wwPDB X-ray Structure Validation Summary Report (i)

Aug 4, 2026 – 05:58 PM EDT

PDB ID	:	3PQ3 / pdb_00003pq3
Title	:	Structure of I274C variant of E. coli KatE[] - Images 7-12
Authors	:	Loewen, P.C.; Jha, V.; Louis, S.; Chelikani, P.; Carpena, X.; Fita, I.
Deposited on	:	2010-11-25
Resolution	:	1.79 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

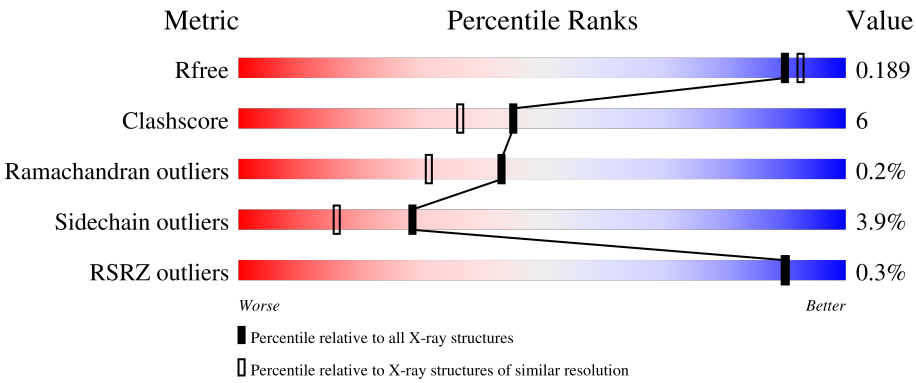
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.79 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	% 85% 11% • •
1	B	753	82% 12% • •
1	C	753	85% 11% • •
1	D	753	84% 11% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HDD	A	760[A]	X	-	-	-
2	HDD	B	760[A]	X	-	-	-
2	HDD	C	760[A]	X	-	-	-
2	HDD	D	760[A]	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 26828 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.

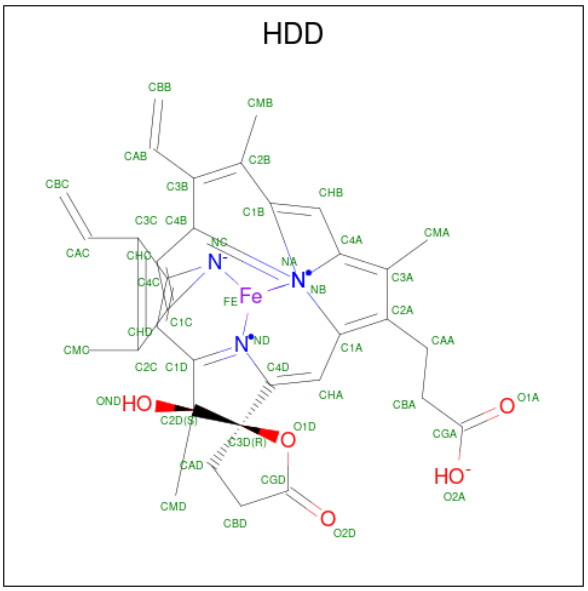
- Molecule 1 is a protein called Catalase HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	726	5755	3652	1009	1083	11	0	5	0
1	B	726	5757	3654	1009	1083	11	0	5	0
1	C	726	5747	3649	1007	1080	11	0	2	0
1	D	726	5771	3662	1013	1085	11	0	9	0

There are 12 discrepancies between the modelled and reference sequences:

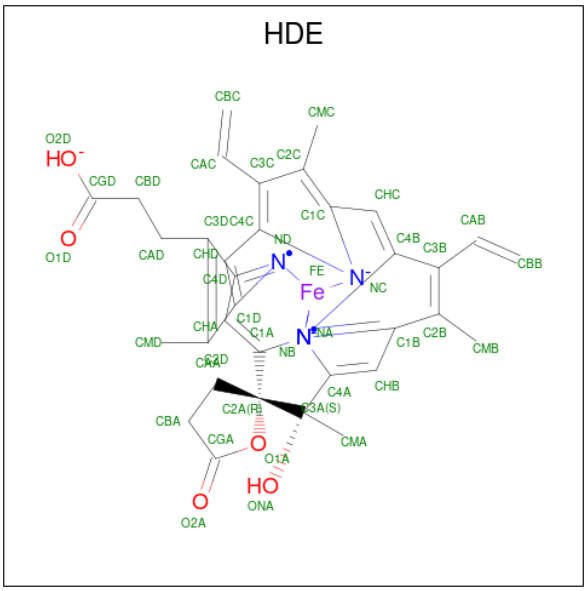
Chain	Residue	Modelled	Actual	Comment	Reference
A	274	CYS	ILE	engineered mutation	UNP P21179
A	438	ALA	CYS	engineered mutation	UNP P21179
A	669	ALA	CYS	engineered mutation	UNP P21179
B	274	CYS	ILE	engineered mutation	UNP P21179
B	438	ALA	CYS	engineered mutation	UNP P21179
B	669	ALA	CYS	engineered mutation	UNP P21179
C	274	CYS	ILE	engineered mutation	UNP P21179
C	438	ALA	CYS	engineered mutation	UNP P21179
C	669	ALA	CYS	engineered mutation	UNP P21179
D	274	CYS	ILE	engineered mutation	UNP P21179
D	438	ALA	CYS	engineered mutation	UNP P21179
D	669	ALA	CYS	engineered mutation	UNP P21179

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula: $C_{34}H_{32}FeN_4O_5$).



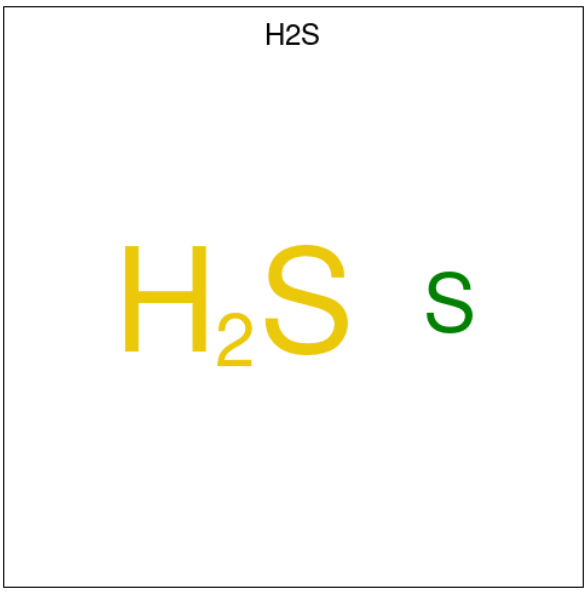
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	44	34	1	4	5	0	1
			Total	C	Fe	N	O		
2	B	1	44	34	1	4	5	0	1
			Total	C	Fe	N	O		
2	C	1	44	34	1	4	5	0	1
			Total	C	Fe	N	O		
2	D	1	44	34	1	4	5	0	1

- Molecule 3 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE 17R, 18S (CCD ID: HDE) (formula: $C_{34}H_{32}FeN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	A	1	44	34	1	4	5	0	1
3	B	1	44	34	1	4	5	0	1
3	C	1	44	34	1	4	5	0	1
3	D	1	44	34	1	4	5	0	1

- Molecule 4 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H_2S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	S		
4	A	1	1	1	0	0
4	B	1	1	1	0	0
4	C	1	1	1	0	0
4	D	1	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	895	895	895	0	0
5	B	791	791	791	0	0

Continued on next page...

Continued from previous page...

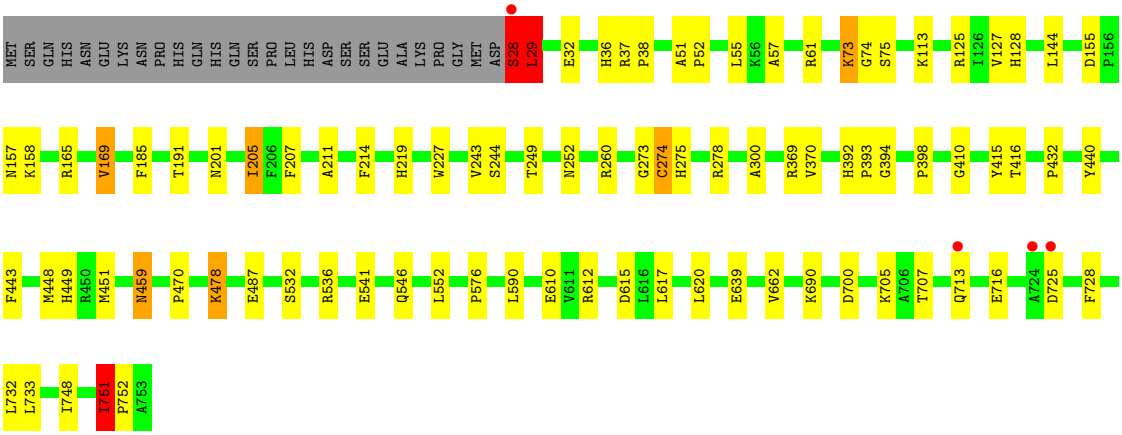
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	C	842	842	842	0	0
			Total	O		
5	D	914	914	914	0	0

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 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.

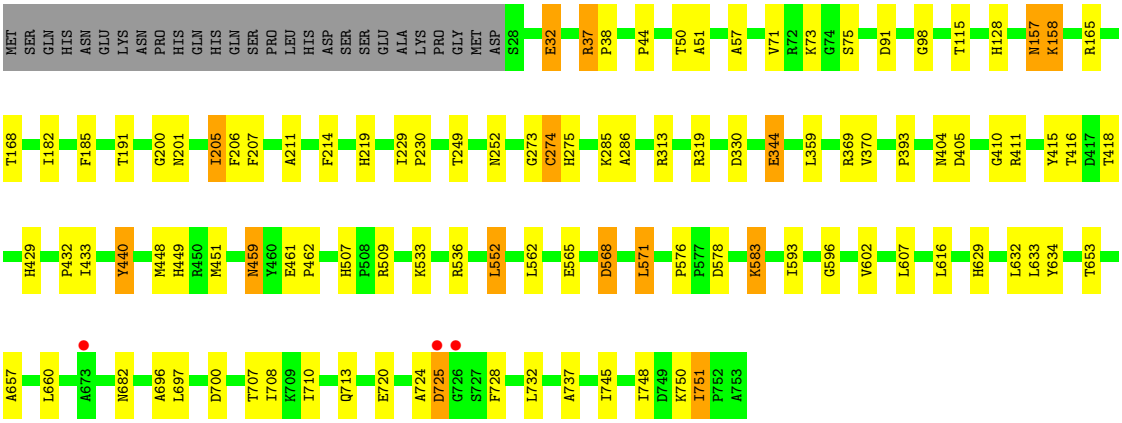
• Molecule 1: Catalase HPII

Chain A:



• Molecule 1: Catalase HPII

Chain B:



• Molecule 1: Catalase HPII

Chain C:

MET SER GLN HIS ASN GLU LYS ASN PRO HIS GLN HIS GLN SER PRO LEU HIS ASP SER SER GLU ALA LYS PRO GLY MET ASP S28 E32 R37 P38 Q48 A51 P52 D59 S75 D91 L104 I109 E124 H128 Y137 K158 I159 T168 V169

Q170 V199 G200 N201 I205 H219 W227 D237 N252 R267 G273 C274 E283 G284 K285 D330 P356 L359 Q368 R377 P393 N404 D405 Y415 Y440 D446 H449 R450 M451 N459 P474 R488 H507 R521

L552 T567 L571 D578 L582 K583 K584 G596 V602 L606 R612 L616 L617 K626 H629 L633 Y634 S635 R636 L648 T653 V662 A669 Y689 A696 L697 A698 F704 T707 I708 Q713 A724 D725 F728 L732 L733

R744 I745 I748 D749 K750 I751 P752 A753

- Molecule 1: Catalase HPII

Chain D: 84% 11% • •

MET SER GLN HIS ASN GLU LYS ASN PRO HIS GLN HIS GLN SER PRO LEU HIS ASP SER SER GLU ALA LYS PRO GLY MET ASP S28 E32 R37 Q48 A51 P52 A57 K73 G74 S75 N83 D91 H128 T168 T178 T191 N201 N202 T203 P204

I205 F206 F207 A211 H219 S244 T249 N252 R260 R267 G273 C274 R278 L296 R313 R319 D330 F331 P332 E333 I341 L359 Q388 P393 N404 D405 G410 R411 Y415 T416 I420 S421 I431 P432 Y440 G447

M448 H449 R450 M451 N459 Y460 E461 P462 Y485 Q486 E487 E490 H507 P508 R509 R536 Q546 L552 Q556 T574 P575 P576 L582 L590 G596 L616 H629 Y634 L648 T653 A657 L660 A696 D700 K709 Q713

F728 E731 L732 A737 I745 P746 K747 I748 D749 K750 I751 P752 A753

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.51Å 133.03Å 122.65Å 90.00° 109.39° 90.00°	Depositor
Resolution (Å)	35.23 – 1.79 35.23 – 1.79	Depositor EDS
% Data completeness (in resolution range)	92.3 (35.23-1.79) 92.3 (35.23-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 1.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.142 , 0.189 0.142 , 0.189	Depositor DCC
R_{free} test set	12198 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	11.4	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26828	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HDE, HDD, H2S

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	1.38	12/5932 (0.2%)	1.15	11/8064 (0.1%)
1	B	1.32	11/5931 (0.2%)	1.13	10/8062 (0.1%)
1	C	1.33	8/5908 (0.1%)	1.14	15/8033 (0.2%)
1	D	1.38	12/5966 (0.2%)	1.13	8/8109 (0.1%)
All	All	1.35	43/23737 (0.2%)	1.14	44/32268 (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	C	0	3

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	745	ILE	CA-CB	8.45	1.58	1.54
1	A	169	VAL	N-CA	7.00	1.52	1.46
1	D	203	THR	N-CA	6.87	1.51	1.45
1	B	57	ALA	CA-CB	6.75	1.61	1.53
1	B	205	ILE	CA-CB	6.63	1.63	1.54

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	449[A]	HIS	CA-C-O	-9.41	107.26	119.59
1	C	449[B]	HIS	CA-C-O	-9.41	107.26	119.59
1	C	159	ILE	CB-CG1-CD1	-7.34	98.38	113.80
1	C	169	VAL	CB-CA-C	-7.30	104.55	111.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	657	ALA	CA-C-N	7.29	127.73	119.92

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	449[A]	HIS	Mainchain
1	C	724	ALA	Peptide
1	C	725	ASP	Peptide

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	5755	0	5582	71	0
1	B	5757	0	5587	73	0
1	C	5747	0	5577	50	1
1	D	5771	0	5598	50	0
2	A	44	0	31	3	0
2	B	44	0	31	13	0
2	C	44	0	30	8	0
2	D	44	0	31	2	0
3	A	44	0	36	8	0
3	B	44	0	36	13	0
3	C	44	0	36	10	0
3	D	44	0	36	8	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	895	0	0	21	2
5	B	791	0	0	13	1
5	C	842	0	0	19	0
5	D	914	0	0	17	0
All	All	26828	0	22611	270	2

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 6.

The worst 5 of 270 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)
3:B:761[B]:HDE:HBCA	3:B:761[B]:HDE:CMC	1.65	1.22
1:A:716:GLU:HG2	5:A:3090:HOH:O	1.40	1.20
1:D:451:MET:SD	5:D:3617:HOH:O	2.05	1.14
1:C:578:ASP:HB3	5:C:2919:HOH:O	1.48	1.12
1:C:451:MET:SD	5:C:3612:HOH:O	2.07	1.11

All (2) 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)
5:A:3348:HOH:O	5:B:2822:HOH:O[2_545]	2.13	0.07
1:C:584:LYS:NZ	5:A:1624:HOH:O[1_554]	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	729/753 (97%)	707 (97%)	21 (3%)	1 (0%)	48	34
1	B	729/753 (97%)	708 (97%)	19 (3%)	2 (0%)	36	25
1	C	726/753 (96%)	700 (96%)	25 (3%)	1 (0%)	48	34
1	D	733/753 (97%)	710 (97%)	22 (3%)	1 (0%)	48	34
All	All	2917/3012 (97%)	2825 (97%)	87 (3%)	5 (0%)	43	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	75	SER
1	C	75	SER
1	B	75	SER
1	D	75	SER

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	614/634 (97%)	593 (97%)	21 (3%)	32	20
1	B	614/634 (97%)	588 (96%)	26 (4%)	26	14
1	C	611/634 (96%)	586 (96%)	25 (4%)	27	15
1	D	618/634 (98%)	594 (96%)	24 (4%)	28	16
All	All	2457/2536 (97%)	2361 (96%)	96 (4%)	28	16

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	552	LEU
1	C	751	ILE
1	C	606	LEU
1	C	708	ILE
1	D	73[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	486	GLN
1	D	629	HIS
1	C	556	GLN
1	D	459	ASN
1	C	546	GLN

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)

Of 12 ligands modelled in this entry, 4 are modelled with single atom - leaving 8 for Mogul analysis.

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	HDD	D	760[A]	1,5	49,52,52	2.34	11 (22%)	62,89,89	2.24	20 (32%)
2	HDD	C	760[A]	4,1,5	49,52,52	2.10	10 (20%)	62,89,89	2.06	23 (37%)
3	HDE	C	761[B]	1,5	50,52,52	2.53	21 (42%)	60,89,89	2.37	22 (36%)
3	HDE	A	761[B]	1,5	50,52,52	2.54	20 (40%)	60,89,89	2.23	18 (30%)
3	HDE	B	761[B]	1,5	50,52,52	2.61	22 (44%)	60,89,89	2.53	27 (45%)
3	HDE	D	761[B]	1,5	50,52,52	2.44	19 (38%)	60,89,89	2.35	23 (38%)
2	HDD	A	760[A]	1,5	49,52,52	2.17	11 (22%)	62,89,89	2.39	24 (38%)
2	HDD	B	760[A]	1,5	49,52,52	2.45	12 (24%)	62,89,89	1.83	13 (20%)

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	HDD	D	760[A]	1,5	1/1/8/14	5/9/89/89	0/1/9/9
2	HDD	C	760[A]	4,1,5	1/1/8/14	3/9/89/89	0/1/9/9
3	HDE	C	761[B]	1,5	-	3/9/89/89	0/1/9/9
3	HDE	A	761[B]	1,5	-	2/9/89/89	0/1/9/9
3	HDE	B	761[B]	1,5	-	2/9/89/89	0/1/9/9
3	HDE	D	761[B]	1,5	-	2/9/89/89	0/1/9/9
2	HDD	A	760[A]	1,5	1/1/8/14	6/9/89/89	0/1/9/9
2	HDD	B	760[A]	1,5	1/1/8/14	2/9/89/89	0/1/9/9

The worst 5 of 126 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	760[A]	HDD	C1D-ND	12.75	1.43	1.35
2	D	760[A]	HDD	FE-ND	9.12	2.23	1.94
2	C	760[A]	HDD	FE-ND	8.67	2.21	1.94
2	A	760[A]	HDD	FE-ND	7.17	2.17	1.94
2	A	760[A]	HDD	C1D-ND	7.07	1.40	1.35

The worst 5 of 170 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	760[A]	HDD	O1D-CGD-CBD	-9.13	101.85	110.17
2	B	760[A]	HDD	O1D-CGD-O2D	7.22	126.89	120.81
3	C	761[B]	HDE	C2D-C1D-ND	6.96	117.85	109.84
3	D	761[B]	HDE	C2D-C1D-ND	6.75	117.60	109.84
3	B	761[B]	HDE	C2D-C1D-ND	6.68	117.52	109.84

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	760[A]	HDD	NC
2	B	760[A]	HDD	NC
2	C	760[A]	HDD	NC
2	D	760[A]	HDD	NC

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	760[A]	HDD	C2B-C3B-CAB-CBB
2	A	760[A]	HDD	C4B-C3B-CAB-CBB
2	D	760[A]	HDD	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	760[A]	HDD	C4B-C3B-CAB-CBB
2	A	760[A]	HDD	C2C-C3C-CAC-CBC

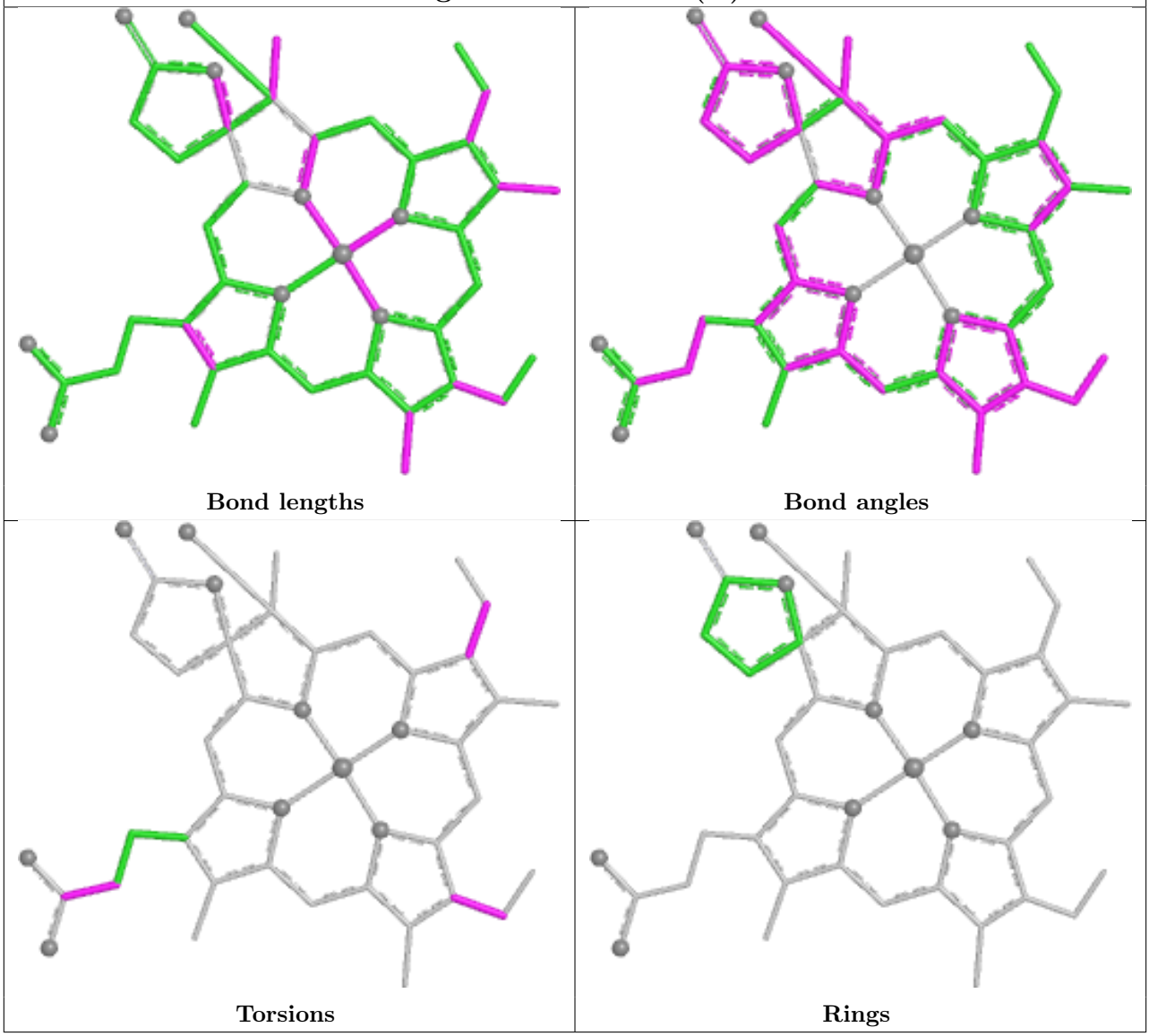
There are no ring outliers.

8 monomers are involved in 65 short contacts:

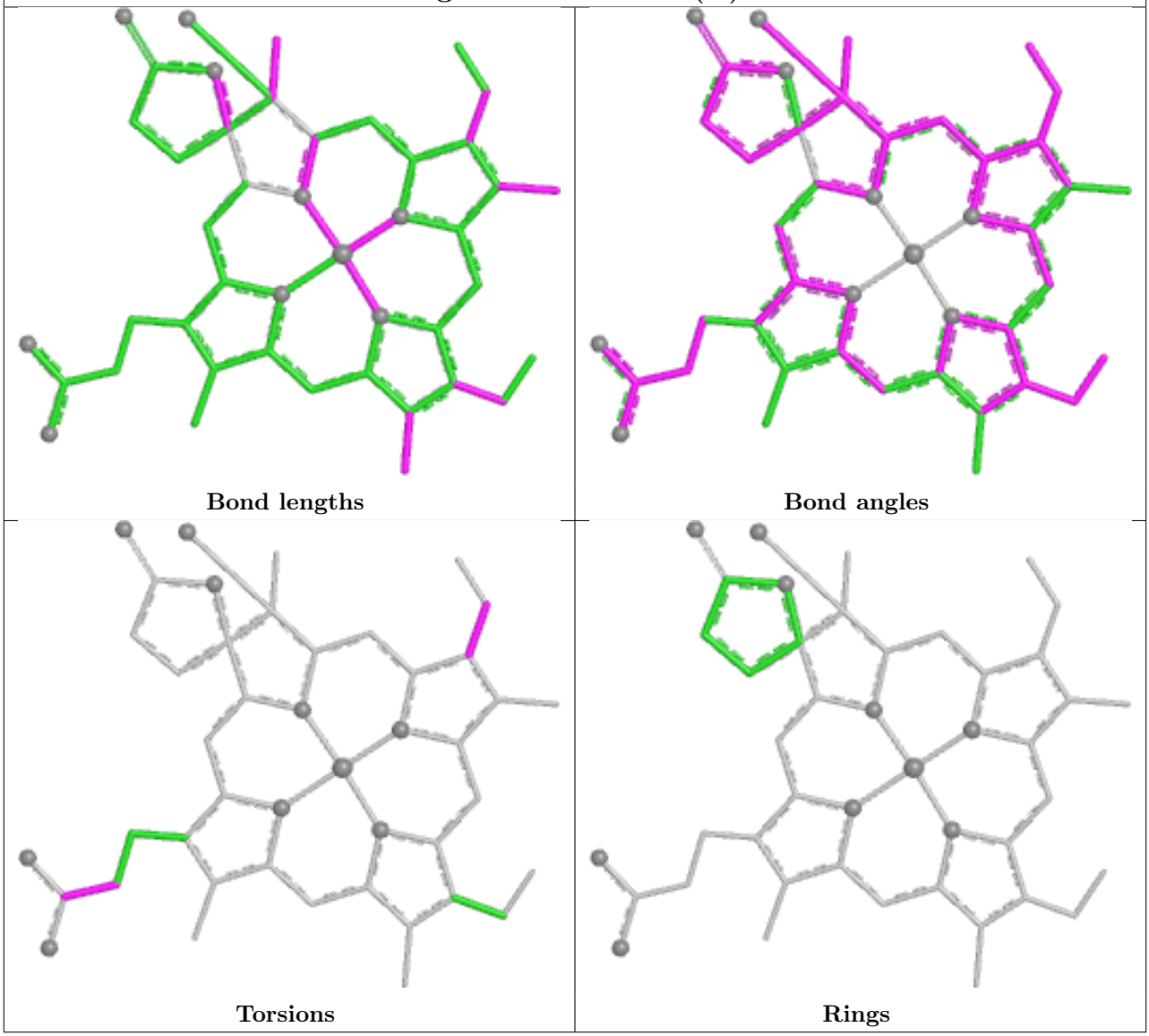
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	760[A]	HDD	2	0
2	C	760[A]	HDD	8	0
3	C	761[B]	HDE	10	0
3	A	761[B]	HDE	8	0
3	B	761[B]	HDE	13	0
3	D	761[B]	HDE	8	0
2	A	760[A]	HDD	3	0
2	B	760[A]	HDD	13	0

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.

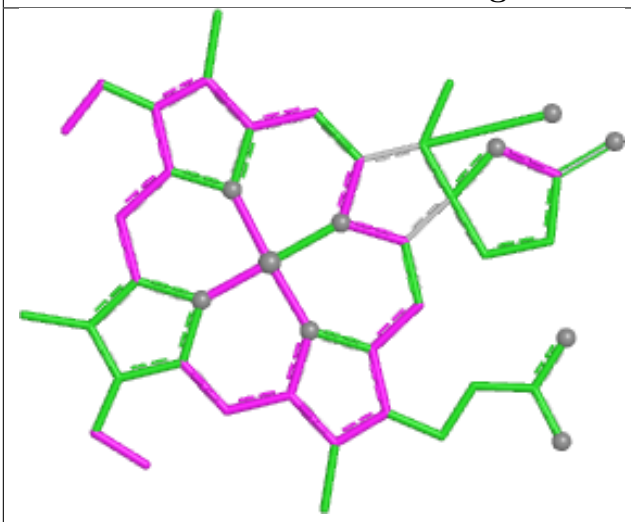
Ligand HDD D 760 (A)



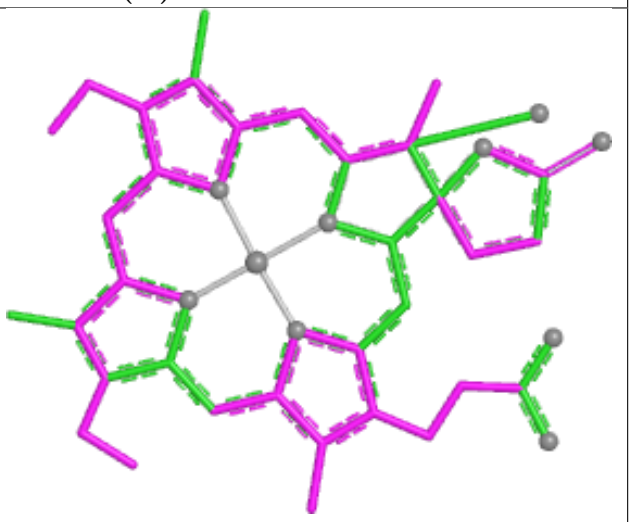
Ligand HDD C 760 (A)



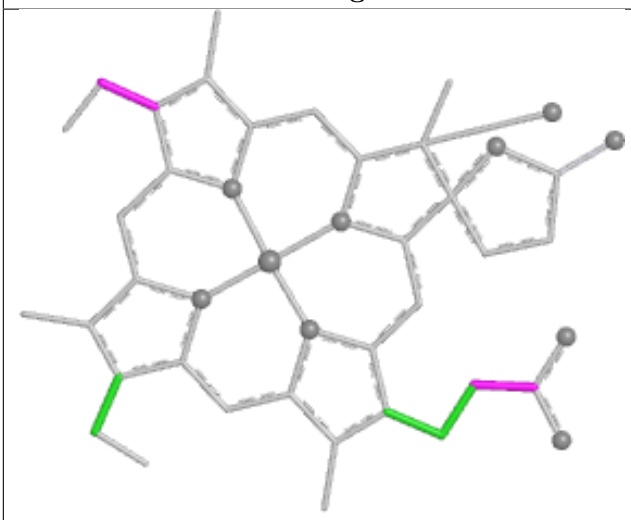
Ligand HDE C 761 (B)



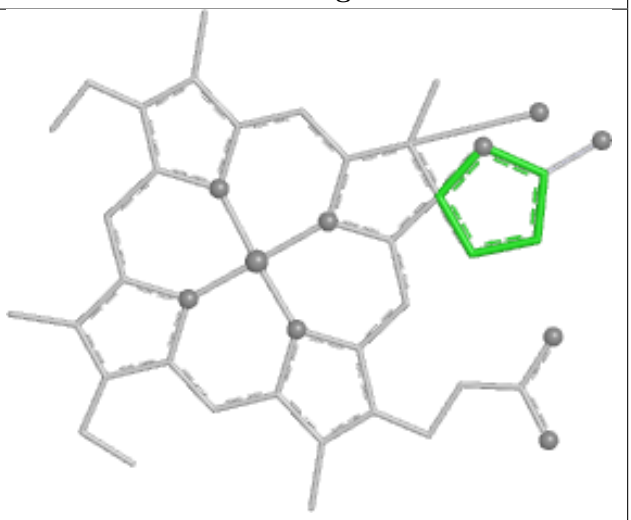
Bond lengths



Bond angles

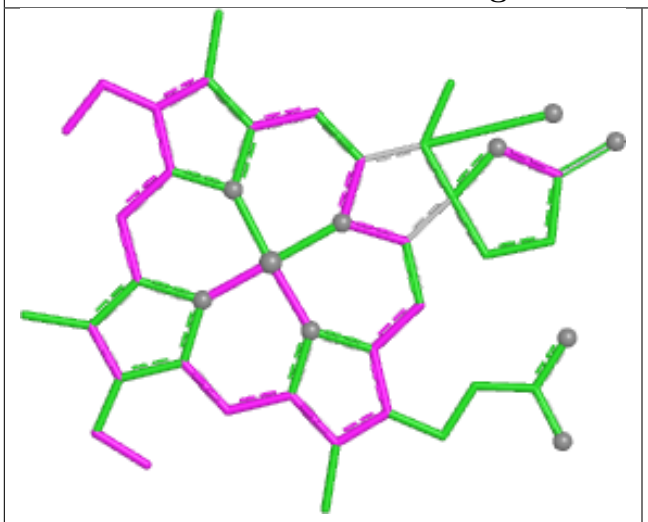


Torsions

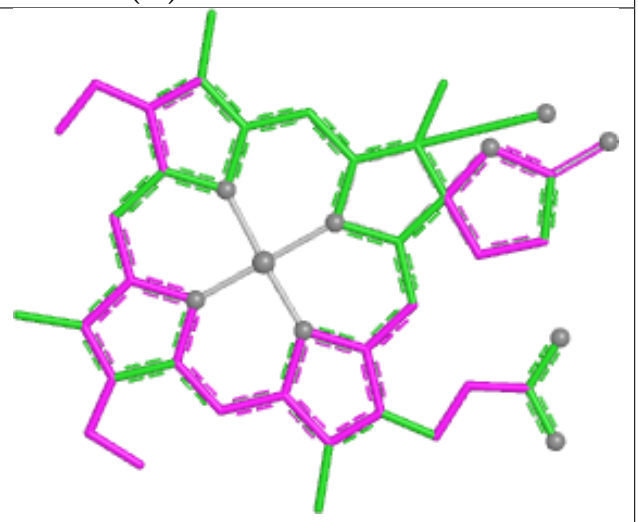


Rings

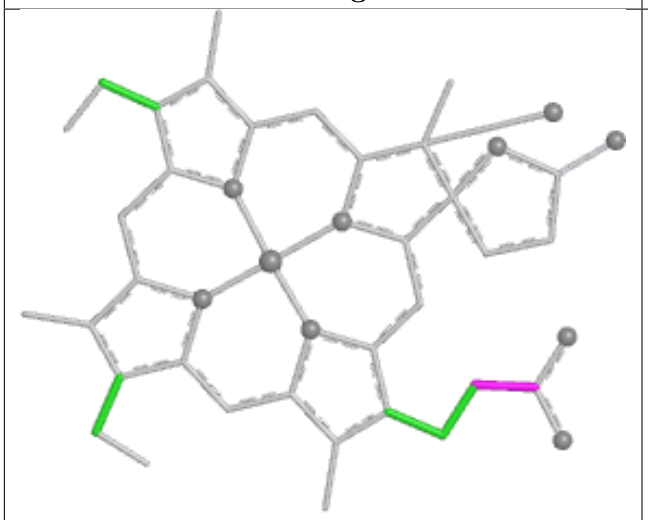
Ligand HDE A 761 (B)



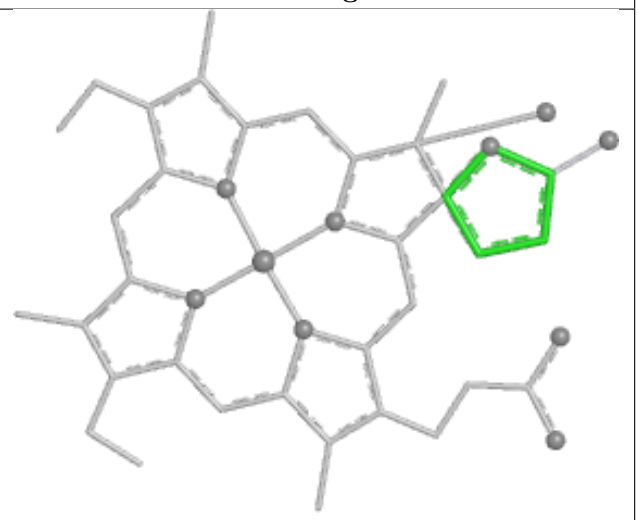
Bond lengths



Bond angles

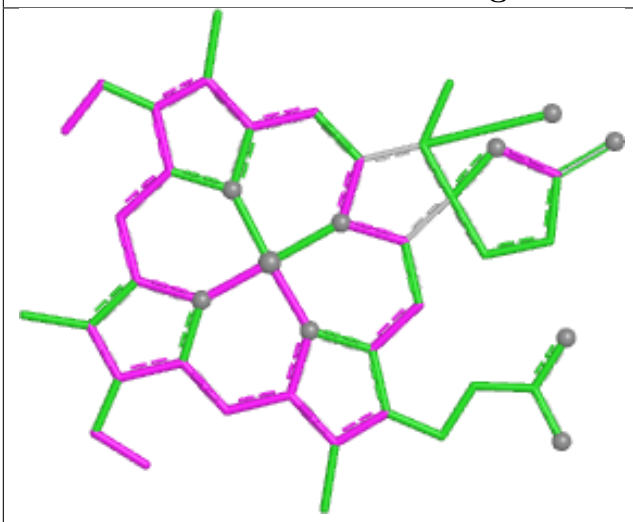


Torsions

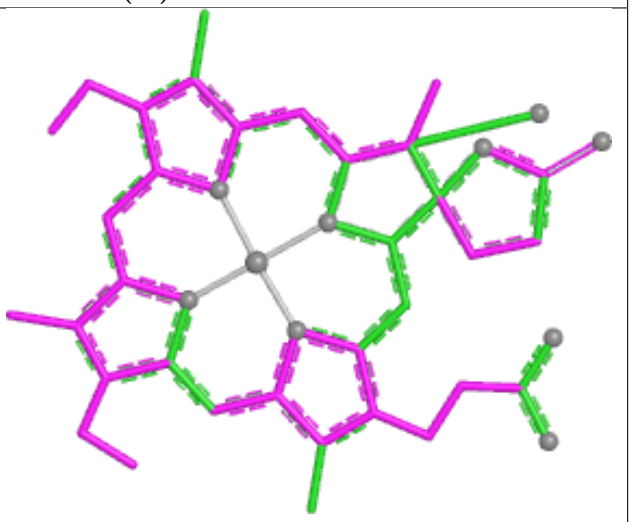


Rings

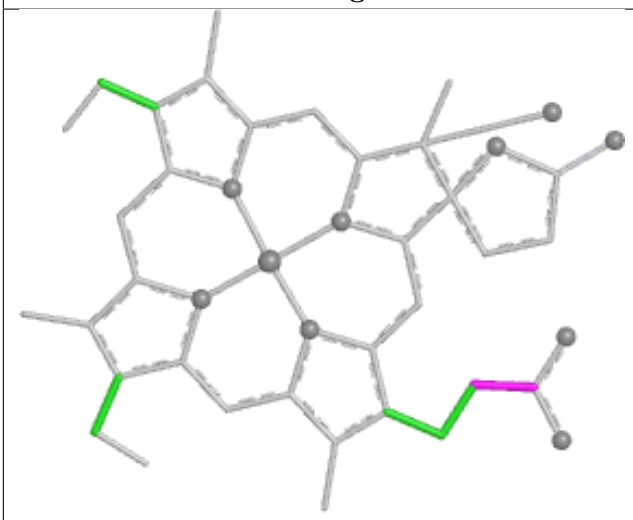
Ligand HDE B 761 (B)



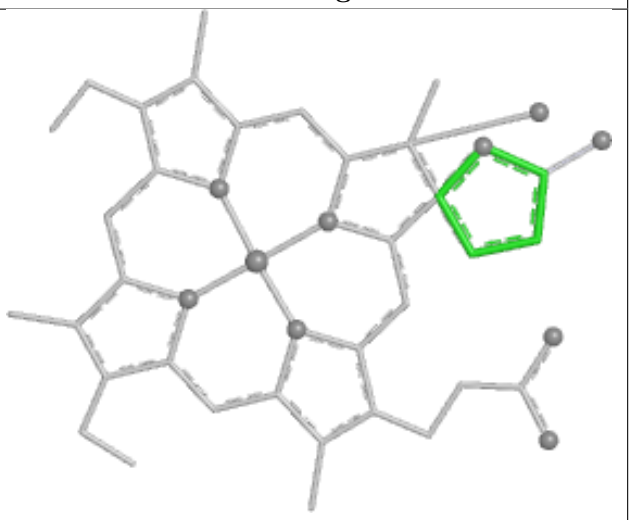
Bond lengths



Bond angles

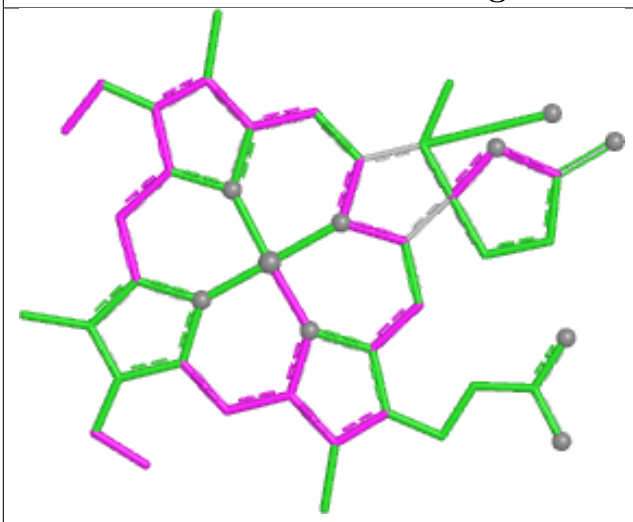


Torsions

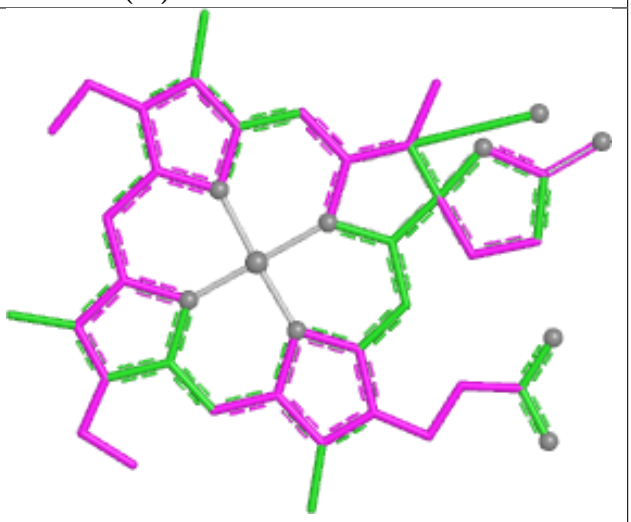


Rings

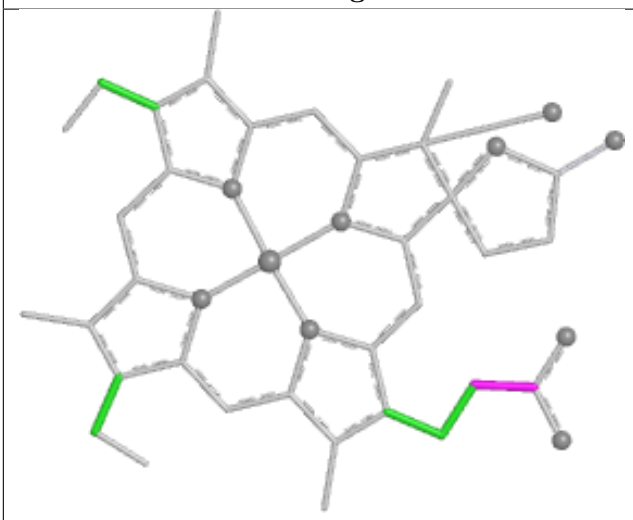
Ligand HDE D 761 (B)



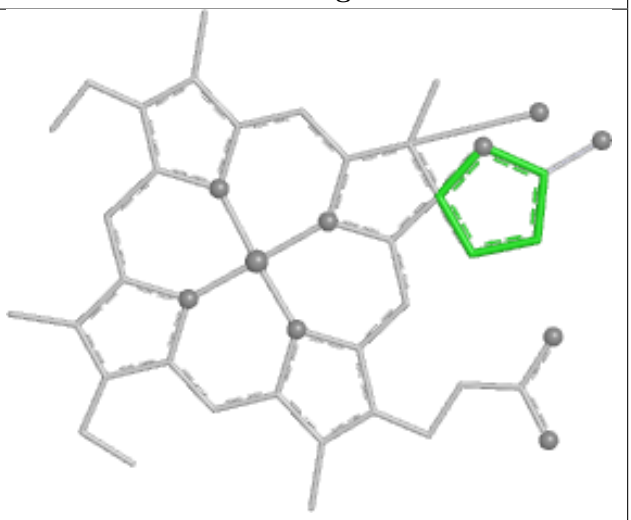
Bond lengths



Bond angles

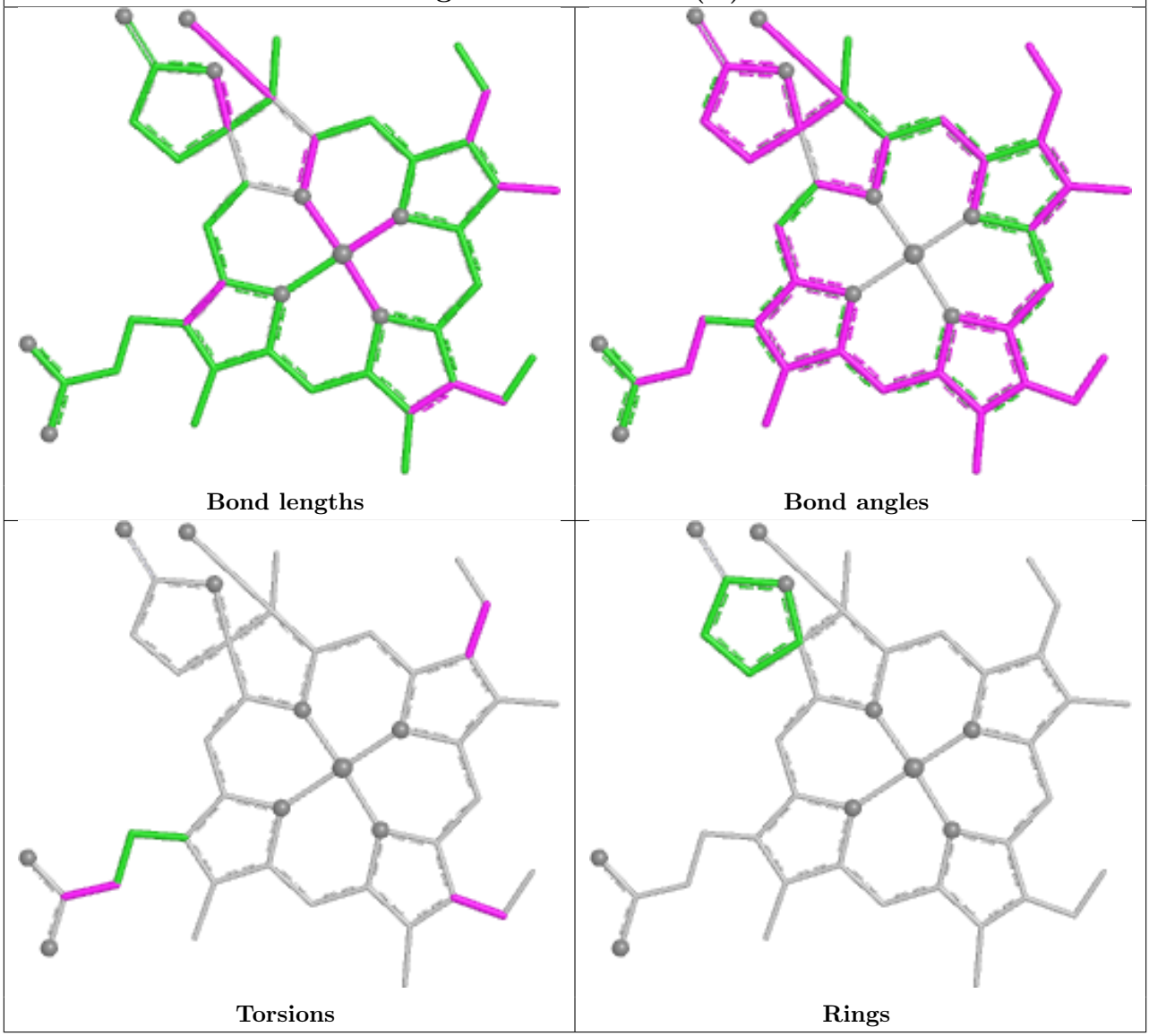


Torsions

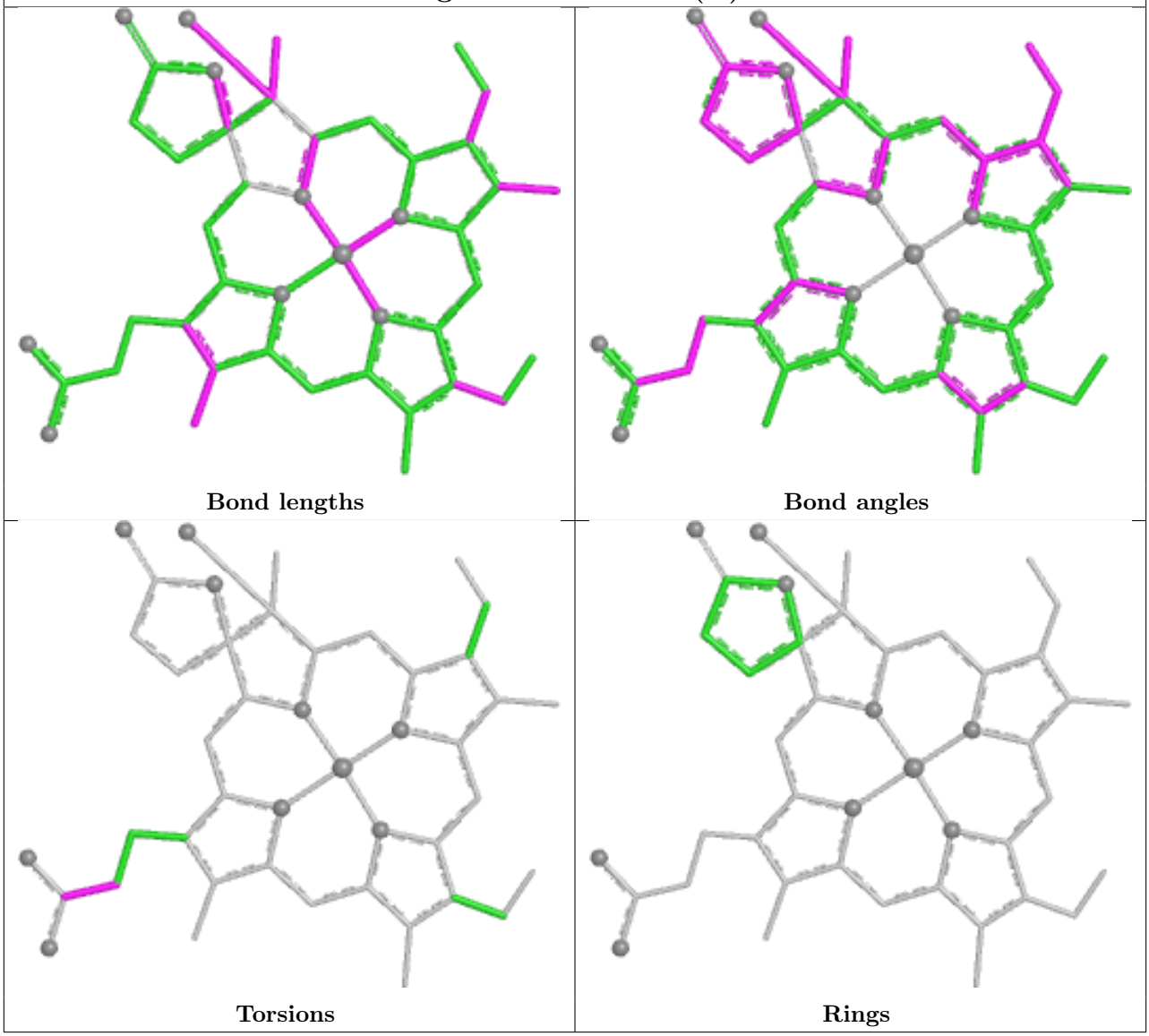


Rings

Ligand HDD A 760 (A)



Ligand HDD B 760 (A)



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, 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	726/753 (96%)	-0.73	4 (0%)	85	86	3, 10, 26, 44	7 (0%)
1	B	726/753 (96%)	-0.58	3 (0%)	88	89	3, 11, 32, 47	7 (0%)
1	C	726/753 (96%)	-0.61	0	100	100	2, 11, 31, 46	4 (0%)
1	D	726/753 (96%)	-0.71	2 (0%)	90	90	3, 10, 27, 44	10 (1%)
All	All	2904/3012 (96%)	-0.66	9 (0%)	90	90	2, 10, 30, 47	28 (0%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	SER	3.3
1	D	28	SER	2.8
1	B	725	ASP	2.5
1	B	726	GLY	2.5
1	A	713	GLN	2.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

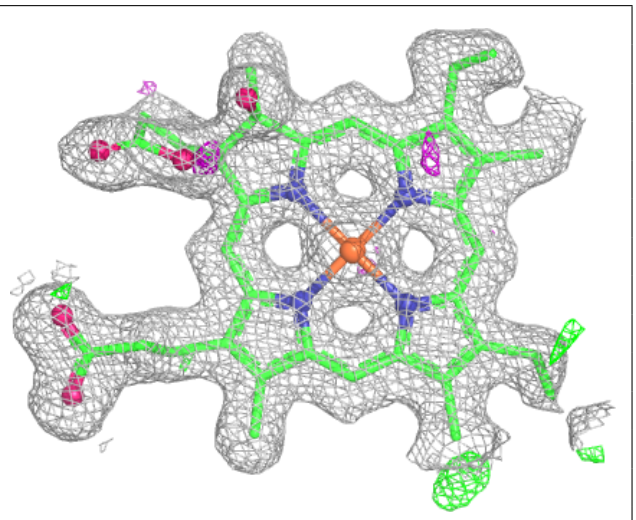
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

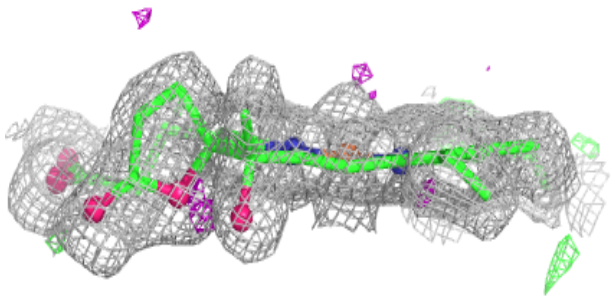
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	H2S	A	754	1/1	0.94	0.15	28,28,28,28	1
4	H2S	D	754	1/1	0.95	0.10	23,23,23,23	1
4	H2S	C	754	1/1	0.96	0.11	20,20,20,20	1
4	H2S	B	754	1/1	0.96	0.06	26,26,26,26	1
2	HDD	C	760[A]	44/44	0.98	0.05	2,4,9,14	44
3	HDE	B	761[B]	44/44	0.98	0.06	2,9,13,14	44
3	HDE	C	761[B]	44/44	0.98	0.06	3,11,13,15	44
3	HDE	D	761[B]	44/44	0.98	0.05	2,8,12,16	44
3	HDE	A	761[B]	44/44	0.99	0.05	2,7,10,13	44
2	HDD	B	760[A]	44/44	0.99	0.05	2,3,6,7	44
2	HDD	A	760[A]	44/44	0.99	0.04	2,3,6,9	44
2	HDD	D	760[A]	44/44	0.99	0.04	2,3,7,12	44

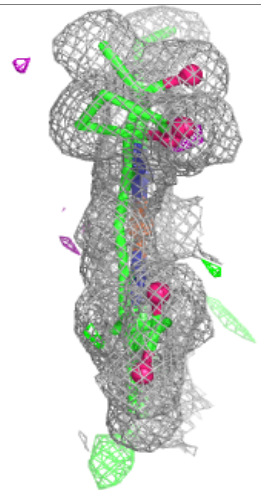
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

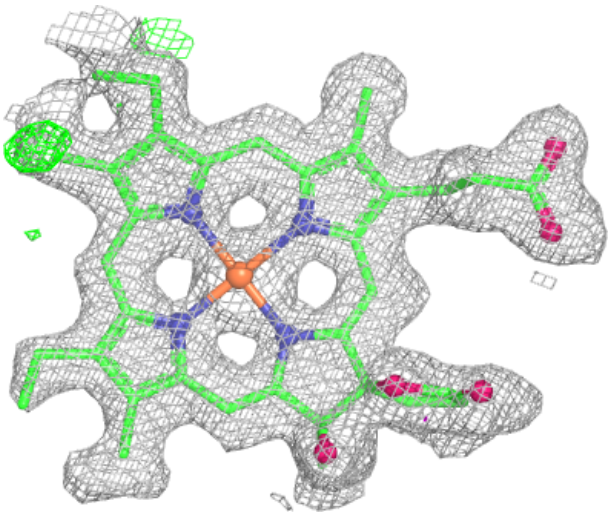
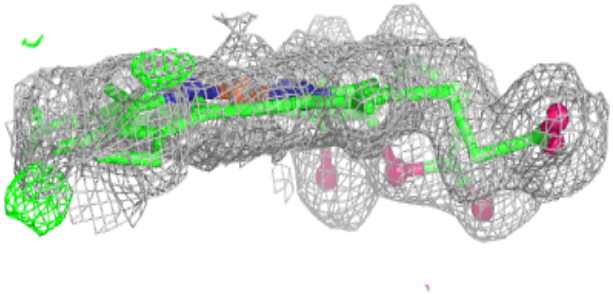
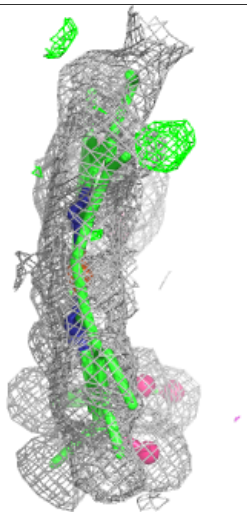
Electron density around HDD C 760 (A):

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



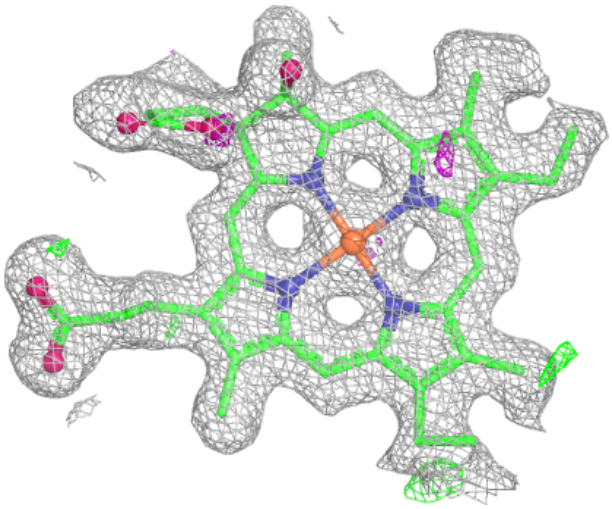


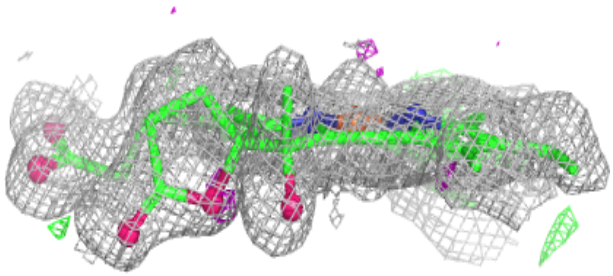


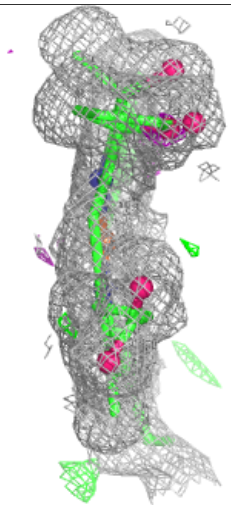
Electron density around HDE B 761 (B): $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around HDE C 761 (B):

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

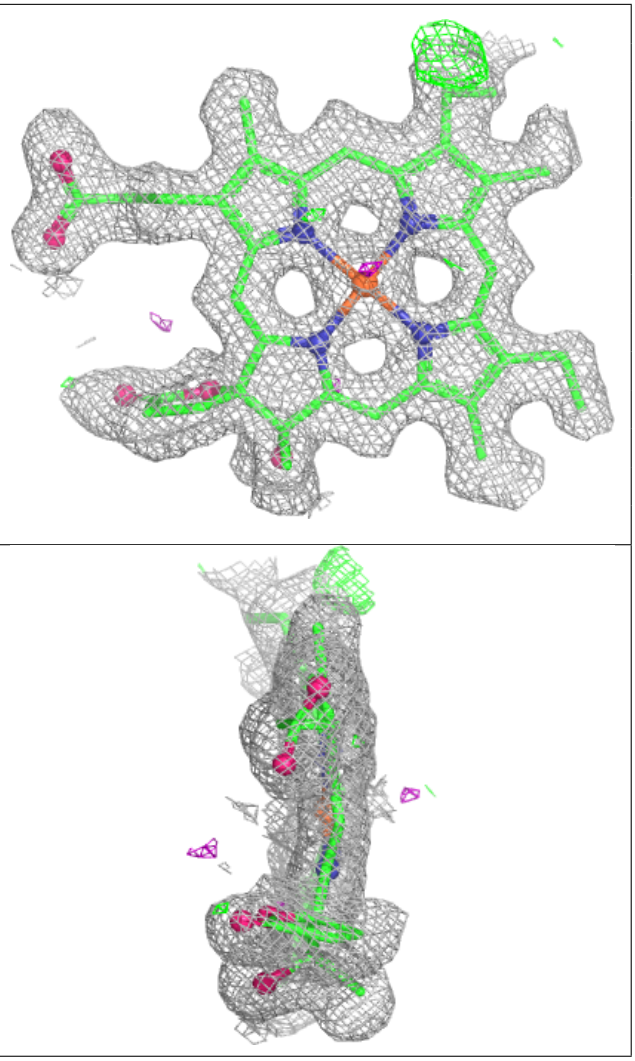


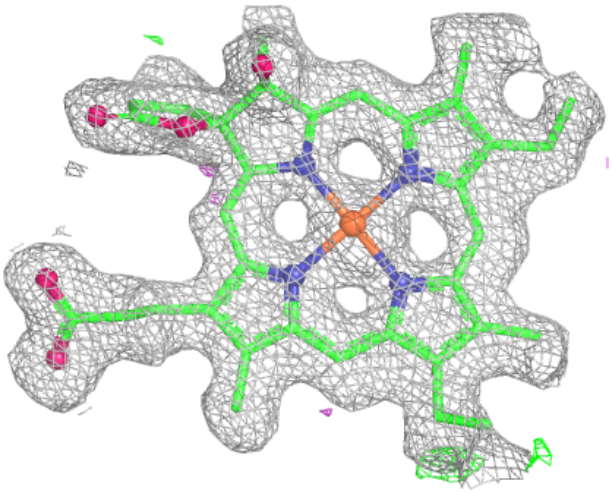
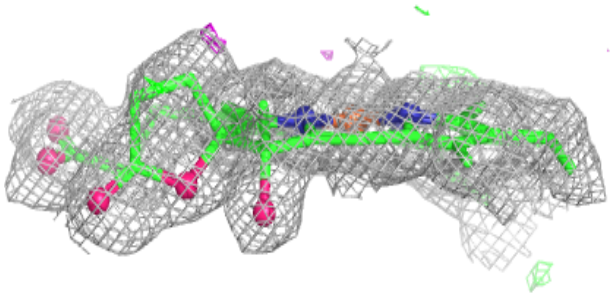
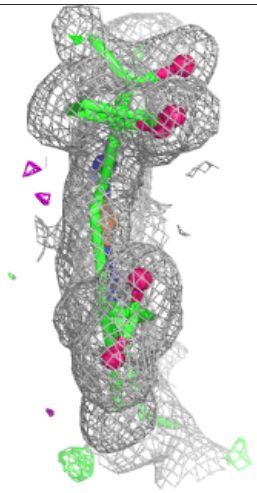




Electron density around HDE D 761 (B):

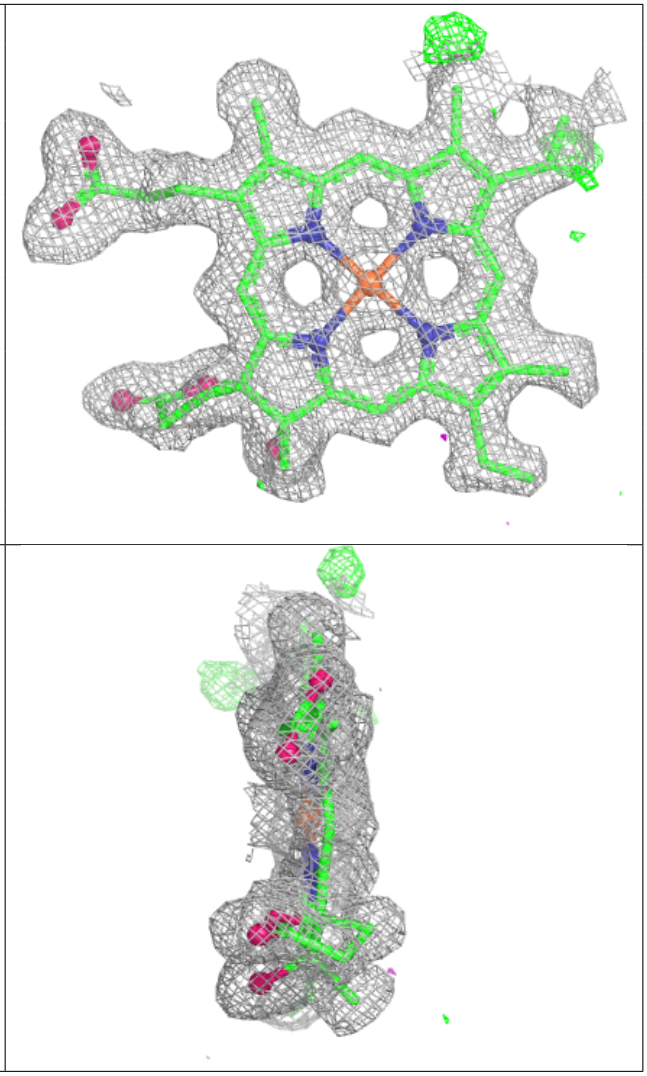
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HDE A 761 (B): $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

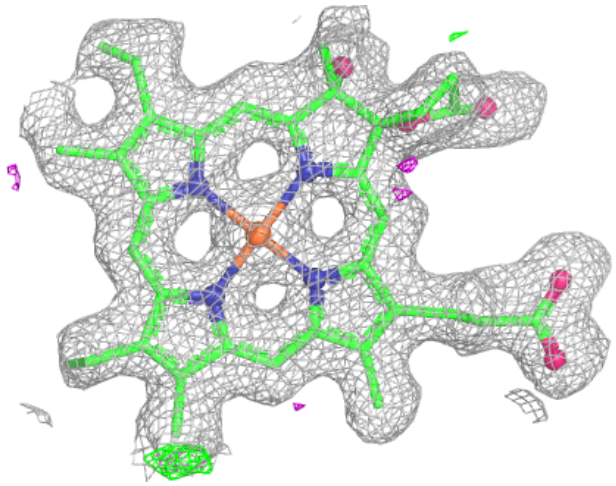
Electron density around HDD B 760 (A):

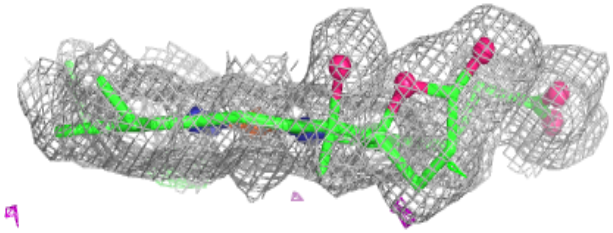
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

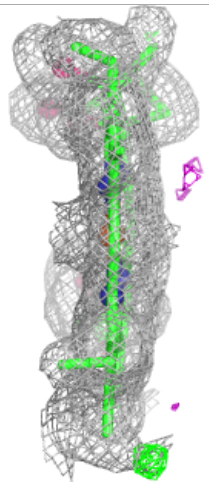


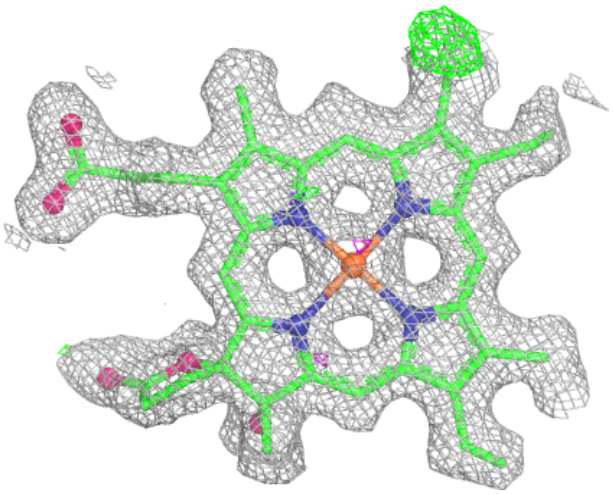
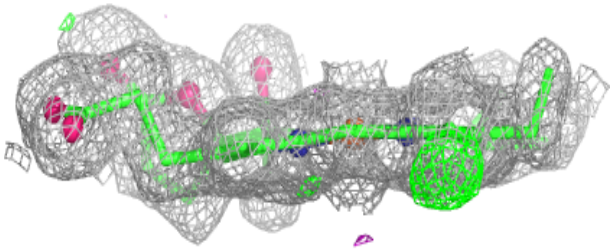
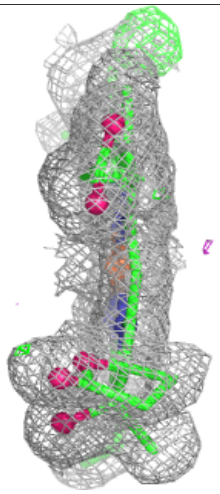
Electron density around HDD A 760 (A):

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







Electron density around HDD D 760 (A): 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.