wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2026 – 10:45 pm BST

PDB ID	:	6ZTW / pdb_00006ztw
Title	:	Crystal Structure of catalase HPII from Escherichia coli (serendipitously crystallized)
Authors	:	Grzechowiak, M.; Sekula, B.; Ruszkowski, M.
Deposited on	:	2020-07-20
Resolution	:	1.84 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:

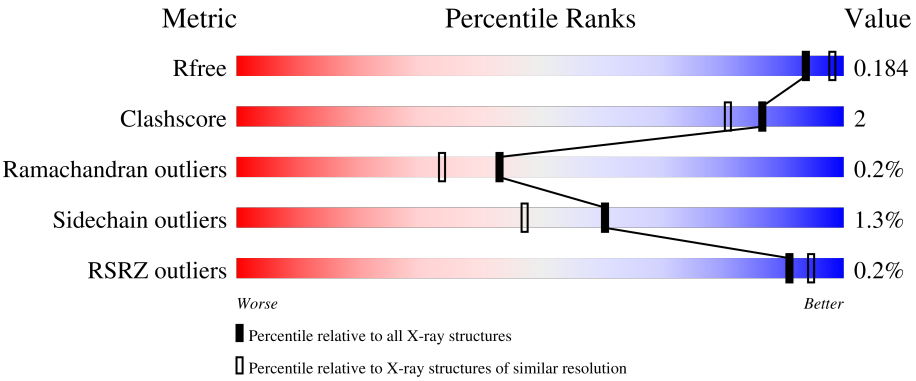
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	91% 5%
1	B	753	91% 5%
1	C	753	92% 5%
1	D	753	92% 5%
1	E	753	89% 7%

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Mol	Chain	Length	Quality of chain
1	F	753	91% 5%
1	G	753	91% 5%
1	H	753	% 90% 6%

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	801	X	-	-	-
2	HDD	B	801	X	-	-	-
2	HDD	C	801	X	-	-	-
2	HDD	D	801	X	-	-	-
2	HDD	E	801	X	-	-	-
2	HDD	F	801	X	-	-	-
2	HDD	G	801	X	-	-	-
2	HDD	H	801	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 51313 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.

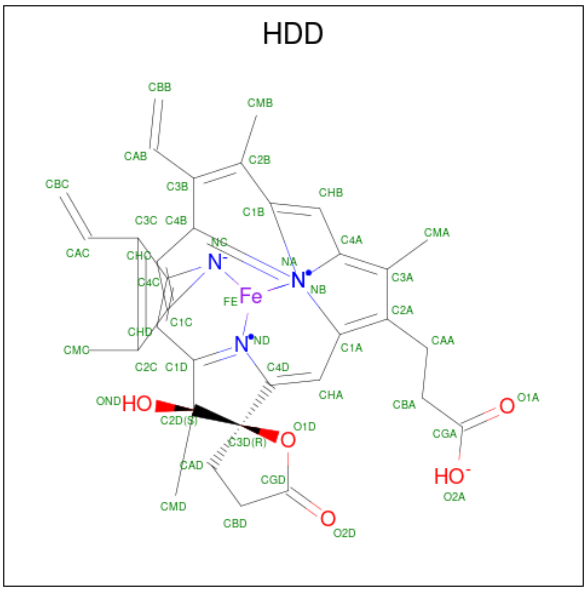
- Molecule 1 is a protein called Catalase HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	1	0
			5750	3649	1007	1082	12			
1	B	726	Total	C	N	O	S	0	3	0
			5770	3663	1011	1084	12			
1	C	726	Total	C	N	O	S	0	1	0
			5763	3656	1011	1084	12			
1	D	726	Total	C	N	O	S	0	3	0
			5773	3664	1015	1082	12			
1	E	726	Total	C	N	O	S	0	3	0
			5769	3660	1014	1083	12			
1	F	726	Total	C	N	O	S	0	2	0
			5758	3654	1010	1082	12			
1	G	727	Total	C	N	O	S	0	3	0
			5772	3661	1012	1087	12			
1	H	726	Total	C	N	O	S	0	3	0
			5767	3662	1010	1083	12			

There are 8 discrepancies between the modelled and reference sequences:

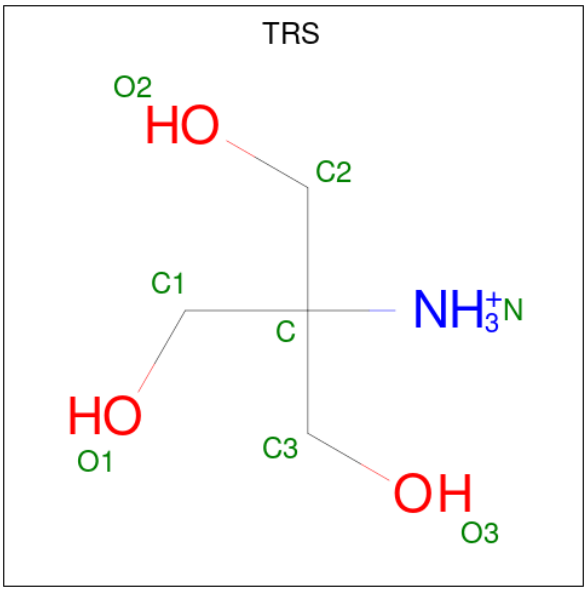
Chain	Residue	Modelled	Actual	Comment	Reference
A	99	ASN	SER	variant	UNP P21179
B	99	ASN	SER	variant	UNP P21179
C	99	ASN	SER	variant	UNP P21179
D	99	ASN	SER	variant	UNP P21179
E	99	ASN	SER	variant	UNP P21179
F	99	ASN	SER	variant	UNP P21179
G	99	ASN	SER	variant	UNP P21179
H	99	ASN	SER	variant	UNP P21179

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula: $C_{34}H_{32}FeN_4O_5$) (labeled as "Ligand of Interest" by depositor).



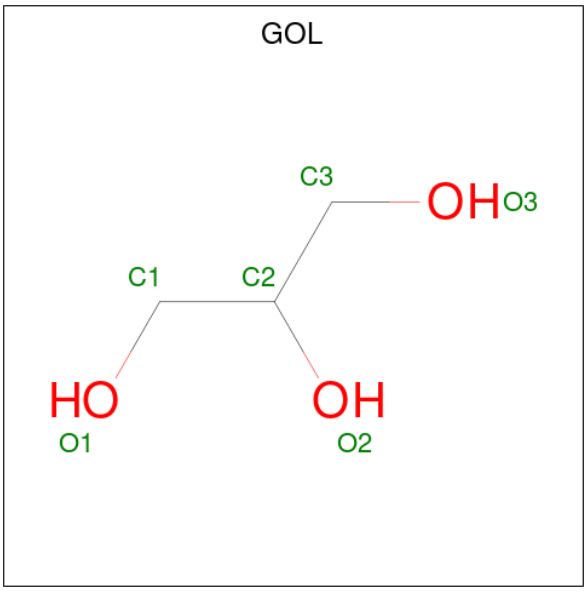
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	B	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	C	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	D	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	E	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	F	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	G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

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



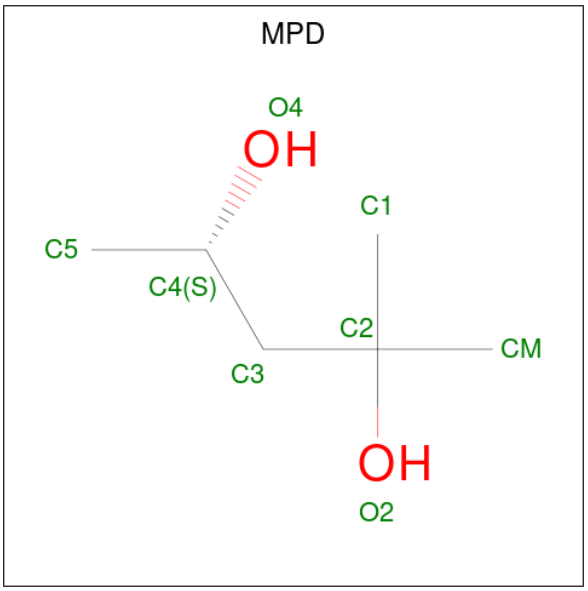
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 8 4 1 3	0	0
3	B	1	Total C N O 8 4 1 3	0	0
3	C	1	Total C N O 8 4 1 3	0	0
3	D	1	Total C N O 8 4 1 3	0	0
3	E	1	Total C N O 8 4 1 3	0	0
3	E	1	Total C N O 8 4 1 3	0	0
3	F	1	Total C N O 8 4 1 3	0	0
3	G	1	Total C N O 8 4 1 3	0	0
3	H	1	Total C N O 8 4 1 3	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



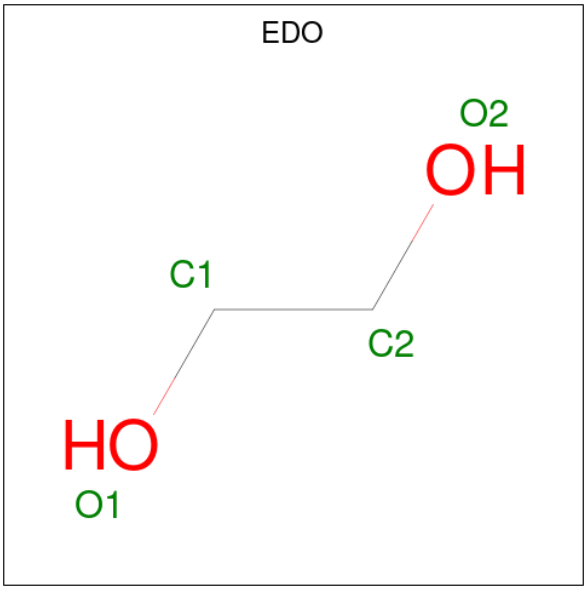
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 8 6 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 4 2 2	0	0
6	E	1	Total C O 4 2 2	0	0
6	F	1	Total C O 4 2 2	0	0
6	F	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

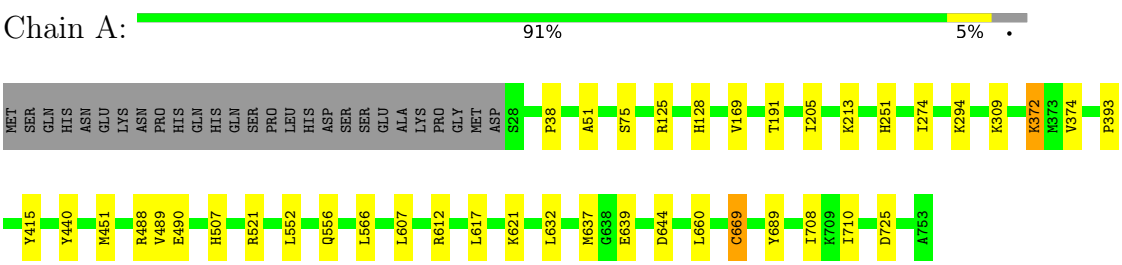
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	593	Total O 593 593	0	0
7	B	602	Total O 602 602	0	0
7	C	581	Total O 581 581	0	0
7	D	659	Total O 659 659	0	0
7	E	571	Total O 571 571	0	0
7	F	569	Total O 569 569	0	0
7	G	588	Total O 588 588	0	0
7	H	532	Total O 532 532	0	0

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.

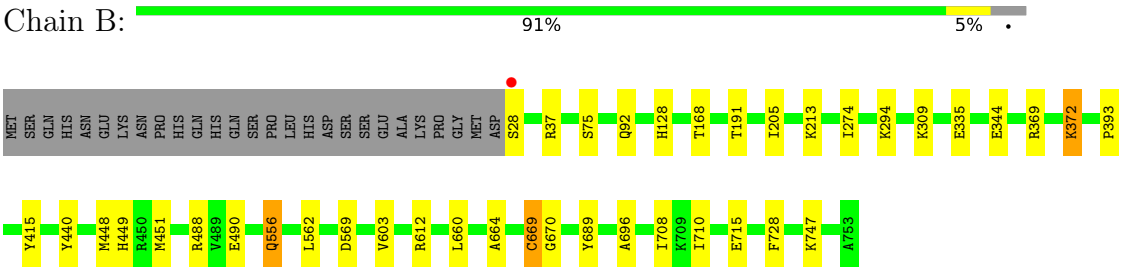
• Molecule 1: Catalase HPII

Chain A:



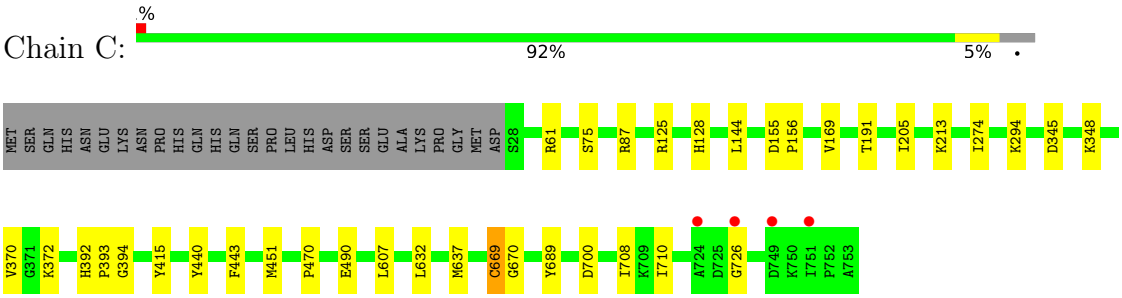
• Molecule 1: Catalase HPII

Chain B:



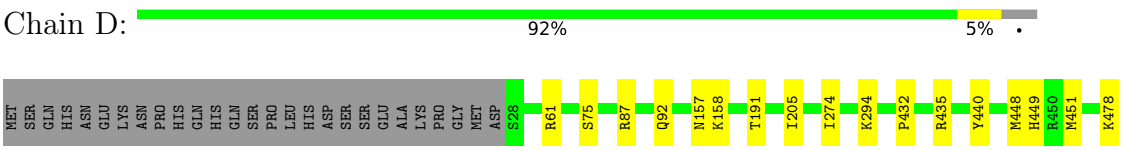
• Molecule 1: Catalase HPII

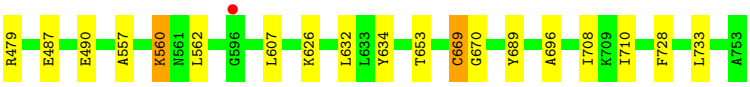
Chain C:



• Molecule 1: Catalase HPII

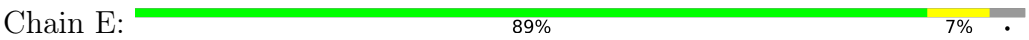
Chain D:





• Molecule 1: Catalase HPII

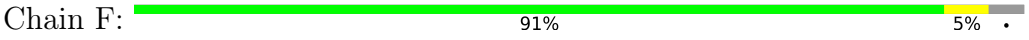
Chain E:

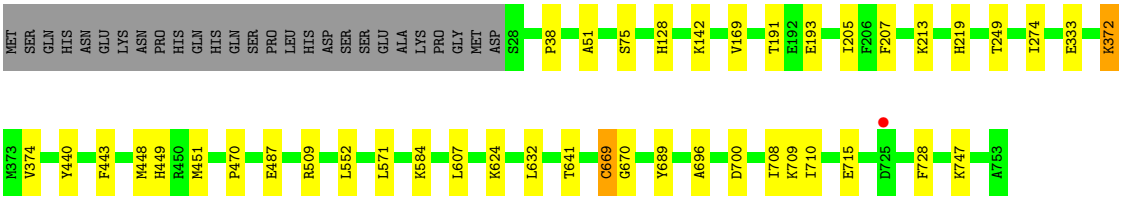




• Molecule 1: Catalase HPII

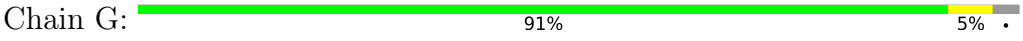
Chain F:

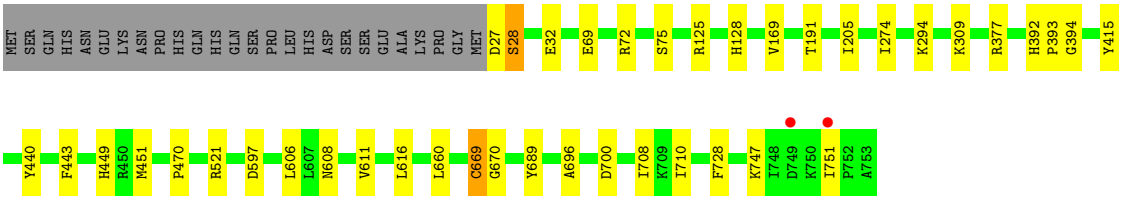




• Molecule 1: Catalase HPII

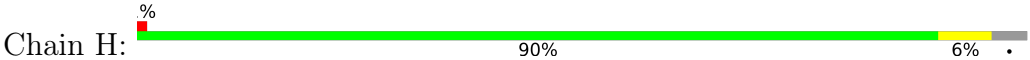
Chain G:

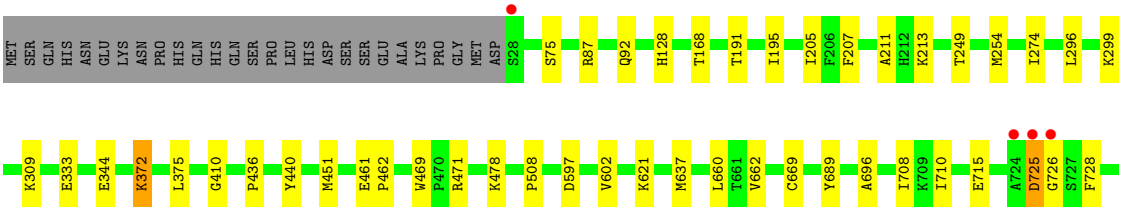




• Molecule 1: Catalase HPII

Chain H:






D749
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	121.19Å 168.07Å 137.98Å 90.00° 105.24° 90.00°	Depositor
Resolution (Å)	78.25 – 1.84 78.25 – 1.84	Depositor EDS
% Data completeness (in resolution range)	98.4 (78.25-1.84) 98.4 (78.25-1.84)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.144 , 0.184 0.145 , 0.184	Depositor DCC
R_{free} test set	2262 reflections (0.49%)	wwPDB-VP
Wilson B-factor (Å^2)	18.2	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	51313	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4531e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: EDO, TRS, GOL, OCS, HDD, MPD

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	0.32	0/5900	0.49	0/8020
1	B	0.32	0/5924	0.49	0/8052
1	C	0.31	0/5911	0.49	0/8035
1	D	0.33	0/5933	0.50	0/8064
1	E	0.30	0/5922	0.48	0/8049
1	F	0.30	0/5911	0.48	0/8034
1	G	0.31	0/5925	0.48	0/8053
1	H	0.29	0/5924	0.47	0/8052
All	All	0.31	0/47350	0.49	0/64359

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5750	0	5581	24	0
1	B	5770	0	5603	26	0
1	C	5763	0	5586	21	0
1	D	5773	0	5615	28	0
1	E	5769	0	5606	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	5758	0	5595	27	0
1	G	5772	0	5601	22	0
1	H	5767	0	5604	24	0
2	A	44	0	31	3	0
2	B	44	0	31	2	0
2	C	44	0	31	2	0
2	D	44	0	31	2	0
2	E	44	0	31	3	0
2	F	44	0	31	1	0
2	G	44	0	31	3	0
2	H	44	0	31	2	0
3	A	8	0	12	0	0
3	B	8	0	12	0	0
3	C	8	0	12	0	0
3	D	8	0	12	1	0
3	E	16	0	24	1	0
3	F	8	0	12	1	0
3	G	8	0	12	0	0
3	H	8	0	12	0	0
4	A	12	0	16	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	E	6	0	8	0	0
4	G	6	0	8	1	0
5	B	8	0	14	0	0
6	B	8	0	12	0	0
6	C	8	0	12	0	0
6	E	4	0	6	0	0
6	F	8	0	12	1	0
7	A	593	0	0	2	0
7	B	602	0	0	3	0
7	C	581	0	0	3	0
7	D	659	0	0	4	0
7	E	571	0	0	4	0
7	F	569	0	0	2	0
7	G	588	0	0	3	0
7	H	532	0	0	1	0
All	All	51313	0	45251	195	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 2.

The worst 5 of 195 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:451:MET:HE2	1:C:451:MET:HE2	1.52	0.90
1:F:451:MET:HE2	1:H:451:MET:HE2	1.59	0.85
1:E:451:MET:HE2	1:G:451:MET:HE2	1.59	0.84
1:B:708:ILE:HG13	1:B:710:ILE:HG12	1.68	0.76
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.69	0.73

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	724/753 (96%)	705 (97%)	18 (2%)	1 (0%)	48	38
1	B	726/753 (96%)	707 (97%)	18 (2%)	1 (0%)	48	38
1	C	725/753 (96%)	707 (98%)	17 (2%)	1 (0%)	48	38
1	D	727/753 (96%)	709 (98%)	17 (2%)	1 (0%)	48	38
1	E	726/753 (96%)	708 (98%)	17 (2%)	1 (0%)	48	38
1	F	725/753 (96%)	709 (98%)	15 (2%)	1 (0%)	48	38
1	G	727/753 (96%)	710 (98%)	15 (2%)	2 (0%)	36	25
1	H	726/753 (96%)	707 (97%)	17 (2%)	2 (0%)	36	25
All	All	5806/6024 (96%)	5662 (98%)	134 (2%)	10 (0%)	43	34

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	28	SER
1	A	75	SER
1	B	75	SER
1	D	75	SER
1	F	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	611/635 (96%)	604 (99%)	7 (1%)	65	54
1	B	613/635 (96%)	602 (98%)	11 (2%)	51	35
1	C	612/635 (96%)	607 (99%)	5 (1%)	73	65
1	D	614/635 (97%)	610 (99%)	4 (1%)	76	68
1	E	613/635 (96%)	603 (98%)	10 (2%)	55	39
1	F	612/635 (96%)	604 (99%)	8 (1%)	61	47
1	G	614/635 (97%)	604 (98%)	10 (2%)	55	39
1	H	613/635 (96%)	602 (98%)	11 (2%)	51	35
All	All	4902/5080 (96%)	4836 (99%)	66 (1%)	61	47

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	213	LYS
1	H	375	LEU
1	H	749	ASP
1	D	205	ILE
1	D	191	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	368	GLN
1	E	556	GLN
1	H	556	GLN
1	H	246	GLN
1	H	368	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)

8 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	D	669	1	7,8,9	1.03	1 (14%)	6,11,13	1.07	1 (16%)
1	OCS	C	669	1	7,8,9	1.48	1 (14%)	6,11,13	1.69	2 (33%)
1	OCS	B	669	1	7,8,9	1.04	1 (14%)	6,11,13	0.92	0
1	OCS	E	669	1	7,8,9	1.51	1 (14%)	6,11,13	1.42	1 (16%)
1	OCS	F	669	1	7,8,9	1.04	1 (14%)	6,11,13	0.69	0
1	OCS	G	669	1	7,8,9	1.55	1 (14%)	6,11,13	2.15	2 (33%)
1	OCS	A	669	1	7,8,9	1.54	1 (14%)	6,11,13	1.82	2 (33%)
1	OCS	H	669	1	7,8,9	1.02	1 (14%)	6,11,13	0.89	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OCS	D	669	1	-	1/4/7/9	-
1	OCS	C	669	1	-	1/4/7/9	-
1	OCS	B	669	1	-	3/4/7/9	-
1	OCS	E	669	1	-	1/4/7/9	-
1	OCS	F	669	1	-	3/4/7/9	-
1	OCS	G	669	1	-	4/4/7/9	-
1	OCS	A	669	1	-	2/4/7/9	-
1	OCS	H	669	1	-	2/4/7/9	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	669	OCS	OD1-SG	3.57	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	669	OCS	OD1-SG	3.53	1.55	1.45
1	A	669	OCS	OD1-SG	3.53	1.55	1.45
1	C	669	OCS	OD1-SG	3.47	1.55	1.45
1	F	669	OCS	OD2-SG	2.28	1.55	1.47

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	669	OCS	OD1-SG-CB	-3.62	102.64	106.94
1	G	669	OCS	OD2-SG-OD3	3.42	119.63	111.27
1	A	669	OCS	OD1-SG-CB	-2.91	103.48	106.94
1	C	669	OCS	OD2-SG-OD3	2.87	118.30	111.27
1	A	669	OCS	OD2-SG-OD3	2.86	118.26	111.27

There are no chirality outliers.

5 of 17 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	E	669	OCS	N-CA-CB-SG

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	669	OCS	1	0
1	C	669	OCS	2	0
1	B	669	OCS	1	0
1	F	669	OCS	2	0
1	G	669	OCS	2	0
1	A	669	OCS	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

31 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	$\#\|Z\| > 2$
6	EDO	C	804	-	3,3,3	0.54	0	2,2,2	0.12	0
3	TRS	B	802	-	7,7,7	0.25	0	9,9,9	0.40	0
2	HDD	F	801	1,7	50,52,52	1.85	13 (26%)	56,89,89	1.75	13 (23%)
6	EDO	C	803	-	3,3,3	0.47	0	2,2,2	0.20	0
3	TRS	G	802	-	7,7,7	0.30	0	9,9,9	0.35	0
2	HDD	H	801	1,7	50,52,52	1.84	11 (22%)	56,89,89	1.75	10 (17%)
2	HDD	G	801	1	50,52,52	1.87	12 (24%)	56,89,89	1.64	11 (19%)
3	TRS	D	802	-	7,7,7	0.28	0	9,9,9	0.32	0
5	MPD	B	803	-	7,7,7	0.29	0	9,10,10	0.32	0
6	EDO	B	804	-	3,3,3	0.54	0	2,2,2	0.29	0
2	HDD	D	801	1	50,52,52	1.83	12 (24%)	56,89,89	1.63	10 (17%)
4	GOL	E	805	-	5,5,5	0.84	0	5,5,5	1.13	0
3	TRS	A	802	-	7,7,7	0.24	0	9,9,9	0.33	0
6	EDO	F	804	-	3,3,3	0.47	0	2,2,2	0.35	0
6	EDO	B	805	-	3,3,3	0.49	0	2,2,2	0.26	0
3	TRS	H	802	-	7,7,7	0.26	0	9,9,9	0.41	0
2	HDD	A	801	1	50,52,52	1.85	12 (24%)	56,89,89	1.63	10 (17%)
4	GOL	G	803	-	5,5,5	0.83	0	5,5,5	1.07	0
4	GOL	C	805	-	5,5,5	0.93	0	5,5,5	0.98	0
3	TRS	E	802	-	7,7,7	0.30	0	9,9,9	0.35	0
6	EDO	E	804	-	3,3,3	0.53	0	2,2,2	0.34	0
3	TRS	E	803	-	7,7,7	0.38	0	9,9,9	0.53	0
2	HDD	B	801	1	50,52,52	1.85	15 (30%)	56,89,89	1.76	12 (21%)
3	TRS	C	802	-	7,7,7	0.24	0	9,9,9	0.53	0
6	EDO	F	803	-	3,3,3	0.46	0	2,2,2	0.34	0
3	TRS	F	802	-	7,7,7	0.26	0	9,9,9	0.31	0
2	HDD	E	801	1	50,52,52	1.80	13 (26%)	56,89,89	1.71	11 (19%)
2	HDD	C	801	1,7	50,52,52	1.86	13 (26%)	56,89,89	1.62	10 (17%)
4	GOL	A	804	-	5,5,5	0.86	0	5,5,5	1.06	0
4	GOL	A	803	-	5,5,5	0.77	0	5,5,5	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	B	806	-	5,5,5	0.85	0	5,5,5	1.01	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	C	804	-	-	0/1/1/1	-
3	TRS	B	802	-	-	3/9/9/9	-
2	HDD	F	801	1,7	1/1/8/14	6/9/89/89	0/1/9/9
6	EDO	C	803	-	-	0/1/1/1	-
3	TRS	G	802	-	-	0/9/9/9	-
2	HDD	H	801	1,7	1/1/8/14	4/9/89/89	0/1/9/9
2	HDD	G	801	1	1/1/8/14	2/9/89/89	0/1/9/9
3	TRS	D	802	-	-	1/9/9/9	-
5	MPD	B	803	-	-	3/5/5/5	-
6	EDO	B	804	-	-	0/1/1/1	-
2	HDD	D	801	1	1/1/8/14	4/9/89/89	0/1/9/9
4	GOL	E	805	-	-	0/4/4/4	-
3	TRS	A	802	-	-	3/9/9/9	-
6	EDO	F	804	-	-	0/1/1/1	-
6	EDO	B	805	-	-	1/1/1/1	-
3	TRS	H	802	-	-	3/9/9/9	-
2	HDD	A	801	1	1/1/8/14	2/9/89/89	0/1/9/9
4	GOL	G	803	-	-	1/4/4/4	-
4	GOL	C	805	-	-	0/4/4/4	-
3	TRS	E	802	-	-	0/9/9/9	-
6	EDO	E	804	-	-	0/1/1/1	-
3	TRS	E	803	-	-	0/9/9/9	-
2	HDD	B	801	1	1/1/8/14	6/9/89/89	0/1/9/9
3	TRS	C	802	-	-	2/9/9/9	-
6	EDO	F	803	-	-	0/1/1/1	-
3	TRS	F	802	-	-	4/9/9/9	-
2	HDD	E	801	1	1/1/8/14	4/9/89/89	0/1/9/9
2	HDD	C	801	1,7	1/1/8/14	4/9/89/89	0/1/9/9
4	GOL	A	804	-	-	4/4/4/4	-
4	GOL	A	803	-	-	4/4/4/4	-
4	GOL	B	806	-	-	2/4/4/4	-

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	HDD	FE-NB	5.09	2.10	1.94
2	B	801	HDD	FE-NB	5.08	2.10	1.94
2	G	801	HDD	FE-NB	5.06	2.10	1.94
2	E	801	HDD	FE-NB	5.01	2.10	1.94
2	G	801	HDD	CHB-C1B	4.99	1.48	1.38

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	801	HDD	C3C-C2C-C1C	-5.29	102.03	107.08
2	E	801	HDD	C2B-C1B-NB	5.22	116.02	109.84
2	F	801	HDD	C2B-C1B-NB	5.18	115.97	109.84
2	A	801	HDD	C2B-C1B-NB	5.16	115.95	109.84
2	H	801	HDD	C3C-C2C-C1C	-5.15	102.16	107.08

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	801	HDD	NC
2	B	801	HDD	NC
2	C	801	HDD	NC
2	D	801	HDD	NC
2	E	801	HDD	NC

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	804	GOL	C1-C2-C3-O3
4	B	806	GOL	O1-C1-C2-C3
5	B	803	MPD	O2-C2-C3-C4
4	A	803	GOL	O1-C1-C2-O2
4	A	803	GOL	O1-C1-C2-C3

There are no ring outliers.

13 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	801	HDD	1	0
2	H	801	HDD	2	0
2	G	801	HDD	3	0
3	D	802	TRS	1	0

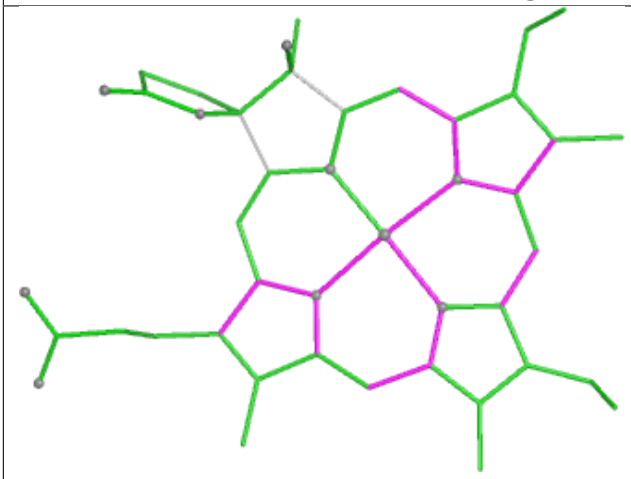
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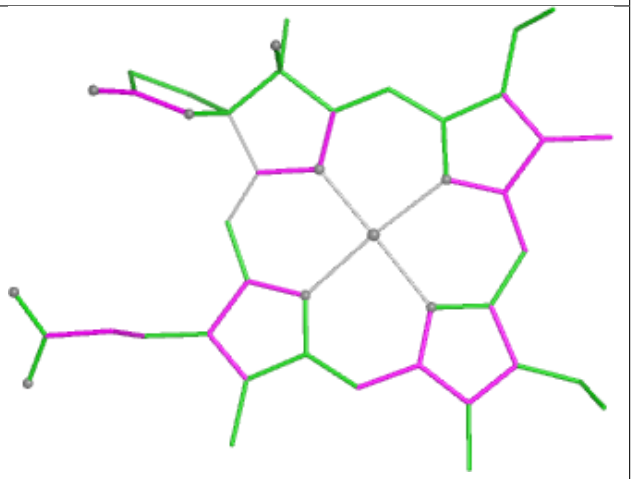
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	HDD	2	0
2	A	801	HDD	3	0
4	G	803	GOL	1	0
3	E	802	TRS	1	0
2	B	801	HDD	2	0
6	F	803	EDO	1	0
3	F	802	TRS	1	0
2	E	801	HDD	3	0
2	C	801	HDD	2	0

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

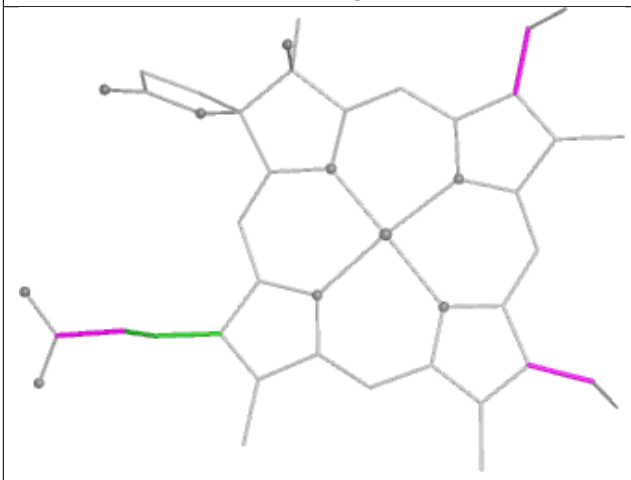
Ligand HDD F 801



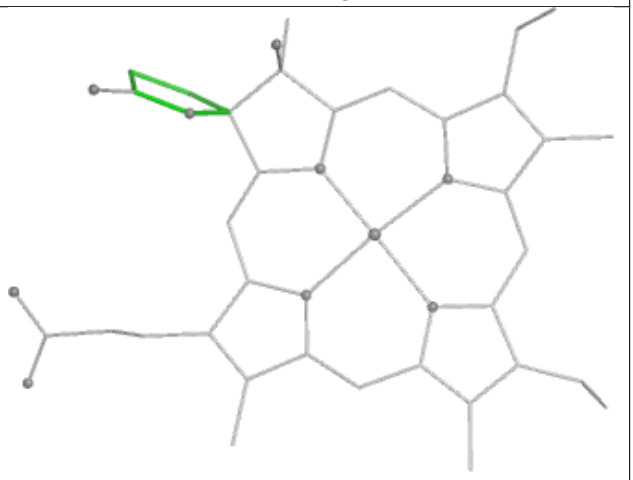
Bond lengths



Bond angles

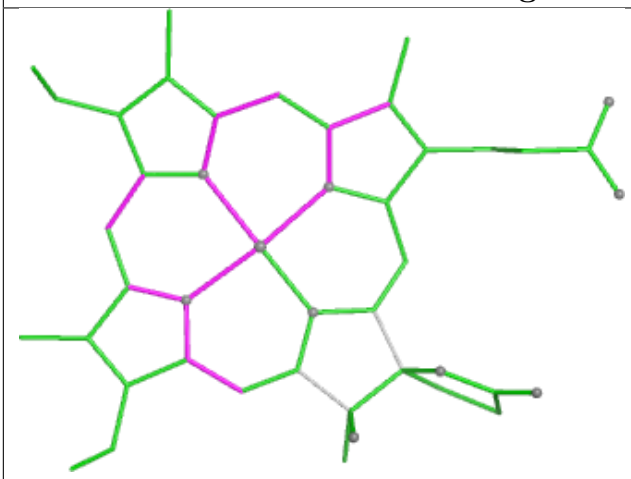


Torsions

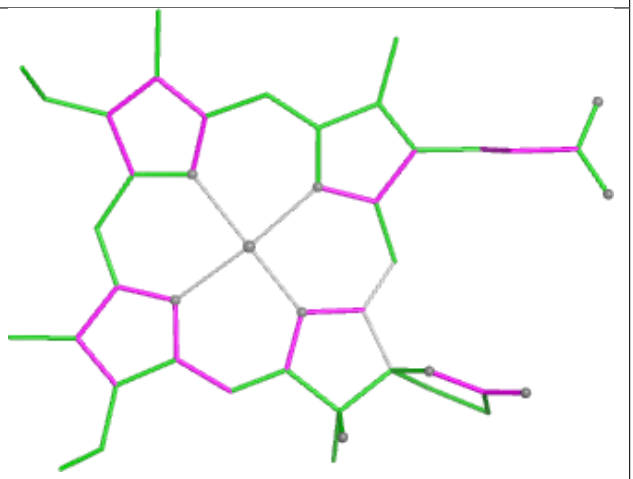


Rings

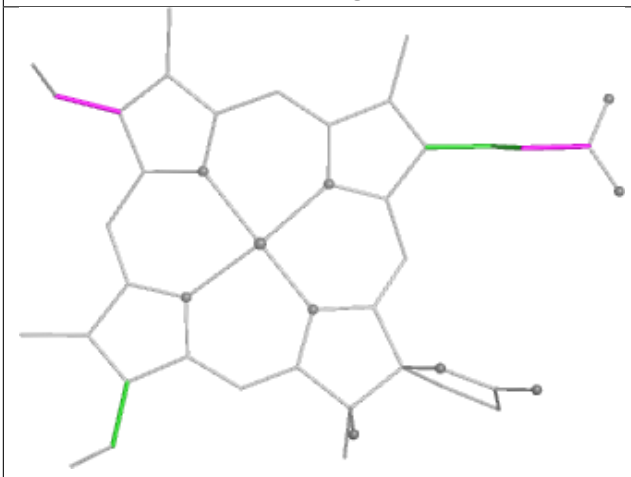
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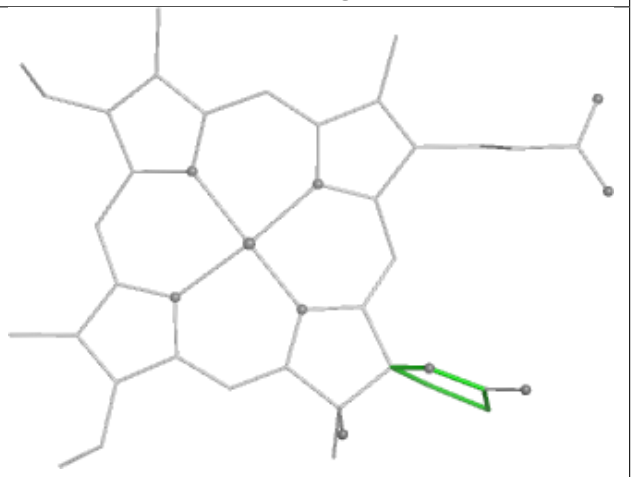
Bond lengths



Bond angles

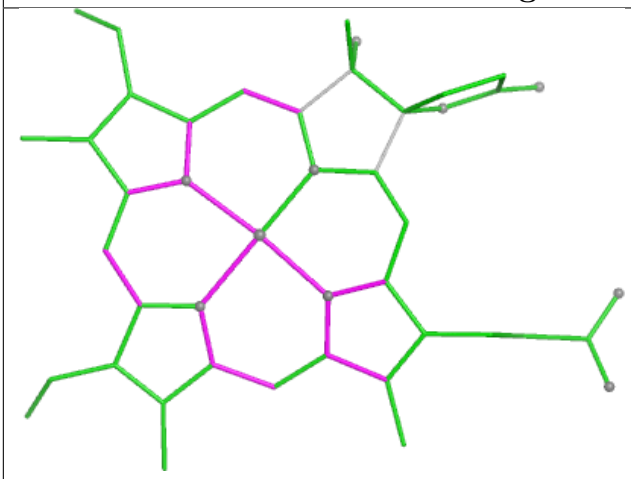


Torsions

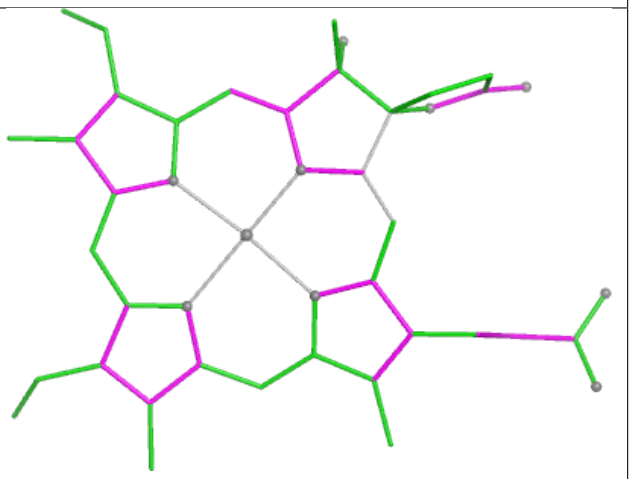


Rings

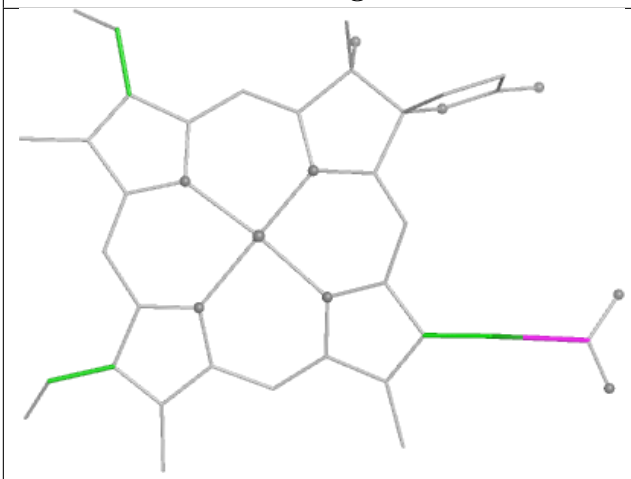
Ligand HDD G 801



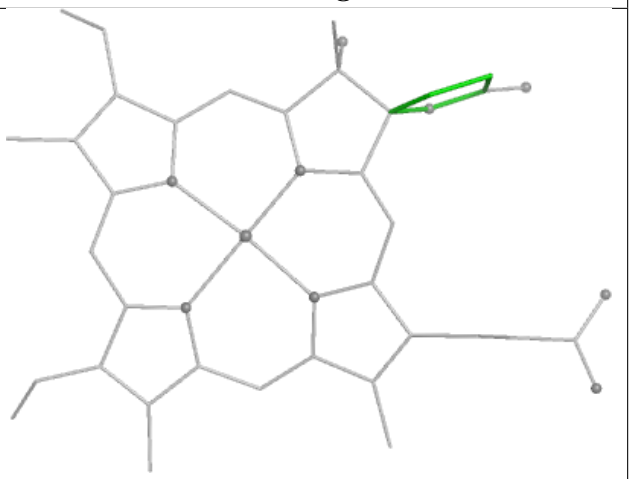
Bond lengths



Bond angles

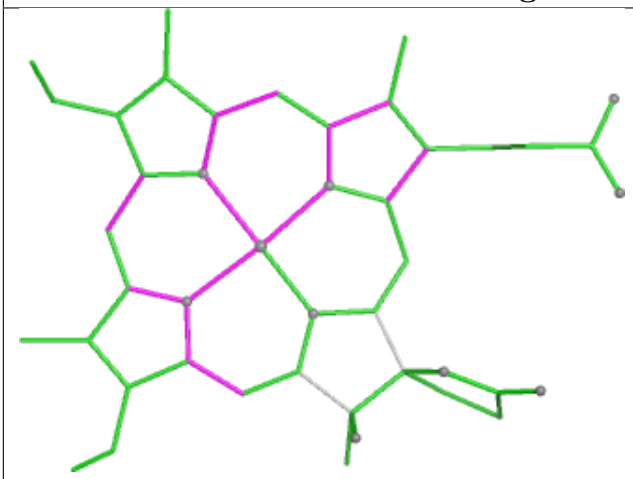


Torsions

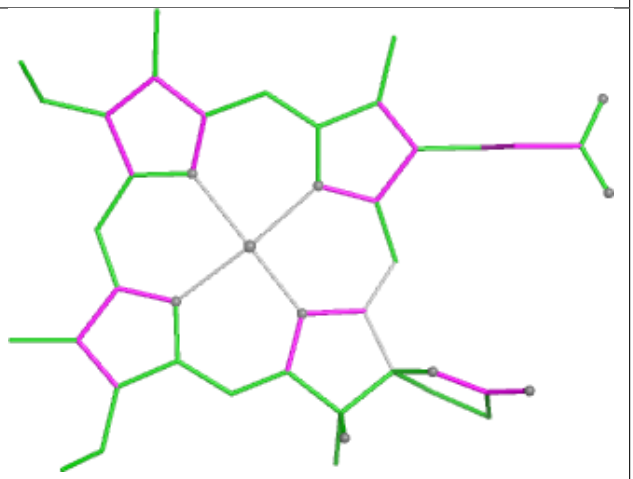


Rings

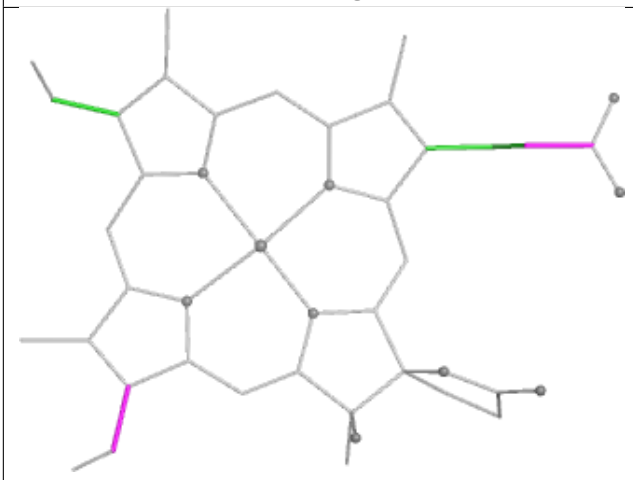
Ligand HDD D 801



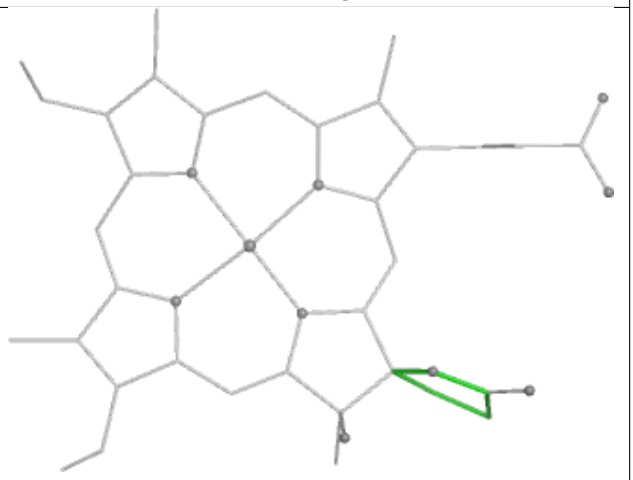
Bond lengths



Bond angles

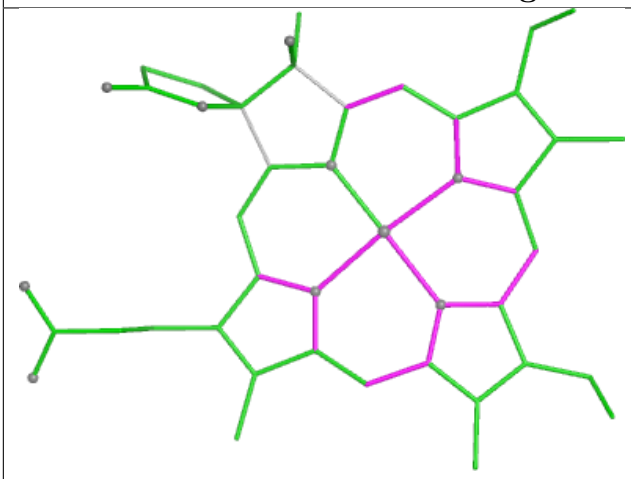


Torsions

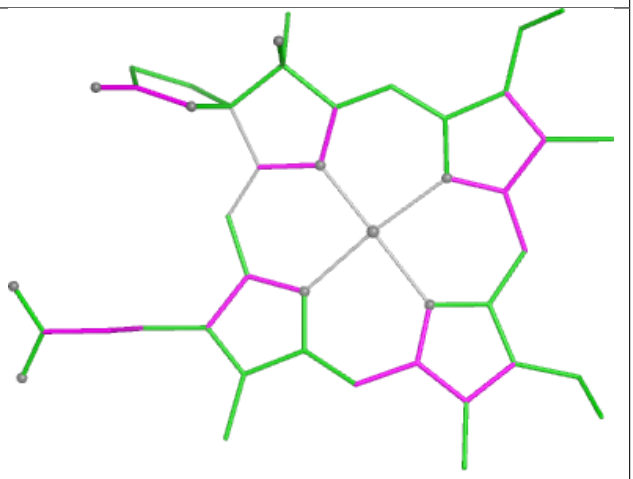


Rings

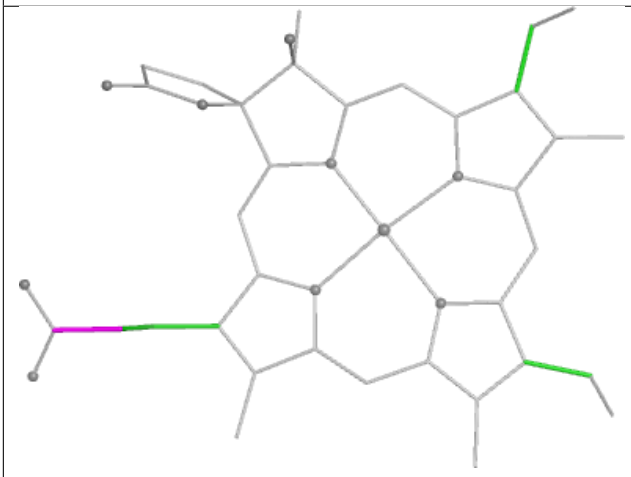
Ligand HDD A 801



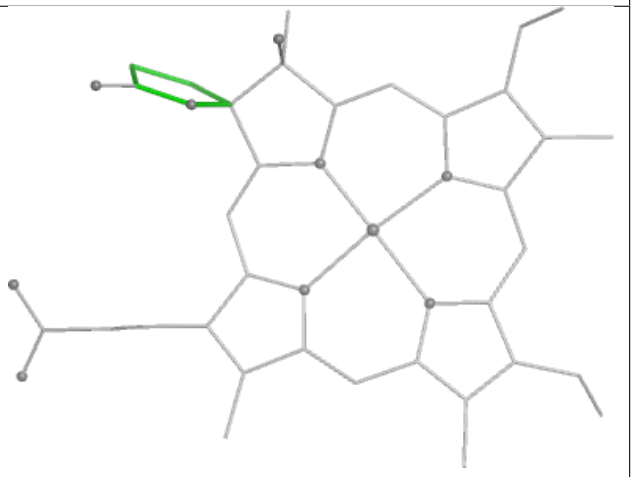
Bond lengths



Bond angles

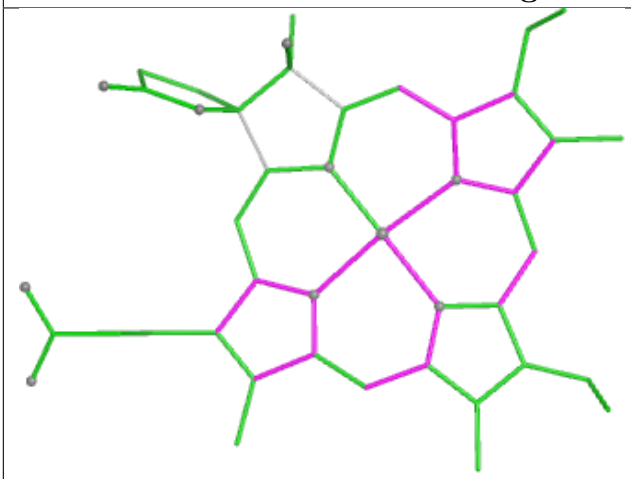


Torsions

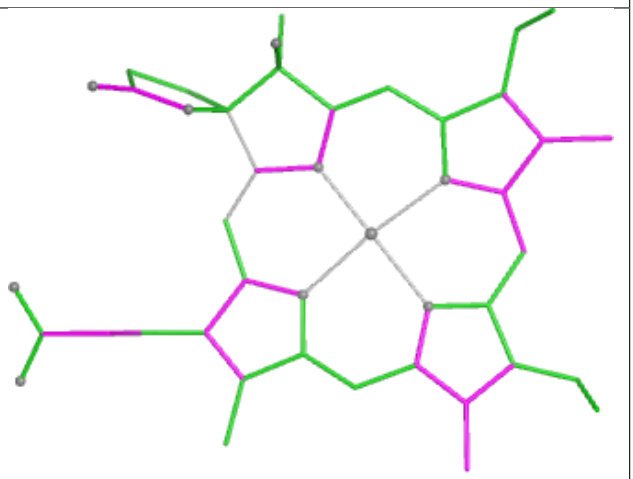


Rings

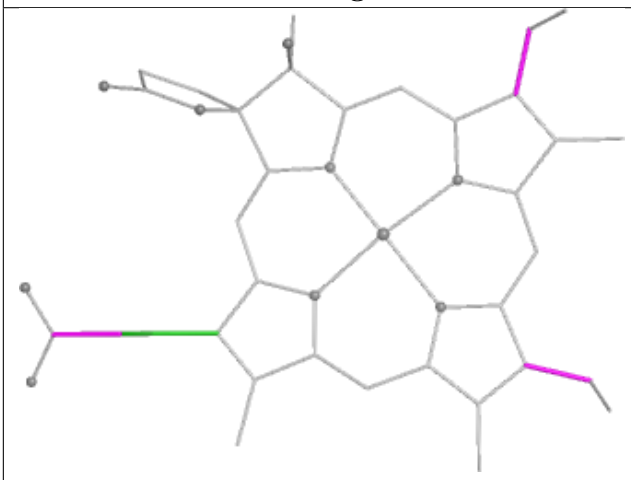
Ligand HDD B 801



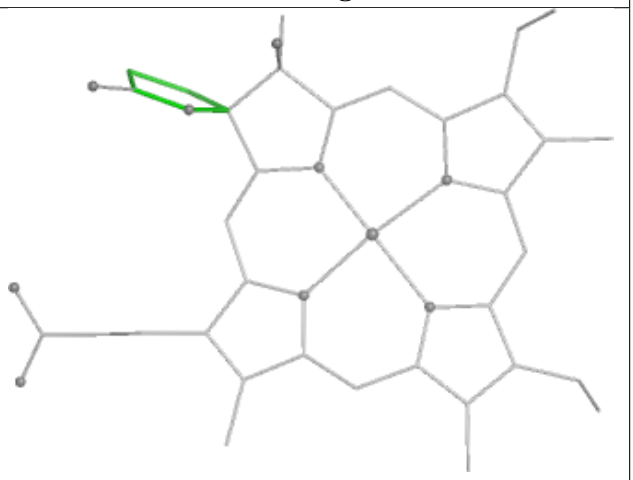
Bond lengths



Bond angles

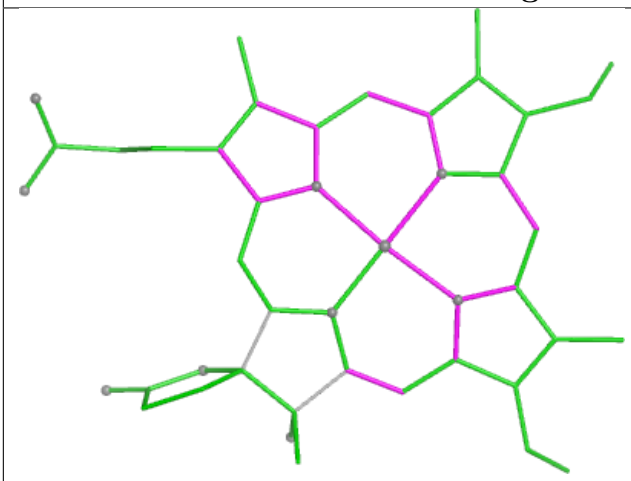


Torsions

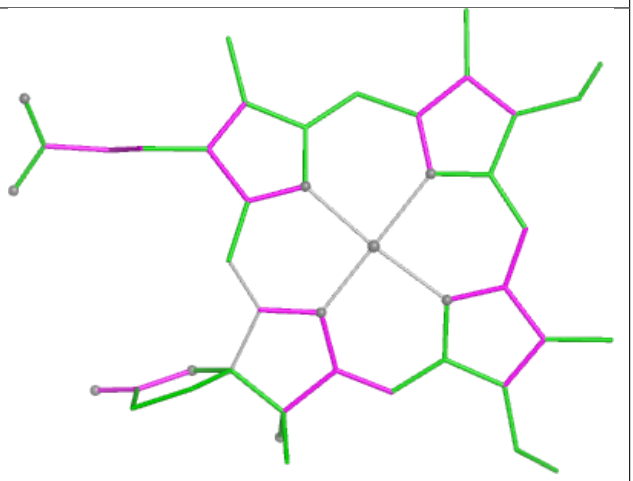


Rings

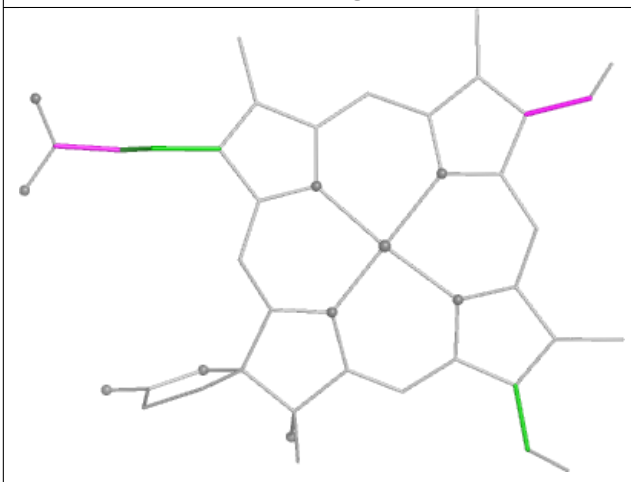
Ligand HDD E 801



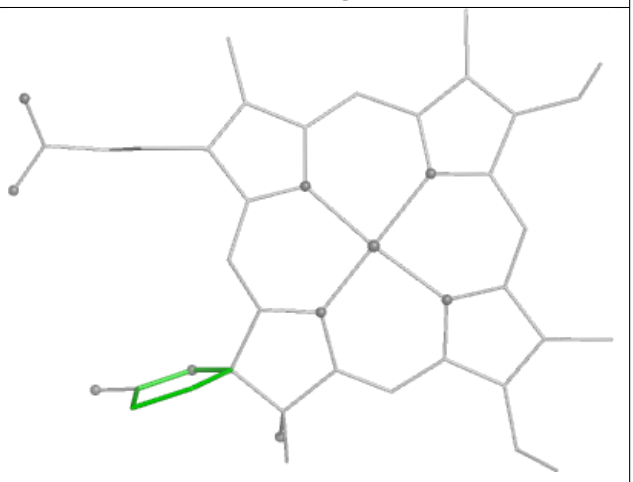
Bond lengths



Bond angles

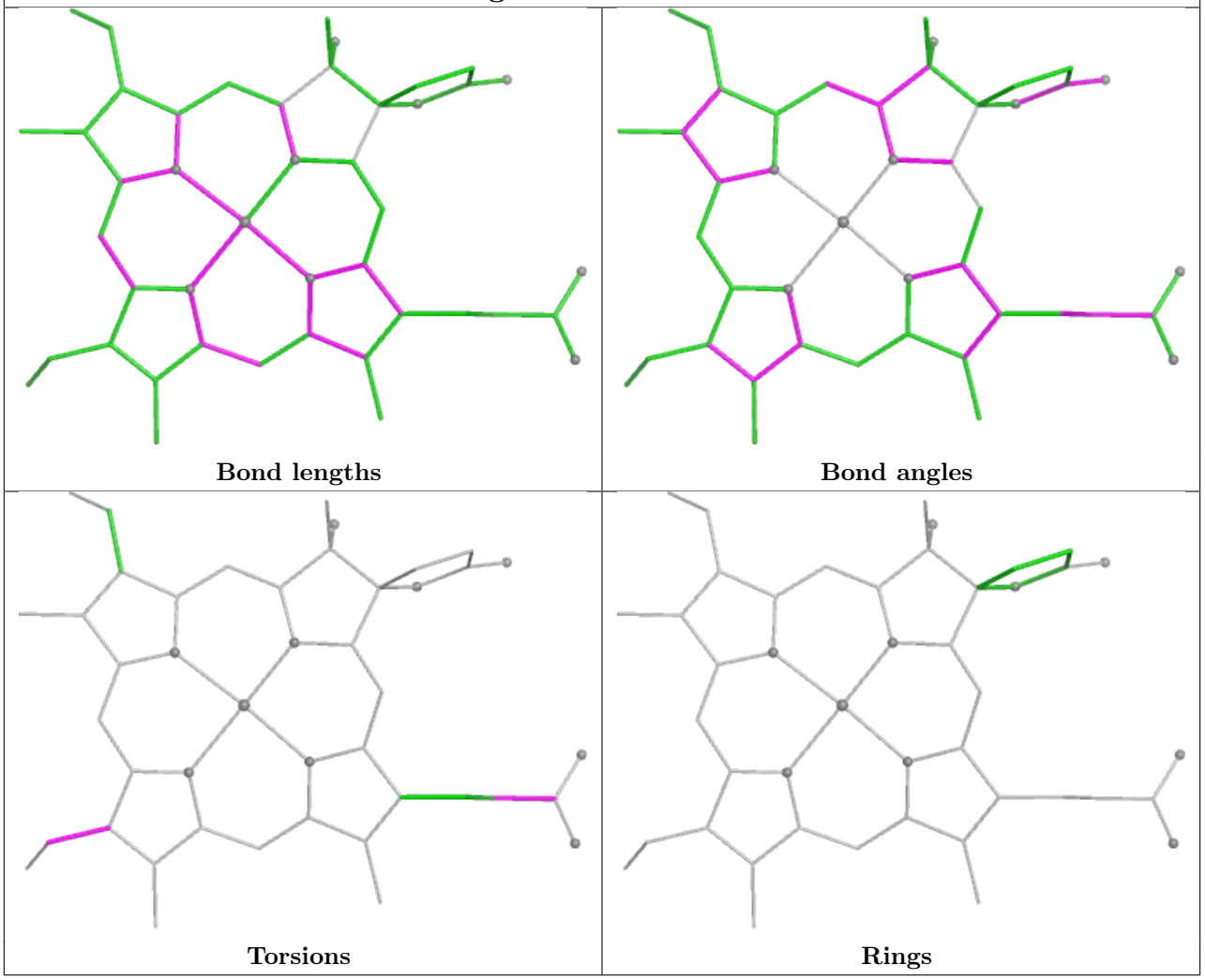


Torsions



Rings

Ligand HDD C 801



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

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^{th} 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%)	-0.68	0 100 100	10, 18, 38, 61	1 (0%)
1	B	725/753 (96%)	-0.68	1 (0%) 92 95	9, 19, 34, 70	4 (0%)
1	C	725/753 (96%)	-0.65	4 (0%) 85 90	5, 19, 38, 87	2 (0%)
1	D	725/753 (96%)	-0.77	1 (0%) 92 95	7, 17, 31, 51	3 (0%)
1	E	725/753 (96%)	-0.64	0 100 100	9, 20, 36, 62	4 (0%)
1	F	725/753 (96%)	-0.60	1 (0%) 92 95	10, 20, 38, 54	3 (0%)
1	G	726/753 (96%)	-0.66	2 (0%) 90 94	9, 20, 38, 88	3 (0%)
1	H	725/753 (96%)	-0.53	4 (0%) 85 90	9, 22, 47, 91	3 (0%)
All	All	5801/6024 (96%)	-0.65	13 (0%) 91 94	5, 19, 39, 91	23 (0%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	749	ASP	3.1
1	H	724	ALA	3.0
1	H	725	ASP	2.8
1	C	751	ILE	2.8
1	D	596	GLY	2.6

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, 95^{th} 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	B	669	9/10	0.93	0.09	23,28,49,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	OCS	G	669	9/10	0.93	0.10	24,32,47,59	0
1	OCS	H	669	9/10	0.94	0.08	41,46,55,56	0
1	OCS	D	669	9/10	0.95	0.07	15,25,37,50	0
1	OCS	F	669	9/10	0.95	0.08	25,29,42,50	0
1	OCS	A	669	9/10	0.95	0.07	25,30,41,53	0
1	OCS	C	669	9/10	0.95	0.08	26,29,42,49	0
1	OCS	E	669	9/10	0.97	0.06	19,21,34,44	0

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
6	EDO	C	804	4/4	0.73	0.15	34,44,50,55	0
4	GOL	G	803	6/6	0.74	0.16	52,54,58,61	0
6	EDO	B	804	4/4	0.77	0.14	36,40,47,51	0
4	GOL	A	804	6/6	0.80	0.12	42,45,49,51	0
4	GOL	B	806	6/6	0.83	0.12	57,61,63,64	0
6	EDO	E	804	4/4	0.83	0.13	41,41,42,45	0
6	EDO	C	803	4/4	0.84	0.13	48,48,49,52	0
4	GOL	A	803	6/6	0.84	0.12	50,53,55,57	0
4	GOL	C	805	6/6	0.84	0.11	50,53,54,57	0
6	EDO	F	804	4/4	0.84	0.13	44,47,49,50	0
5	MPD	B	803	8/8	0.87	0.11	39,41,43,47	0
4	GOL	E	805	6/6	0.88	0.10	36,43,51,52	0
6	EDO	F	803	4/4	0.88	0.10	49,49,51,52	0
3	TRS	E	803	8/8	0.88	0.09	33,38,40,40	0
6	EDO	B	805	4/4	0.90	0.10	41,43,47,48	0
3	TRS	H	802	8/8	0.91	0.09	21,31,35,36	0
3	TRS	D	802	8/8	0.92	0.09	21,31,35,39	0
3	TRS	F	802	8/8	0.92	0.08	23,27,31,31	0
3	TRS	G	802	8/8	0.92	0.07	20,25,28,34	0
3	TRS	C	802	8/8	0.95	0.07	16,22,24,26	0
3	TRS	A	802	8/8	0.95	0.06	18,26,31,31	0

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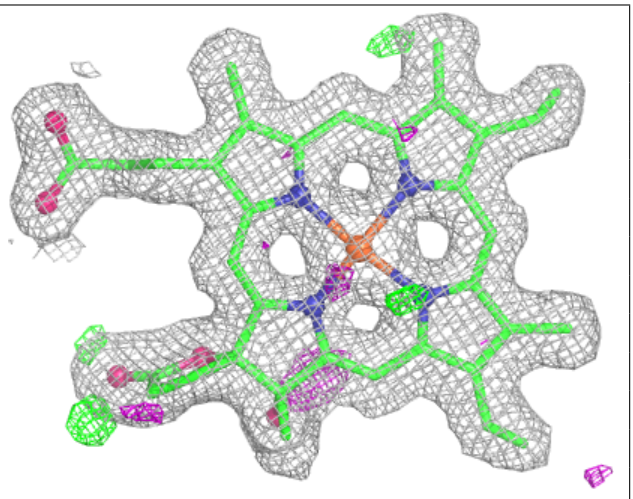
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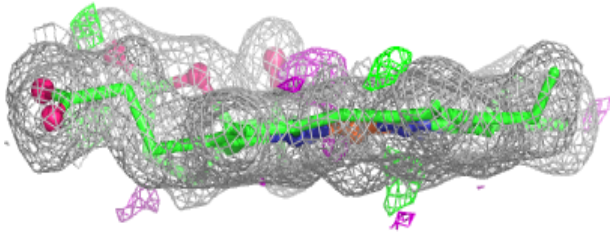
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TRS	E	802	8/8	0.95	0.06	20,25,32,36	0
3	TRS	B	802	8/8	0.96	0.08	20,22,23,24	0
2	HDD	H	801	44/44	0.98	0.05	9,15,21,25	0
2	HDD	A	801	44/44	0.98	0.05	10,13,21,24	0
2	HDD	B	801	44/44	0.98	0.06	9,14,22,23	0
2	HDD	C	801	44/44	0.98	0.06	7,14,20,25	0
2	HDD	D	801	44/44	0.98	0.06	7,12,19,21	0
2	HDD	E	801	44/44	0.98	0.06	9,14,20,26	0
2	HDD	F	801	44/44	0.98	0.05	10,16,24,25	0
2	HDD	G	801	44/44	0.98	0.05	8,14,19,23	0

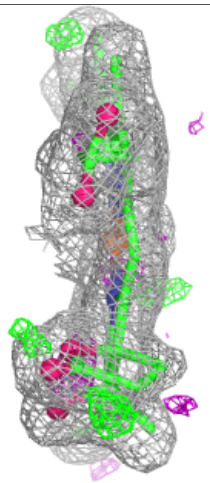
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HDD H 801:

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

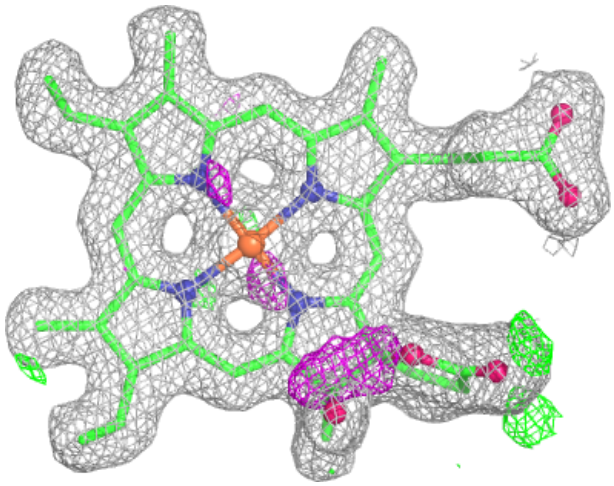


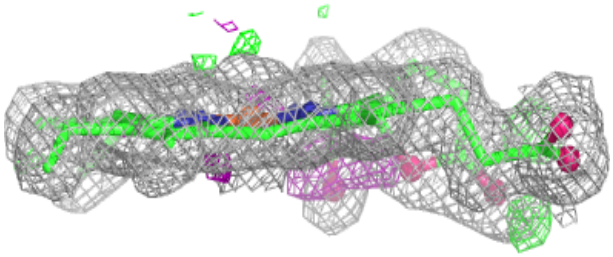


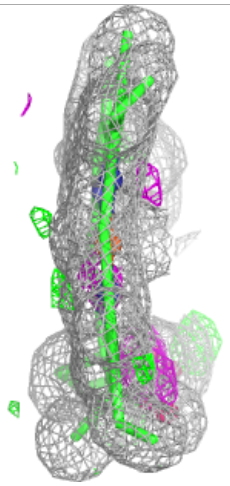


Electron density around HDD A 801:

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

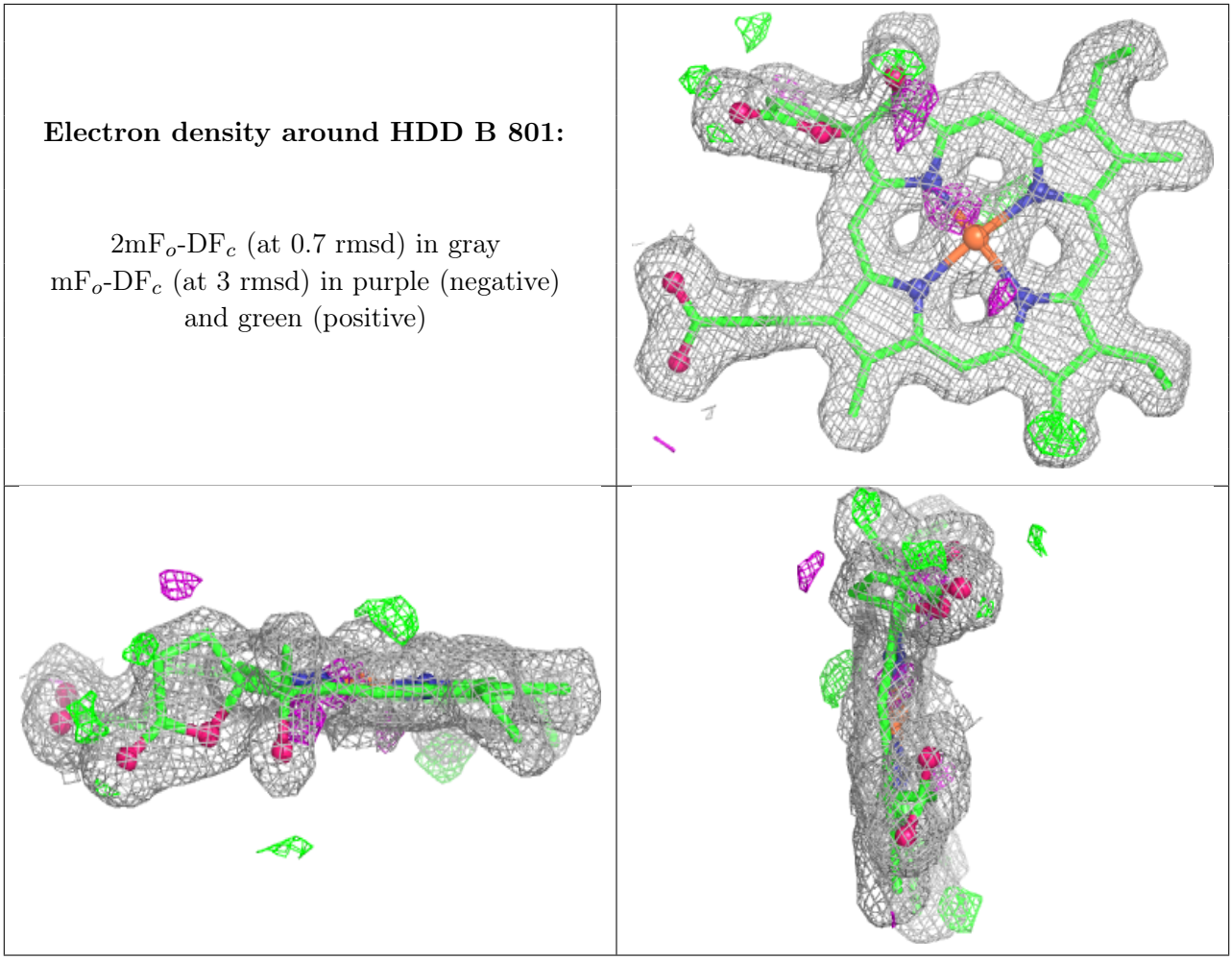






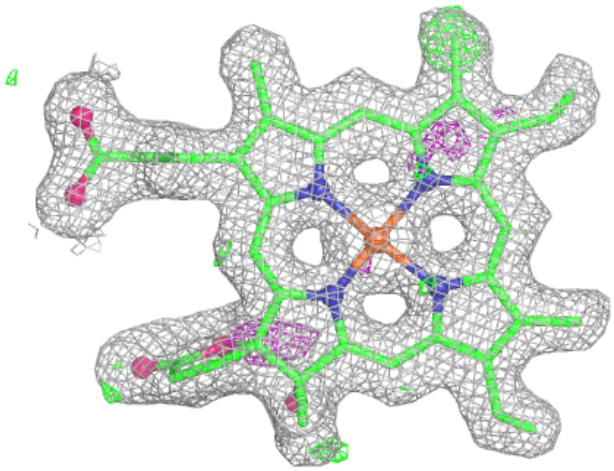
Electron density around HDD B 801:

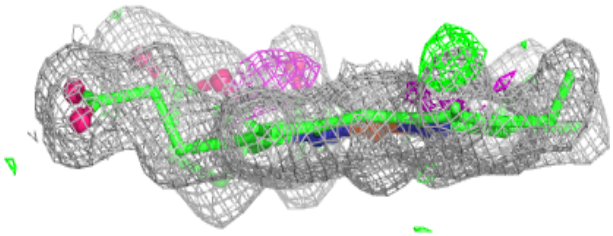
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

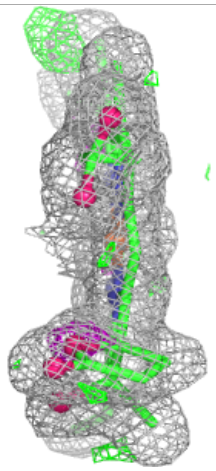


Electron density around HDD C 801:

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

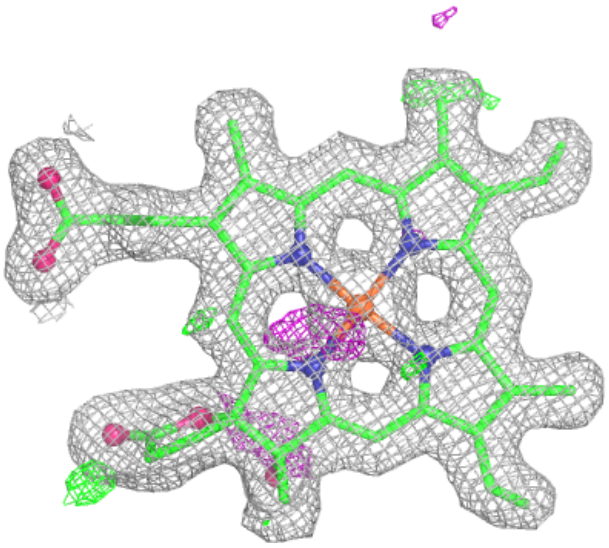


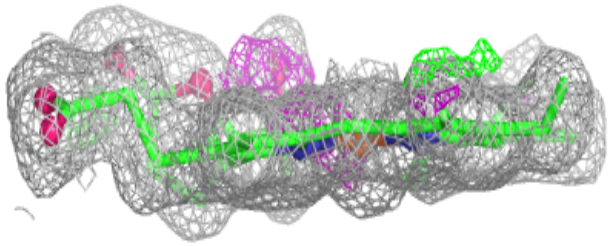


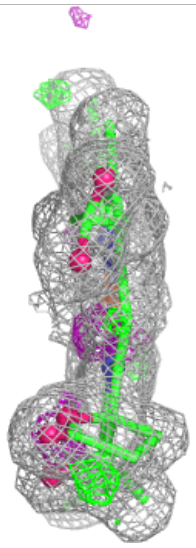


Electron density around HDD D 801:

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

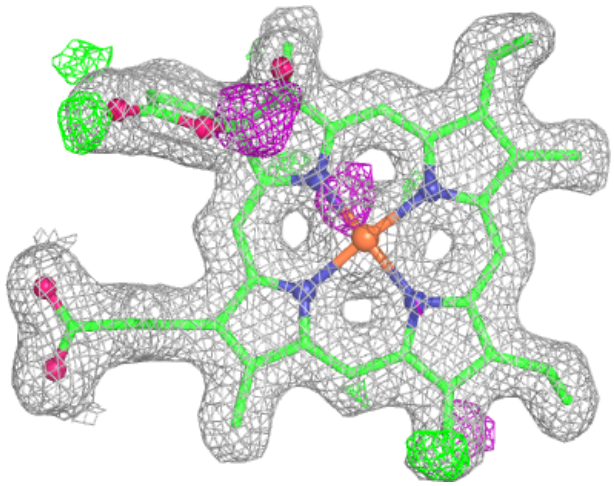


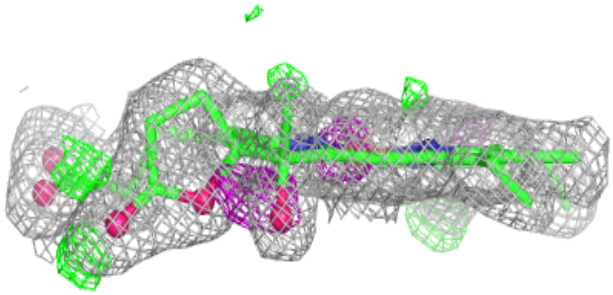


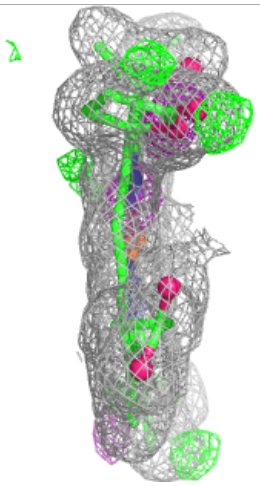


Electron density around HDD E 801:

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

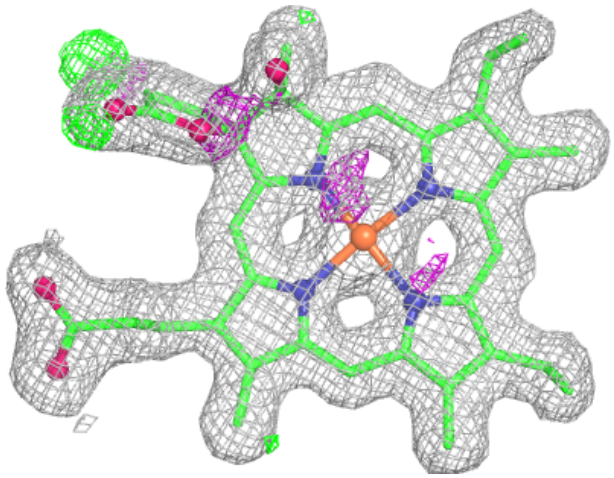


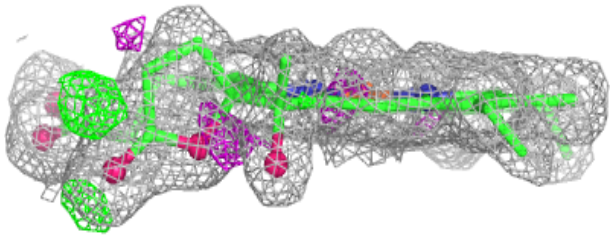


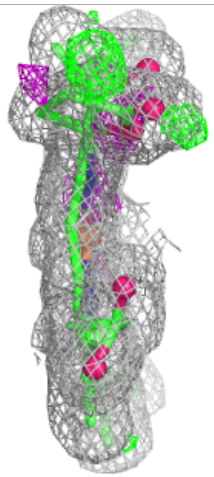


Electron density around HDD F 801:

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

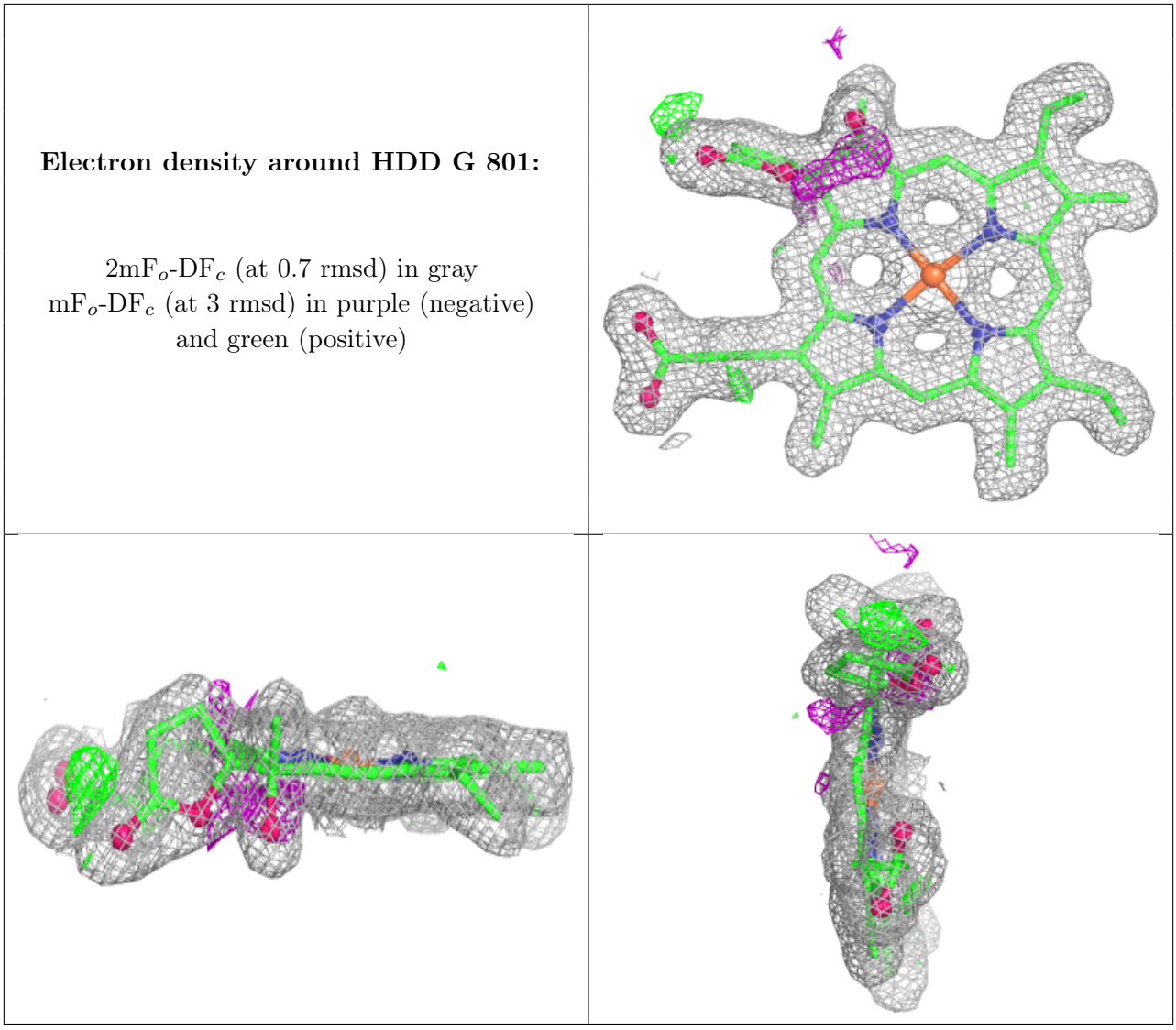






Electron density around HDD G 801:

$2mF_o$-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.