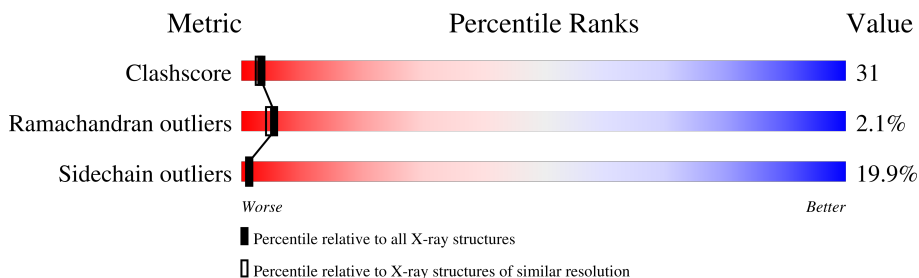
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	506	53% 38% 8% .
1	B	506	36% 45% 17% ..
1	C	506	40% 43% 15% ..
1	D	506	43% 45% 10% ..

2 Entry composition [i](#)

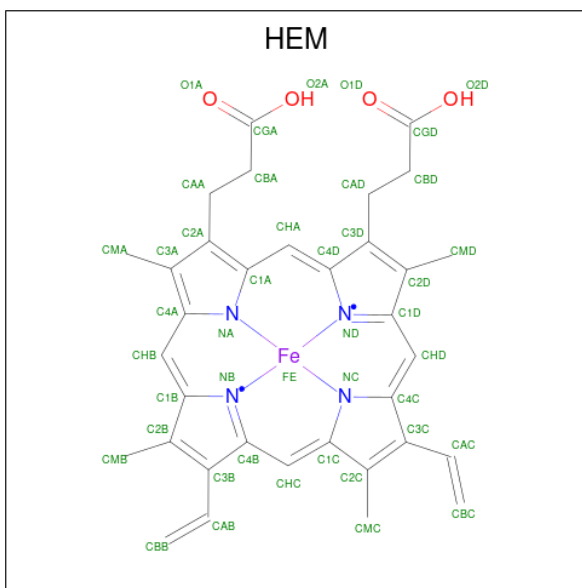
There are 4 unique types of molecules in this entry. The entry contains 16816 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (CATALASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	499	Total 4017	C 2548	N 715	O 740	S 14	0	0	0
1	B	499	Total 4017	C 2548	N 715	O 740	S 14	0	0	0
1	C	499	Total 4017	C 2548	N 715	O 740	S 14	0	0	0
1	D	499	Total 4017	C 2548	N 715	O 740	S 14	0	0	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



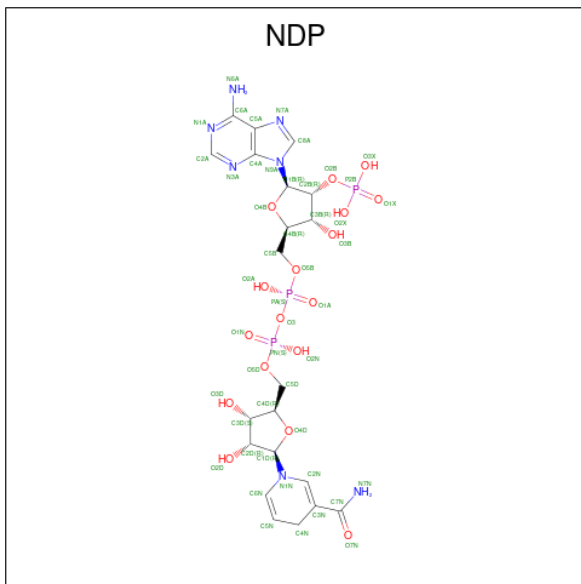
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total	O	0	0
			119	119		
4	B	89	Total	O	0	0
			89	89		
4	C	83	Total	O	0	0
			83	83		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	93	Total	O	0	0
			93	93		

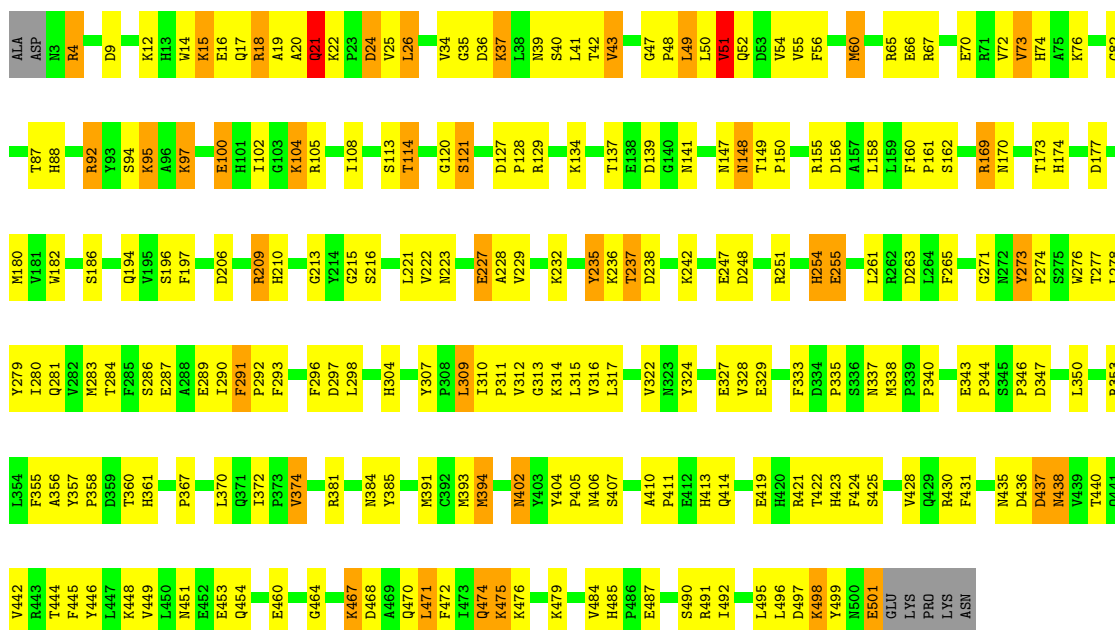
3 Residue-property plots [i](#)

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 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.

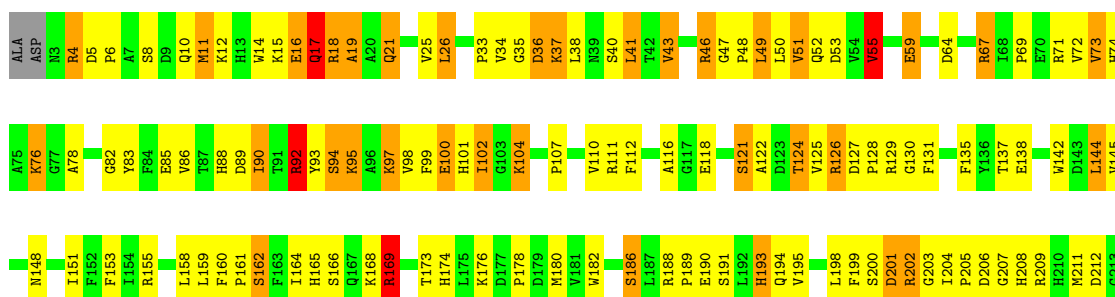
- Molecule 1: PROTEIN (CATALASE)

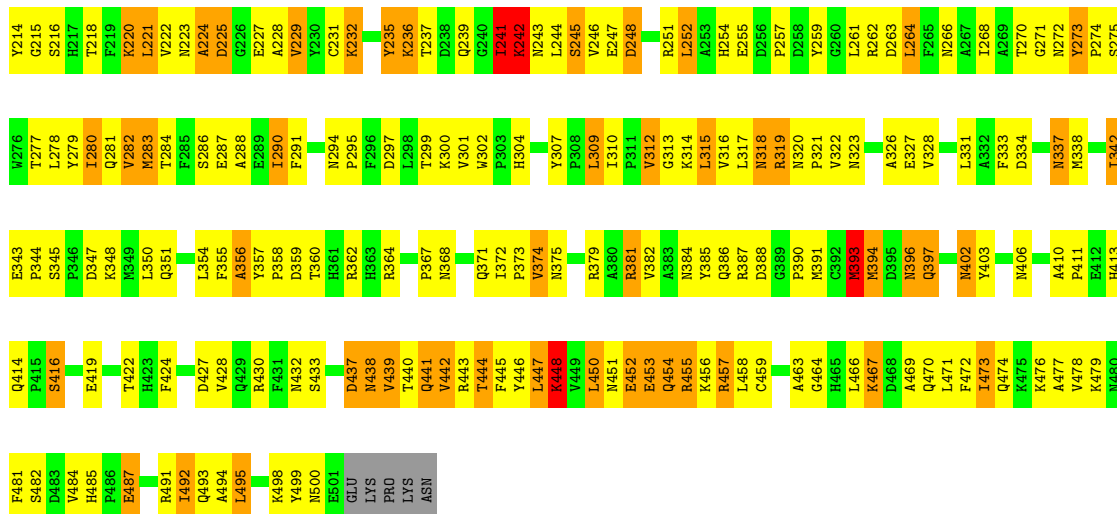
Chain A: 



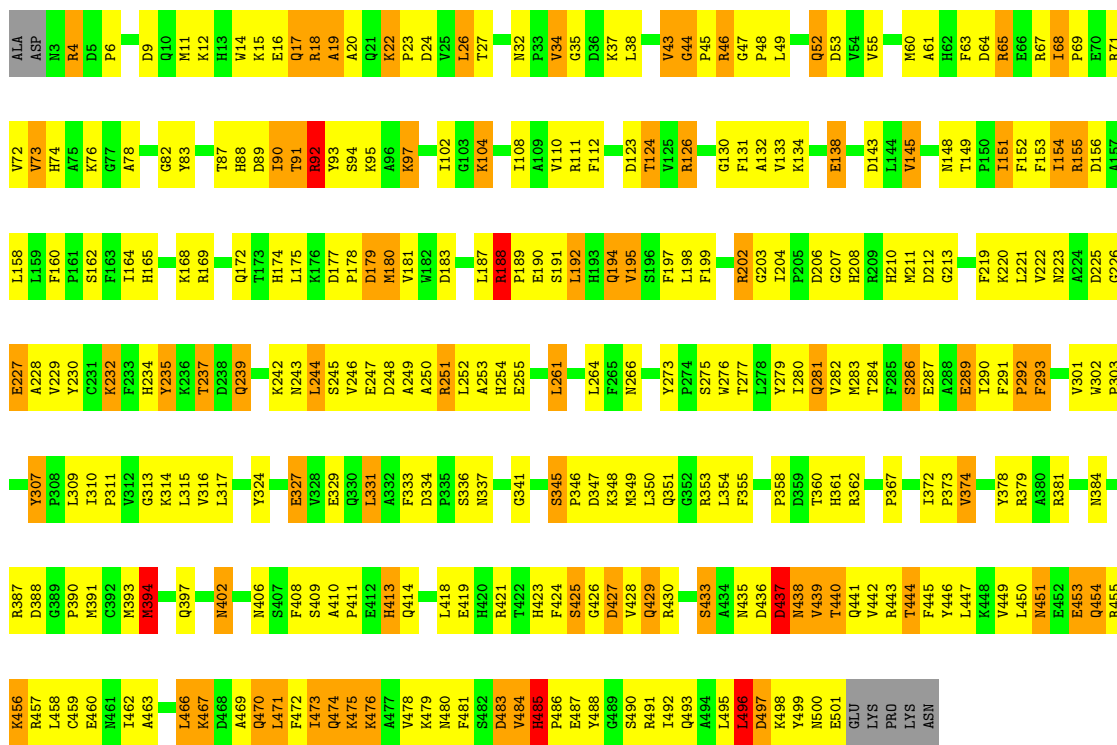
- Molecule 1: PROTEIN (CATALASE)

Chain B: 





● Molecule 1: PROTEIN (CATALASE)



● Molecule 1: PROTEIN (CATALASE)



F84	F160	T237	N320	Y385	E452
E85	P161	I241	N323	Q386	R455
V86	P164	K242	N327	R387	K456
D89	I164	N243	E327	P390	E460
I90	K168	L244	V328	M391	K467
T91	R169	S245	E329	C392	L471
R92	M170	V246	Q330	M393	Q474
Y93	P171	E247	L331	R394	K475
S94	Q172	D248	A332	Q397	K476
K95	T173	L252	F333	P401	A477
A96	D177	A253	D334	M402	V478
K97	F178	L261	F335	Y403	K479
V96	M180	R262	N337	Y404	N480
F99	V181	D263	M338	P405	V484
E100	V181	F265	P339	F408	H485
H101	W185	L264	P340	S409	P486
I102	R188	F266	G341	A410	E487
G103	P189	N266	I342	E411	Y488
K104	E190	A257	E343	E412	G489
R105	E190	G271	P344	H413	S490
T106	S191	N272	S345	Q414	R491
P107	L192	Y273	P346	P415	I492
I108	L193	E274	D347	R415	Q493
R111	H193	S275	K348	S416	A494
F112	F197	W276	M349	A417	L495
S113	F197	T277	L350	L418	L496
P107	T114	L278	R353	E419	D497
I108	R202	Y279	L354	H420	K498
R111	P205	Y279	L355	R421	Y499
F112	D206	L280	L356	S425	N500
S119	R209	Q281	F355	G426	E501
G120	H210	V282	A356	D427	GLU
G130	M211	M283	Y357	W428	LYS
K134	D212	T284	T360	Q429	PRO
T137	G213	F285	H361	R430	LYS
E138	Y214	E287	R362	F431	ASN
D139	G215	A288	R363	N432	
D139	S216	E289	R364	S433	
W142	H217	I290	L365	A434	
D143	K220	F291	G366	M435	
L144	L221	P292	P367	D436	
V145	V222	F293	M368	D437	
V145	N223	F296	Y369	N438	
M148	A224	D297	I372	V439	
T149	D225	L298	P373	T440	
P150	G226	T299	V374	Q441	
I151	E227	K300	M375	V442	
F152	A228	V301	P377	R443	
F153	V229	W302	P377	T444	
I154	V230	P303	Y378	F445	
R155	Y230	L309	R379	Y446	
D156	C231	A300	A380	L447	
A157	K232	L309	R381	K448	
L158	Y235	G313	V382	V449	
L159	K236	K314	A383	L450	
		L315	N384	N451	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.80Å 140.60Å 232.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	87.5 (20.00-2.30)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.205 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	16816	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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: NDP, 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	0.49	0/4137	0.96	11/5619 (0.2%)
1	B	0.45	0/4137	0.94	12/5619 (0.2%)
1	C	0.46	0/4137	0.98	26/5619 (0.5%)
1	D	0.47	0/4137	0.94	12/5619 (0.2%)
All	All	0.47	0/16548	0.96	61/22476 (0.3%)

There are no bond length outliers.

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	ILE	N-CA-C	-8.30	103.14	111.77
1	D	356	ALA	N-CA-C	8.22	121.28	111.33
1	C	55	VAL	N-CA-C	-8.13	102.89	110.53
1	A	356	ALA	N-CA-C	7.56	121.43	111.75
1	B	55	VAL	N-CA-C	-7.35	103.62	110.53

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	4017	0	3839	185	0
1	B	4017	0	3839	319	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4017	0	3839	292	0
1	D	4017	0	3839	276	0
2	A	43	0	30	5	0
2	B	43	0	30	0	0
2	C	43	0	30	4	0
2	D	43	0	30	2	0
3	A	48	0	26	3	0
3	B	48	0	26	3	0
3	C	48	0	26	2	0
3	D	48	0	26	1	0
4	A	119	0	0	8	0
4	B	89	0	0	16	0
4	C	83	0	0	8	0
4	D	93	0	0	11	0
All	All	16816	0	15580	979	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 31.

The worst 5 of 979 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:D:223:ASN:HD21	1:D:227:GLU:HB3	0.98	1.12
1:A:451:ASN:H	1:A:454:GLN:HE21	1.06	1.01
1:D:223:ASN:ND2	1:D:227:GLU:HB3	1.79	0.98
1:B:169:ARG:HG2	1:B:169:ARG:HH11	1.30	0.95
1:B:457:ARG:HH11	1:B:457:ARG:HB2	1.28	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	497/506 (98%)	442 (89%)	50 (10%)	5 (1%)	12	15
1	B	497/506 (98%)	423 (85%)	58 (12%)	16 (3%)	3	2
1	C	497/506 (98%)	417 (84%)	65 (13%)	15 (3%)	3	2
1	D	497/506 (98%)	442 (89%)	49 (10%)	6 (1%)	10	12
All	All	1988/2024 (98%)	1724 (87%)	222 (11%)	42 (2%)	5	4

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ALA
1	A	437	ASP
1	B	124	THR
1	B	242	LYS
1	B	394	MET

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	431/437 (99%)	359 (83%)	72 (17%)	2	2
1	B	431/437 (99%)	320 (74%)	111 (26%)	0	0
1	C	431/437 (99%)	347 (80%)	84 (20%)	1	1
1	D	431/437 (99%)	355 (82%)	76 (18%)	2	2
All	All	1724/1748 (99%)	1381 (80%)	343 (20%)	1	1

5 of 343 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	331	LEU
1	D	148	ASN
1	C	413	HIS
1	C	474	GLN
1	D	245	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	193	HIS
1	D	254	HIS
1	D	500	ASN
1	B	272	ASN
1	B	243	ASN

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](#)

8 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	HEM	C	507	1	50,50,50	1.25	5 (10%)	67,82,82	1.00	1 (1%)
3	NDP	B	1202	-	51,52,52	1.66	10 (19%)	71,80,80	2.06	18 (25%)
2	HEM	D	507	1	50,50,50	1.25	5 (10%)	67,82,82	1.25	6 (8%)
3	NDP	A	1102	-	51,52,52	1.51	7 (13%)	71,80,80	1.91	14 (19%)
2	HEM	B	507	1	50,50,50	1.13	4 (8%)	67,82,82	1.07	5 (7%)
3	NDP	D	1402	-	51,52,52	1.59	10 (19%)	71,80,80	1.85	12 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NDP	C	1302	-	51,52,52	1.53	10 (19%)	71,80,80	2.08	16 (22%)
2	HEM	A	507	1	50,50,50	1.15	5 (10%)	67,82,82	0.94	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
2	HEM	C	507	1	-	5/14/54/54	-
3	NDP	B	1202	-	-	10/34/77/77	0/5/5/5
2	HEM	D	507	1	-	4/14/54/54	-
3	NDP	A	1102	-	-	7/34/77/77	0/5/5/5
2	HEM	B	507	1	-	8/14/54/54	-
3	NDP	D	1402	-	-	9/34/77/77	0/5/5/5
3	NDP	C	1302	-	-	7/34/77/77	0/5/5/5
2	HEM	A	507	1	-	5/14/54/54	-

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1202	NDP	PN-O3	4.31	1.64	1.59
3	D	1402	NDP	P2B-O1X	4.20	1.63	1.50
3	C	1302	NDP	P2B-O1X	3.94	1.62	1.50
3	A	1102	NDP	P2B-O1X	3.91	1.62	1.50
3	B	1202	NDP	C4N-C3N	-3.84	1.42	1.50

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1402	NDP	C5A-C4A-N3A	-6.37	117.95	126.72
3	C	1302	NDP	O4D-C1D-N1N	6.20	119.91	108.08
3	A	1102	NDP	C5A-C4A-N3A	-5.95	118.52	126.72
3	C	1302	NDP	C5A-C4A-N3A	-5.94	118.54	126.72
3	B	1202	NDP	C2B-C1B-N9A	5.78	123.26	113.75

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

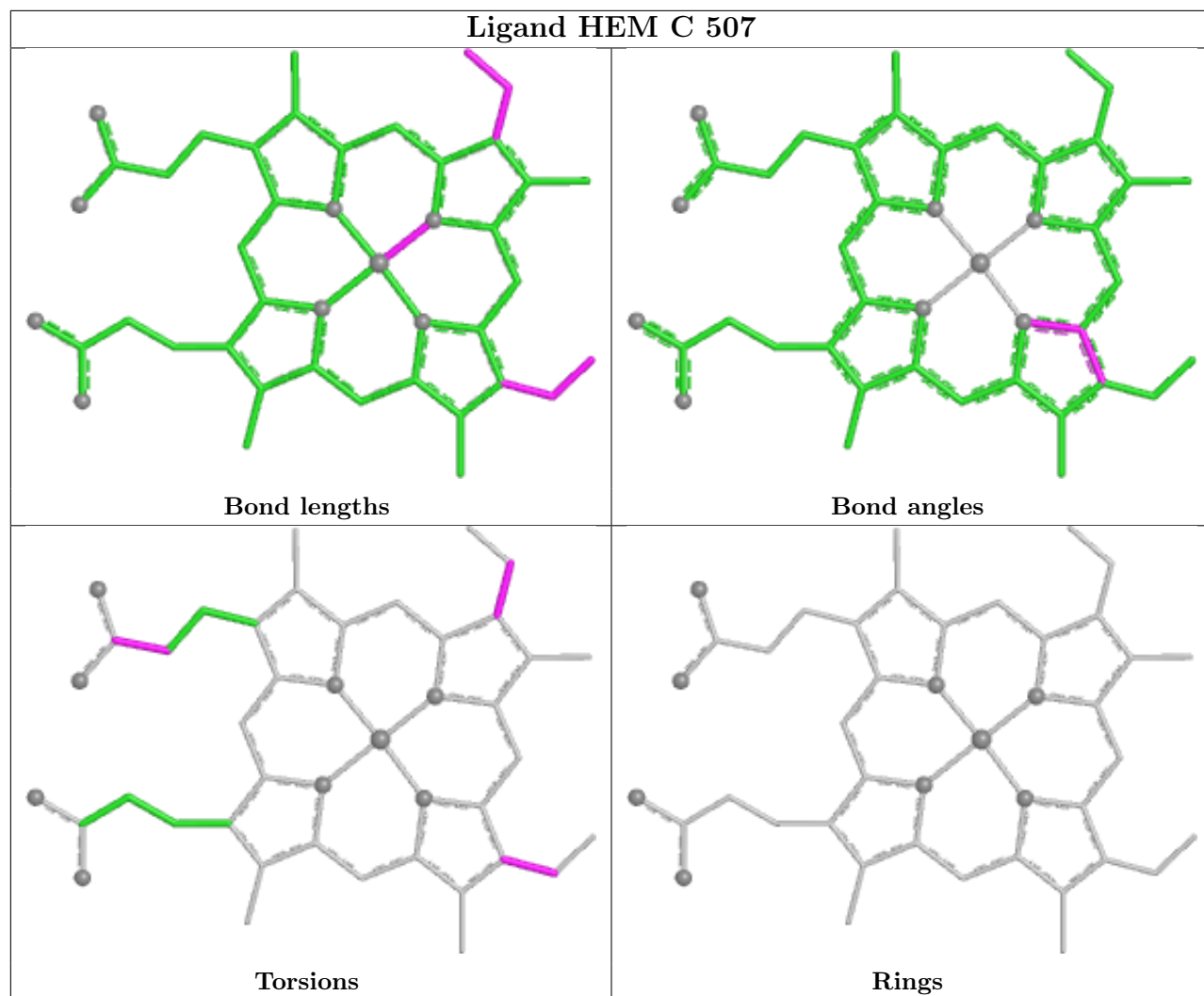
Mol	Chain	Res	Type	Atoms
2	A	507	HEM	C2B-C3B-CAB-CBB
2	A	507	HEM	C4B-C3B-CAB-CBB
2	A	507	HEM	C2C-C3C-CAC-CBC
2	B	507	HEM	C2B-C3B-CAB-CBB
2	D	507	HEM	C2B-C3B-CAB-CBB

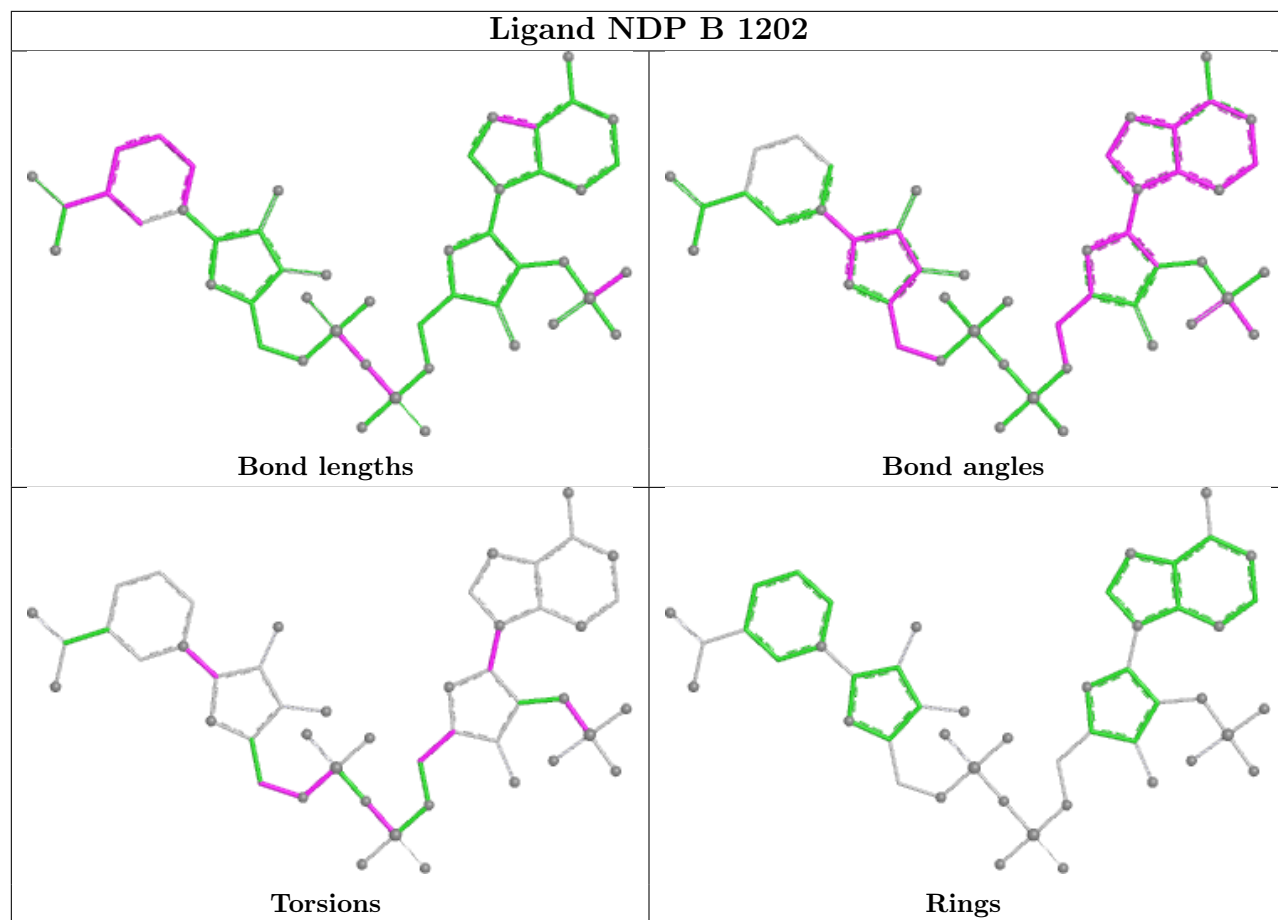
There are no ring outliers.

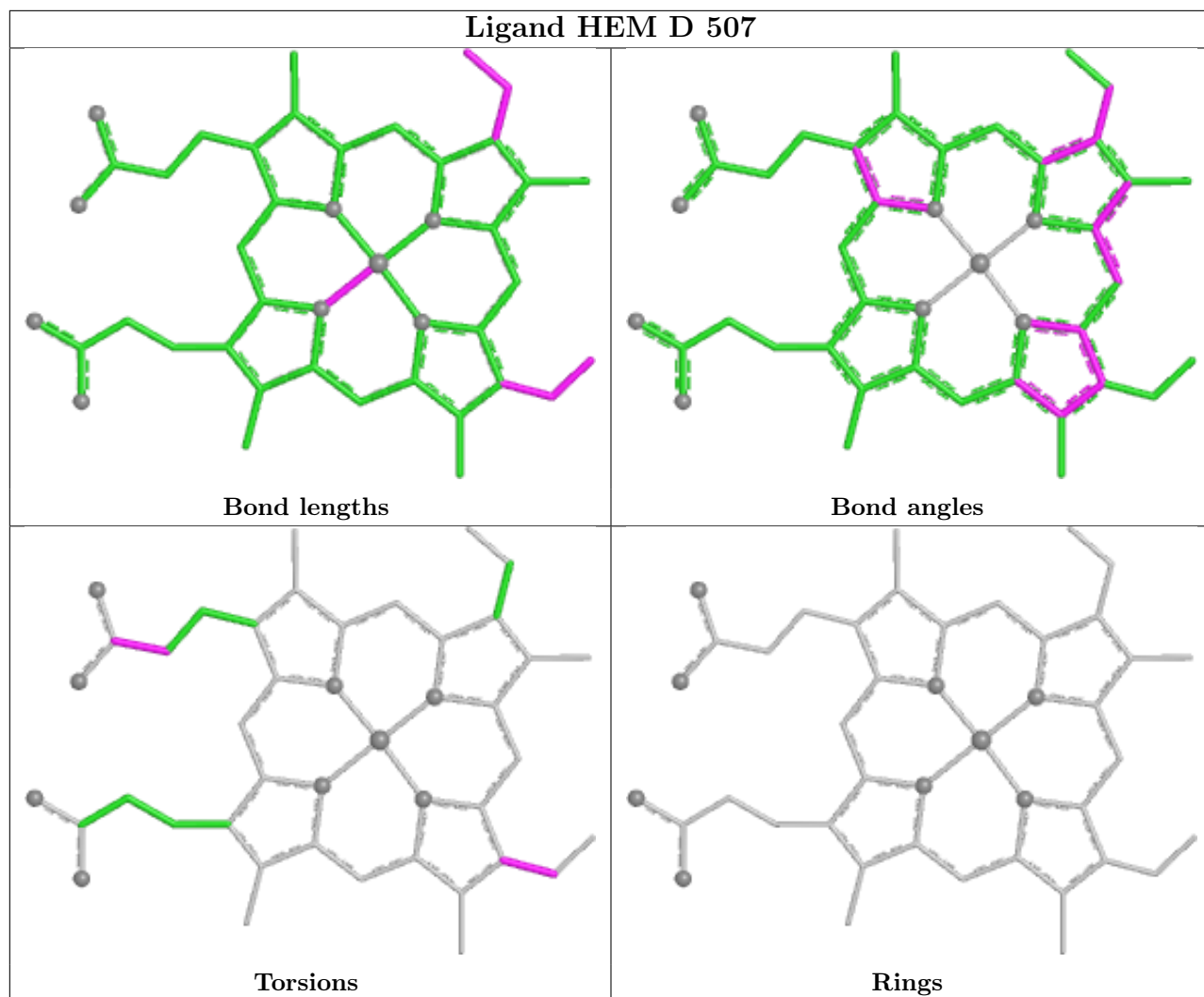
7 monomers are involved in 20 short contacts:

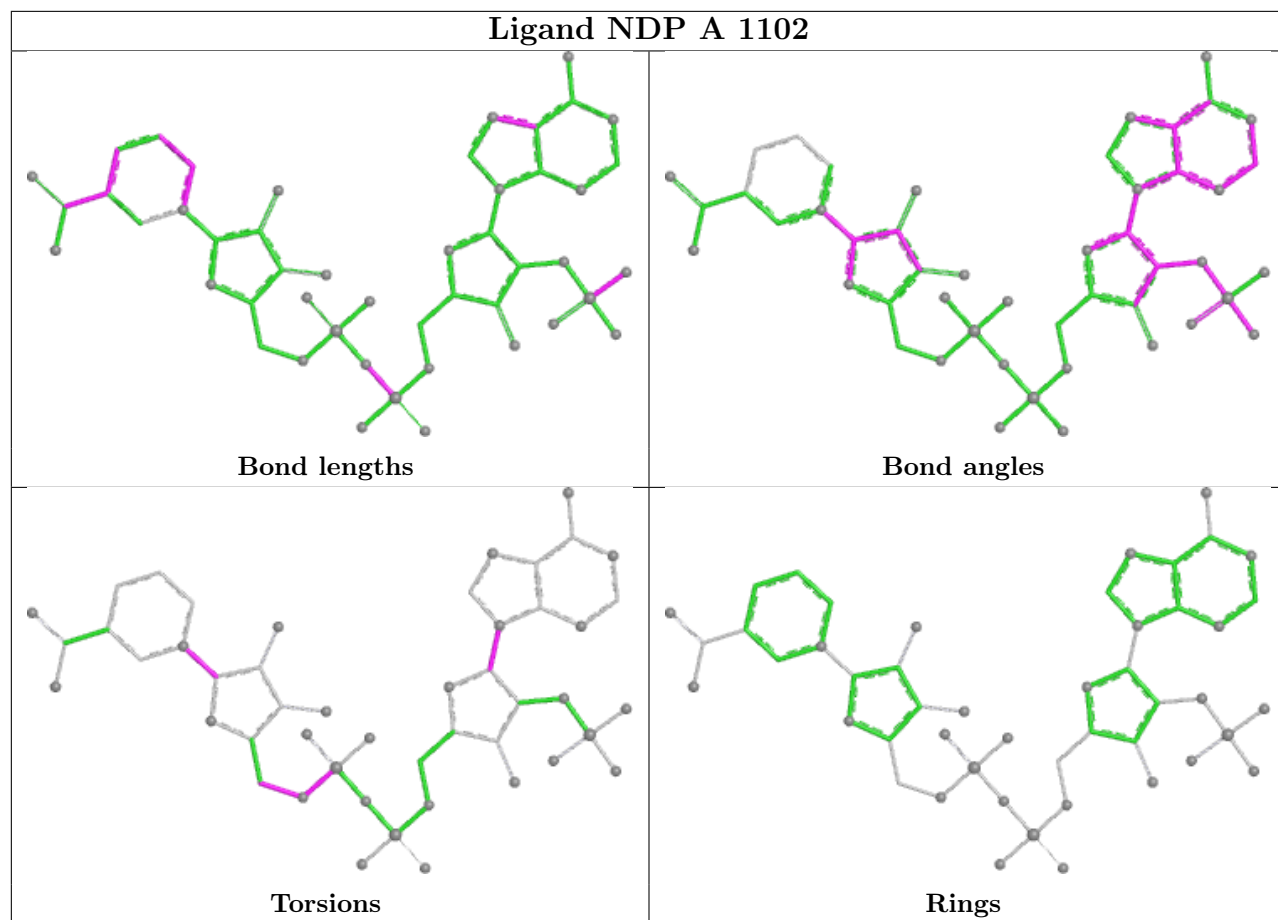
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	507	HEM	4	0
3	B	1202	NDP	3	0
2	D	507	HEM	2	0
3	A	1102	NDP	3	0
3	D	1402	NDP	1	0
3	C	1302	NDP	2	0
2	A	507	HEM	5	0

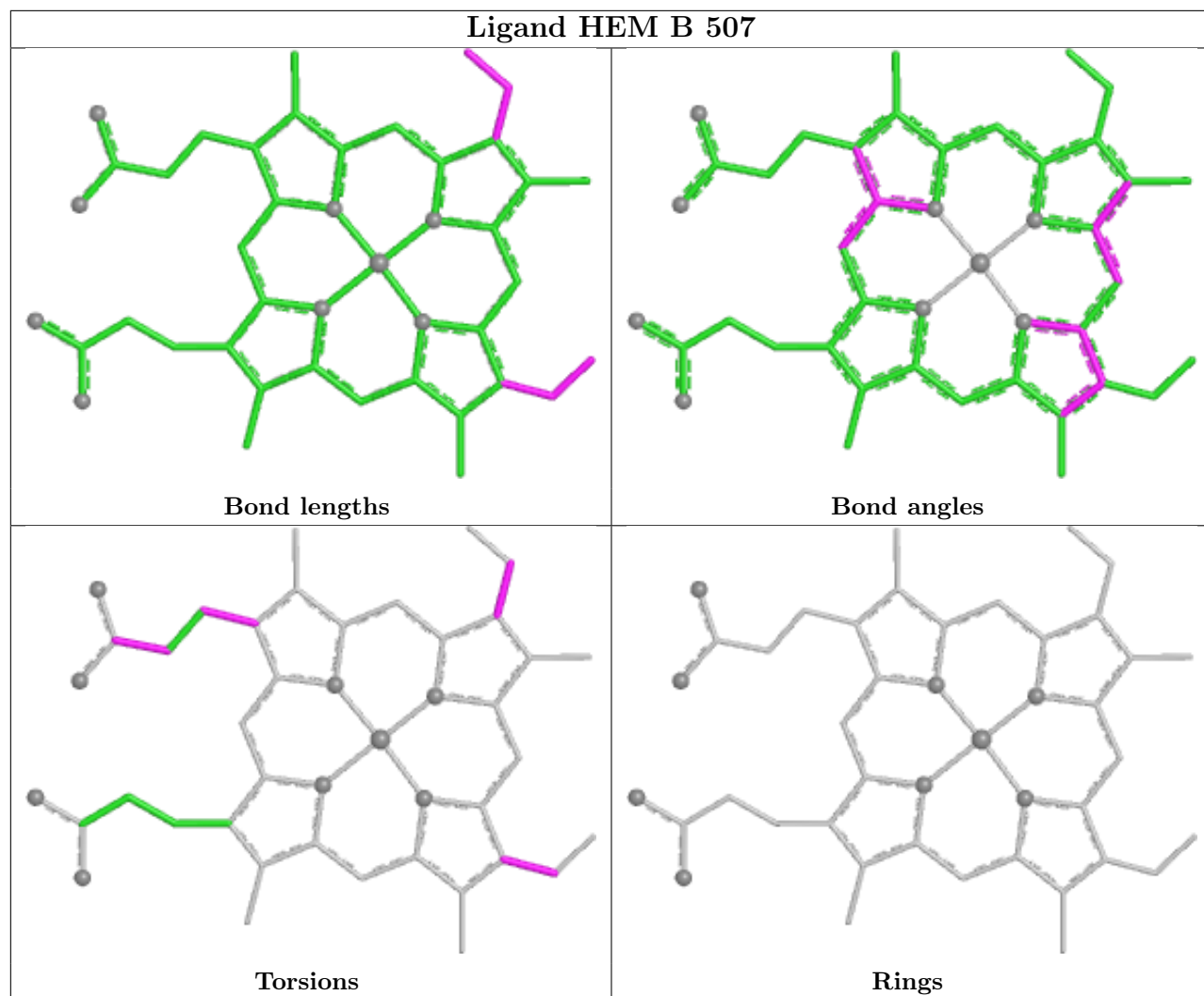
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

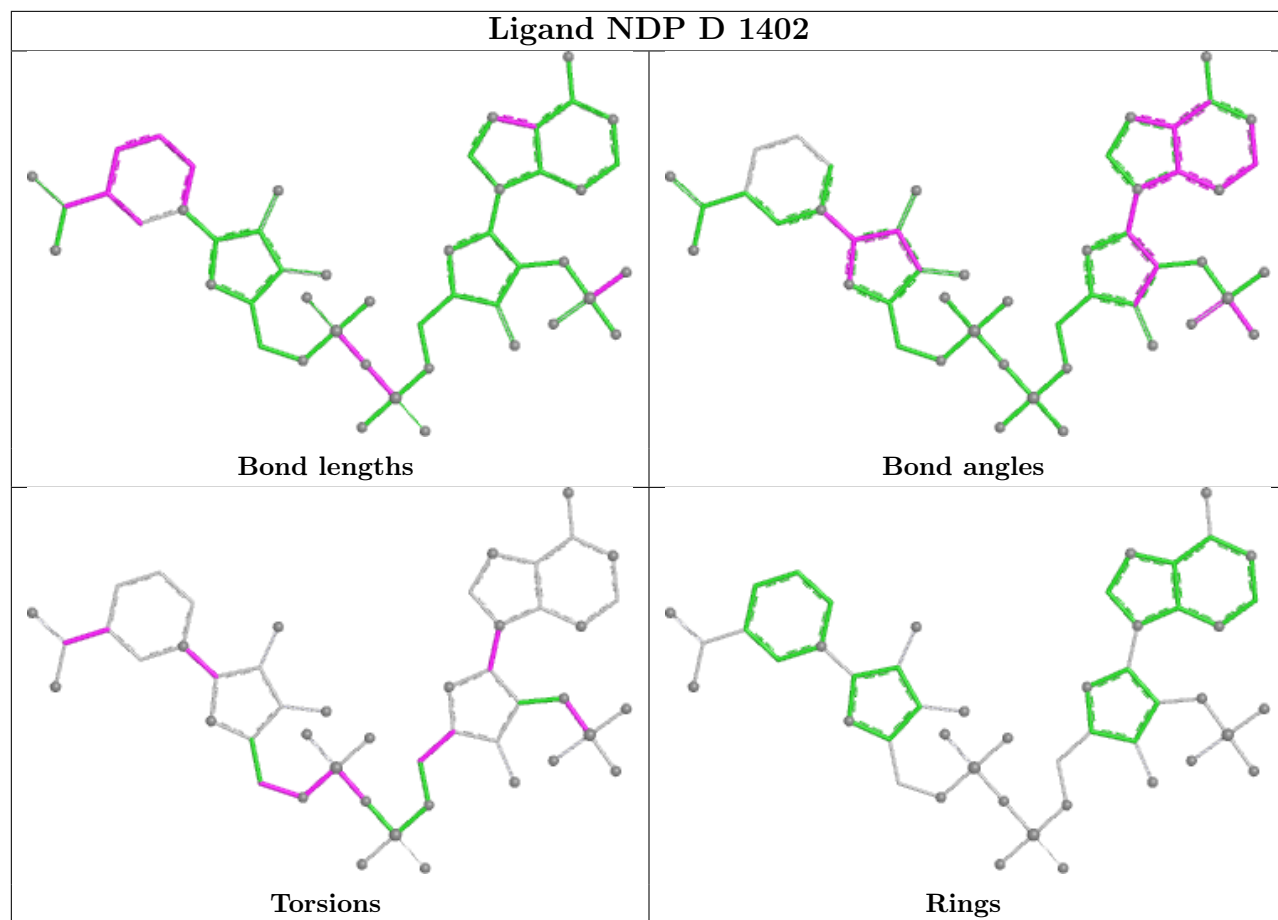


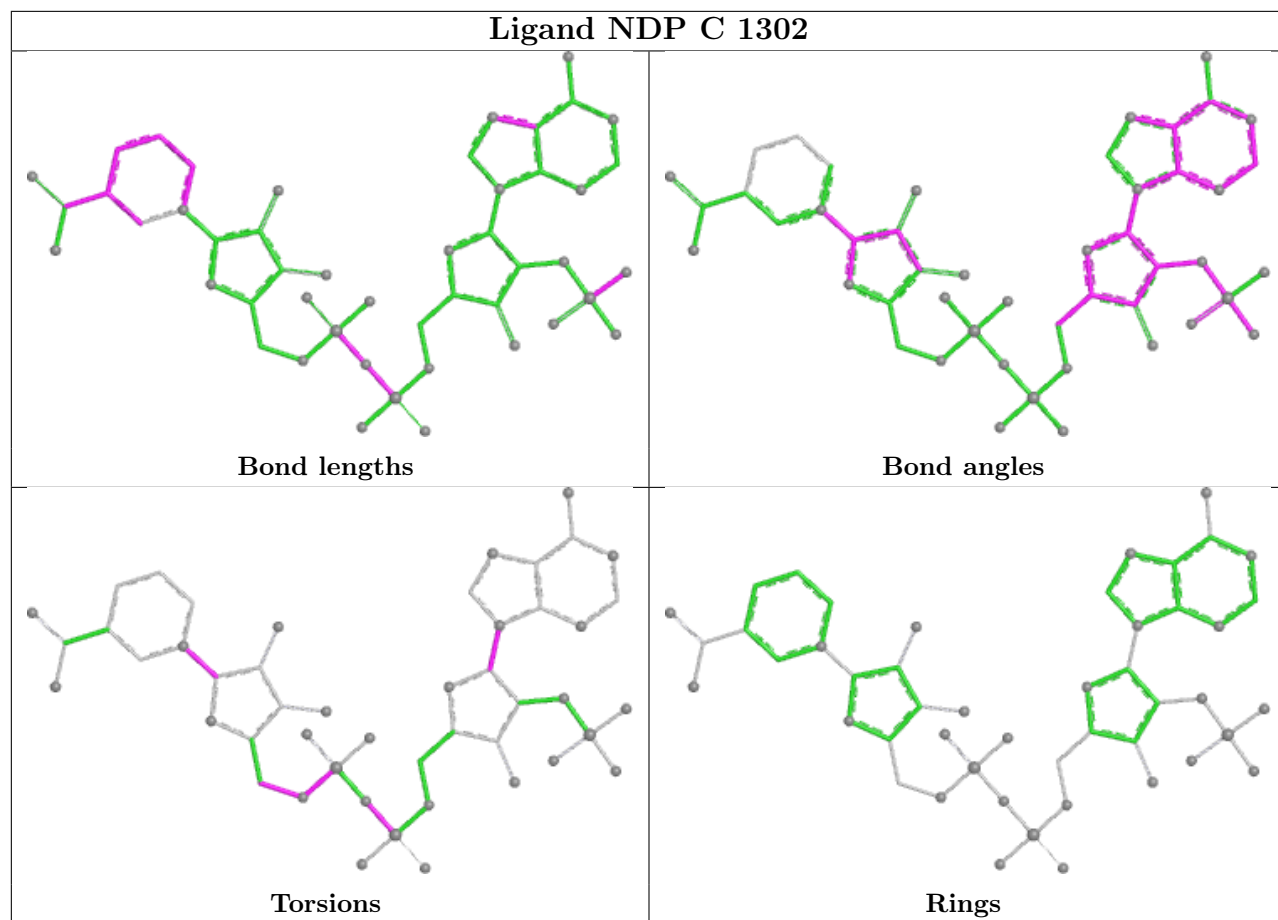


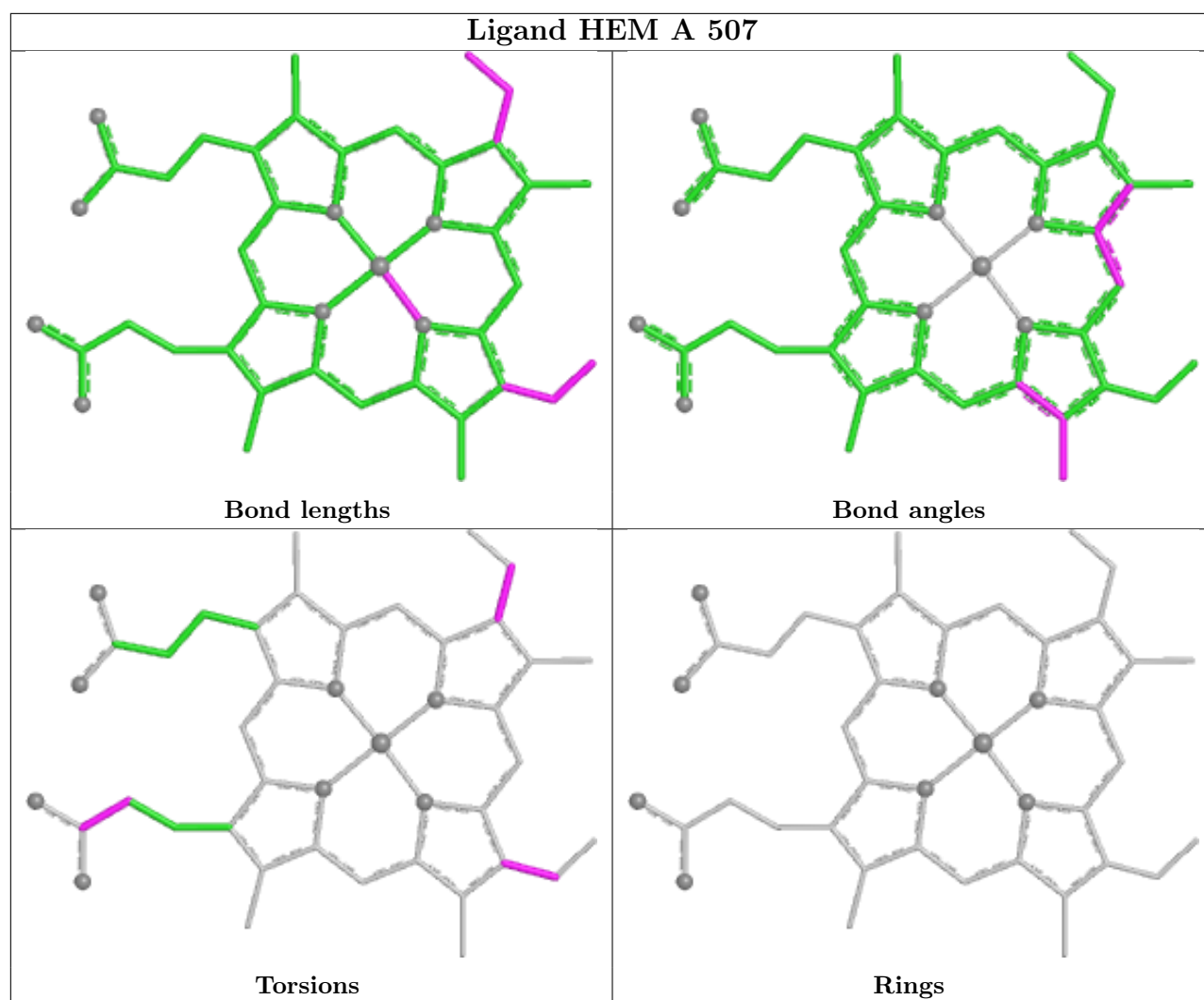












5.7 Other polymers [i](#)

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.