



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 01:25 am BST

PDB ID : 3TTV  
Title : Structure of the F413E variant of E. coli KatE  
Authors : Loewen, P.C.; Jha, V.  
Deposited on : 2011-09-15  
Resolution : 1.45 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](mailto: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.

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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	:	2.11
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)	:	2.11

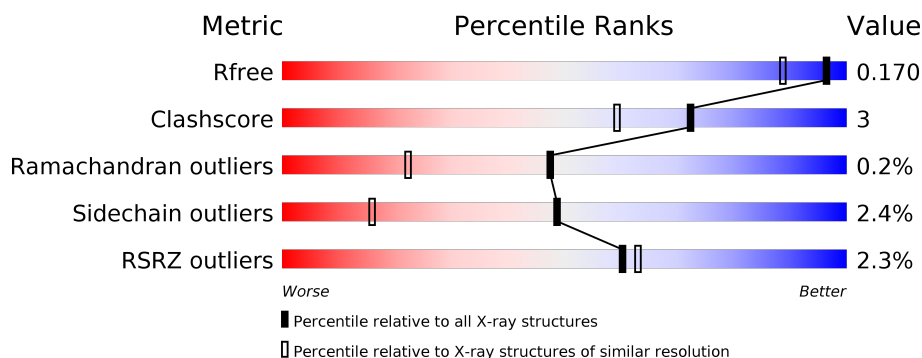
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	753	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>• •</div> </div> </div>
1	B	753	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>• •</div> </div> </div>
1	C	753	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• •</div> </div> </div>
1	D	753	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26511 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 Catalase HPIL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	3	0
			5755	3652	1006	1085	12			
1	B	726	Total	C	N	O	S	0	3	0
			5758	3654	1006	1086	12			
1	C	726	Total	C	N	O	S	0	2	0
			5750	3649	1006	1083	12			
1	D	726	Total	C	N	O	S	0	2	0
			5750	3649	1006	1083	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	ALA	THR	ENGINEERED MUTATION	UNP P21179
A	413	TYR	PHE	ENGINEERED MUTATION	UNP P21179
B	115	ALA	THR	ENGINEERED MUTATION	UNP P21179
B	413	TYR	PHE	ENGINEERED MUTATION	UNP P21179
C	115	ALA	THR	ENGINEERED MUTATION	UNP P21179
C	413	TYR	PHE	ENGINEERED MUTATION	UNP P21179
D	115	ALA	THR	ENGINEERED MUTATION	UNP P21179
D	413	TYR	PHE	ENGINEERED MUTATION	UNP P21179

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



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

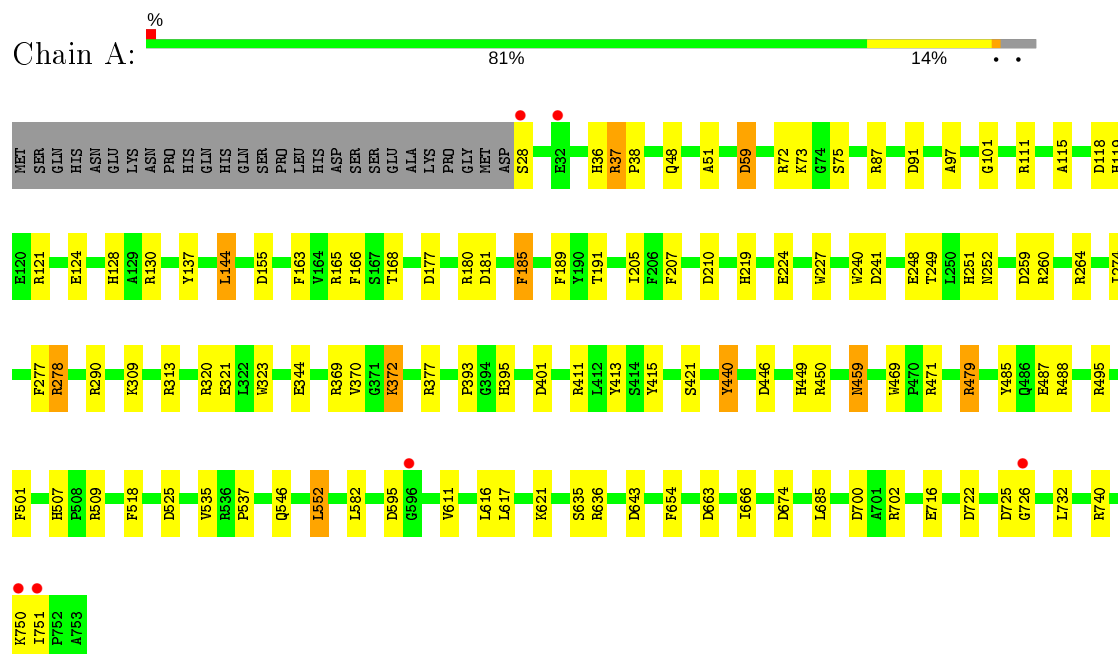
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	864	Total	O	0	0
			864	864		
3	B	775	Total	O	0	0
			775	775		
3	C	797	Total	O	0	0
			797	797		
3	D	890	Total	O	0	0
			890	890		

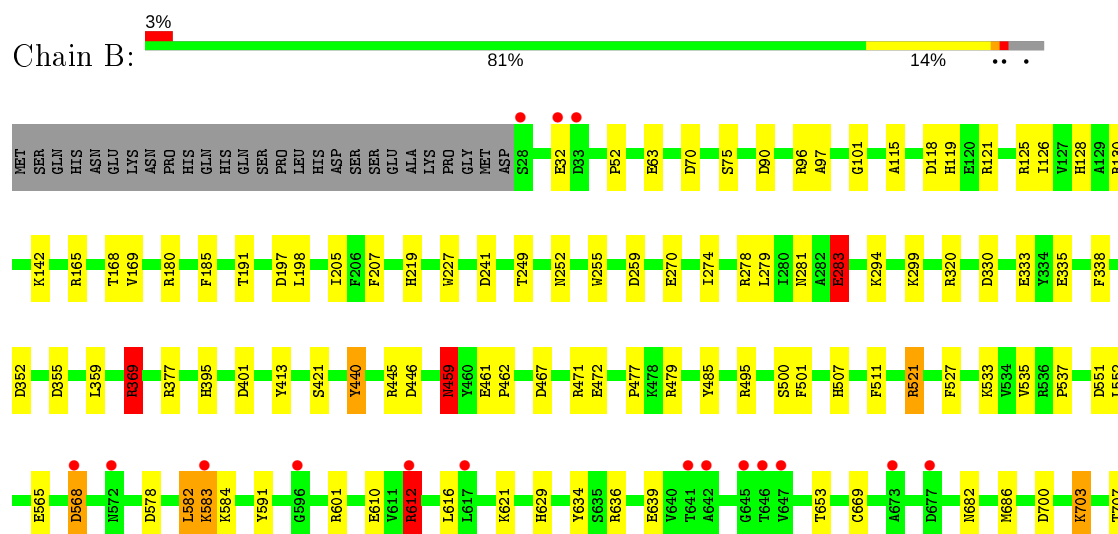
### 3 Residue-property plots

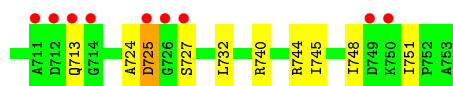
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: Catalase HPII

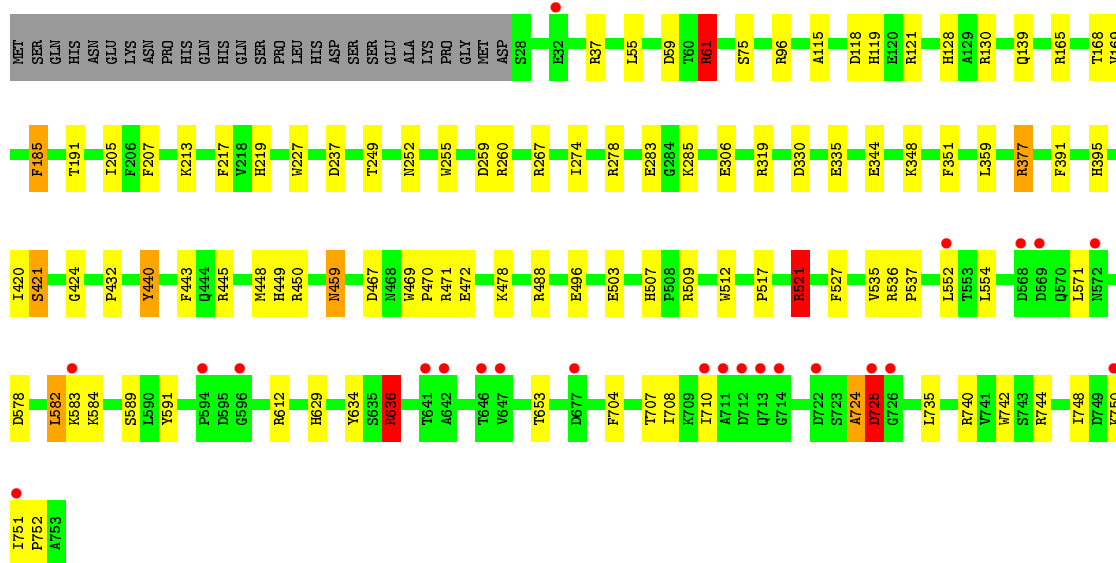
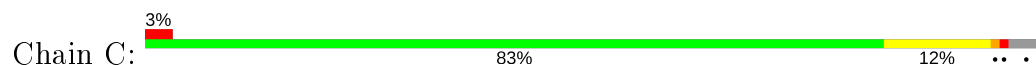


#### • Molecule 1: Catalase HPII

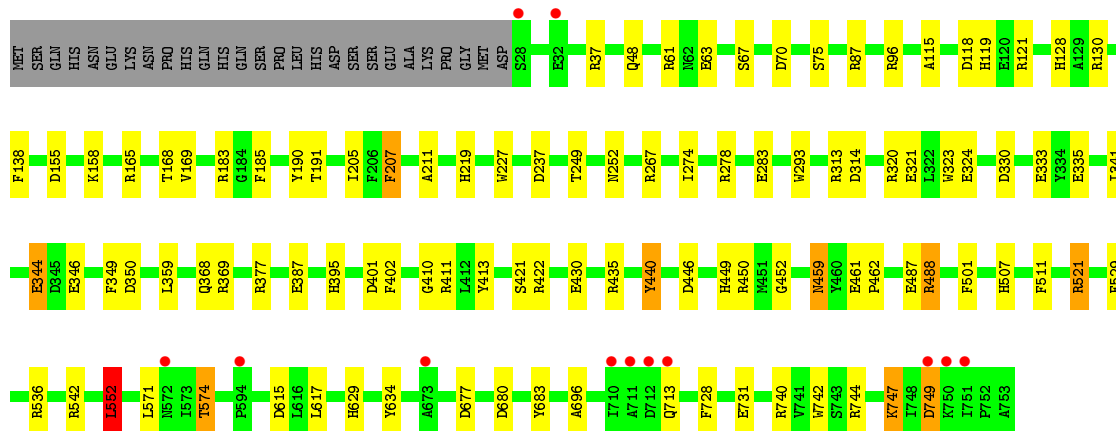
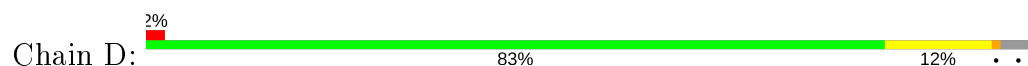




● Molecule 1: Catalase HP1I



● Molecule 1: Catalase HP1I



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.56Å 133.05Å 122.64Å 90.00° 109.29° 90.00°	Depositor
Resolution (Å)	32.16 – 1.45 32.16 – 1.45	Depositor EDS
% Data completeness (in resolution range)	96.8 (32.16-1.45) 96.8 (32.16-1.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 1.45Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.145 , 0.172 0.144 , 0.170	Depositor DCC
$R_{free}$ test set	24236 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.4	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	26511	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, OCS

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	1.35	14/5911 (0.2%)	1.39	72/8035 (0.9%)
1	B	1.29	12/5914 (0.2%)	1.30	53/8040 (0.7%)
1	C	1.31	24/5903 (0.4%)	1.29	39/8024 (0.5%)
1	D	1.37	22/5903 (0.4%)	1.33	46/8024 (0.6%)
All	All	1.33	72/23631 (0.3%)	1.33	210/32123 (0.7%)

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	1
1	C	0	3
All	All	0	4

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321	GLU	CD-OE1	10.68	1.37	1.25
1	D	321	GLU	CD-OE1	9.68	1.36	1.25
1	A	440	TYR	CE1-CZ	8.67	1.49	1.38
1	C	59	ASP	CB-CG	8.35	1.69	1.51
1	D	440	TYR	CE1-CZ	8.06	1.49	1.38

The worst 5 of 210 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	37	ARG	NE-CZ-NH2	-12.96	113.82	120.30
1	A	130	ARG	NE-CZ-NH2	-12.87	113.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	495	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	A	636	ARG	NE-CZ-NH2	10.75	125.67	120.30
1	A	740	ARG	NE-CZ-NH2	-10.61	114.99	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	121	ARG	Sidechain
1	C	121	ARG	Sidechain
1	C	724	ALA	Peptide
1	C	725	ASP	Peptide

## 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	5755	0	5587	37	2
1	B	5758	0	5589	53	2
1	C	5750	0	5583	35	0
1	D	5750	0	5583	41	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
2	C	43	0	30	1	0
2	D	43	0	30	1	0
3	A	864	0	0	9	1
3	B	775	0	0	15	0
3	C	797	0	0	9	0
3	D	890	0	0	16	1
All	All	26511	0	22462	153	3

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 3.

The worst 5 of 153 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:B:521:ARG:HD3	3:B:3047:HOH:O	1.27	1.33
1:B:533:LYS:HE3	3:C:2623:HOH:O	1.28	1.26
1:D:449[B]:HIS:NE2	3:D:2501:HOH:O	1.65	1.24
1:A:546:GLN:HG3	3:A:3434:HOH:O	1.45	1.16
1:A:479:ARG:NH2	3:A:2607:HOH:O	1.89	1.05

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2805:HOH:O	3:D:2468:HOH:O[1_455]	1.97	0.23
1:A:59:ASP:OD1	1:B:369:ARG:NH2[2_545]	1.97	0.23
1:A:59:ASP:OD1	1:B:369:ARG:NH1[2_545]	2.19	0.01

## 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	726/753 (96%)	709 (98%)	16 (2%)	1 (0%)	51 24
1	B	726/753 (96%)	706 (97%)	17 (2%)	3 (0%)	34 13
1	C	725/753 (96%)	705 (97%)	18 (2%)	2 (0%)	41 18
1	D	725/753 (96%)	708 (98%)	16 (2%)	1 (0%)	51 24
All	All	2902/3012 (96%)	2828 (98%)	67 (2%)	7 (0%)	47 22

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	C	75	SER
1	A	75	SER
1	B	75	SER

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Mol	Chain	Res	Type
1	C	725	ASP

### 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	612/634 (96%)	603 (98%)	9 (2%)	65	35
1	B	612/634 (96%)	594 (97%)	18 (3%)	42	10
1	C	611/634 (96%)	593 (97%)	18 (3%)	42	10
1	D	611/634 (96%)	597 (98%)	14 (2%)	50	17
All	All	2446/2536 (96%)	2387 (98%)	59 (2%)	49	16

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	732	LEU
1	C	252	ASN
1	D	459	ASN
1	C	61	ARG
1	C	191	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	459	ASN
1	C	572	ASN
1	D	629	HIS
1	C	507	HIS
1	C	556	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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
1	OCS	A	669	1	7,8,9	2.20	2 (28%)	6,11,13	1.74	2 (33%)
1	OCS	D	669	1	7,8,9	2.14	2 (28%)	6,11,13	2.10	2 (33%)
1	OCS	B	669	1	7,8,9	1.96	1 (14%)	6,11,13	4.22	3 (50%)
1	OCS	C	669	1	7,8,9	1.58	2 (28%)	6,11,13	2.10	2 (33%)

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
1	OCS	A	669	1	-	3/4/7/9	-
1	OCS	D	669	1	-	1/4/7/9	-
1	OCS	B	669	1	-	3/4/7/9	-
1	OCS	C	669	1	-	1/4/7/9	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	669	OCS	OD2-SG	4.71	1.64	1.47
1	D	669	OCS	CB-CA	4.43	1.58	1.53
1	A	669	OCS	OD2-SG	4.42	1.63	1.47
1	D	669	OCS	OD2-SG	3.05	1.58	1.47
1	C	669	OCS	OD2-SG	2.88	1.57	1.47

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	669	OCS	OD1-SG-CB	7.33	115.65	106.94
1	B	669	OCS	OD3-SG-CB	-5.80	100.04	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	669	OCS	OD1-SG-CB	-4.40	101.72	106.94
1	D	669	OCS	OD3-SG-CB	-4.15	102.01	106.94
1	B	669	OCS	OD2-SG-CB	-4.03	99.32	105.74

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	669	OCS	N-CA-CB-SG
1	D	669	OCS	N-CA-CB-SG
1	B	669	OCS	N-CA-CB-SG
1	C	669	OCS	N-CA-CB-SG
1	A	669	OCS	CA-CB-SG-OD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	669	OCS	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	D	760	1	27,50,50	1.35	4 (14%)	17,82,82	2.90	6 (35%)
2	HEM	A	760	1	27,50,50	1.90	6 (22%)	17,82,82	3.48	9 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	C	760	1	27,50,50	1.60	6 (22%)	17,82,82	2.66	6 (35%)
2	HEM	B	760	1	27,50,50	1.68	7 (25%)	17,82,82	2.54	8 (47%)

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	D	760	1	-	0/6/54/54	-
2	HEM	A	760	1	-	0/6/54/54	-
2	HEM	C	760	1	-	0/6/54/54	-
2	HEM	B	760	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)
2	A	760	HEM	C4A-NA	5.33	1.47	1.36
2	A	760	HEM	C1A-NA	4.57	1.45	1.36
2	B	760	HEM	C4A-NA	3.67	1.43	1.36
2	B	760	HEM	C1A-NA	3.44	1.43	1.36
2	C	760	HEM	C4A-NA	3.43	1.43	1.36

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	760	HEM	C1D-C2D-C3D	-8.01	101.42	107.00
2	A	760	HEM	CBD-CAD-C3D	-6.41	100.67	112.48
2	A	760	HEM	CAA-CBA-CGA	-5.83	102.89	112.67
2	B	760	HEM	CAA-CBA-CGA	-5.79	102.95	112.67
2	D	760	HEM	CBD-CAD-C3D	-5.73	101.92	112.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

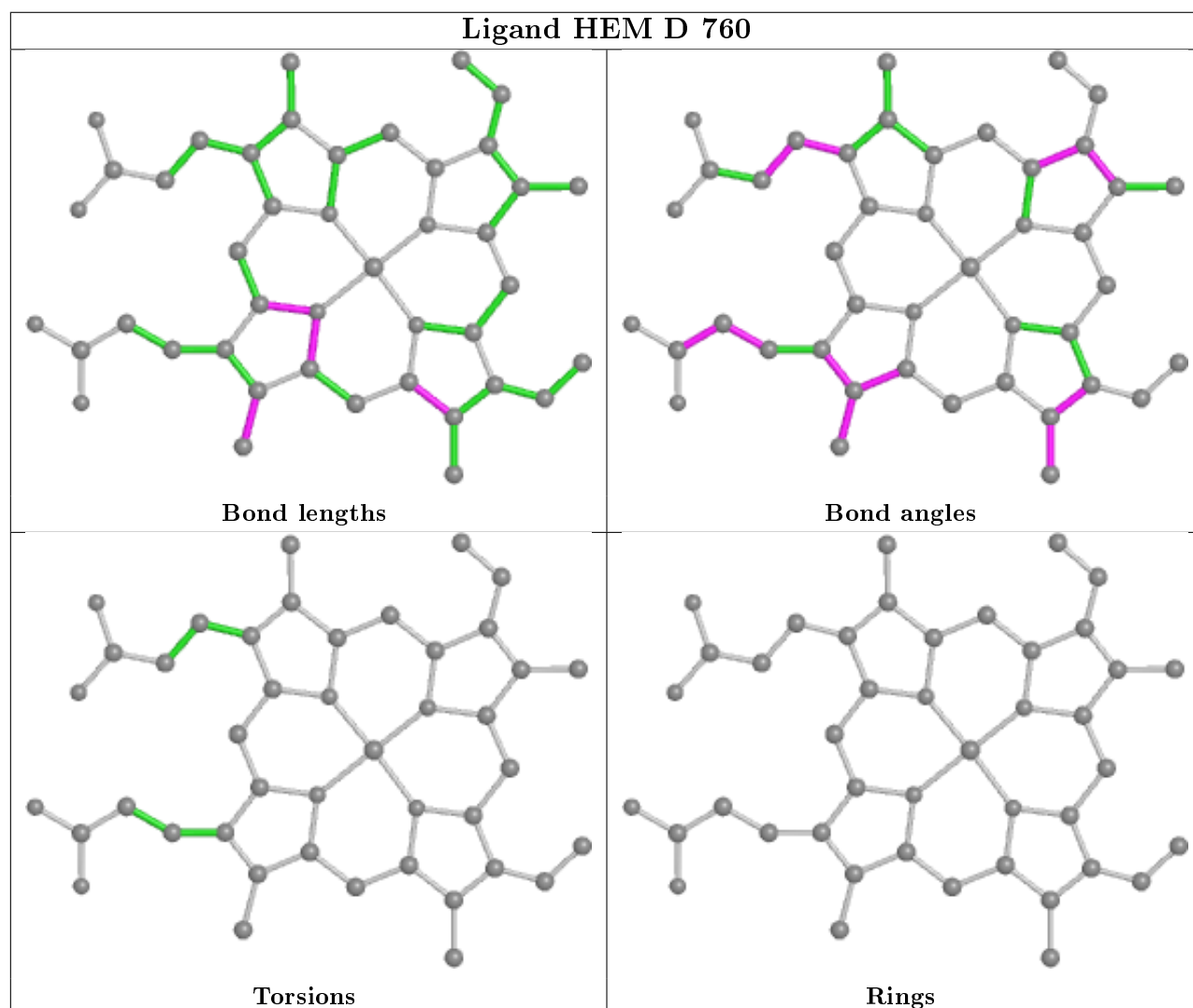
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	760	HEM	1	0
2	A	760	HEM	1	0

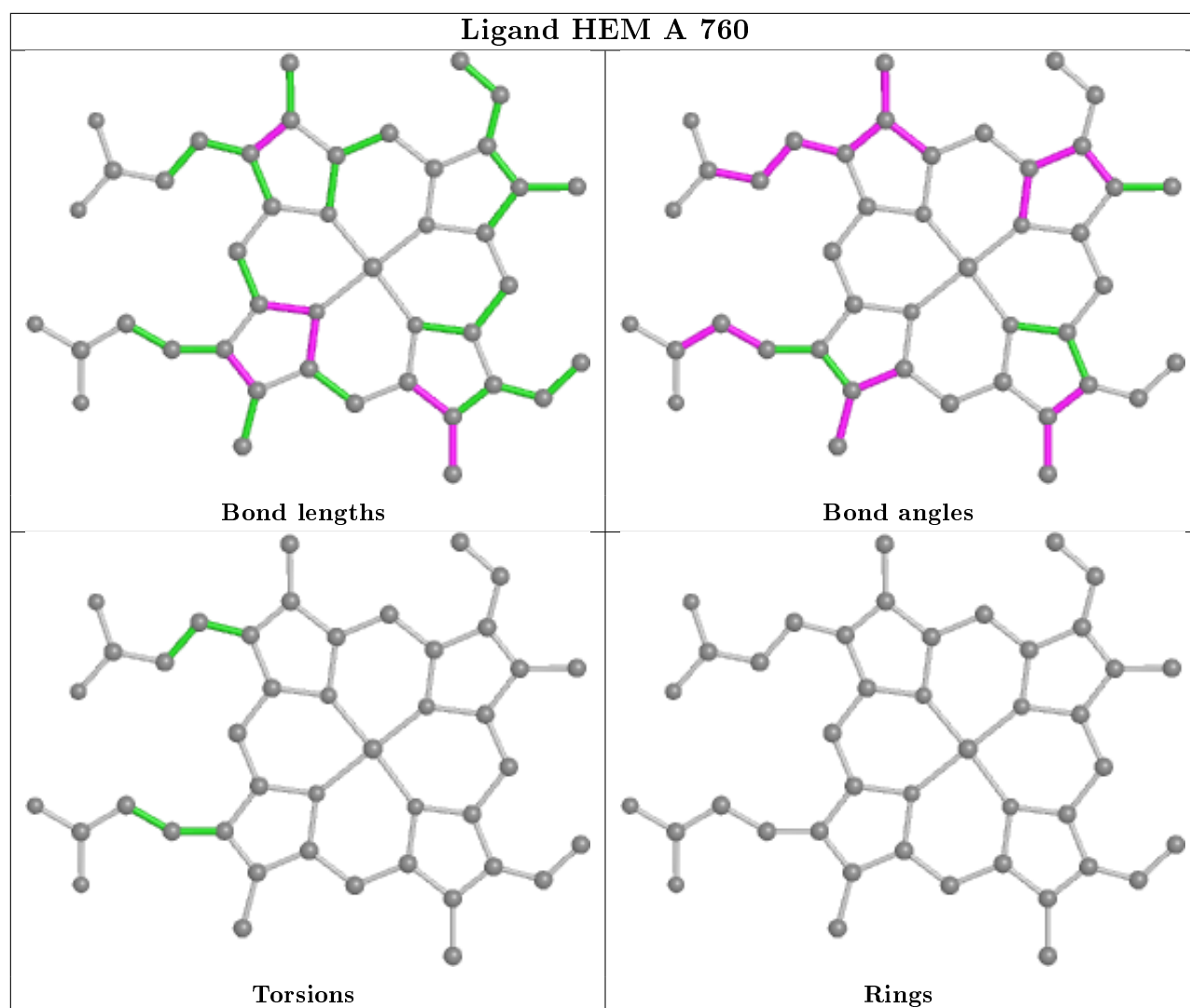
*Continued on next page...*

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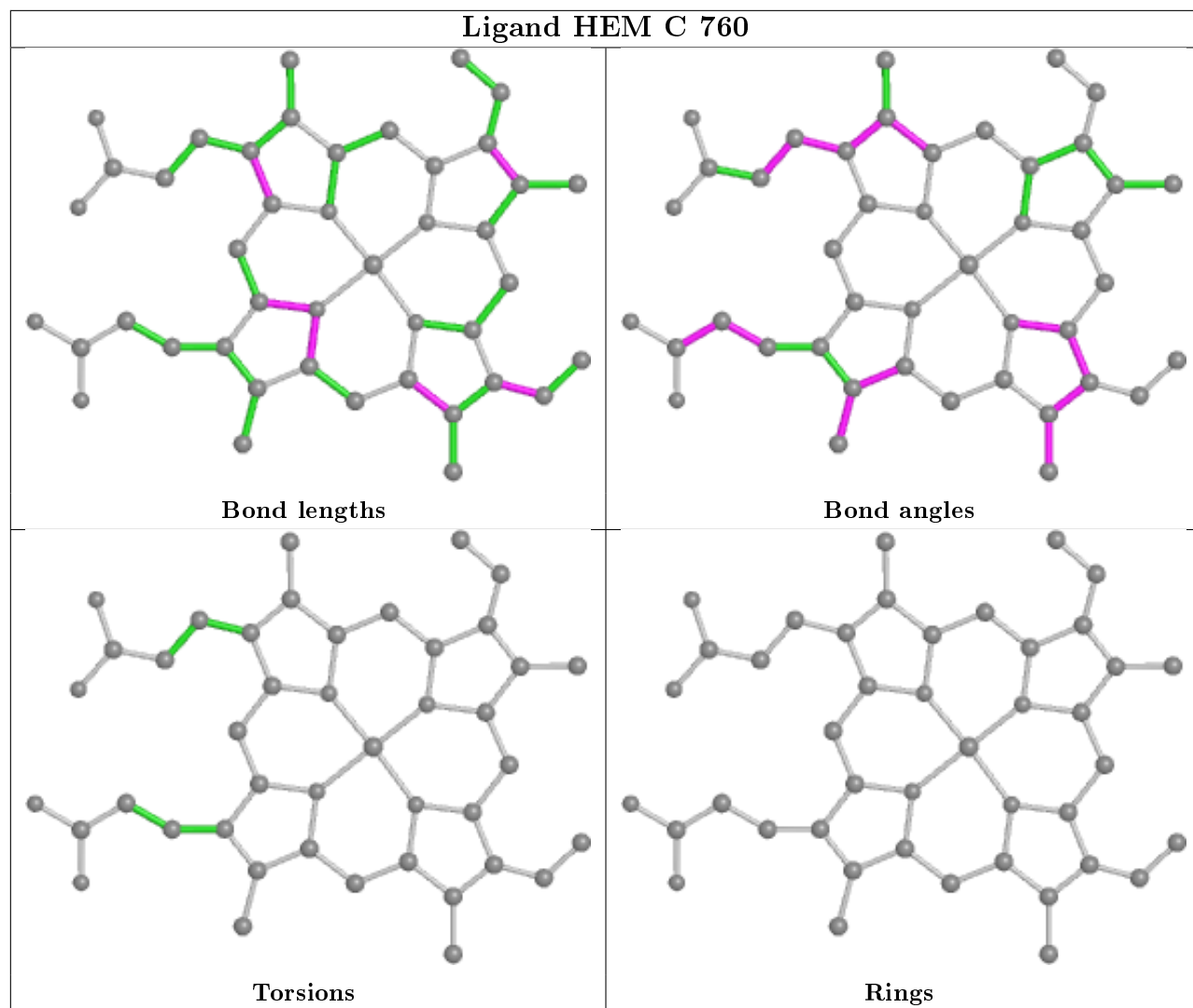
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	760	HEM	1	0
2	B	760	HEM	1	0

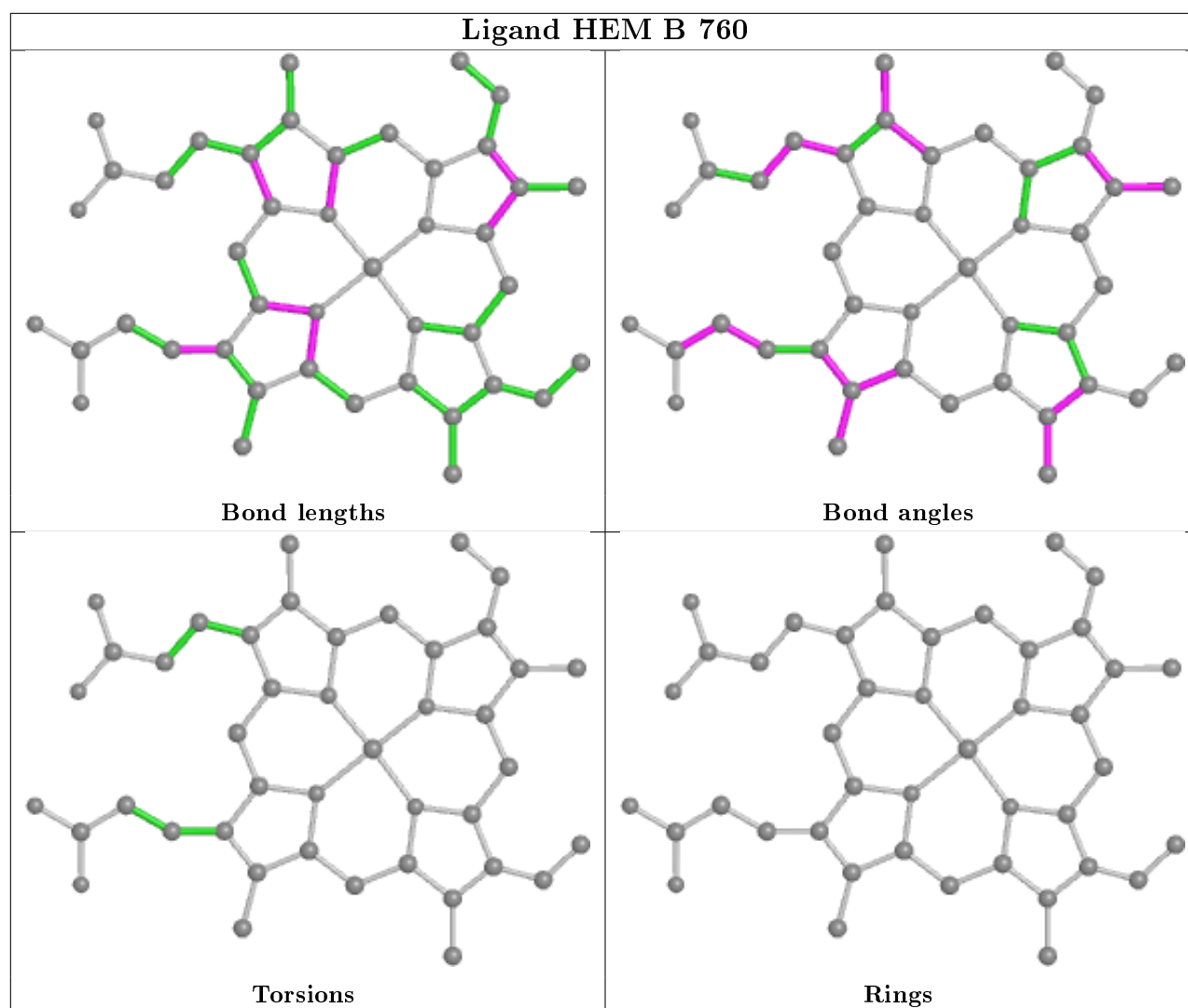
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	725/753 (96%)	-0.35	6 (0%) 86 87	6, 11, 25, 52	1 (0%)
1	B	725/753 (96%)	-0.20	25 (3%) 45 48	7, 13, 34, 57	1 (0%)
1	C	725/753 (96%)	-0.25	23 (3%) 47 50	7, 13, 33, 53	1 (0%)
1	D	725/753 (96%)	-0.31	12 (1%) 70 70	6, 11, 27, 56	1 (0%)
All	All	2900/3012 (96%)	-0.28	66 (2%) 60 63	6, 12, 31, 57	4 (0%)

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	GLY	5.6
1	D	750	LYS	4.4
1	C	726	GLY	4.3
1	B	713	GLN	4.2
1	C	711	ALA	4.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	OCS	B	669	9/10	0.93	0.13	27,28,33,38	0
1	OCS	D	669	9/10	0.94	0.12	19,21,27,29	0
1	OCS	C	669	9/10	0.94	0.14	27,30,36,39	0
1	OCS	A	669	9/10	0.95	0.11	16,19,26,29	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

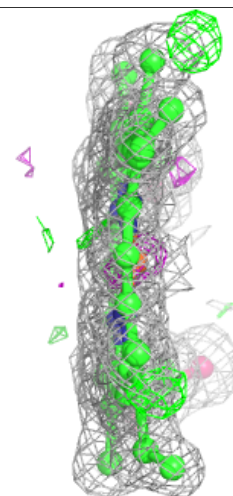
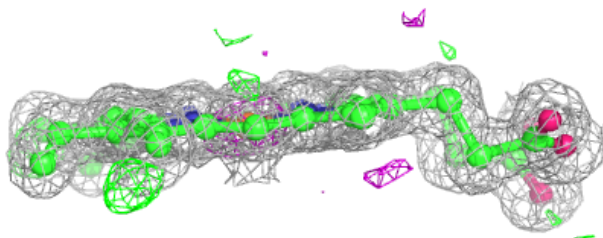
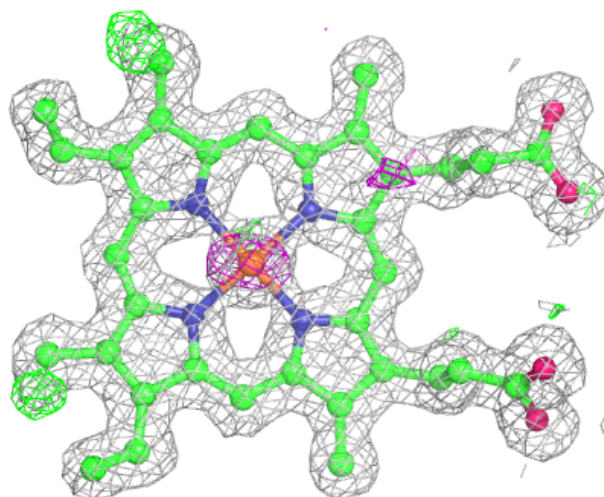
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	D	760	43/43	0.99	0.05	5,7,8,14	0
2	HEM	A	760	43/43	0.99	0.06	5,7,9,15	0
2	HEM	C	760	43/43	0.99	0.05	6,8,10,17	0
2	HEM	B	760	43/43	0.99	0.06	6,8,10,16	0

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.

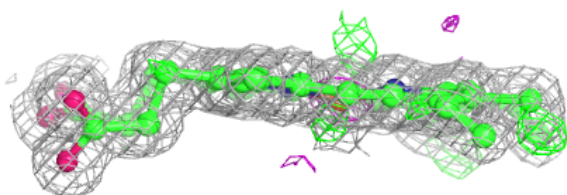
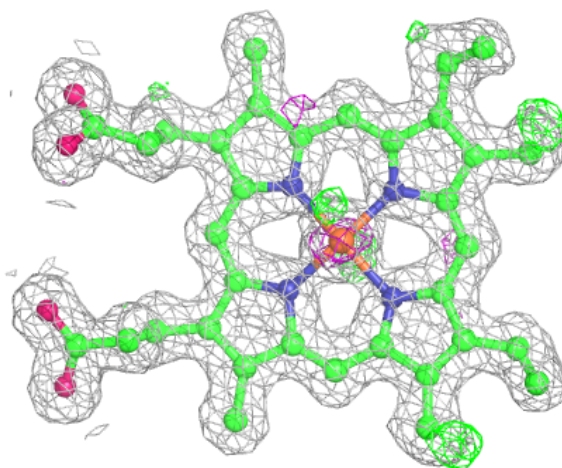
**Electron density around HEM D 760:**

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



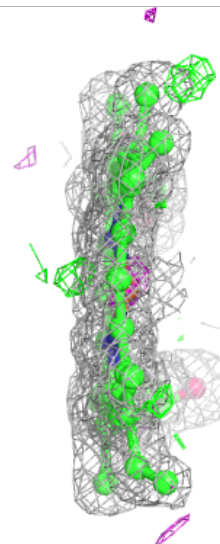
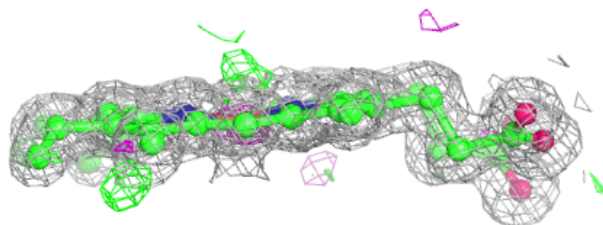
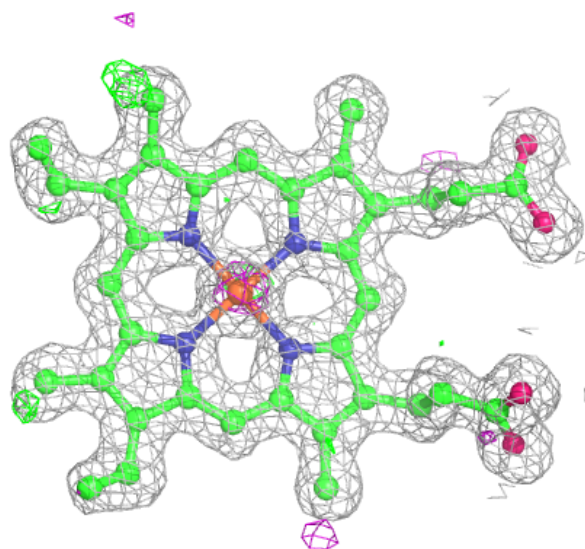
**Electron density around HEM A 760:**

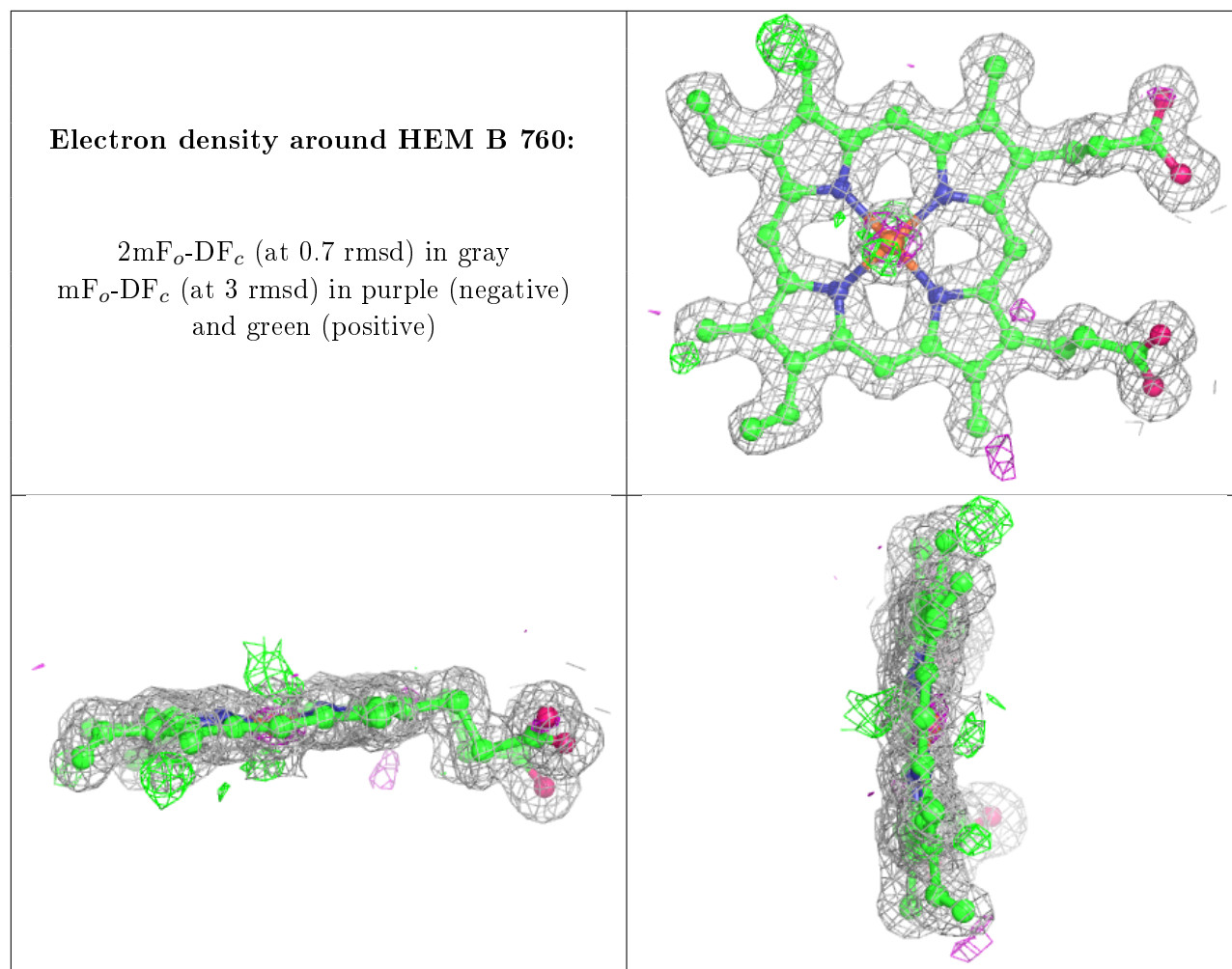
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM C 760:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.