



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 10:02 AM EDT

PDB ID : 1NIR / pdb_00001nir
Title : OXYDIZED NITRITE REDUCTASE FROM PSEUDOMONAS AERUGINOSA
Authors : Nurizzo, D.; Tegoni, M.; Cambillau, C.
Deposited on : 1997-06-17
Resolution : 2.15 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

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

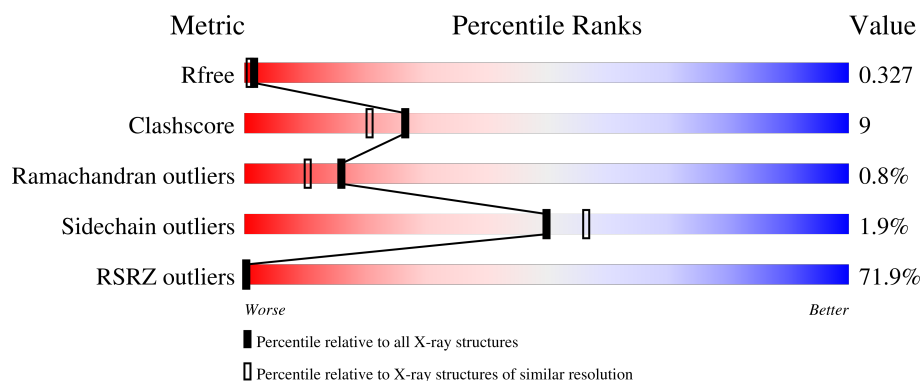
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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 $\leq 5\%$. 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	543	
1	B	543	

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	PO4	A	604	-	X	-	-
2	PO4	B	604	-	X	-	-
5	HEC	A	601	X	-	-	-
5	HEC	B	601	X	-	-	-
6	DHE	A	602	X	-	-	-
6	DHE	B	602	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9483 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 NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4203	2665	733	793	12			
1	B	539	Total	C	N	O	S	0	0	0
			4212	2671	735	794	12			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

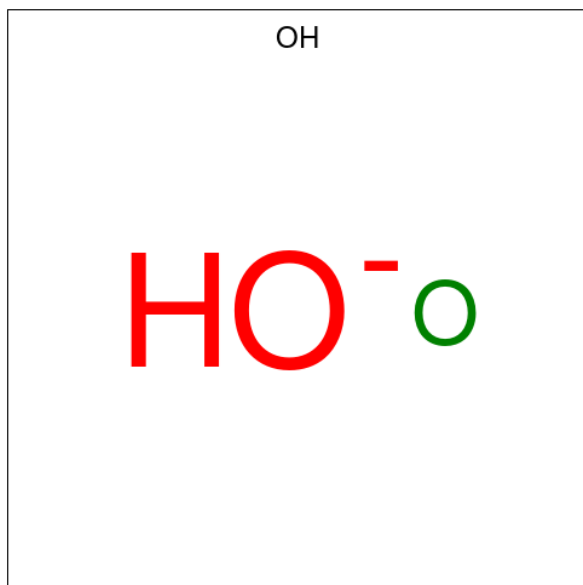


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

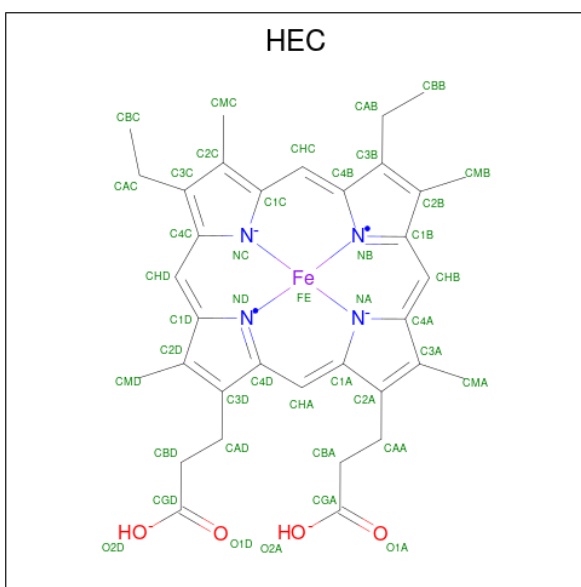
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



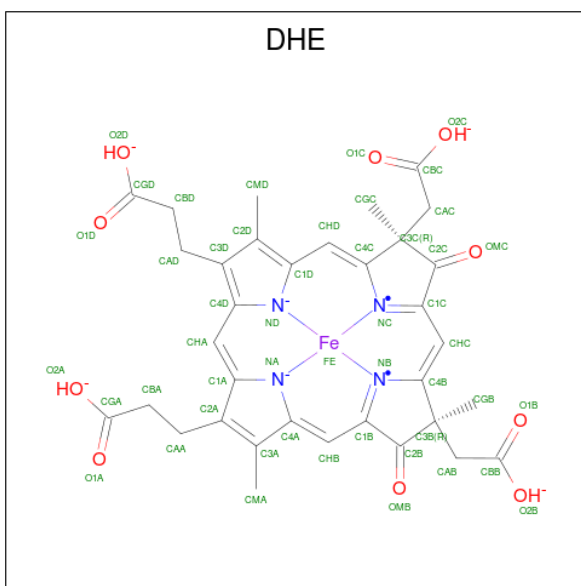
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		

- Molecule 5 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



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

- Molecule 6 is HEME D (CCD ID: DHE) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_{10}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 49	C 34	Fe 1	N 4	O 10	0	0
6	B	1	Total 49	C 34	Fe 1	N 4	O 10	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	449	Total 449	O 449	0	0
7	B	421	Total 421	O 421	0	0

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.

Chain A:

The figure displays a sequence logo for Chain A, showing the relative frequency of various amino acids across different positions (T54 to P25). The y-axis labels include Lys, Asp, Asn, Met, Lys, Ala, Arg, Glu, Gln, His, Ile, Val, Leu, Phe, Thr, Ser, Pro, Gly, Tyr, Cys, Trp, and others. The x-axis represents positions from T54 to P25. The legend indicates a scale from 57% (red) to 23% (yellow).

Chain B:

Position	Amino Acid
K5	Met
A6	Met
A7	Met
E8	Met
Q9	Met
Y10	Met
Q11	Met
G12	Met
A13	Met
A14	Met
S15	Met
S16	Met
A17	Met
A18	Met
A19	Met
P19	Met
A20	Met
H21	Met
V22	Met
V23	Met
R24	Met
T25	Met
N26	Met
A27	Met
G28	Met
P29	Met
D30	Met
M31	Met
S32	Met
S33	Met
S34	Met
E35	Met
F36	Met
N37	Met
E38	Met
A39	Met
K40	Met
Q41	Met
I42	Met
Y43	Met
F44	Met
Q45	Met
R46	Met
C47	Met
A48	Met
C49	Met
C50	Met
G51	Met
H52	Met
G53	Met
L54	Met
R55	Met
K56	Met
G57	Met
A58	Met
T59	Met
G60	Met

G500	K380	S319	F250	S184	M124	P62
N501	X381	A251	T252	R185	R125	L63
S502	G382	A322	L253	M186	E126	T64
D503	P383	A323	G253	S187	S127	P65
S504	V384	P324	D254	A188	W128	D66
S505	W385	F325	G255	S189	K129	I67
A506	S386	L326	E256	G190	V130	T68
L507	T387	H327	T257	R191	L131	Q69
V508	S388	D328	L258	Y192	V132	R70
V509	H389	G329	E259	L193	K133	W71
V510	L390	G330	P260	L194	P134	G72
D511	G391	W331		V195	E135	Q73
D512	D392	D332	T263	I196	D136	Q74
K513	G393	S333	V264	G197	R137	Y75
T514	S394	S334	S265	R198	P138	L76
L515	I395	H335	T266	D199	K139	E77
K516	S396	R336	R267	A200	K140	A78
L517	L397	Y337	G268	R201	Q141	L79
K518	T398	F338	T269	I202	L142	
A519	G399	K339	T270	D203	N143	T81
V520	D400	T340	V271	M204	D144	Y82
V521	D401	A341	D272	L205	G83	G83
K522	P402	A342	T273	D206	D146	T84
D523	K403	R343	Q274	L207	P85	
P524	N404	N344	T275	W208	L86	
R525	H405	Y345	G276	A209	N149	G87
L526	P406	N346	H277	K210	L150	M88
T527	Q407	K347	P278	E211	F151	P89
V528	Y408	V348	E279	P212	S152	N90
P529	A409	A349	P280	T213	V153	Y91
T530	W410	V350	R281		T154	G92
G531	K411	I351	V282	A216	L155	S93
K532	K412	D352	A283	E217	R156	S94
F533	V413	S353	A284	I218	D157	G95
N534	A414	K354	I285	K219	A158	E96
V535	E415	D355	I286	I220	G159	L97
F536	L416	R356	A287	G221	Q160	S98
G477	Q417	F357	S288	I222	I161	
N537	G418	L358	H289	E223	A162	E100
T538	K419	S359		A224	L163	K101
Q539	Q420	A360		R225	V164	I102
H540	D421	L361	F294	S226	D165	T103
D541	G422	V362	I295	V227	G166	L104
V542	S423	D363			D167	M105
Y543	P434	L424	K299	S230	A168	A106
E485	F425	G365	E300	K231	K169	K107
Y486	I426	K366	T301	F232	I170	I108
N487	K427	T367			I171	I109
K488	T428	P368	L305	Y235	V172	Q110
R489	H429	H369	L306	E236	K173	H111
G490	P430	P370	V307	D237	W174	T112
D491	K431	G371	N308	D237	I175	P113
E492	S432	R372	Y309	I241	D176	P114
V493	S433	G373	K310		T177	Q115
W494	H434	A374	D311	A244	G178	P116
F495	L435	N375	I312	Y245	Y179	
S496	V436	F376	D313	W246	A180	W119
V497	V437	V377	N314	P247	V181	G120
W498	D438	H378	L315	P248	H182	M121
N499	T439	P379		T249	I183	

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	163.07Å 90.07Å 111.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.15 30.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	89.0 (30.00-2.15) 89.5 (30.00-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.31 (at 2.14Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.209 , 0.242 0.318 , 0.327	Depositor DCC
R_{free} test set	3270 reflections (3.57%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9483	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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 47.40 % 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 9.9823e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: DHE, HEC, CL, OH, PO4

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	0.93	9/4308 (0.2%)	1.20	34/5854 (0.6%)
1	B	0.82	8/4317 (0.2%)	1.14	22/5865 (0.4%)
All	All	0.88	17/8625 (0.2%)	1.17	56/11719 (0.5%)

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	B	0	2
All	All	0	3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	248	PRO	C-N	-11.17	1.19	1.33
1	A	244	ALA	C-N	-8.90	1.22	1.33
1	B	244	ALA	C-N	-8.02	1.22	1.33
1	B	483	GLN	C-N	6.17	1.41	1.33
1	B	331	TRP	NE1-CE2	-5.73	1.31	1.37

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	VAL	N-CA-C	8.54	120.58	108.36
1	A	27	GLY	N-CA-C	-8.23	103.37	115.63
1	B	244	ALA	O-C-N	-7.70	113.46	123.16
1	B	23	VAL	N-CA-C	7.64	119.61	108.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	309	TYR	O-C-N	-7.45	113.10	122.26

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	385	TRP	Mainchain
1	B	309	TYR	Mainchain
1	B	483	GLN	Mainchain

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	4203	0	4158	87	0
1	B	4212	0	4171	78	2
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	43	0	30	0	0
5	B	43	0	30	2	0
6	A	49	0	24	3	0
6	B	49	0	24	3	0
7	A	449	0	0	5	1
7	B	421	0	0	7	2
All	All	9483	0	8437	158	5

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 9.

The worst 5 of 158 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:B:488:LYS:HB3	7:B:1008:HOH:O	1.62	0.98
1:A:277:HIS:O	1:A:280:PRO:HD3	1.84	0.78
1:A:114:PRO:HB2	1:B:22:VAL:HG12	1.64	0.78
1:B:211:GLU:O	1:B:213:THR:HG23	1.87	0.75
1:B:489:ARG:HG2	7:B:1008:HOH:O	1.88	0.73

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:GLN:NE2	1:B:473:ASP:O[3_556]	1.93	0.27
7:A:616:HOH:O	7:A:772:HOH:O[3_545]	2.01	0.19
7:B:706:HOH:O	7:B:874:HOH:O[3_546]	2.07	0.13
1:B:74:GLN:OE1	1:B:169:LYS:O[3_556]	2.08	0.12
7:B:768:HOH:O	7:B:898:HOH:O[3_556]	2.18	0.02

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	536/543 (99%)	496 (92%)	35 (6%)	5 (1%)	14	9
1	B	537/543 (99%)	502 (94%)	31 (6%)	4 (1%)	18	13
All	All	1073/1086 (99%)	998 (93%)	66 (6%)	9 (1%)	16	10

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	156	ARG
1	A	299	LYS
1	B	156	ARG
1	B	299	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	453/458 (99%)	442 (98%)	11 (2%)	43	47
1	B	454/458 (99%)	448 (99%)	6 (1%)	61	68
All	All	907/916 (99%)	890 (98%)	17 (2%)	50	56

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	413	VAL
1	B	439	THR
1	A	336	ARG
1	A	413	VAL
1	A	424	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	327	HIS
1	B	289	HIS
1	A	540	HIS
1	B	115	GLN
1	A	344	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic and 2 are modelled with single atom - leaving 6 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	$\# Z > 2$
5	HEC	A	601	1	50,50,50	0.88	0	68,82,82	1.11	4 (5%)
6	DHE	B	602	4,1	52,56,56	1.88	8 (15%)	68,94,94	1.73	14 (20%)
5	HEC	B	601	1	50,50,50	0.84	0	68,82,82	1.16	4 (5%)
2	PO4	B	604	-	4,4,4	3.35	4 (100%)	6,6,6	1.23	1 (16%)
6	DHE	A	602	4,1	52,56,56	1.90	8 (15%)	68,94,94	1.71	10 (14%)
2	PO4	A	604	-	4,4,4	3.39	4 (100%)	6,6,6	0.58	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
5	HEC	A	601	1	1/1/3/7	6/14/54/54	-
6	DHE	A	602	4,1	1/1/15/19	6/20/108/108	-
5	HEC	B	601	1	1/1/3/7	6/14/54/54	-
6	DHE	B	602	4,1	1/1/15/19	8/20/108/108	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	602	DHE	CBD-CAD	-6.52	1.29	1.51
6	B	602	DHE	CBD-CAD	-6.44	1.29	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	604	PO4	P-O1	5.15	1.62	1.50
2	B	604	PO4	P-O1	4.69	1.61	1.50
6	A	602	DHE	FE-NC	4.55	2.08	1.94

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	602	DHE	CBD-CAD-C3D	5.25	127.06	112.53
6	A	602	DHE	CAD-CBD-CGD	5.05	127.07	113.67
6	B	602	DHE	C1C-NC-C4C	4.87	110.98	105.21
6	A	602	DHE	C1C-NC-C4C	4.82	110.91	105.21
6	A	602	DHE	CBD-CAD-C3D	4.72	125.58	112.53

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	601	HEC	NA
5	B	601	HEC	NA
6	A	602	DHE	NA
6	B	602	DHE	NA

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	602	DHE	C2D-C3D-CAD-CBD
6	A	602	DHE	C4D-C3D-CAD-CBD
6	B	602	DHE	C2D-C3D-CAD-CBD
6	B	602	DHE	C4D-C3D-CAD-CBD
5	B	601	HEC	C4B-C3B-CAB-CBB

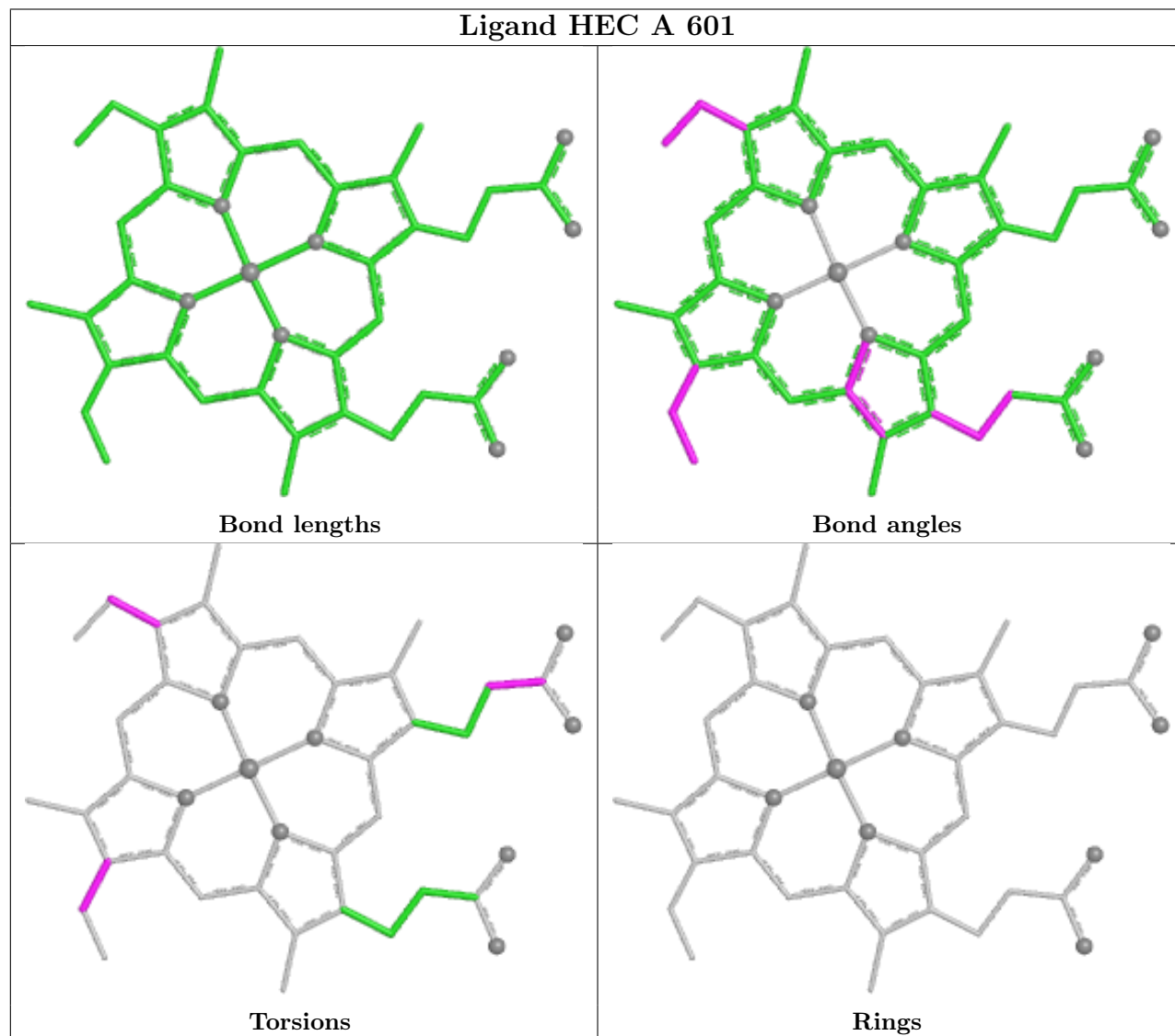
There are no ring outliers.

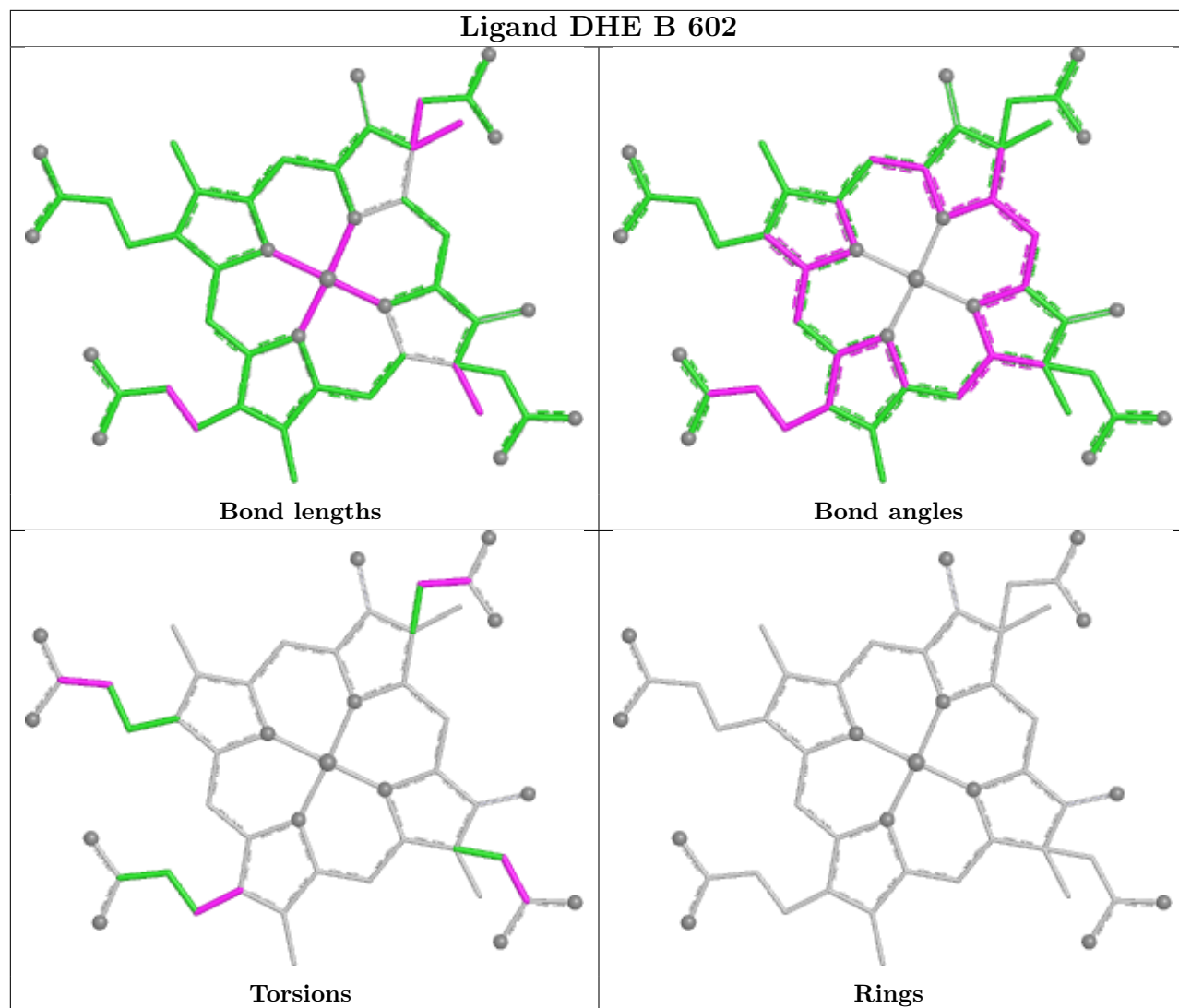
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	602	DHE	3	0
5	B	601	HEC	2	0
6	A	602	DHE	3	0

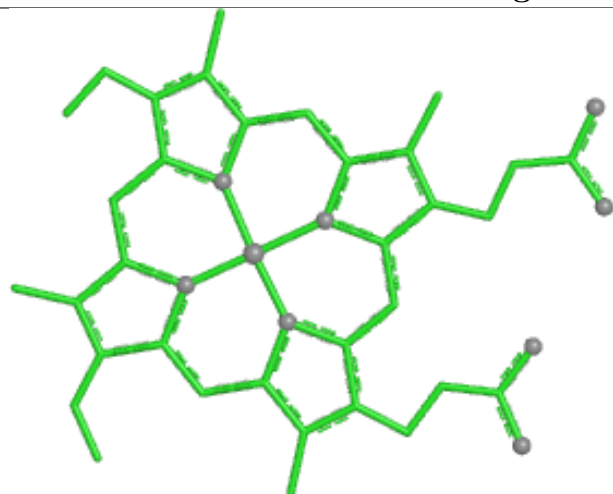
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

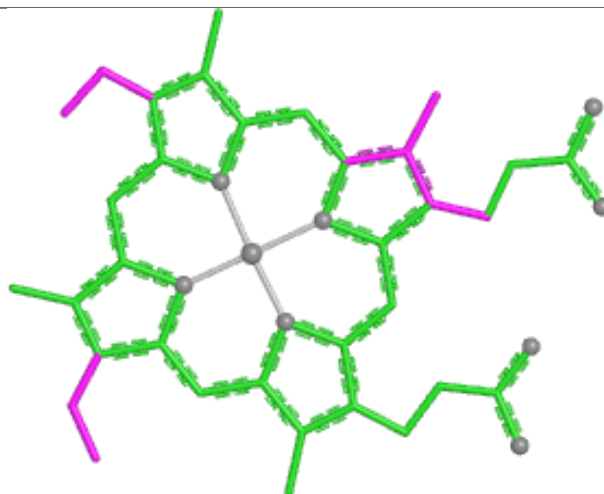




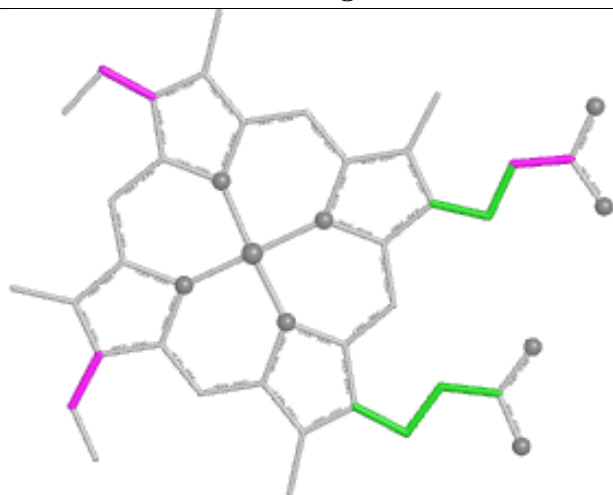
Ligand HEC B 601



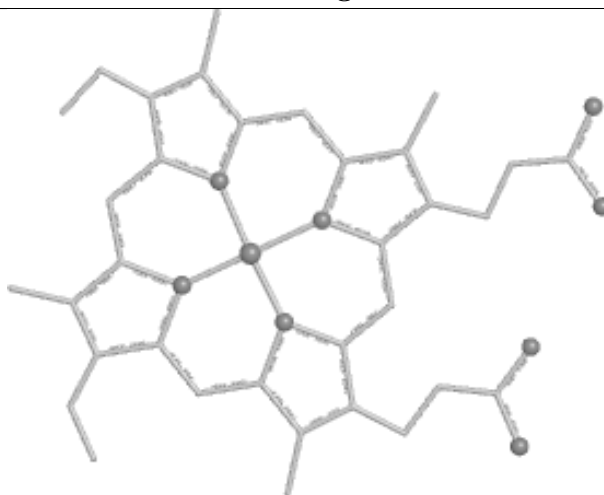
Bond lengths



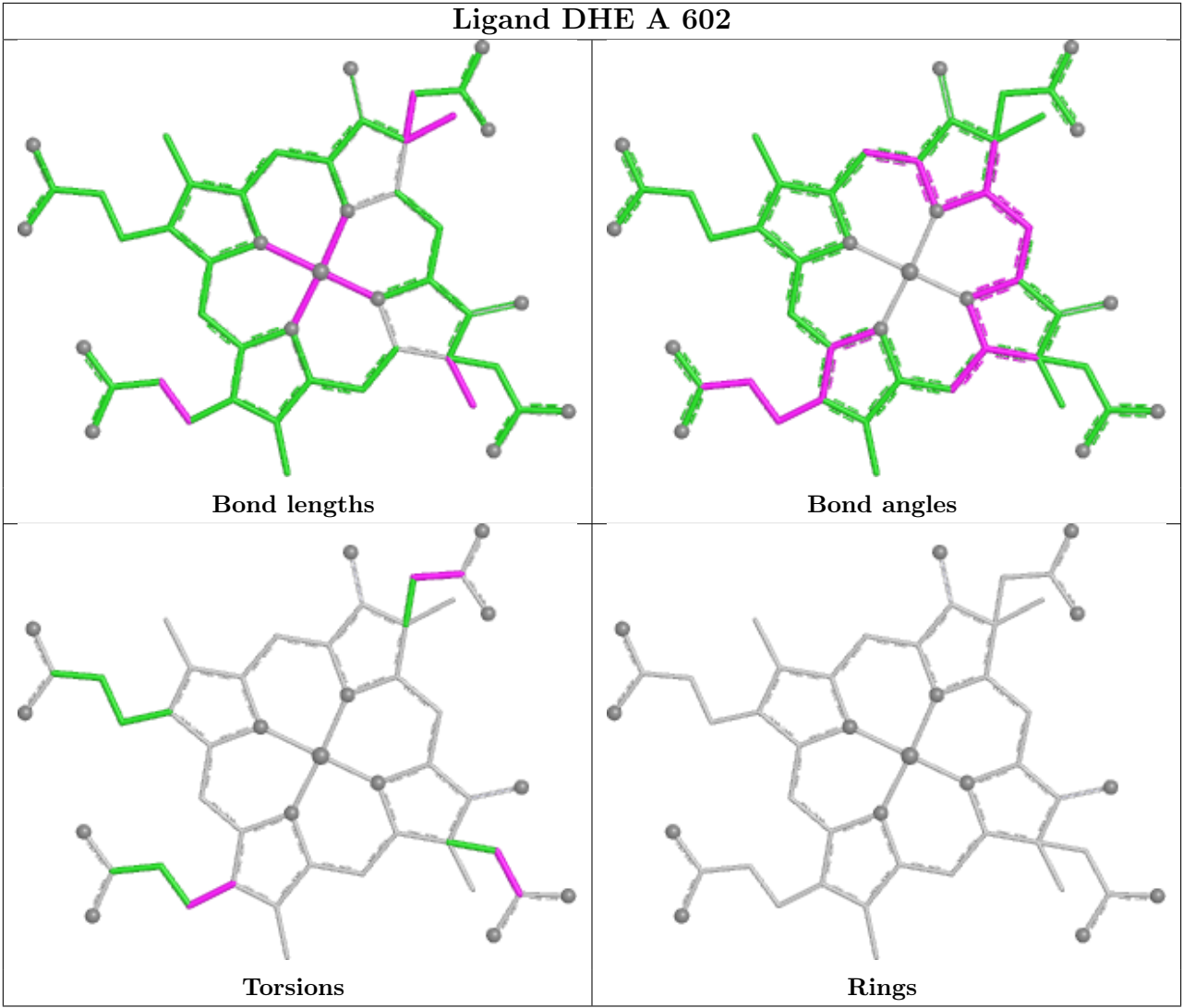
Bond angles



Torsions



Rings



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	248:PRO	C	249:GLN	N	1.19

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	538/543 (99%)	2.35	307 (57%) 0 0	22, 36, 54, 71	0
1	B	539/543 (99%)	3.32	467 (86%) 0 0	23, 37, 56, 72	0
All	All	1077/1086 (99%)	2.83	774 (71%) 0 0	22, 36, 55, 72	0

The worst 5 of 774 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	312	ILE	7.6
1	B	454	PHE	7.3
1	A	99	LYS	7.2
1	B	475	GLY	7.1
1	B	370	PRO	6.9

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

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

6.3 Carbohydrates [i](#)

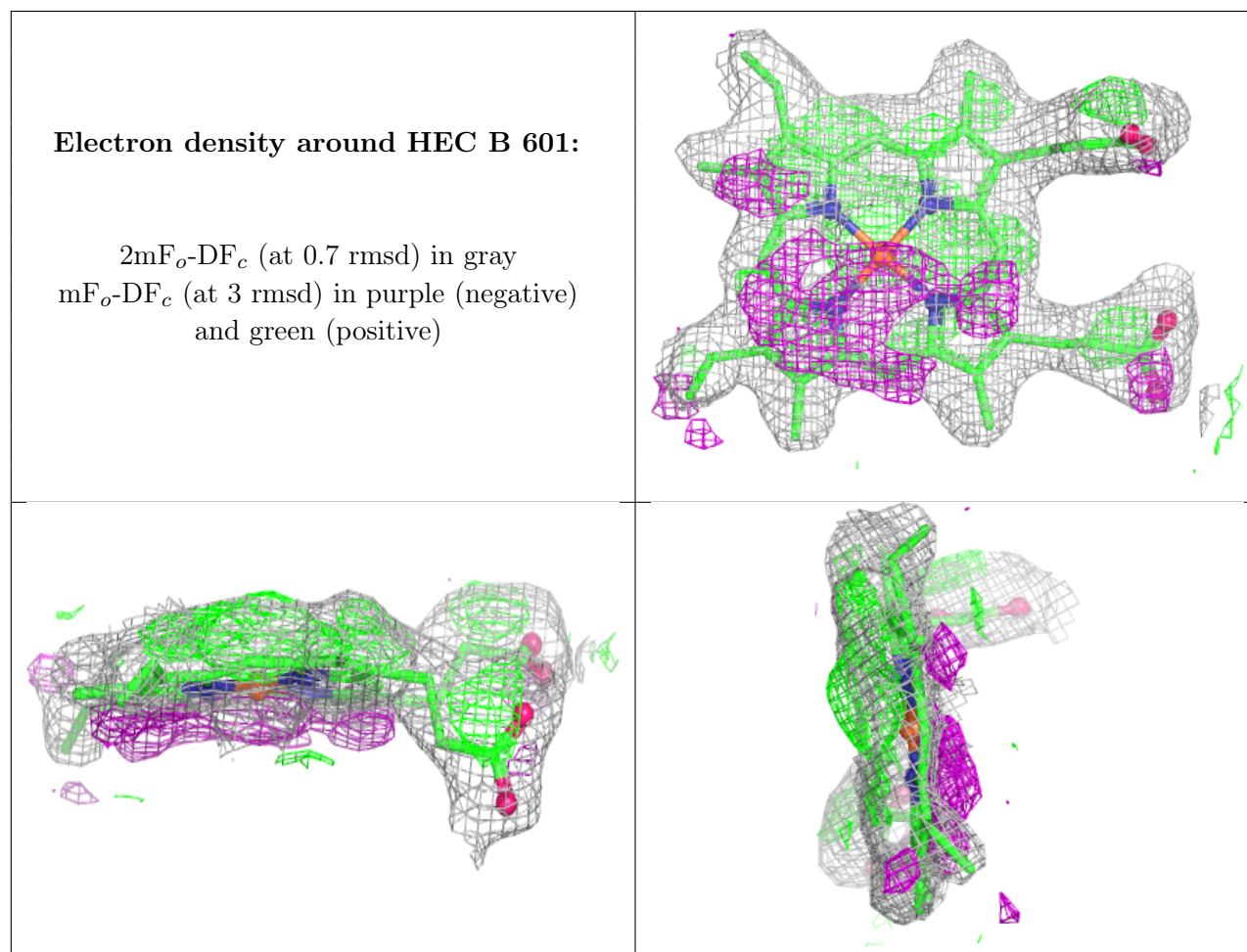
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

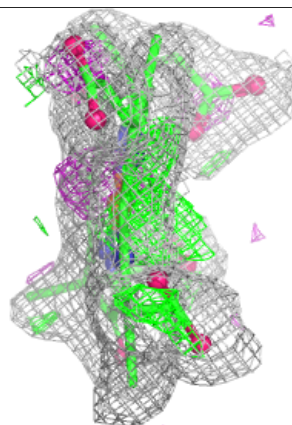
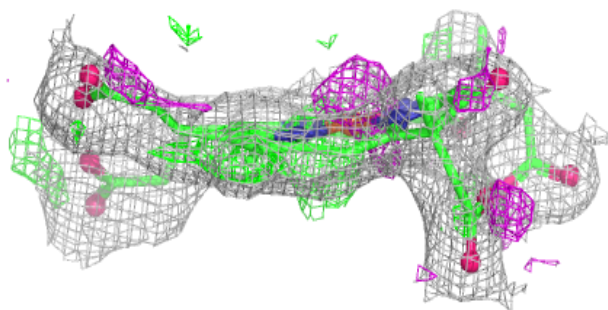
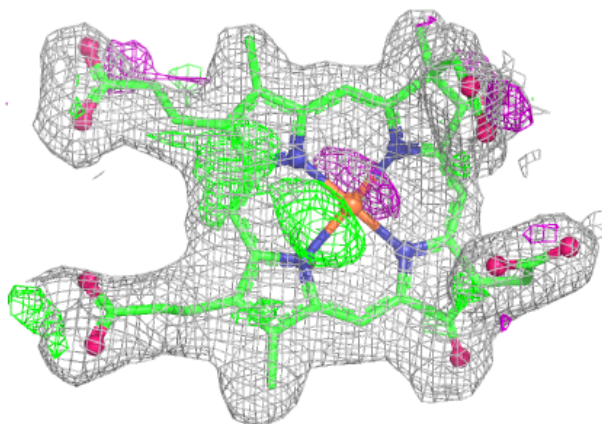
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	OH	B	603	1/1	0.44	0.40	39,39,39,39	0
2	PO4	A	604	5/5	0.73	0.19	75,75,78,78	0
5	HEC	B	601	43/43	0.77	0.24	24,31,34,41	0
2	PO4	B	604	5/5	0.83	0.15	82,82,84,85	0
3	CL	A	605	1/1	0.83	0.13	28,28,28,28	0
6	DHE	B	602	49/49	0.84	0.18	25,30,39,50	0
5	HEC	A	601	43/43	0.89	0.16	24,29,38,42	0
6	DHE	A	602	49/49	0.90	0.14	22,29,36,47	0
4	OH	A	603	1/1	0.93	0.28	36,36,36,36	0
3	CL	B	605	1/1	0.93	0.08	27,27,27,27	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.



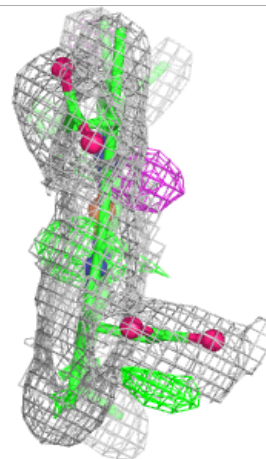
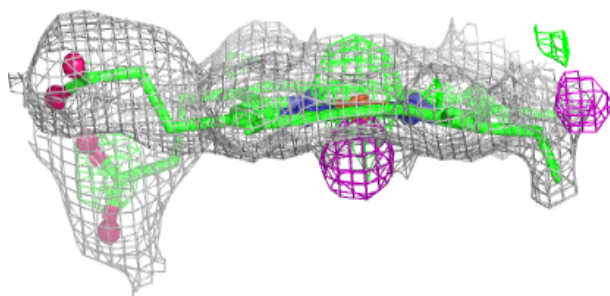
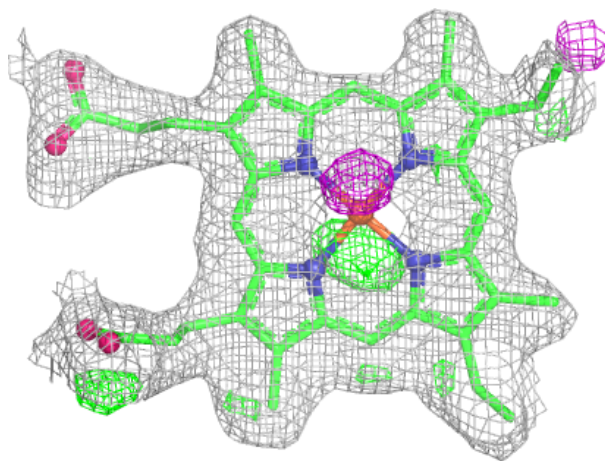
Electron density around DHE B 602:

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



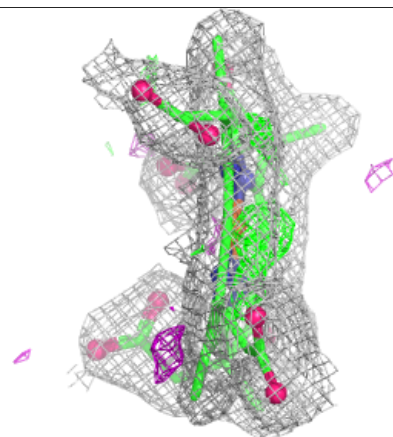
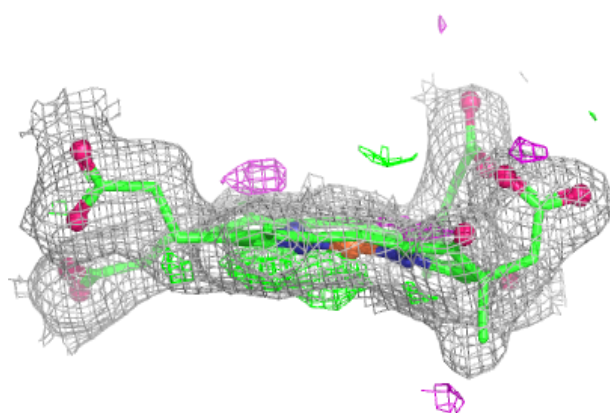
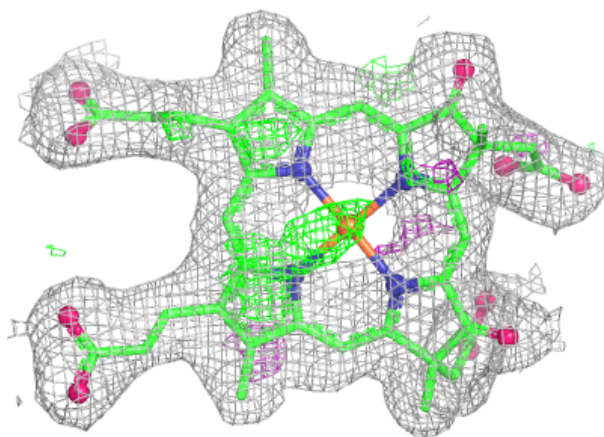
Electron density around HEC A 601:

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



Electron density around DHE A 602:

$2mF_o-DF_c$ (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.