Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:36 am BST

PDB ID	:	6QPZ
Title	:	Crystal structure of as isolated Y323E mutant of haem-Cu containing nitrite reductase from Ralstonia pickettii
Authors	:	Antonyuk, S.V.; Shenoy, R.T.; Hedison, T.M.; Eady, R.R.; Hasnain, S.S.; Scrutton, N.S.
Deposited on	:	2019-02-16
Resolution	:	1.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

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

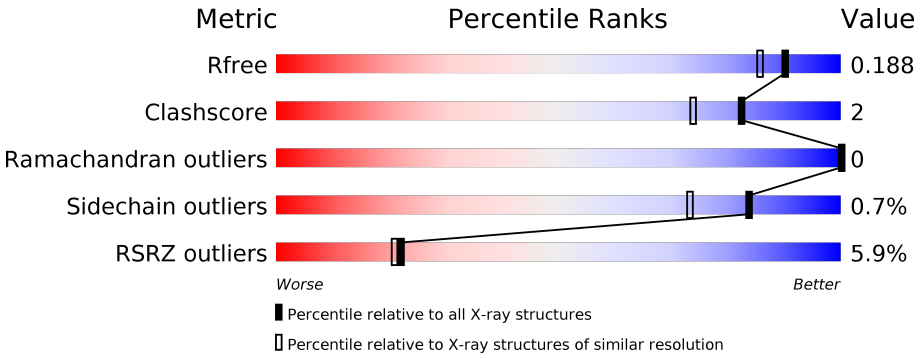
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	468	7% 93%
1	I	468	4% 92% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8341 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 Copper-containing nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	13	0
			3497	2227	600	654	16			
1	I	456	Total	C	N	O	S	0	22	0
			3555	2265	609	664	17			

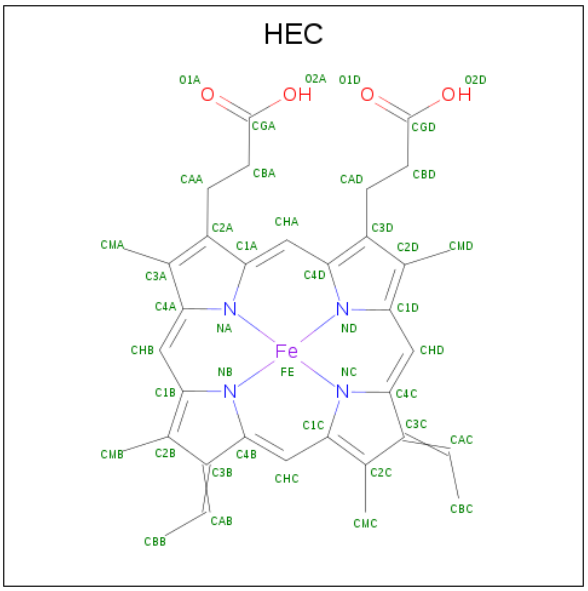
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	GLU	TYR	engineered mutation	UNP I6NAW4
I	323	GLU	TYR	engineered mutation	UNP I6NAW4

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

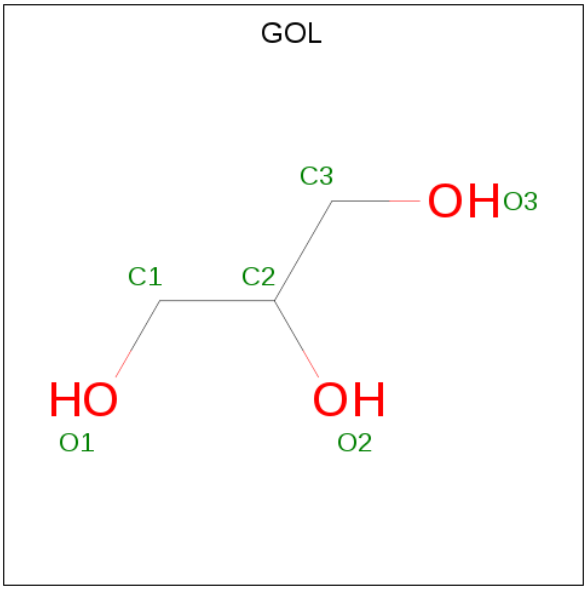
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	2	Total	Cu	0	0
			2	2		
2	A	2	Total	Cu	0	0
			2	2		

- Molecule 3 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	I	1	Total	C	O		0	1
			6	3	3			

- Molecule 5 is water.

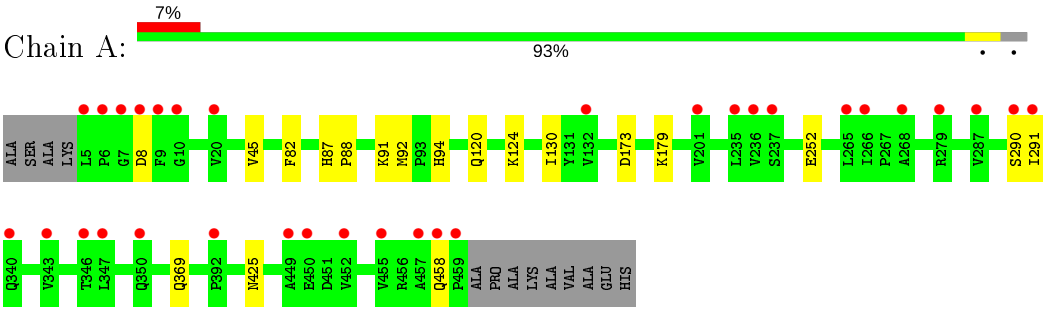
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	556	Total O 567 567	0	11
5	I	609	Total O 626 626	0	22

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

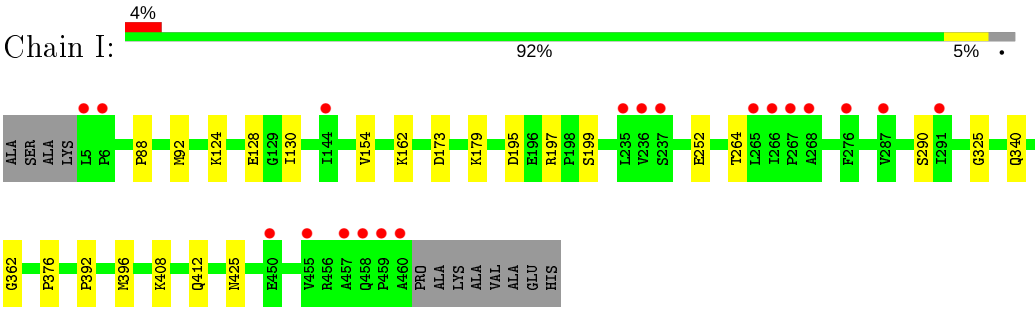
- Molecule 1: Copper-containing nitrite reductase

Chain A:



- Molecule 1: Copper-containing nitrite reductase

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	127.55Å 127.55Å 172.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.73 – 1.65 42.73 – 1.45	Depositor EDS
% Data completeness (in resolution range)	98.8 (42.73-1.65) 98.5 (42.73-1.45)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.158 , 0.178 0.172 , 0.188	Depositor DCC
R_{free} test set	9197 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	22.5	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	8341	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 72.50 % 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 2.1782e-06. 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: GOL, CU, HEC

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	0.71	0/3624	0.84	0/4923
1	I	0.76	1/3706 (0.0%)	0.88	0/5030
All	All	0.74	1/7330 (0.0%)	0.86	0/9953

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	A	0	1
1	I	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	199	SER	CA-CB	-5.95	1.44	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	SER	Peptide
1	I	264	THR	Mainchain
1	I	290	SER	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	3497	0	3493	12	0
1	I	3555	0	3564	17	0
2	A	2	0	0	0	0
2	I	2	0	0	0	0
3	A	43	0	30	2	0
3	I	43	0	30	2	0
4	I	6	0	8	2	0
5	A	567	0	0	5	0
5	I	626	0	0	8	0
All	All	8341	0	7125	35	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.

All (35) 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:I:195[B]:ASP:OD2	1:I:197[B]:ARG:HD3	1.72	0.90
1:I:408[A]:LYS:NZ	5:I:601:HOH:O	2.22	0.72
1:A:369:GLN:NE2	5:A:602:HOH:O	2.26	0.67
4:I:503[A]:GOL:H11	5:I:1070:HOH:O	1.94	0.66
1:I:357[B]:ARG:NH1	5:I:603:HOH:O	2.33	0.61
1:I:195[B]:ASP:HB3	1:I:197[B]:ARG:HG3	1.87	0.55
1:A:130:ILE:O	1:A:252:GLU:HA	2.07	0.55
3:A:503:HEC:HMC1	3:A:503:HEC:HBC3	1.89	0.54
1:I:340[A]:GLN:HG3	5:I:854:HOH:O	2.07	0.54
1:I:197[B]:ARG:NH2	5:I:604:HOH:O	2.34	0.52
1:A:179[A]:LYS:HE2	1:A:425:ASN:OD1	2.10	0.52
1:I:130:ILE:O	1:I:252:GLU:HA	2.10	0.51
1:I:392:PRO:O	1:I:396[B]:MET:HG3	2.13	0.48
3:A:503:HEC:HBB3	3:A:503:HEC:HMB1	1.95	0.48
1:I:197[B]:ARG:HD2	5:I:1125:HOH:O	2.14	0.48
3:I:504:HEC:HBC3	3:I:504:HEC:HMC1	1.96	0.48
1:A:458:GLN:O	1:A:458:GLN:HG3	2.14	0.47
1:A:124:LYS:NZ	5:A:601:HOH:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:PHE:O	1:A:120:GLN:HA	2.14	0.47
1:A:91[B]:LYS:NZ	5:A:607:HOH:O	2.45	0.46
1:A:45:VAL:HG11	1:A:94:HIS:CD2	2.50	0.46
1:I:376:PRO:HB3	1:I:412:GLN:HE22	1.80	0.45
3:I:504:HEC:HMB1	3:I:504:HEC:HBB3	1.98	0.45
1:A:291:ILE:HD13	1:A:291:ILE:HA	1.92	0.44
1:A:8:ASP:HA	5:A:910:HOH:O	2.18	0.43
1:I:325:GLY:HA2	1:I:362:GLY:HA3	2.01	0.43
1:I:162:LYS:NZ	5:I:612:HOH:O	2.46	0.42
1:A:369:GLN:CD	5:A:602:HOH:O	2.57	0.42
1:A:87:HIS:CG	1:A:88:PRO:HD2	2.54	0.42
1:I:179:LYS:HE2	1:I:425:ASN:OD1	2.20	0.42
1:I:128[A]:GLU:HG2	1:I:154:VAL:O	2.21	0.41
4:I:503[A]:GOL:C1	5:I:1070:HOH:O	2.62	0.41

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	467/468 (100%)	456 (98%)	11 (2%)	0	100	100
1	I	476/468 (102%)	464 (98%)	12 (2%)	0	100	100
All	All	943/936 (101%)	920 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	378/371 (102%)	376 (100%)	2 (0%)	88 81
1	I	386/371 (104%)	383 (99%)	3 (1%)	81 70
All	All	764/742 (103%)	759 (99%)	5 (1%)	84 73

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	MET
1	A	173	ASP
1	I	88	PRO
1	I	92	MET
1	I	173	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	412	GLN
1	I	412	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
3	HEC	I	504	1	26,50,50	1.33	5 (19%)	18,82,82	1.75	4 (22%)
4	GOL	I	503[A]	-	5,5,5	0.18	0	5,5,5	0.26	0
3	HEC	A	503	1	26,50,50	1.37	3 (11%)	18,82,82	1.73	6 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	I	504	1	-	0/6/54/54	-
4	GOL	I	503[A]	-	-	0/4/4/4	-
3	HEC	A	503	1	-	0/6/54/54	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	HEC	CBC-CAC	-3.52	1.36	1.49
3	A	503	HEC	C3B-C4B	3.15	1.48	1.43
3	A	503	HEC	CBB-CAB	-3.12	1.37	1.49
3	I	504	HEC	CBC-CAC	-3.00	1.38	1.49
3	I	504	HEC	CBB-CAB	-2.79	1.39	1.49
3	I	504	HEC	C3B-C2B	-2.63	1.38	1.40
3	I	504	HEC	C3C-C2C	-2.47	1.38	1.40
3	I	504	HEC	C3B-C4B	2.33	1.47	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	504	HEC	CAA-CBA-CGA	3.97	119.33	112.67
3	I	504	HEC	C1D-C2D-C3D	-3.18	104.78	107.00
3	A	503	HEC	CAA-CBA-CGA	3.15	117.95	112.67
3	I	504	HEC	CMB-C2B-C1B	-2.86	124.07	128.46
3	A	503	HEC	CMB-C2B-C1B	-2.68	124.35	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	504	HEC	CMC-C2C-C1C	-2.28	124.96	128.46
3	A	503	HEC	C4B-C3B-C2B	-2.25	103.93	106.35
3	A	503	HEC	CAD-CBD-CGD	2.23	116.42	112.67
3	A	503	HEC	C1D-C2D-C3D	-2.22	105.45	107.00
3	A	503	HEC	CMC-C2C-C1C	-2.17	125.12	128.46

There are no chirality outliers.

There are no torsion outliers.

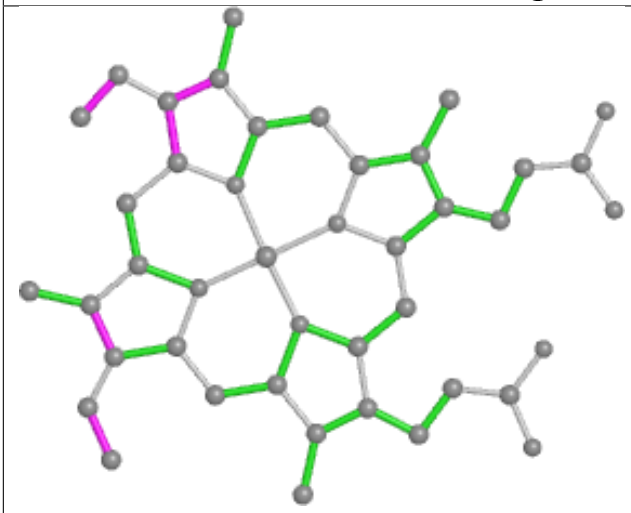
There are no ring outliers.

3 monomers are involved in 6 short contacts:

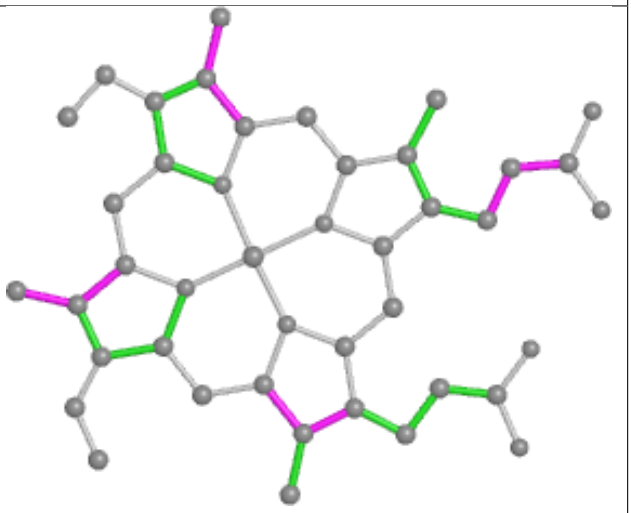
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	504	HEC	2	0
4	I	503[A]	GOL	2	0
3	A	503	HEC	2	0

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.

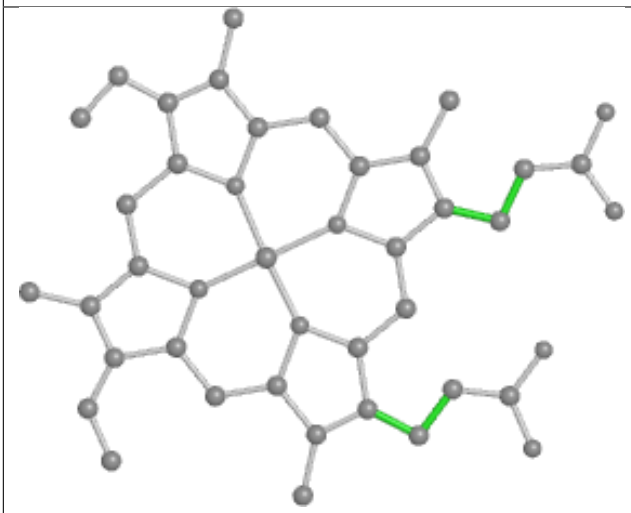
Ligand HEC I 504



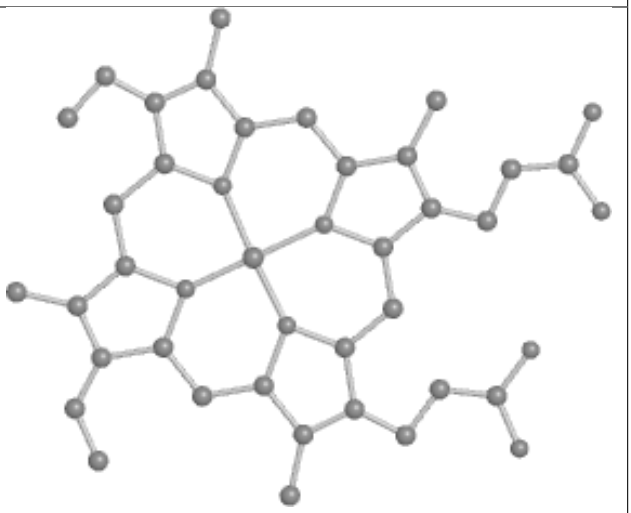
Bond lengths



Bond angles

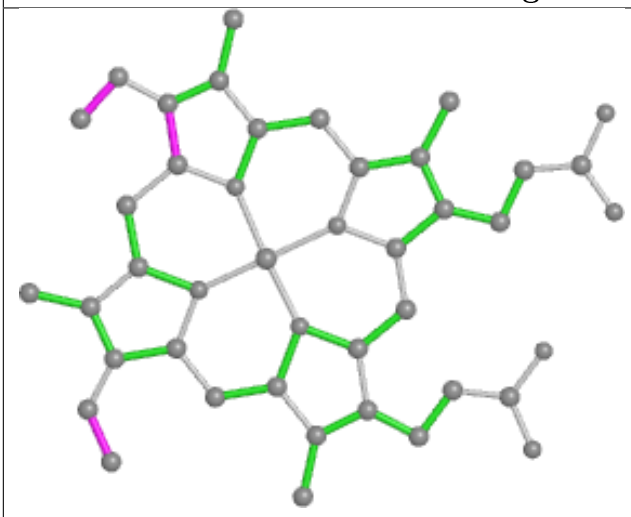


Torsions

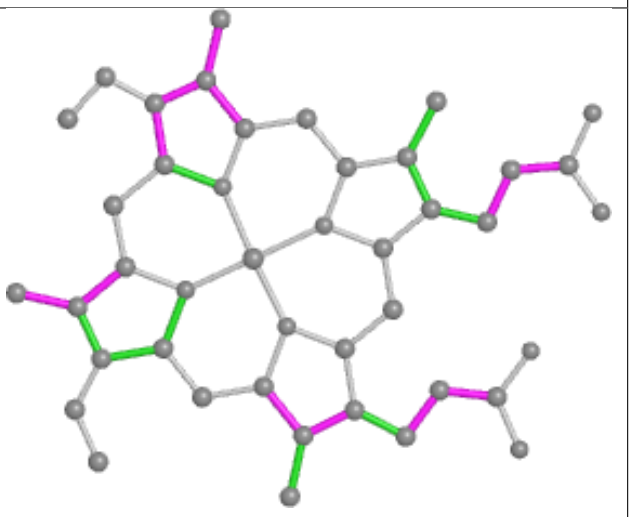


Rings

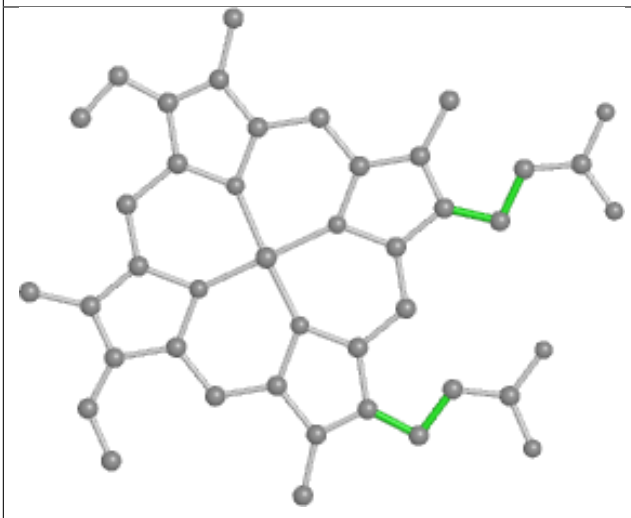
Ligand HEC A 503



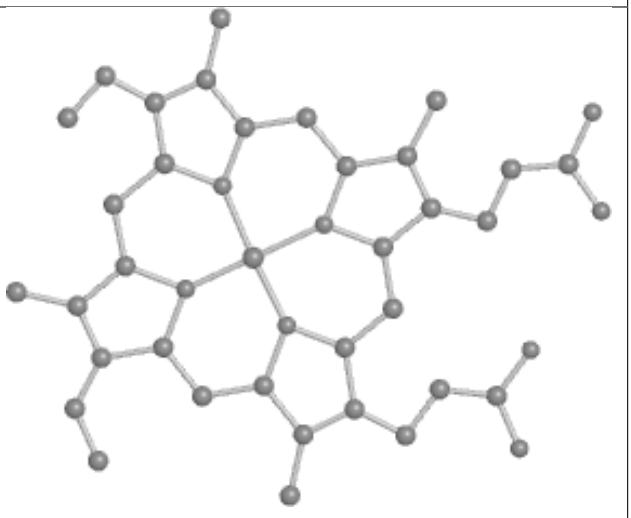
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	455/468 (97%)	0.65	34 (7%)	14	14	17, 23, 34, 79	4 (0%)
1	I	456/468 (97%)	0.51	20 (4%)	34	34	10, 16, 26, 75	7 (1%)
All	All	911/936 (97%)	0.58	54 (5%)	22	21	10, 20, 31, 79	11 (1%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	460	ALA	8.1
1	I	459	PRO	7.8
1	I	5	LEU	7.6
1	A	459	PRO	6.5
1	A	458	GLN	6.1
1	A	8	ASP	5.7
1	A	6	PRO	5.3
1	I	458	GLN	5.1
1	I	6	PRO	4.9
1	A	265	LEU	4.5
1	A	236	VAL	4.3
1	A	266	ILE	4.0
1	A	235	LEU	3.8
1	A	455	VAL	3.8
1	I	457	ALA	3.8
1	A	343	VAL	3.6
1	I	265	LEU	3.5
1	I	236	VAL	3.5
1	A	457	ALA	3.4
1	I	266	ILE	3.4
1	A	5	LEU	3.2
1	I	450	GLU	3.1
1	A	291	ILE	3.1
1	A	10	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	287	VAL	3.0
1	A	268	ALA	3.0
1	I	276	PHE	2.8
1	A	132	VAL	2.8
1	A	449	ALA	2.7
1	I	235	LEU	2.7
1	I	291	ILE	2.6
1	A	201	VAL	2.6
1	I	268	ALA	2.6
1	A	20	VAL	2.6
1	A	452	VAL	2.6
1	A	9	PHE	2.5
1	A	450	GLU	2.4
1	A	347	LEU	2.4
1	A	237	SER	2.3
1	I	237	SER	2.3
1	I	287	VAL	2.3
1	I	267	PRO	2.3
1	I	144	ILE	2.3
1	A	350	GLN	2.3
1	I	345	GLY	2.2
1	A	7	GLY	2.2
1	I	455	VAL	2.2
1	A	290	SER	2.1
1	A	279	ARG	2.1
1	A	346	THR	2.1
1	A	292	PHE	2.1
1	A	392	PRO	2.1
1	A	340	GLN	2.0
1	A	294	ALA	2.0

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 carbohydrates in this entry.

6.4 Ligands (i)

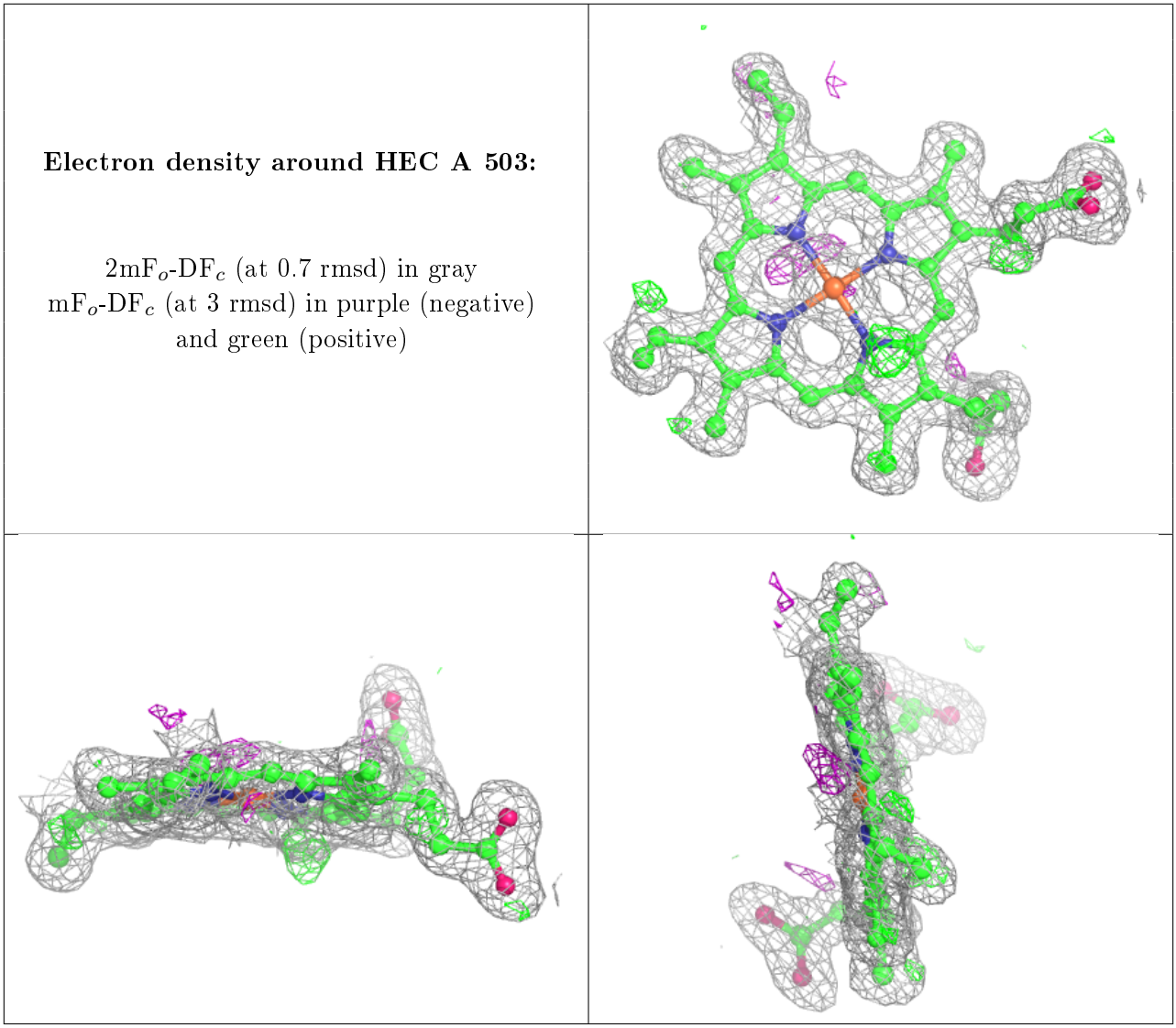
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	GOL	I	503[A]	6/6	0.85	0.32	14,17,19,20	6
3	HEC	A	503	43/43	0.95	0.11	20,21,22,23	0
3	HEC	I	504	43/43	0.96	0.11	13,13,14,15	0
2	CU	A	502	1/1	0.99	0.09	20,20,20,20	0
2	CU	A	501	1/1	1.00	0.09	18,18,18,18	0
2	CU	I	502	1/1	1.00	0.07	13,13,13,13	0
2	CU	I	501	1/1	1.00	0.09	12,12,12,12	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.

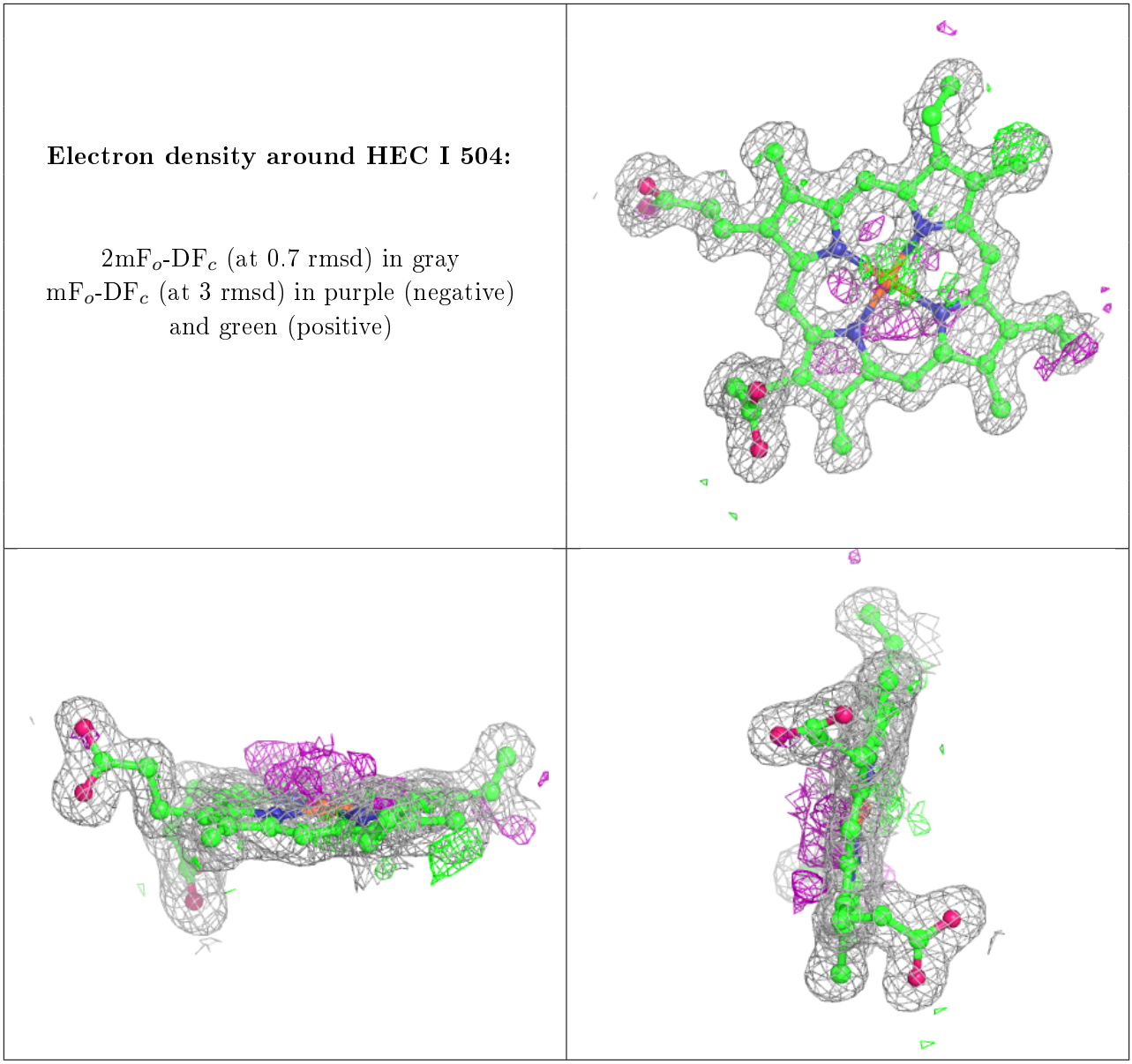
Electron density around HEC A 503:

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



Electron density around HEC I 504:

$2mF_o$-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.