wwPDB X-ray Structure Validation Summary Report (i)

Nov 20, 2023 – 12:23 PM EST

PDB ID	:	2HRE
Title	:	Structure of human ferrochelatase variant E343K with protoporphyrin IX bound
Authors	:	Medlock, A.; Swartz, L.; Dailey, T.A.; Dailey, H.A.; Lanzilotta, W.N.
Deposited on	:	2006-07-20
Resolution	:	2.50 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:

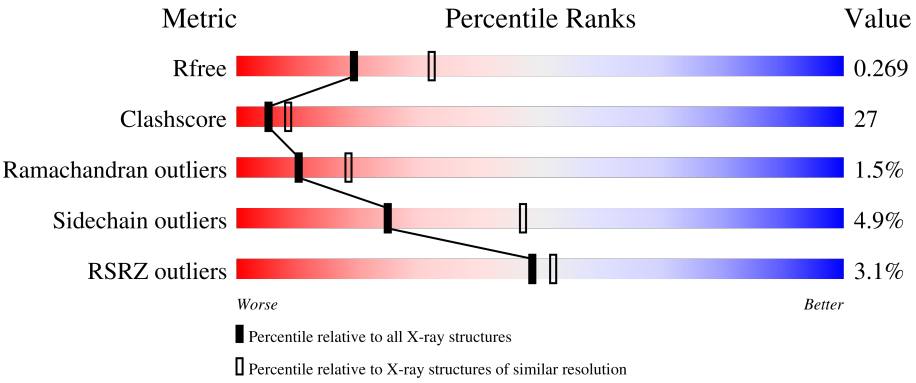
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	359	4% 56% 41% .
1	B	359	3% 52% 44% . .
1	C	359	3% 58% 38% .
1	D	359	3% 54% 41% 5%

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
3	FES	B	502	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12228 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.

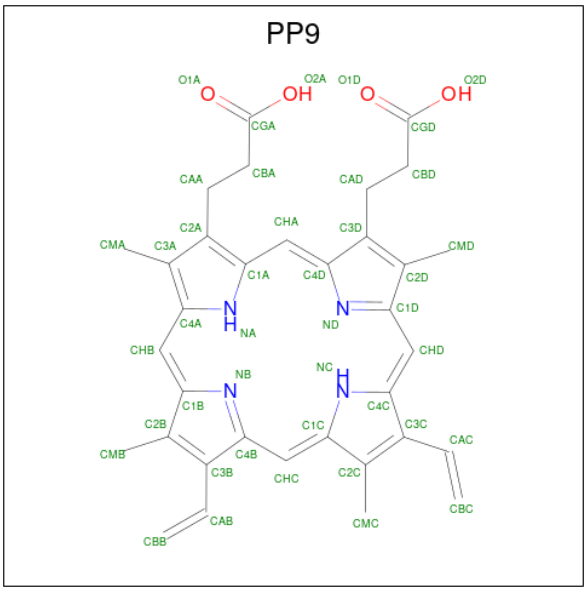
- Molecule 1 is a protein called Ferrochelatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2891	1842	504	527	18			
1	B	359	Total	C	N	O	S	0	0	0
			2891	1842	504	527	18			
1	C	359	Total	C	N	O	S	0	0	0
			2891	1842	504	527	18			
1	D	359	Total	C	N	O	S	0	0	0
			2891	1842	504	527	18			

There are 4 discrepancies between the modelled and reference sequences:

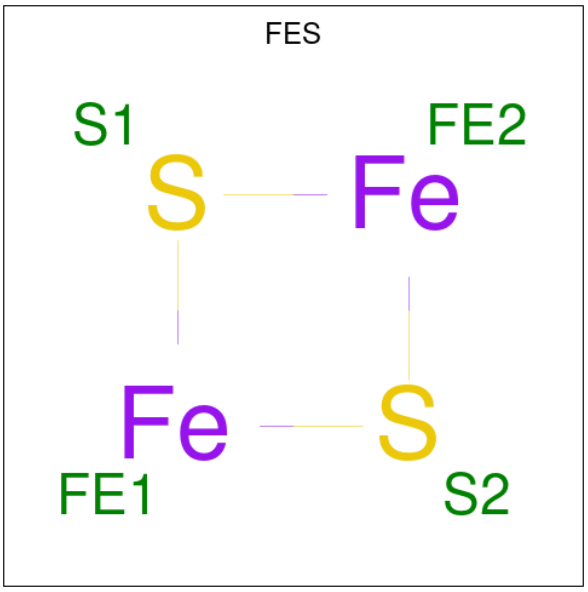
Chain	Residue	Modelled	Actual	Comment	Reference
A	343	LYS	GLU	engineered mutation	UNP P22830
B	343	LYS	GLU	engineered mutation	UNP P22830
C	343	LYS	GLU	engineered mutation	UNP P22830
D	343	LYS	GLU	engineered mutation	UNP P22830

- Molecule 2 is PROTOPORPHYRIN IX (three-letter code: PP9) (formula: $C_{34}H_{34}N_4O_4$).



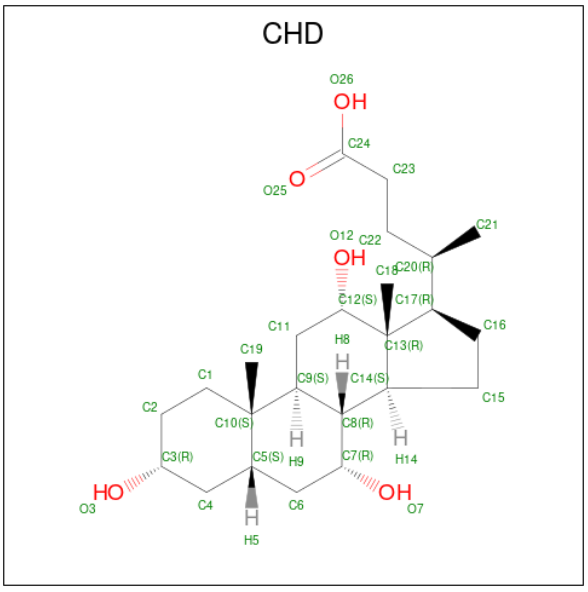
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 42 34 4 4	0	0
2	B	1	Total C N O 42 34 4 4	0	0
2	B	1	Total C N O 42 34 4 4	0	0
2	C	1	Total C N O 42 34 4 4	0	0
2	D	1	Total C N O 42 34 4 4	0	0
2	D	1	Total C N O 42 34 4 4	0	0

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 4 2 2	0	0
3	B	1	Total Fe S 4 2 2	0	0
3	C	1	Total Fe S 4 2 2	0	0
3	D	1	Total Fe S 4 2 2	0	0

- Molecule 4 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 29 24 5	0	0
4	D	1	Total C O 29 24 5	0	0

- Molecule 5 is water.

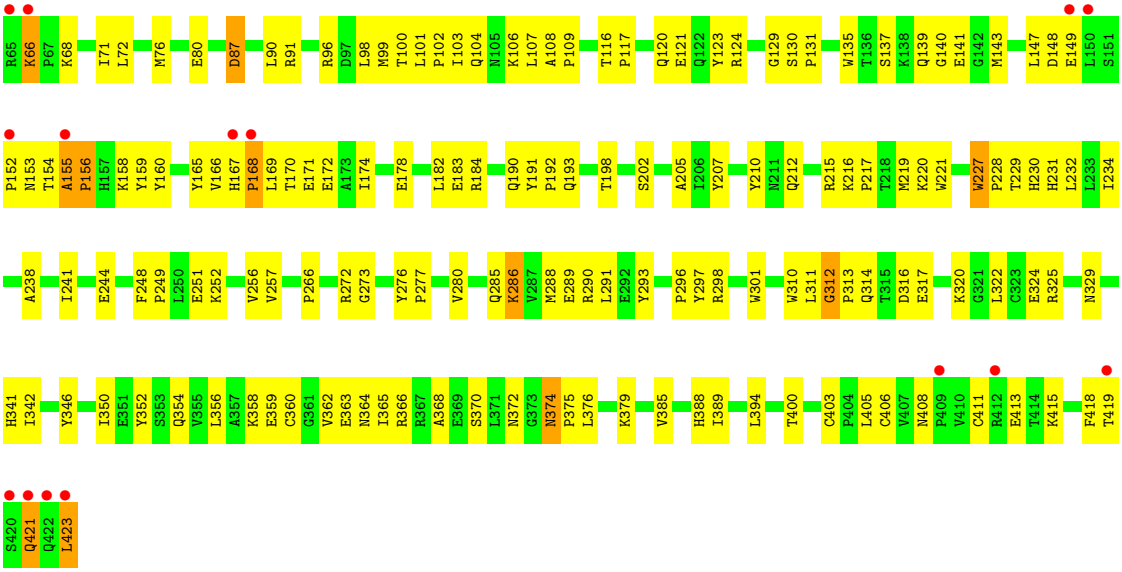
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	120	Total O 120 120	0	0
5	B	99	Total O 99 99	0	0
5	C	91	Total O 91 91	0	0
5	D	28	Total O 28 28	0	0

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.

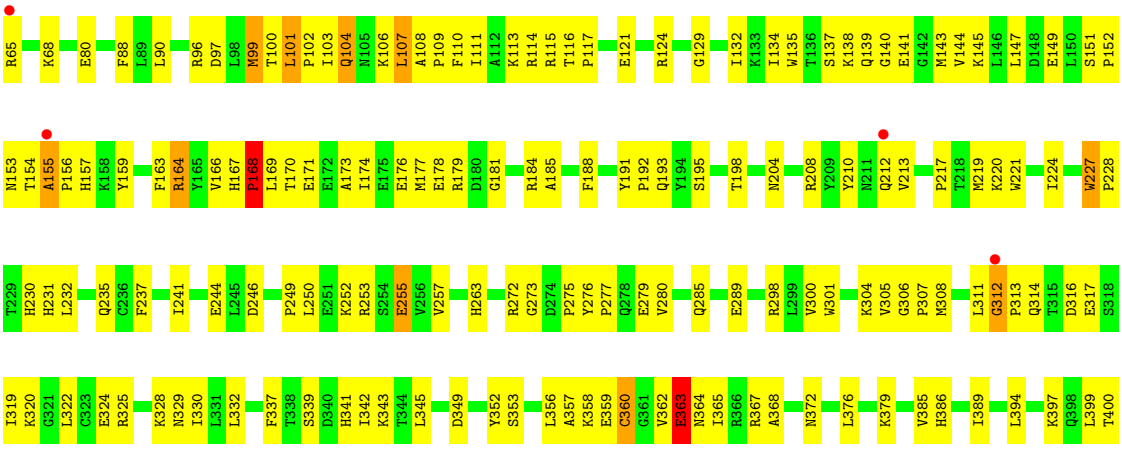
• Molecule 1: Ferrochelatase

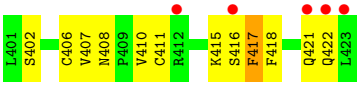
Chain A:



• Molecule 1: Ferrochelatase

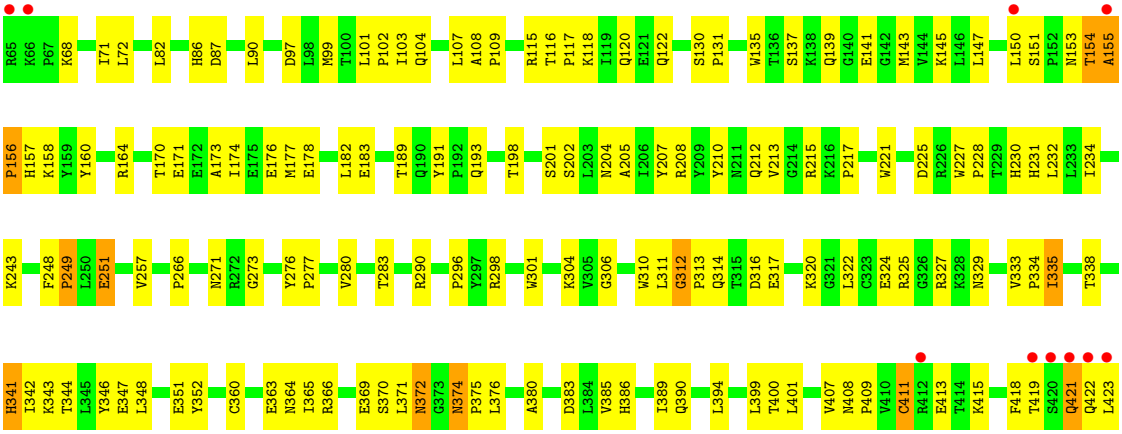
Chain B:





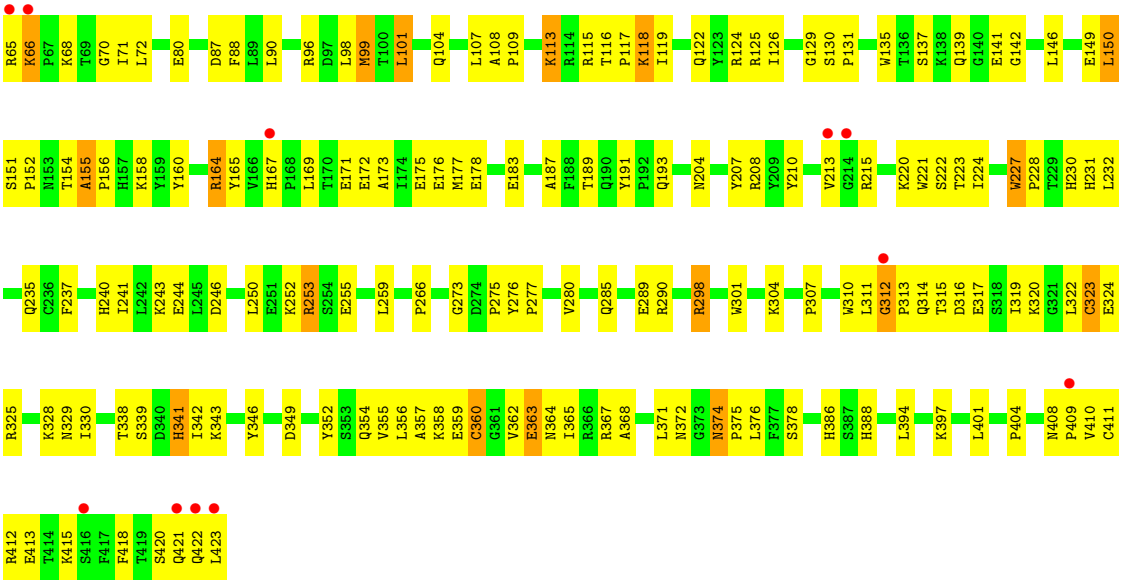
• Molecule 1: Ferrochelatase

Chain C:



• Molecule 1: Ferrochelatase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.95Å 88.39Å 93.25Å 102.41° 109.34° 105.58°	Depositor
Resolution (Å)	43.66 – 2.50 43.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.7 (43.66-2.50) 91.7 (43.66-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.68 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.216 , 0.279 0.207 , 0.269	Depositor DCC
R_{free} test set	2869 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.0	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	0.92	EDS
Total number of atoms	12228	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, PP9, CHD

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	0.48	0/2961	0.72	0/4010
1	B	0.47	1/2961 (0.0%)	0.82	5/4010 (0.1%)
1	C	0.49	1/2961 (0.0%)	0.70	0/4010
1	D	0.46	0/2961	0.72	0/4010
All	All	0.48	2/11844 (0.0%)	0.74	5/16040 (0.0%)

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	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	GLU	CD-OE1	-5.31	1.19	1.25
1	C	171	GLU	CD-OE1	-5.22	1.20	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	167	HIS	C-N-CD	-20.58	75.33	120.60
1	B	167	HIS	C-N-CA	13.72	179.62	122.00
1	B	168	PRO	N-CA-C	-6.42	95.40	112.10
1	B	224	ILE	N-CA-C	-5.62	95.83	111.00
1	B	168	PRO	CA-N-CD	-5.06	104.41	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	346	TYR	Sidechain

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	2891	0	2904	150	0
1	B	2891	0	2904	174	0
1	C	2891	0	2904	156	0
1	D	2891	0	2905	165	0
2	A	42	0	32	5	0
2	B	84	0	64	11	0
2	C	42	0	32	5	0
2	D	84	0	64	10	0
3	A	4	0	0	0	0
3	B	4	0	0	2	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	B	29	0	39	4	0
4	D	29	0	39	1	0
5	A	120	0	0	5	0
5	B	99	0	0	13	0
5	C	91	0	0	3	0
5	D	28	0	0	0	0
All	All	12228	0	11887	632	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 27.

The worst 5 of 632 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:ALA:HB1	1:D:156:PRO:CD	1.66	1.24
1:D:155:ALA:HB1	1:D:156:PRO:HD3	1.08	1.07
1:D:311:LEU:HD12	1:D:312:GLY:H	1.22	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:ALA:CB	1:D:156:PRO:CD	2.37	1.02
1:B:155:ALA:HB1	1:B:156:PRO:CD	1.93	0.99

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	357/359 (99%)	331 (93%)	22 (6%)	4 (1%)	14 26
1	B	357/359 (99%)	313 (88%)	37 (10%)	7 (2%)	7 12
1	C	357/359 (99%)	325 (91%)	26 (7%)	6 (2%)	9 16
1	D	357/359 (99%)	326 (91%)	26 (7%)	5 (1%)	11 20
All	All	1428/1436 (99%)	1295 (91%)	111 (8%)	22 (2%)	10 18

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ALA
1	A	168	PRO
1	A	312	GLY
1	B	155	ALA
1	B	168	PRO

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	324/324 (100%)	309 (95%)	15 (5%)	27	50
1	B	324/324 (100%)	308 (95%)	16 (5%)	25	47
1	C	324/324 (100%)	311 (96%)	13 (4%)	31	56
1	D	324/324 (100%)	305 (94%)	19 (6%)	19	37
All	All	1296/1296 (100%)	1233 (95%)	63 (5%)	25	47

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	339	SER
1	D	253	ARG
1	C	249	PRO
1	D	227	TRP
1	D	360	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	278	GLN
1	D	388	HIS
1	D	285	GLN
1	D	354	GLN
1	B	390	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	PP9	D	604	-	31,46,46	1.73	5 (16%)	25,68,68	1.74	2 (8%)
4	CHD	D	702	-	32,32,32	2.12	15 (46%)	51,51,51	1.93	16 (31%)
2	PP9	C	605	-	31,46,46	1.80	8 (25%)	25,68,68	2.01	4 (16%)
2	PP9	D	606	-	31,46,46	1.78	7 (22%)	25,68,68	2.10	4 (16%)
3	FES	C	503	1	0,4,4	-	-	-		
3	FES	D	504	1	0,4,4	-	-	-		
4	CHD	B	701	-	32,32,32	2.08	12 (37%)	51,51,51	1.91	17 (33%)
3	FES	B	502	1	0,4,4	-	-	-		
2	PP9	A	601	-	31,46,46	1.78	9 (29%)	25,68,68	1.99	5 (20%)
2	PP9	B	602	-	31,46,46	1.76	10 (32%)	25,68,68	2.05	5 (20%)
3	FES	A	501	1	0,4,4	-	-	-		
2	PP9	B	603	-	31,46,46	1.69	6 (19%)	25,68,68	1.68	2 (8%)

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	PP9	D	604	-	-	6/12/62/62	0/4/5/5
4	CHD	D	702	-	-	4/9/74/74	0/4/4/4
3	FES	B	502	1	-	-	0/1/1/1
2	PP9	C	605	-	-	5/12/62/62	0/4/5/5
2	PP9	D	606	-	-	3/12/62/62	0/4/5/5
3	FES	C	503	1	-	-	0/1/1/1
3	FES	D	504	1	-	-	0/1/1/1
4	CHD	B	701	-	-	3/9/74/74	0/4/4/4
2	PP9	A	601	-	-	5/12/62/62	0/4/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PP9	B	602	-	-	1/12/62/62	0/4/5/5
3	FES	A	501	1	-	-	0/1/1/1
2	PP9	B	603	-	-	10/12/62/62	0/4/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	702	CHD	O25-C24	4.71	1.37	1.22
4	B	701	CHD	O25-C24	4.67	1.37	1.22
2	D	604	PP9	CBB-CAB	4.51	1.52	1.30
2	B	602	PP9	CBB-CAB	4.49	1.52	1.30
2	B	603	PP9	CBB-CAB	4.49	1.52	1.30

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	606	PP9	CBA-CAA-C2A	-5.98	102.52	112.60
2	C	605	PP9	CBA-CAA-C2A	-5.78	102.87	112.60
2	B	602	PP9	CBA-CAA-C2A	-5.64	103.10	112.60
2	D	606	PP9	CAA-CBA-CGA	5.49	129.14	113.76
2	B	602	PP9	CAA-CBA-CGA	5.39	128.87	113.76

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	PP9	C2B-C3B-CAB-CBB
2	A	601	PP9	C4B-C3B-CAB-CBB
2	B	603	PP9	C1A-C2A-CAA-CBA
2	B	603	PP9	C3A-C2A-CAA-CBA
2	B	603	PP9	C4D-C3D-CAD-CBD

There are no ring outliers.

9 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	604	PP9	1	0
4	D	702	CHD	1	0
2	C	605	PP9	5	0
2	D	606	PP9	9	0
4	B	701	CHD	4	0

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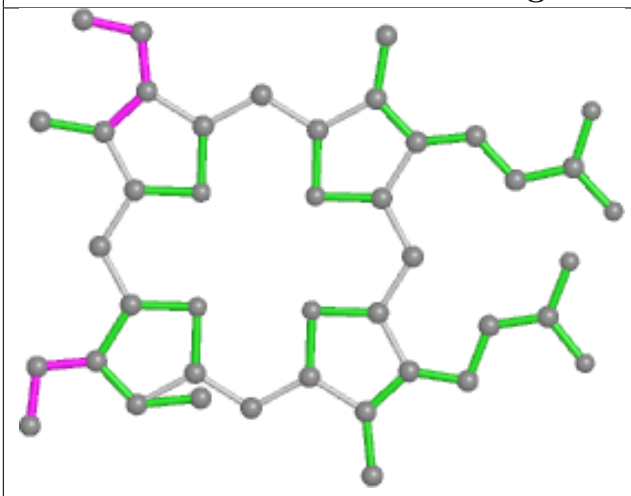
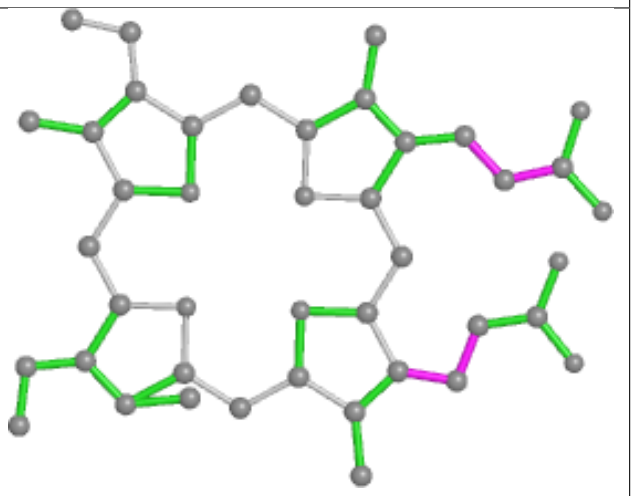
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	FES	2	0
2	A	601	PP9	5	0
2	B	602	PP9	7	0
2	B	603	PP9	4	0

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.

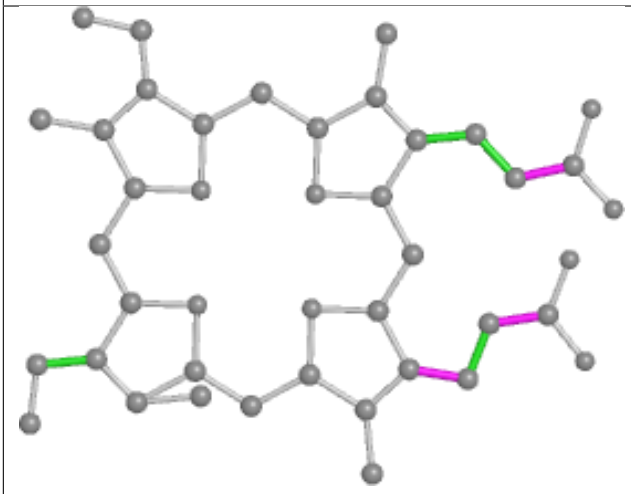
Ligand PP9 D 604



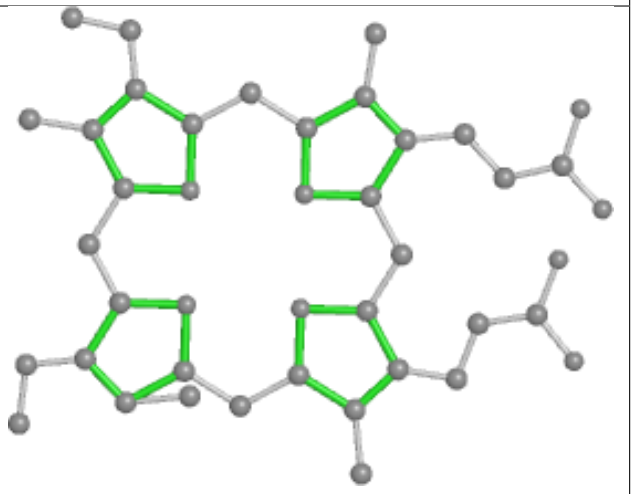
Bond lengths



Bond angles

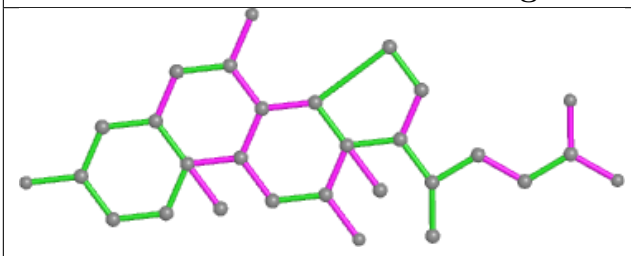


Torsions

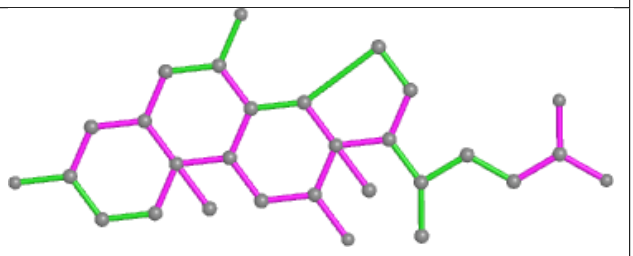


Rings

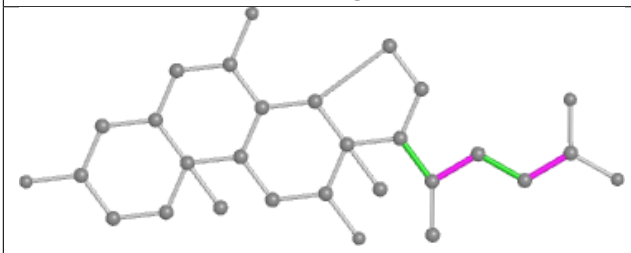
Ligand CHD D 702



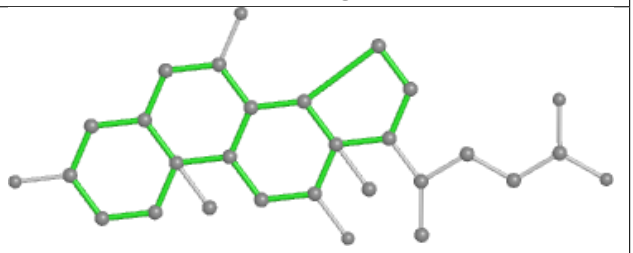
Bond lengths



Bond angles

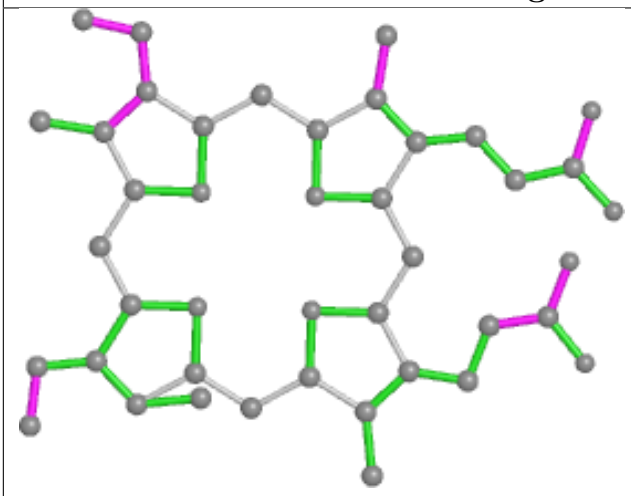


Torsions

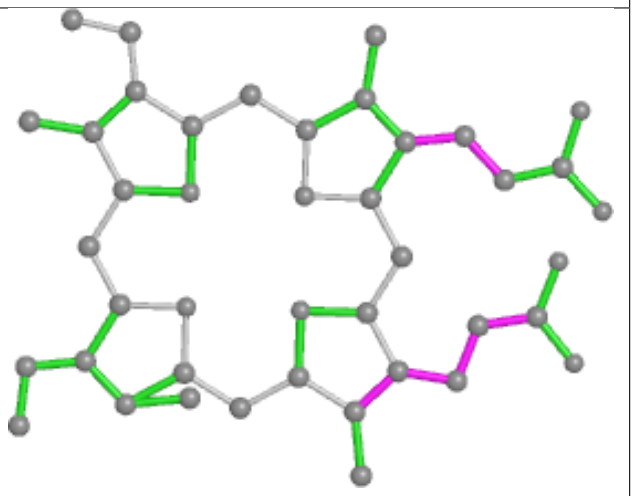


Rings

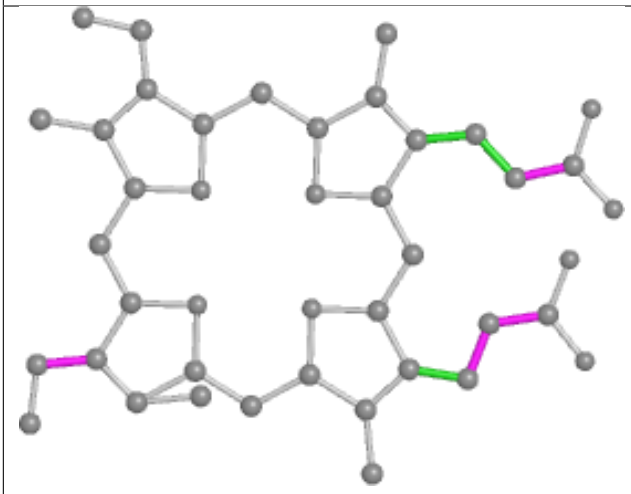
Ligand PP9 C 605



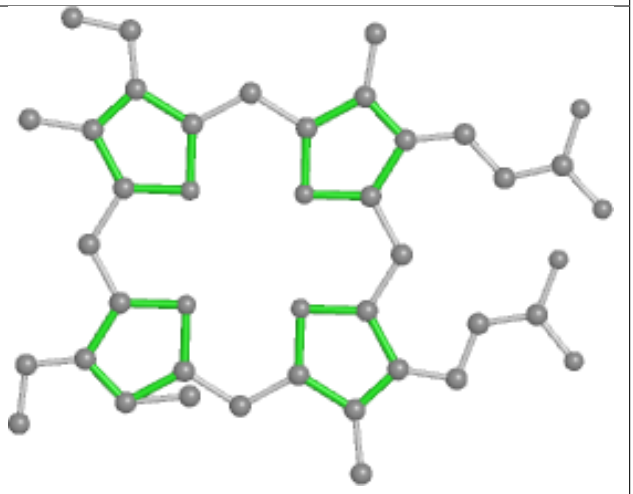
Bond lengths



Bond angles

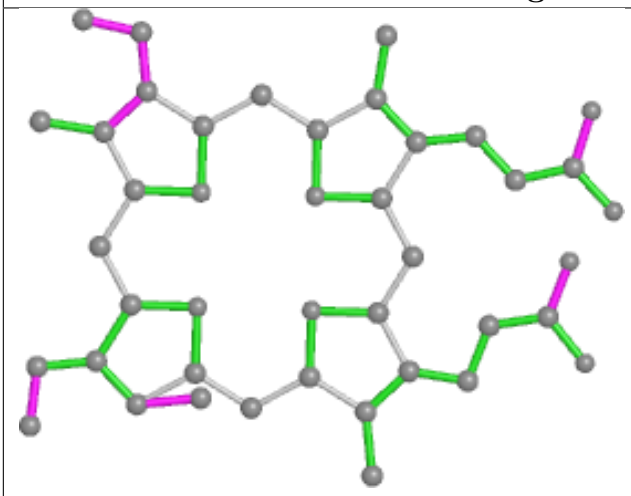


Torsions

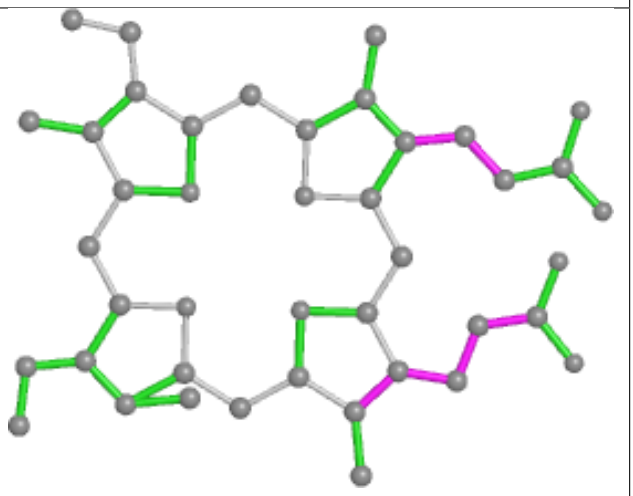


Rings

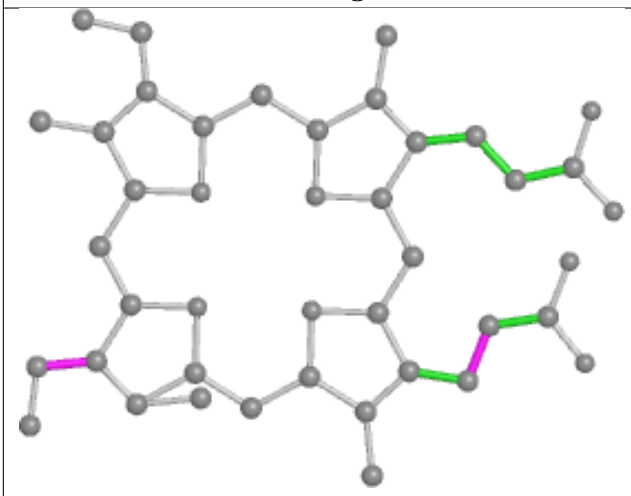
Ligand PP9 D 606



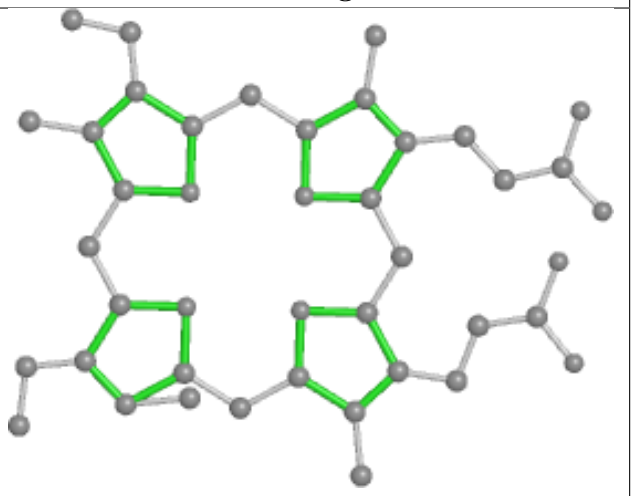
Bond lengths



Bond angles

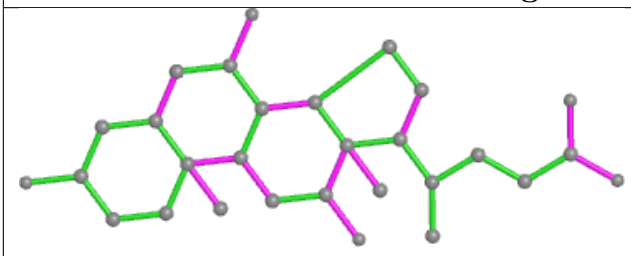


Torsions

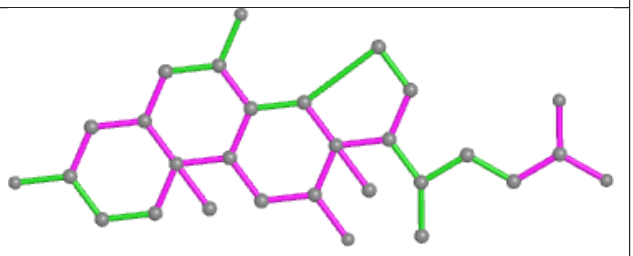


Rings

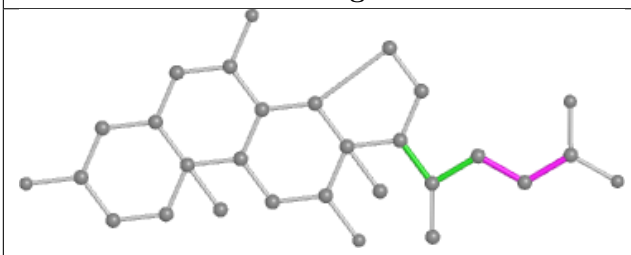
Ligand CHD B 701



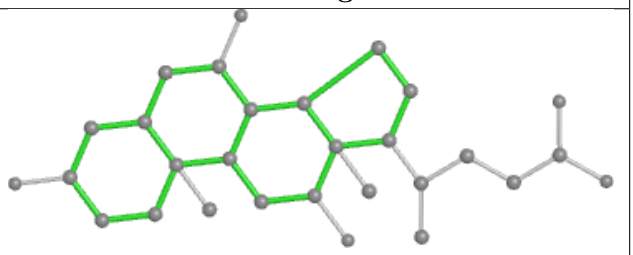
Bond lengths



Bond angles

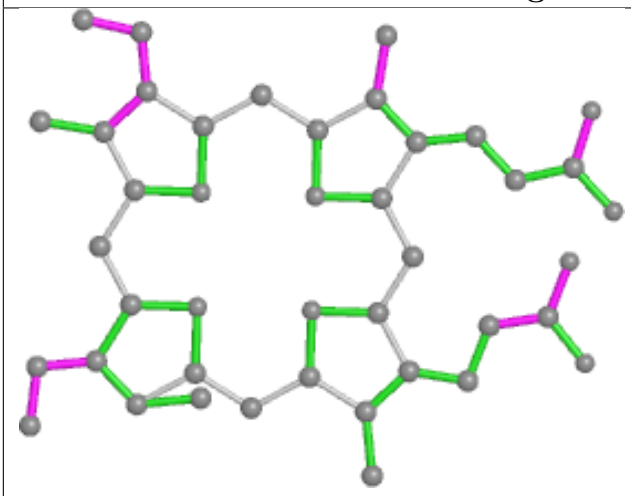


Torsions

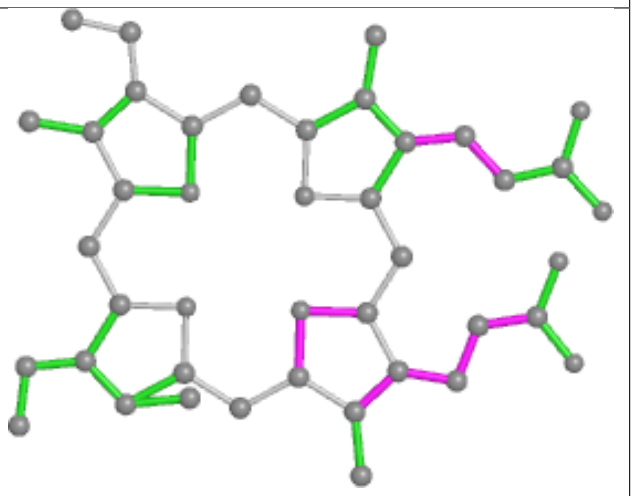


Rings

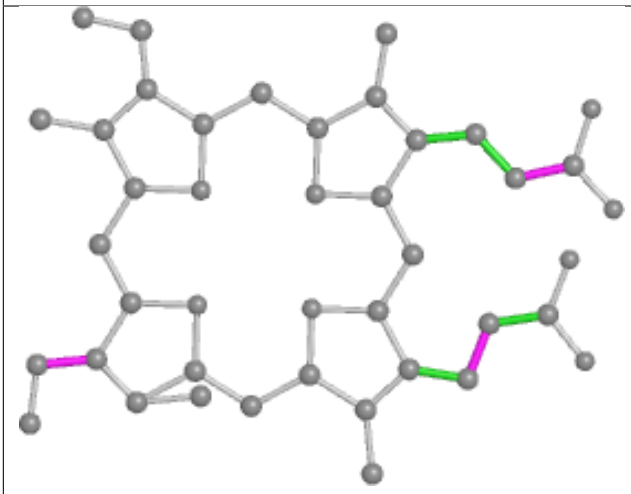
Ligand PP9 A 601



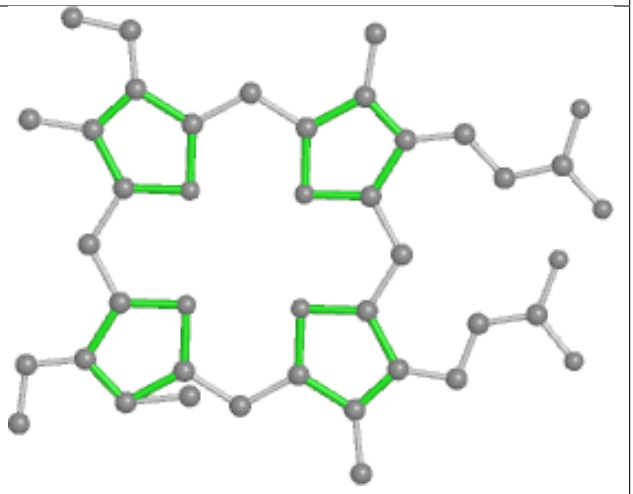
Bond lengths



Bond angles

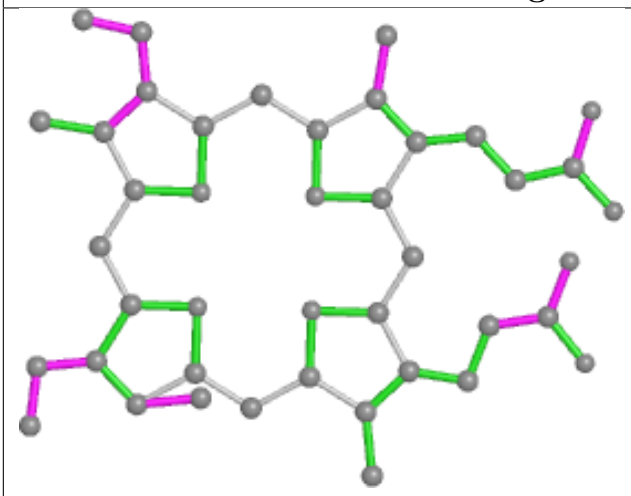


Torsions

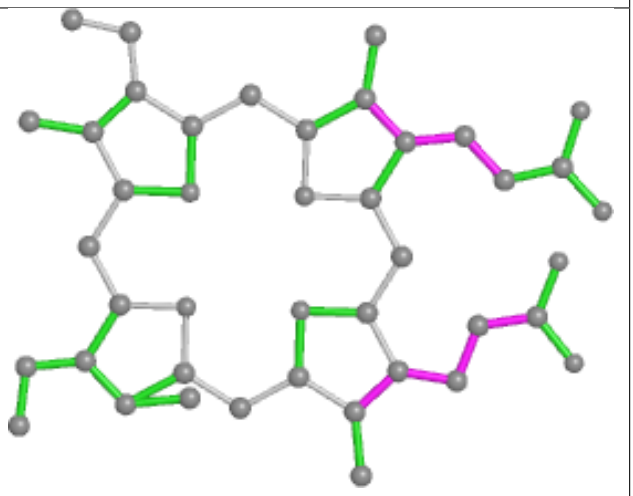


Rings

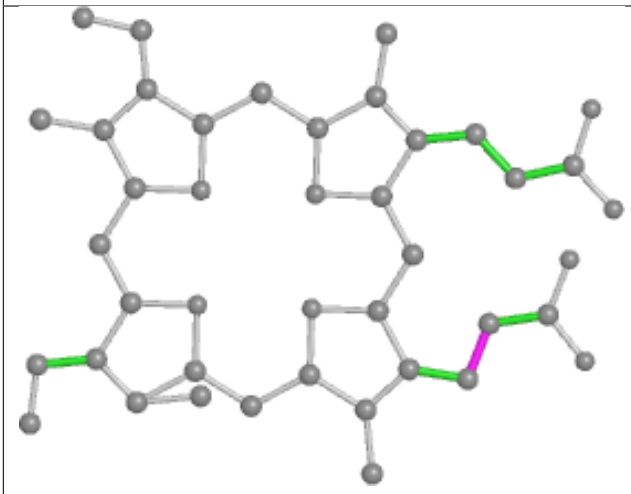
Ligand PP9 B 602



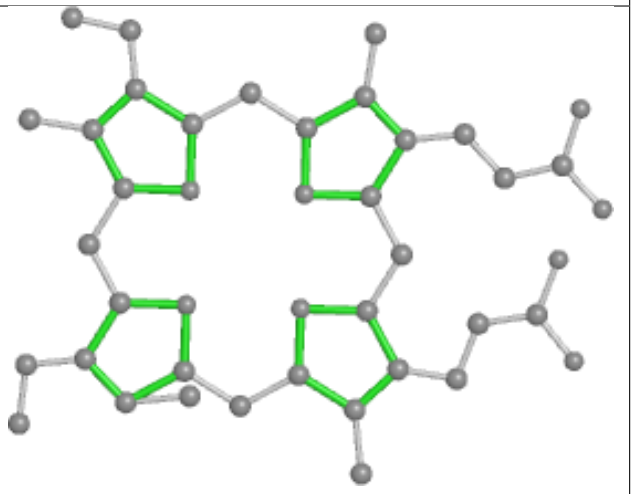
Bond lengths



Bond angles

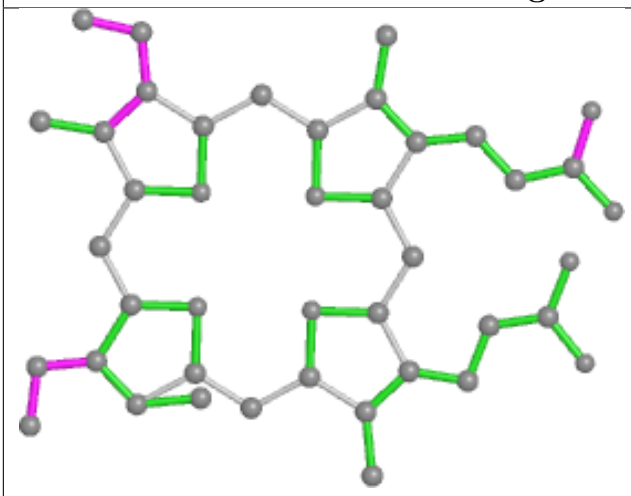


Torsions

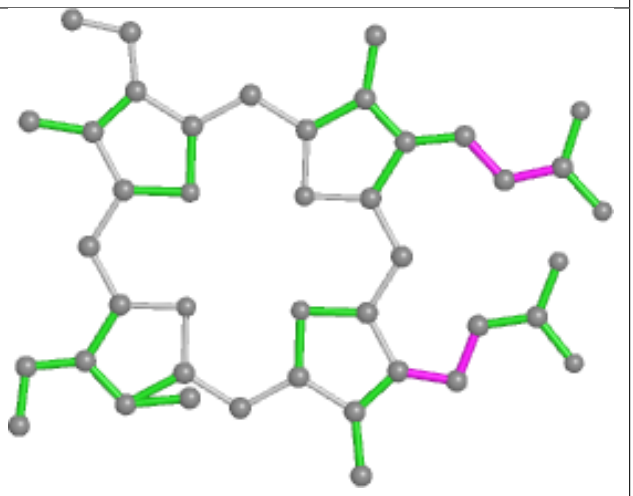


Rings

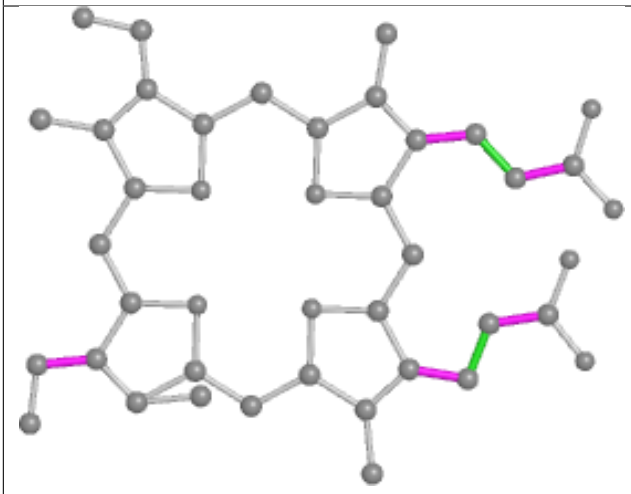
Ligand PP9 B 603



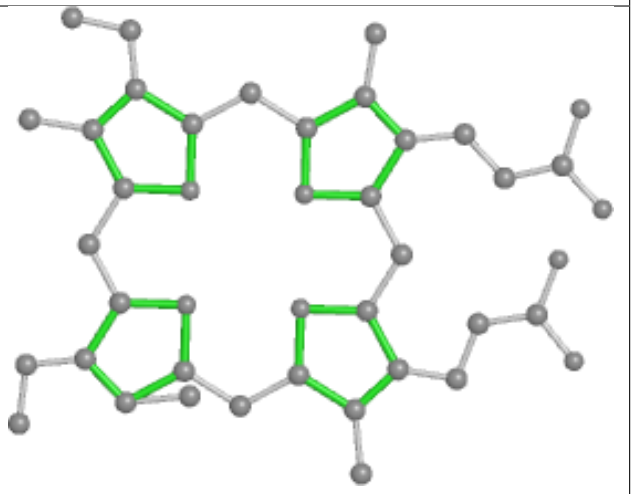
Bond lengths



Bond angles



Torsions



Rings

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	359/359 (100%)	0.11	15 (4%) 36 39	10, 28, 54, 90	0
1	B	359/359 (100%)	0.10	9 (2%) 57 61	7, 30, 54, 100	0
1	C	359/359 (100%)	-0.03	10 (2%) 53 56	11, 28, 57, 90	0
1	D	359/359 (100%)	0.08	11 (3%) 49 52	8, 28, 56, 92	0
All	All	1436/1436 (100%)	0.07	45 (3%) 49 52	7, 28, 56, 100	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	423	LEU	10.1
1	B	422	GLN	9.2
1	D	423	LEU	8.5
1	A	423	LEU	7.9
1	C	423	LEU	7.3

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

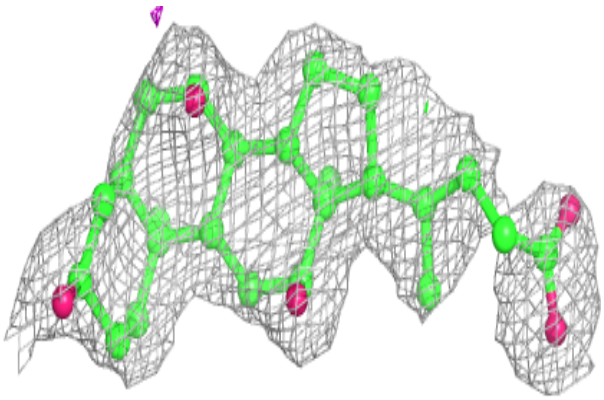
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

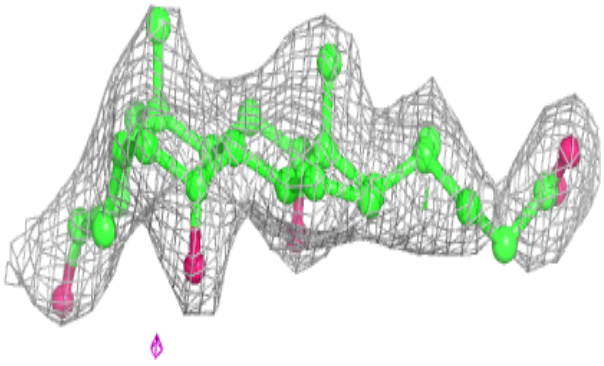
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CHD	D	702	29/29	0.82	0.22	40,42,47,47	0
4	CHD	B	701	29/29	0.84	0.24	39,42,48,49	0
2	PP9	D	604	42/42	0.86	0.24	36,46,56,60	0
2	PP9	B	603	42/42	0.89	0.24	41,48,55,57	0
2	PP9	B	602	42/42	0.91	0.15	14,17,24,26	0
2	PP9	A	601	42/42	0.92	0.16	11,15,27,30	0
2	PP9	D	606	42/42	0.93	0.17	9,17,24,26	0
2	PP9	C	605	42/42	0.94	0.16	19,22,24,25	0
3	FES	D	504	4/4	0.94	0.07	49,50,50,50	0
3	FES	A	501	4/4	0.95	0.06	52,52,53,53	0
3	FES	C	503	4/4	0.97	0.05	46,47,47,47	0
3	FES	B	502	4/4	0.98	0.05	49,49,51,51	0

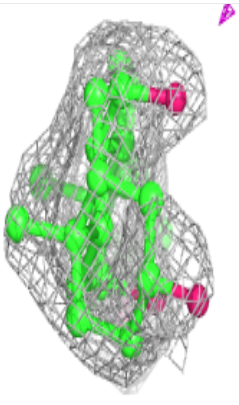
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CHD D 702:

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

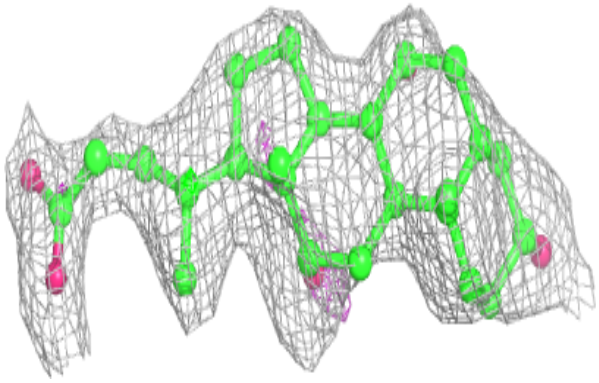


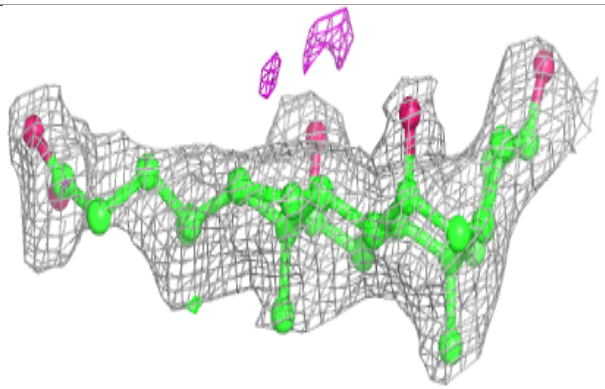


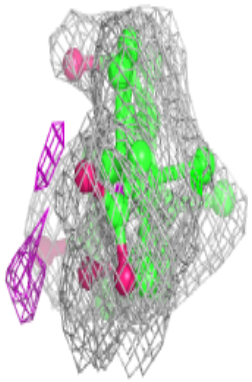


Electron density around CHD B 701:

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

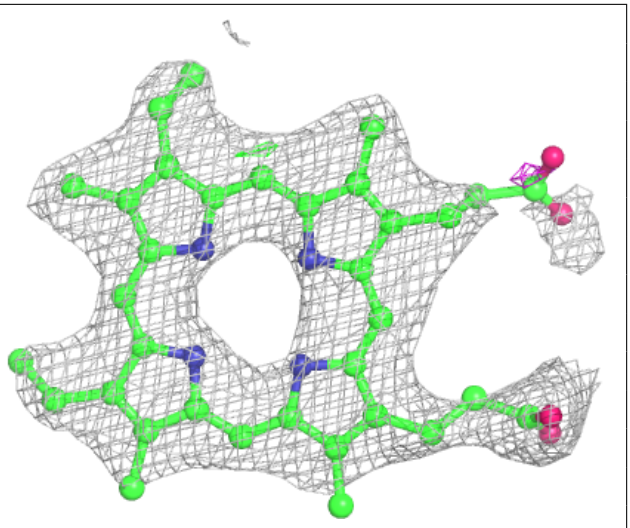


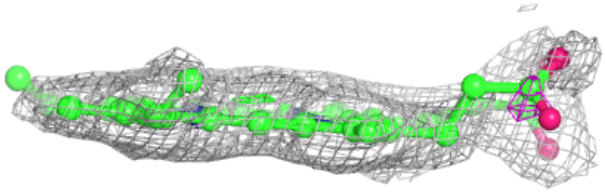


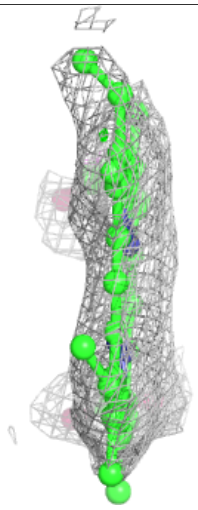


Electron density around PP9 D 604:

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

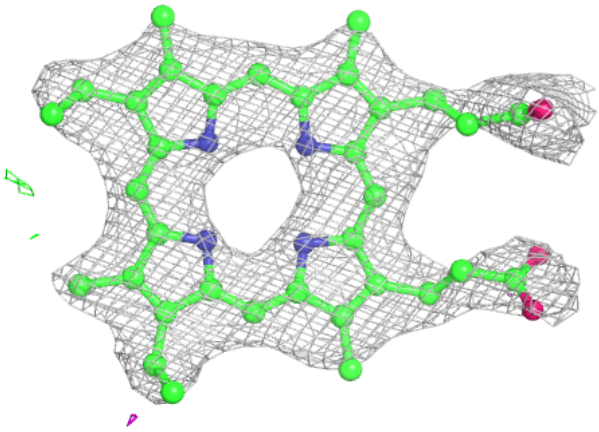


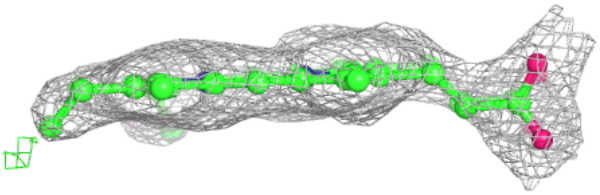


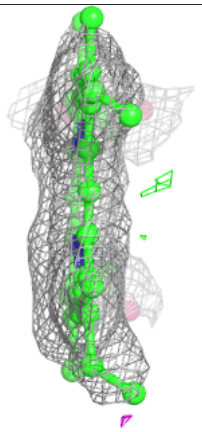


Electron density around PP9 B 603:

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

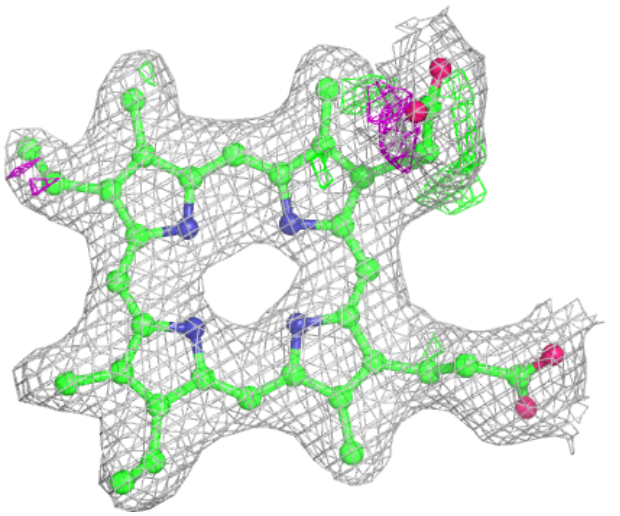


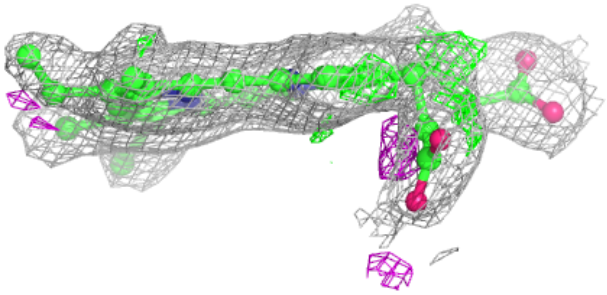


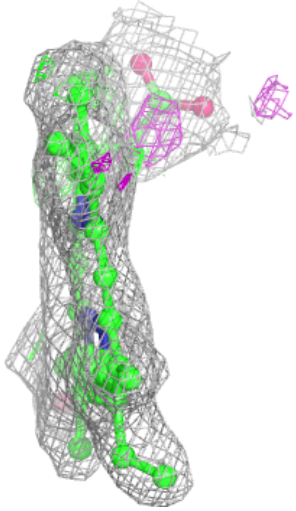


Electron density around PP9 B 602:

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

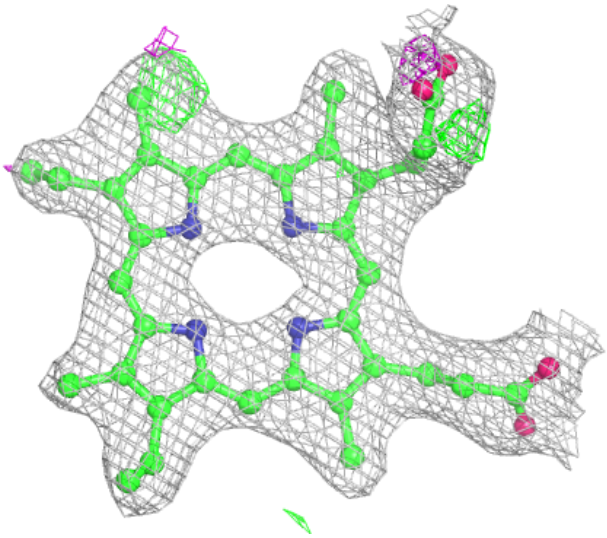


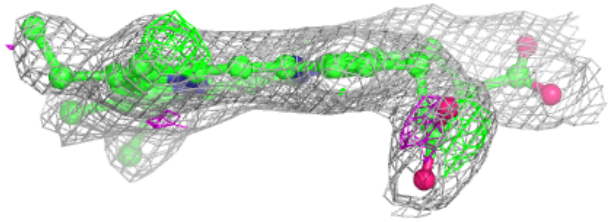


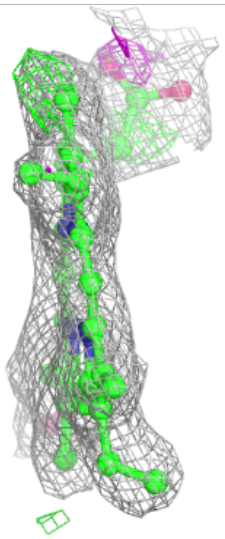


Electron density around PP9 A 601:

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

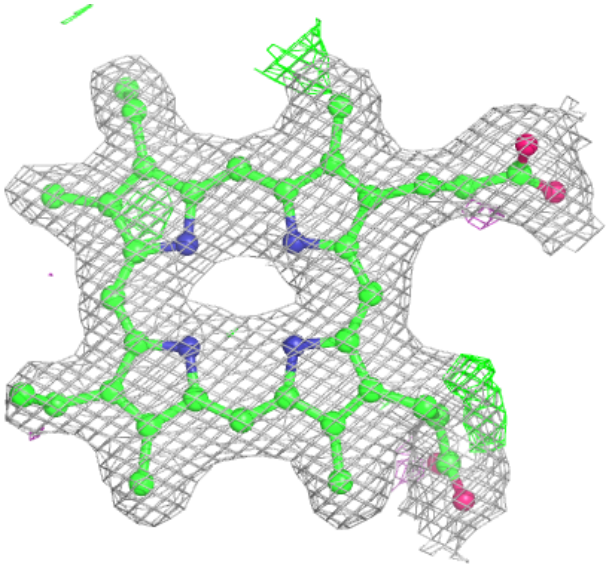


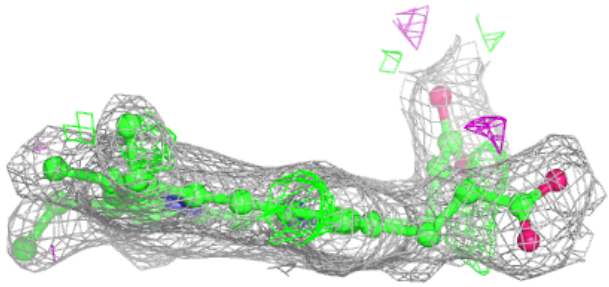


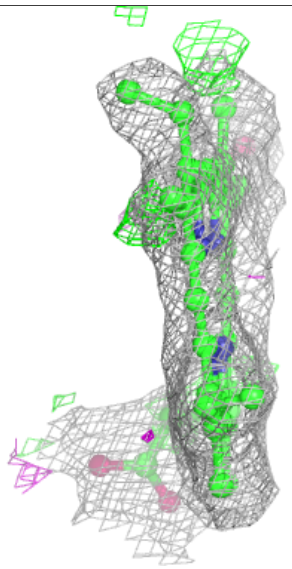


Electron density around PP9 D 606:

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

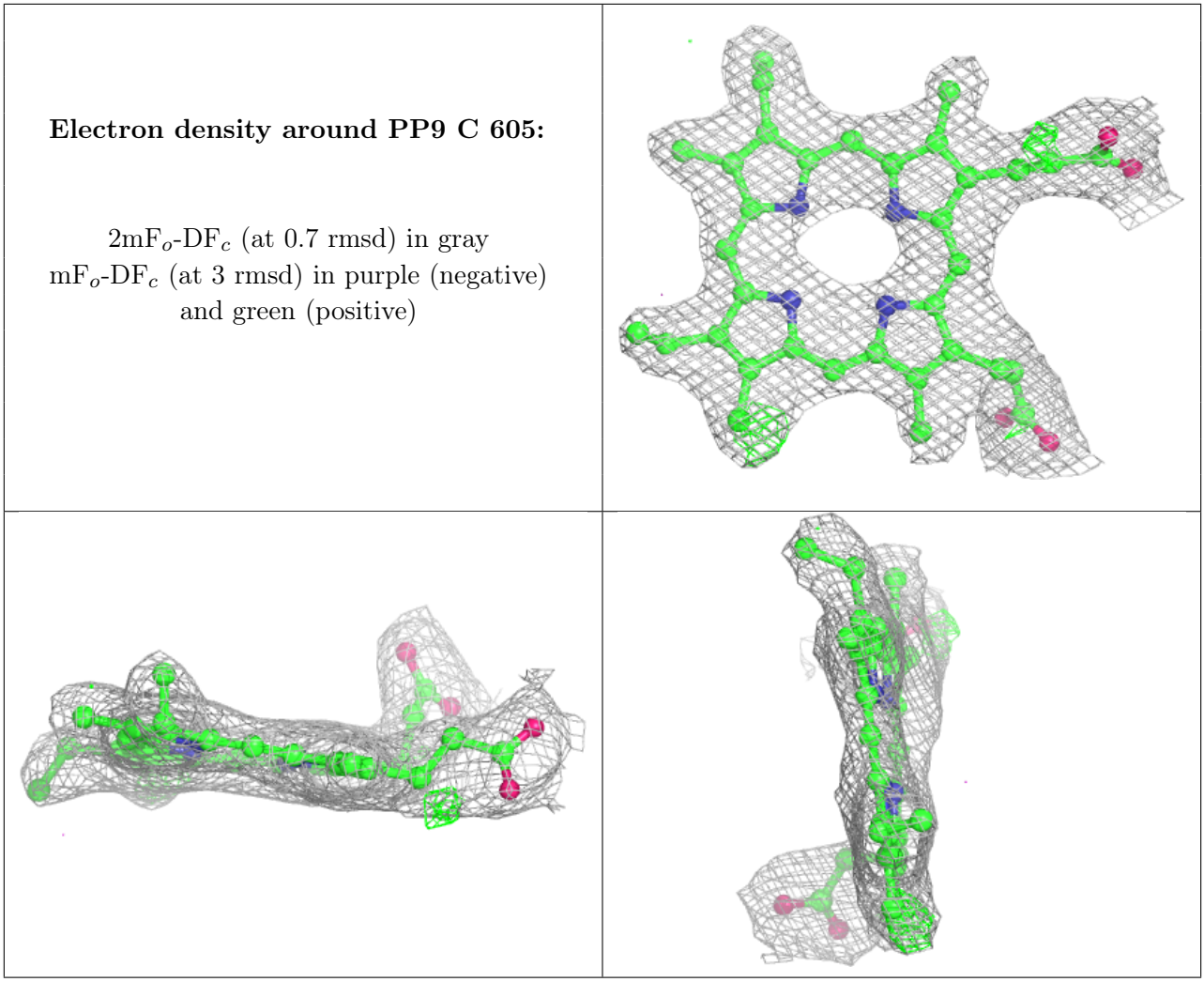






Electron density around PP9 C 605:

$2mF_o$-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.