wwPDB X-ray Structure Validation Summary Report (i)

Sep 5, 2023 – 06:34 AM EDT

PDB ID	:	3TTW
Title	:	Structure of the F413E variant of E. coli KatE
Authors	:	Loewen, P.C.; Jha, V.
Deposited on	:	2011-09-15
Resolution	:	1.62 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

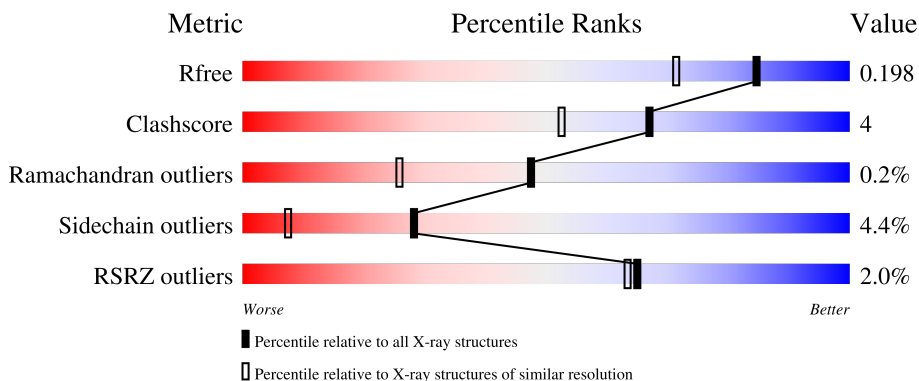|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

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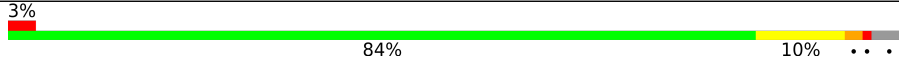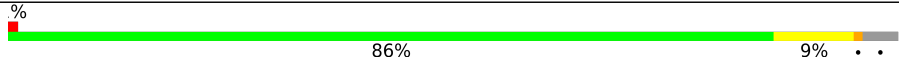*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.62 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	Percentile Ranks	Value
Rfree		0.198
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		4.4%
RSRZ outliers		2.0%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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% 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	% 86% 9% · ·
1	B	753	3% 84% 11% · ·
1	C	753	3% 84% 10% · · ·
1	D	753	% 86% 9% · ·

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 25988 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 HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	1	0
			5745	3643	1006	1084	12			
1	B	726	Total	C	N	O	S	0	1	0
			5746	3644	1006	1084	12			
1	C	726	Total	C	N	O	S	0	1	0
			5745	3643	1006	1084	12			
1	D	726	Total	C	N	O	S	0	1	0
			5746	3644	1006	1084	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	413	GLU	PHE	engineered mutation	UNP P21179
B	413	GLU	PHE	engineered mutation	UNP P21179
C	413	GLU	PHE	engineered mutation	UNP P21179
D	413	GLU	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	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	768	Total	O	0	0
			768	768		
3	B	643	Total	O	0	0
			643	643		
3	C	693	Total	O	0	0
			693	693		
3	D	730	Total	O	0	0
			730	730		

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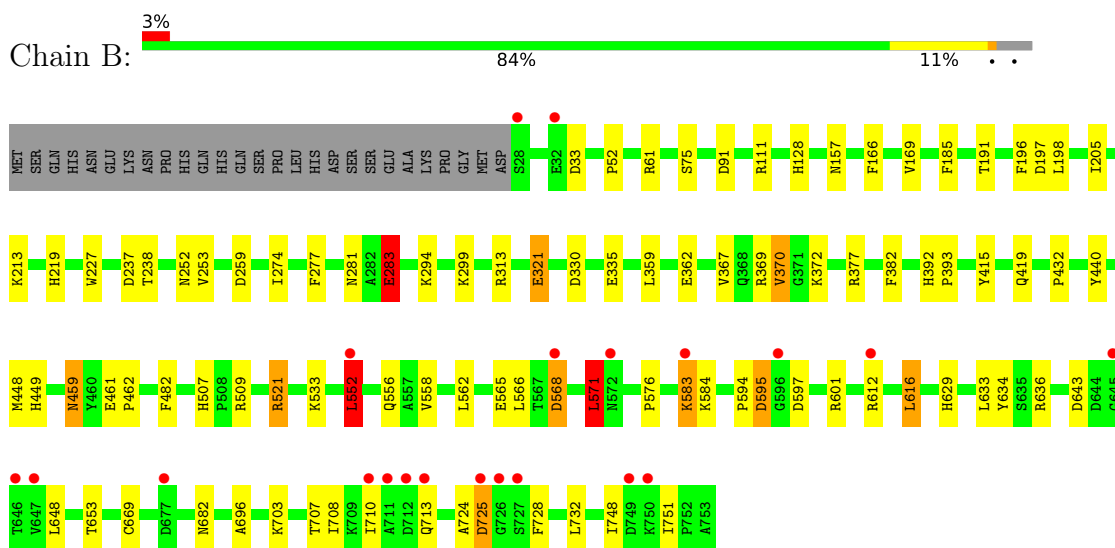 outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 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.
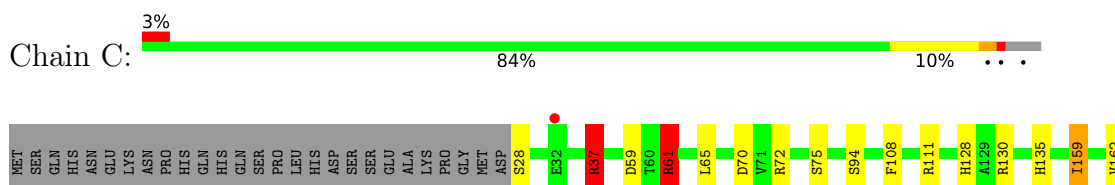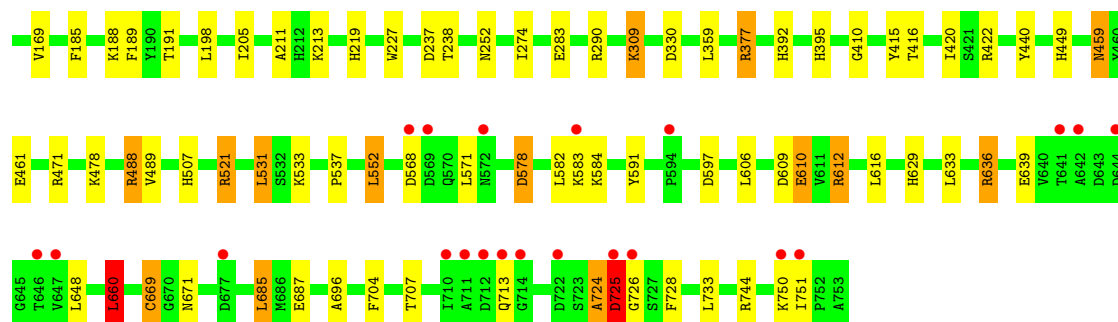
- Molecule 1: Catalase HPII

Chain A:

- Molecule 1: Catalase HPII

Chain B:

- Molecule 1: Catalase HPII

Chain C:

V169 F185 K188 F189 Y190 T191 L198 I205 A211 H212 K213 H219 W227 D237 T238 N252 I274 E283 R290 K309 D330 L359 R377 H392 H395 G410 Y415 T416 I420 S421 R422 Y440 H449 N459 Y460

E461 R471 K478 R488 V489 H507 R521 L531 S532 K533 P537 L552 D568 D569 Q570 L571 N572 D578 L582 K583 K584 Y591 P594 D597 L606 D609 E610 V611 R612 L616 H629 L633 R636 E639 V640 T641 A642 D643 D644

G645 T646 V647 L648 L660 C669 G670 N671 D677 L685 M686 E687 A696 F704 T707 I710 A711 D712 Q713 G714 D722 S723 A724 D725 G726 S727 F728 L733 R744 K750 I751 P752 A753

• Molecule 1: Catalase HPII

%

Chain D:

86% 9% • •

MET SER GLN HIS ASN GLU LYS ASN PRO HIS GLN HIS GLN SER PRO LEU HIS ASP SER GLU ALA LYS PRO GLY MET ASP S28 E32 Q48 R61 N66 E69 K73 G74 S75 R96 R100 K158 D181 F185 T191 I205 A211 H212 K213

H219 W227 G232 D237 Y242 N252 T268 I274 G298 D330 L340 I341 E344 L359 H392 D401 G410 Y415 Q419 P432 Y440 F443 Q444 R445 M448 H449 R450 M451 N459 Y460 E461 P470 R471 K478

R488 V489 E490 R495 E496 H507 P508 R509 W512 R521 L552 T553 L554 L571 T574 P575 P576 L582 L590 D597 V598 V602 R612 L616 V628 H629 D643 L648 C669 A696 A711 D712 Q713 D725 F728 E731 R740

K747 I748 D749 K750 I751 P752 A753

4　Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.49Å　132.85Å　122.68Å 90.00°　109.36°　90.00°	Depositor
Resolution (Å)	31.25　–　1.62 31.25　–　1.62	Depositor EDS
% Data completeness (in resolution range)	87.1 (31.25-1.62) 87.1 (31.25-1.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 1.62Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.156　,　0.199 0.155　,　0.198	Depositor DCC
R_{free} test set	15716 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	15.0	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.2	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	25988	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	1.22	6/5895 (0.1%)	1.11	27/8013 (0.3%)
1	B	1.21	14/5895 (0.2%)	1.08	23/8013 (0.3%)
1	C	1.20	6/5895 (0.1%)	1.07	24/8013 (0.3%)
1	D	1.23	11/5895 (0.2%)	1.10	21/8013 (0.3%)
All	All	1.21	37/23580 (0.2%)	1.09	95/32052 (0.3%)

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	C	0	2

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	321	GLU	CB-CG	10.32	1.71	1.52
1	B	157	ASN	CB-CG	7.22	1.67	1.51
1	A	440	TYR	CE1-CZ	7.17	1.47	1.38
1	B	321	GLU	CG-CD	-6.85	1.41	1.51
1	B	283	GLU	CG-CD	6.67	1.61	1.51

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	61	ARG	NE-CZ-NH2	14.05	127.33	120.30
1	A	740	ARG	NE-CZ-NH1	10.29	125.44	120.30
1	D	61	ARG	NE-CZ-NH1	-10.22	115.19	120.30
1	A	377	ARG	NE-CZ-NH2	-9.12	115.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	521	ARG	NE-CZ-NH2	8.91	124.75	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	5745	0	5572	49	0
1	B	5746	0	5577	46	0
1	C	5745	0	5573	52	0
1	D	5746	0	5577	41	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	2	0
2	D	43	0	30	1	0
3	A	768	0	0	6	0
3	B	643	0	0	9	0
3	C	693	0	0	21	0
3	D	730	0	0	10	0
All	All	25988	0	22419	177	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 4.

The worst 5 of 177 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:392:HIS:ND1	1:A:415:TYR:CB	1.67	1.54
1:B:392:HIS:ND1	1:B:415:TYR:CB	1.70	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:HIS:ND1	1:D:415:TYR:CB	1.69	1.51
1:C:392:HIS:ND1	1:C:415:TYR:CB	1.70	1.48
1:C:449[A]:HIS:CE1	3:C:3266:HOH:O	1.71	1.31

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	724/753 (96%)	706 (98%)	16 (2%)	2 (0%)	41	21
1	B	724/753 (96%)	701 (97%)	21 (3%)	2 (0%)	41	21
1	C	724/753 (96%)	703 (97%)	19 (3%)	2 (0%)	41	21
1	D	724/753 (96%)	707 (98%)	16 (2%)	1 (0%)	51	28
All	All	2896/3012 (96%)	2817 (97%)	72 (2%)	7 (0%)	47	26

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	711	ALA
1	B	725	ASP
1	A	75	SER
1	B	75	SER
1	C	75	SER

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	611/635 (96%)	590 (97%)	21 (3%)	37	12
1	B	611/635 (96%)	584 (96%)	27 (4%)	28	7
1	C	611/635 (96%)	573 (94%)	38 (6%)	18	3
1	D	611/635 (96%)	589 (96%)	22 (4%)	35	11
All	All	2444/2540 (96%)	2336 (96%)	108 (4%)	28	7

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	252	ASN
1	C	584	LYS
1	D	574	THR
1	C	440	TYR
1	C	537	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	671	ASN
1	D	459	ASN
1	D	252	ASN
1	D	507	HIS
1	B	507	HIS

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	0.70	0	6,11,13	2.21	1 (16%)
1	OCS	B	669	1	7,8,9	1.06	0	6,11,13	1.44	1 (16%)
1	OCS	C	669	1	7,8,9	0.80	0	6,11,13	2.42	2 (33%)
1	OCS	D	669	1	7,8,9	0.94	0	6,11,13	1.39	1 (16%)

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	669	OCS	OD1-SG-CB	4.65	112.47	106.94
1	C	669	OCS	OD3-SG-CB	4.52	112.31	106.94
1	C	669	OCS	OD1-SG-CB	-3.43	102.86	106.94
1	B	669	OCS	OD3-SG-CB	-3.25	103.08	106.94
1	D	669	OCS	OD2-SG-OD3	2.24	116.75	111.27

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	669	OCS	N-CA-CB-SG
1	B	669	OCS	N-CA-CB-SG
1	C	669	OCS	N-CA-CB-SG
1	D	669	OCS	N-CA-CB-SG
1	A	669	OCS	CA-CB-SG-OD1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	669	OCS	1	0
1	D	669	OCS	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	C	760	1	41,50,50	1.60	10 (24%)	45,82,82	2.44	17 (37%)
2	HEM	B	760	1	41,50,50	1.78	9 (21%)	45,82,82	2.29	18 (40%)
2	HEM	A	760	1	41,50,50	1.73	9 (21%)	45,82,82	2.39	20 (44%)
2	HEM	D	760	1	41,50,50	1.77	10 (24%)	45,82,82	2.35	19 (42%)

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	760	1	-	2/12/54/54	-
2	HEM	B	760	1	-	2/12/54/54	-
2	HEM	A	760	1	-	2/12/54/54	-
2	HEM	D	760	1	-	2/12/54/54	-

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HEM	C3D-C2D	5.60	1.48	1.36
2	D	760	HEM	C3D-C2D	5.56	1.48	1.36
2	B	760	HEM	C3D-C2D	4.74	1.46	1.36
2	B	760	HEM	C3C-C2C	-4.34	1.34	1.40
2	C	760	HEM	C3D-C2D	4.15	1.45	1.36

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	760	HEM	CBD-CAD-C3D	-7.07	92.98	112.63
2	A	760	HEM	CBD-CAD-C3D	-7.06	93.00	112.63
2	D	760	HEM	CBD-CAD-C3D	-6.59	94.33	112.63
2	C	760	HEM	C1B-NB-C4B	6.16	111.43	105.07
2	B	760	HEM	CBD-CAD-C3D	-5.62	97.01	112.63

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	760	HEM	CAA-CBA-CGA-O1A
2	B	760	HEM	CAA-CBA-CGA-O1A
2	D	760	HEM	CAA-CBA-CGA-O1A
2	C	760	HEM	CAA-CBA-CGA-O2A
2	C	760	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.
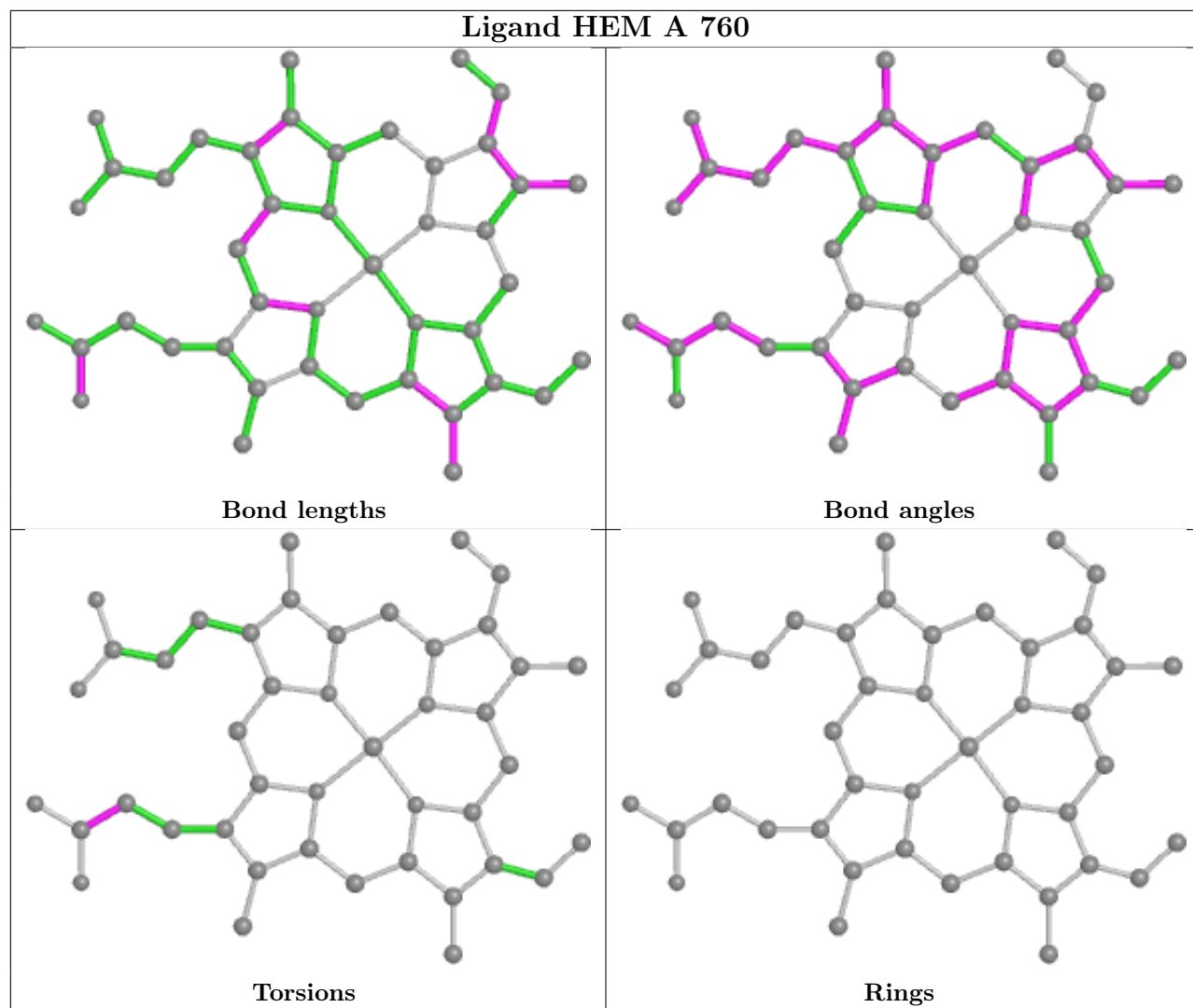
4 monomers are involved in 6 short contacts:

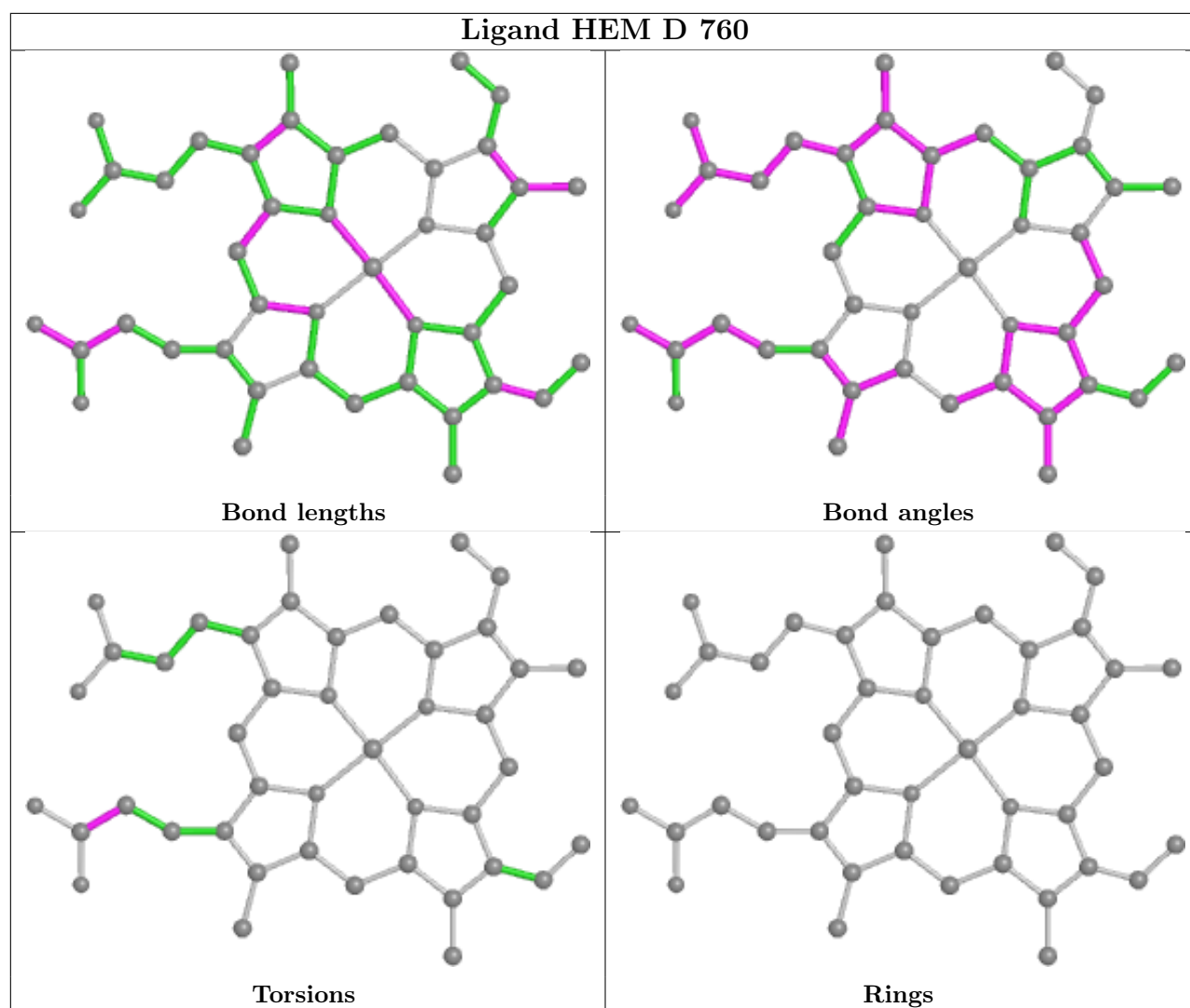| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	760	HEM	2	0
2	B	760	HEM	1	0
2	A	760	HEM	2	0
2	D	760	HEM	1	0

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 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 HEM C 760

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 760

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 760

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM D 760

Bond lengths

Bond angles

Torsions

Rings
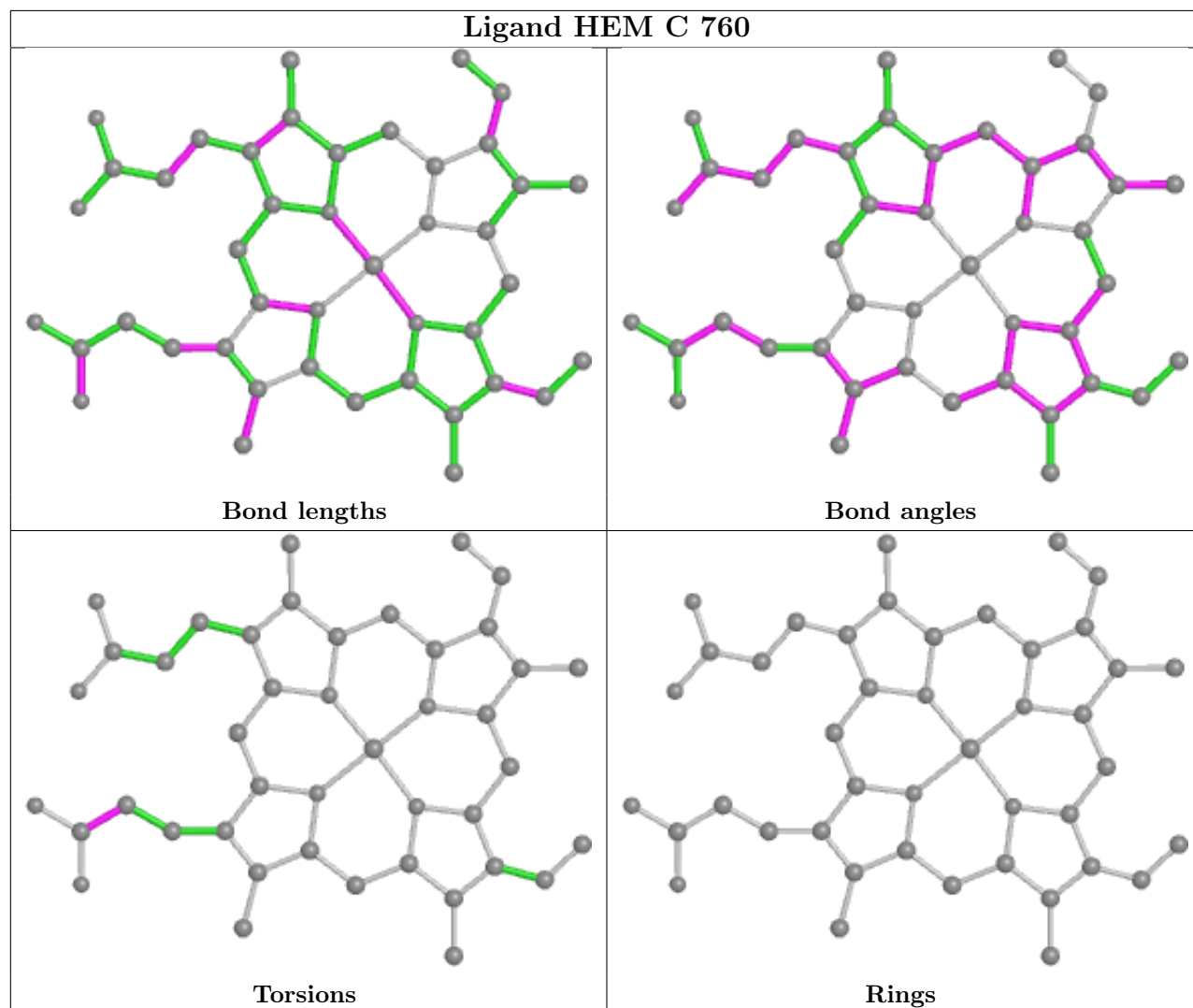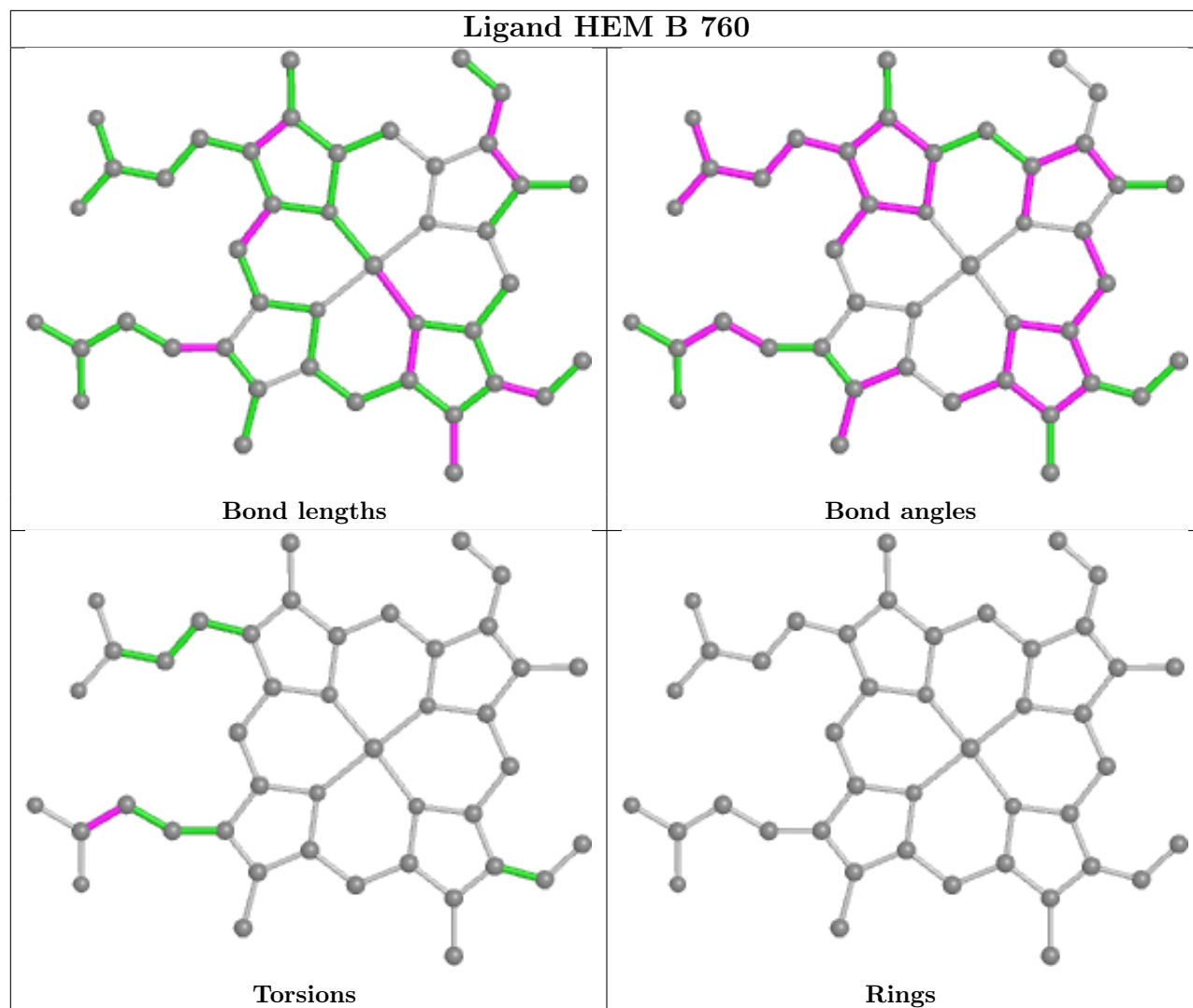
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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^2)	Q<0.9
1	A	725/753 (96%)	-0.42	7 (0%)	82	82	7, 13, 28, 45	1 (0%)
1	B	725/753 (96%)	-0.31	21 (2%)	51	48	8, 15, 33, 48	1 (0%)
1	C	725/753 (96%)	-0.29	22 (3%)	50	47	8, 15, 34, 48	1 (0%)
1	D	725/753 (96%)	-0.39	7 (0%)	82	82	7, 13, 30, 47	1 (0%)
All	All	2900/3012 (96%)	-0.35	57 (1%)	65	63	7, 14, 31, 48	4 (0%)

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	710	ILE	6.7
1	B	726	GLY	5.3
1	D	28	SER	4.3
1	C	711	ALA	3.9
1	B	713	GLN	3.8

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

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, 95th 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.

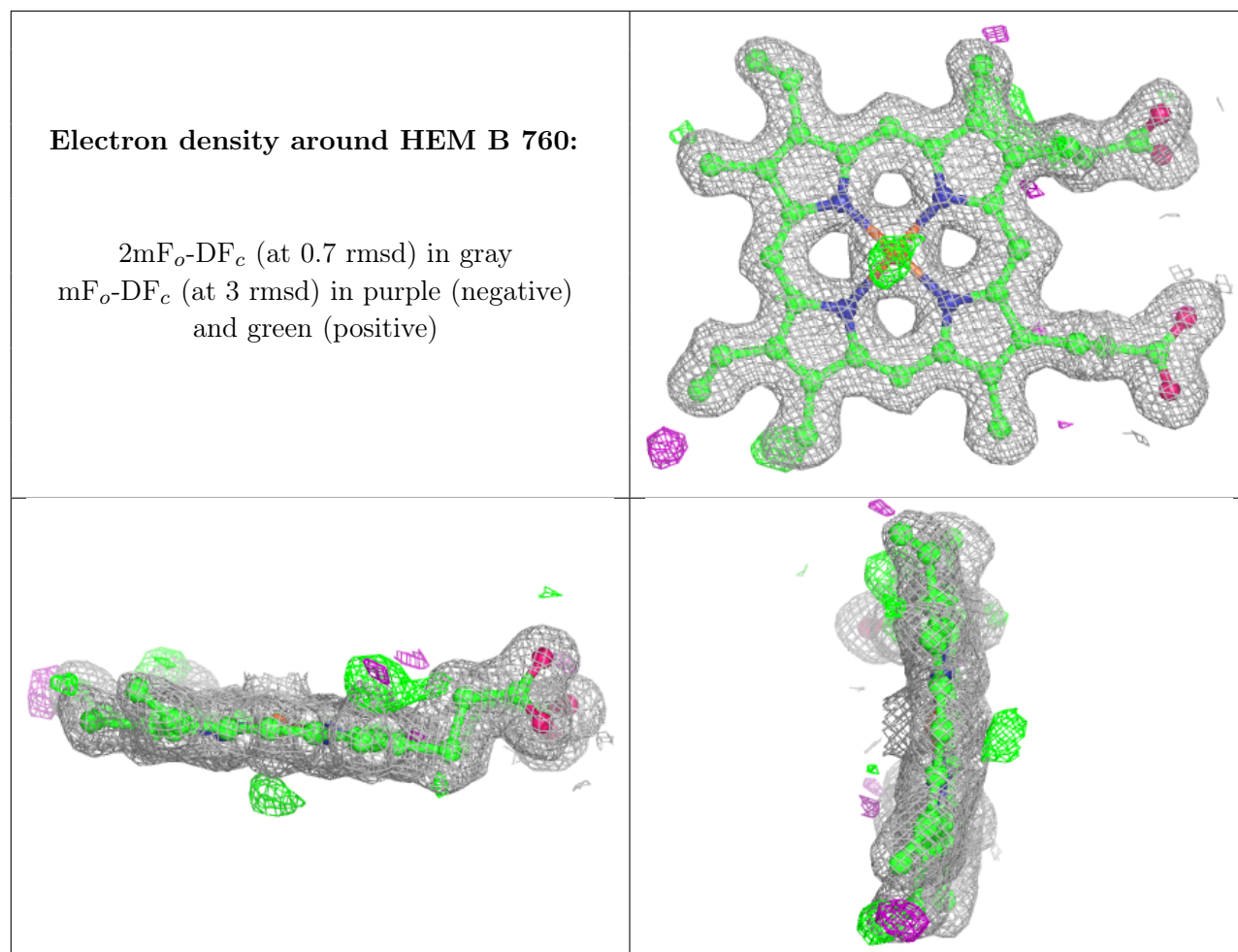| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	OCS	A	669	9/10	0.96	0.10	19,21,26,29	0
1	OCS	B	669	9/10	0.96	0.11	26,27,33,33	0
1	OCS	C	669	9/10	0.96	0.14	28,29,32,34	0
1	OCS	D	669	9/10	0.96	0.10	22,23,27,29	0

6.3   Carbohydrates (i)

There are no monosaccharides 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, 95th 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.
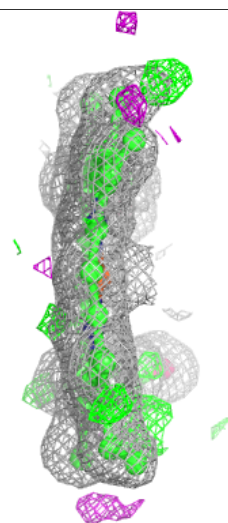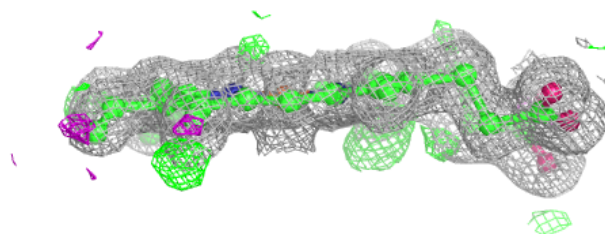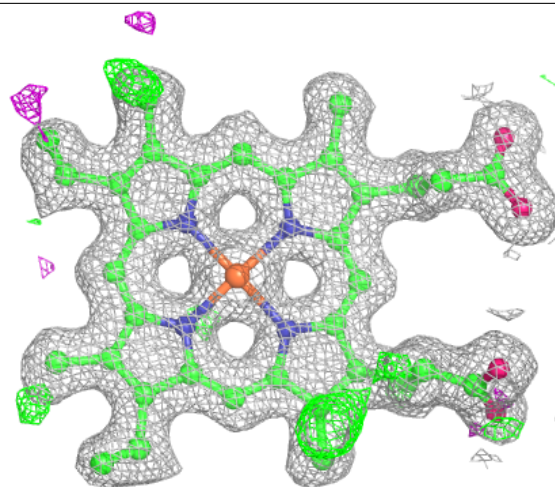
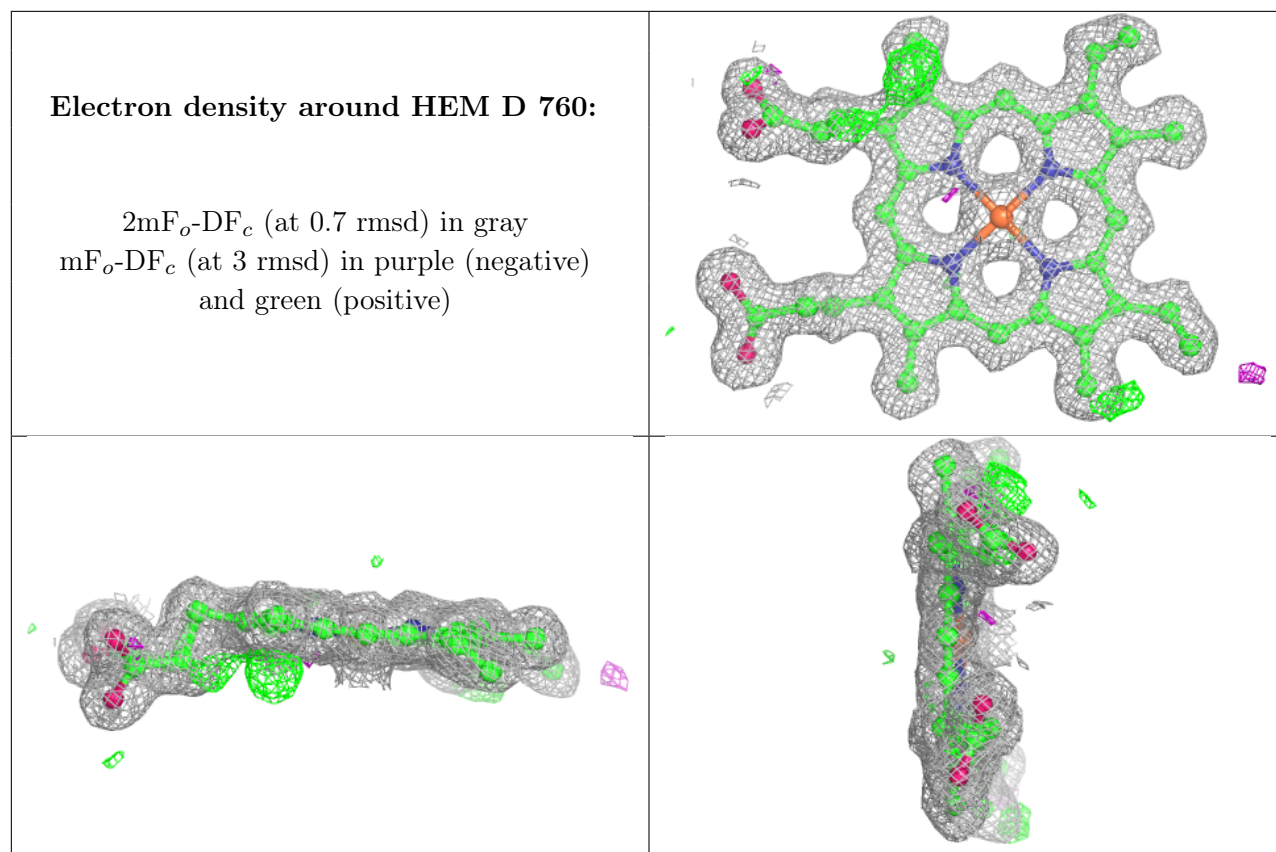| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	B	760	43/43	0.98	0.07	7,11,16,23	0
2	HEM	C	760	43/43	0.98	0.08	8,11,20,21	0
2	HEM	D	760	43/43	0.98	0.07	5,10,17,21	0
2	HEM	A	760	43/43	0.99	0.07	6,9,14,18	0

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.
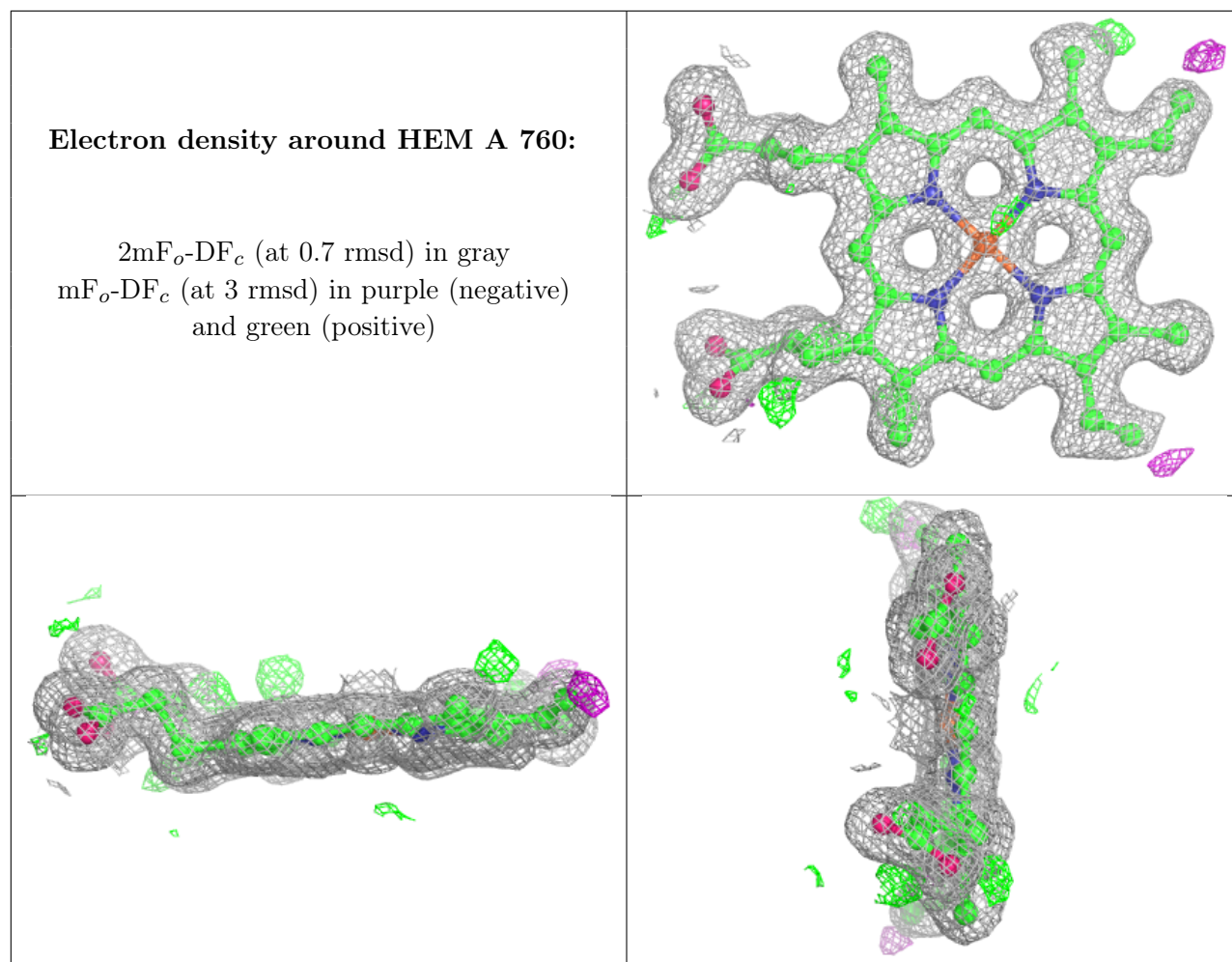
Electron density around HEM B 760:

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

Electron density around HEM C 760:

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

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)

6.5   Other polymers ⓘ

There are no such residues in this entry.