



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 08:03 pm BST

PDB ID : 1H9Y
Title : Cytochrome cd1 Nitrite Reductase, reduced form complexed to CN
Authors : Sjogren, T.; Hajdu, J.
Deposited on : 2001-03-23
Resolution : 2.40 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

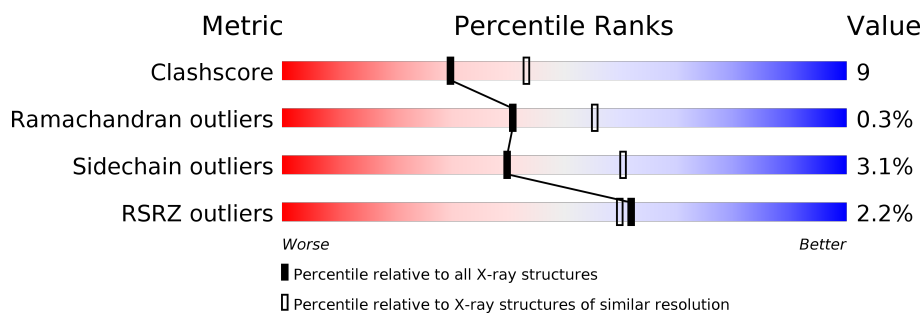
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 $\leq 5\%$. 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	567	<div> <div>2%</div> <div>74%</div> <div>17%</div> <div>• 8%</div> </div>
1	B	567	<div> <div>2%</div> <div>71%</div> <div>19%</div> <div>• 8%</div> </div>

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
5	SO4	B	621	-	-	X	-

2 Entry composition [i](#)

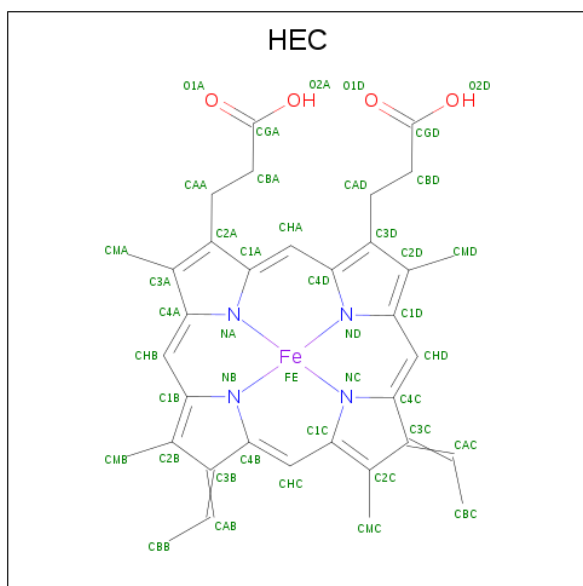
There are 6 unique types of molecules in this entry. The entry contains 8551 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CYTOCHROME CD1 NITRITE REDUCTASE.

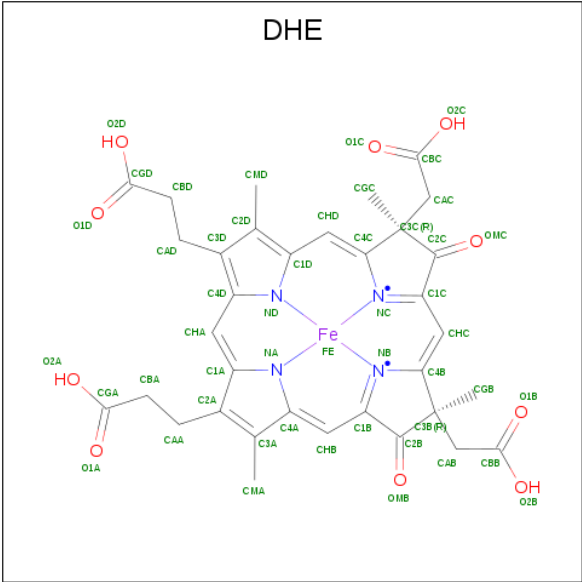
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			4056	2570	676	796	14			
1	B	519	Total	C	N	O	S	0	0	0
			4051	2567	675	795	14			

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



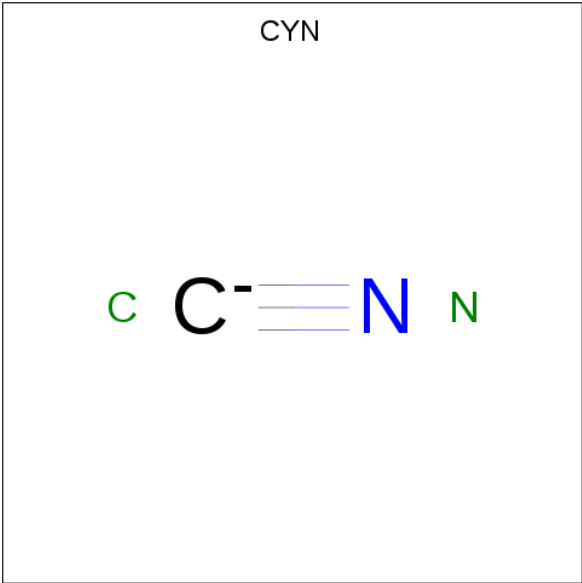
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is HEME D (three-letter code: DHE) (formula: $C_{34}H_{32}FeN_4O_{10}$).



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

- Molecule 4 is CYANIDE ION (three-letter code: CYN) (formula: CN).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			2	1	1		
4	B	1	Total	C	N	0	0
			2	1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	118	Total O 118 118	0	0
6	B	124	Total O 124 124	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	127.57Å 127.57Å 263.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.40) 97.8 (19.98-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.238 , 0.269 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.0	EDS
L-test for twinning ¹	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8551	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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, CYN, SO4

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	0.41	0/4156	1.09	17/5651 (0.3%)
1	B	0.43	0/4151	1.10	11/5644 (0.2%)
All	All	0.42	0/8307	1.09	28/11295 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	ARG	CD-NE-CZ	12.46	141.05	123.60
1	A	87	ARG	NE-CZ-NH2	-11.55	114.52	120.30
1	B	174	ARG	NE-CZ-NH2	-9.69	115.46	120.30
1	B	174	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	A	363	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	B	363	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	A	363	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	B	199	VAL	CB-CA-C	-7.36	97.42	111.40
1	A	309	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	A	255	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	64	ARG	CD-NE-CZ	6.61	132.86	123.60
1	B	484	ASP	CA-CB-CG	6.38	127.45	113.40
1	B	390	GLY	N-CA-C	-6.20	97.61	113.10
1	A	143	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	87	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	143	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	A	269	VAL	CB-CA-C	-5.71	100.54	111.40
1	B	92	ASP	CA-CB-CG	-5.66	100.95	113.40
1	B	203	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	229	GLU	OE1-CD-OE2	-5.47	116.73	123.30
1	A	404	TRP	CA-CB-CG	5.40	123.97	113.70
1	A	64	ARG	NE-CZ-NH1	5.39	123.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	557	PHE	CB-CG-CD2	-5.24	117.13	120.80
1	B	547	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	390	GLY	N-CA-C	-5.09	100.38	113.10
1	A	557	PHE	CB-CG-CD1	5.08	124.36	120.80
1	A	285	ARG	CD-NE-CZ	5.04	130.65	123.60
1	A	285	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	4056	0	3913	59	0
1	B	4051	0	3908	87	0
2	A	43	0	30	4	0
2	B	43	0	30	4	0
3	A	49	0	28	5	0
3	B	49	0	28	3	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	5	0	0	1	0
5	B	9	0	0	5	0
6	A	118	0	0	0	0
6	B	124	0	0	2	0
All	All	8551	0	7937	153	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 9.

All (153) 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:108:ASN:HD22	1:A:111:THR:HG22	1.22	1.03
1:B:342:ARG:HH21	1:B:363:ARG:HH22	1.04	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:PRO:HA	1:B:86:THR:HG22	1.52	0.91
1:A:167:ASN:HD21	1:A:511:ASN:HB2	1.40	0.85
1:B:159:GLN:HE21	1:B:161:ASN:ND2	1.79	0.81
1:B:342:ARG:NH2	1:B:363:ARG:HH22	1.81	0.76
1:A:108:ASN:ND2	1:A:111:THR:HG22	2.00	0.73
1:A:198:ALA:HB1	1:A:216:ARG:HB2	1.71	0.73
1:A:236:ILE:HG21	1:A:271:MET:HE3	1.72	0.71
1:B:342:ARG:HH21	1:B:363:ARG:NH2	1.84	0.70
1:A:165:LEU:HA	1:A:168:LEU:HD12	1.72	0.70
1:A:167:ASN:ND2	1:A:512:LYS:H	1.90	0.69
1:A:167:ASN:HD22	1:A:512:LYS:H	1.44	0.66
1:B:109:TRP:CE2	2:B:601:HEC:HBB2	2.31	0.66
1:B:537:LYS:HZ2	1:B:537:LYS:H	1.43	0.66
1:B:83:PRO:HA	1:B:86:THR:CG2	2.27	0.64
1:A:109:TRP:CE2	2:A:601:HEC:HBB2	2.33	0.64
1:B:161:ASN:HD22	1:B:163:TRP:H	1.46	0.64
1:B:86:THR:HG21	1:B:127:LEU:O	1.98	0.64
1:A:280:LYS:HE2	1:A:282:GLN:NE2	2.14	0.62
1:B:49:LEU:HD22	1:B:122:LEU:HD23	1.82	0.62
1:B:537:LYS:NZ	1:B:537:LYS:H	1.97	0.62
1:A:271:MET:CE	1:A:276:LEU:HD22	2.31	0.61
1:A:195:THR:HG21	1:A:213:VAL:HG21	1.83	0.59
1:B:60:ILE:HG23	1:B:64:ARG:HD3	1.85	0.59
1:A:179:ILE:HD13	1:A:213:VAL:HG11	1.85	0.59
1:A:202:SER:HB3	1:A:211:LEU:HD11	1.86	0.58
3:A:602:DHE:HBD2	3:A:602:DHE:HMD1	1.85	0.57
1:A:155:ARG:HB3	1:A:156:PRO:HD2	1.86	0.57
1:A:271:MET:HE2	1:A:276:LEU:HD22	1.87	0.57
1:A:236:ILE:HG21	1:A:271:MET:CE	2.34	0.57
1:B:280:LYS:HE3	1:B:330:LEU:O	2.06	0.56
1:B:82:THR:O	1:B:86:THR:HB	2.07	0.54
1:B:222:MET:HE2	1:B:234:ALA:HB3	1.90	0.54
1:A:57:ALA:HB2	1:A:122:LEU:HD22	1.90	0.53
1:B:201:ILE:CD1	1:B:203:ARG:HG2	2.38	0.53
1:B:420:ASP:OD2	1:B:424:HIS:HD2	1.91	0.53
1:B:195:THR:HG21	1:B:213:VAL:HG21	1.90	0.53
1:A:498:ILE:HD12	1:A:521:VAL:HG11	1.91	0.52
1:B:109:TRP:NE1	2:B:601:HEC:HBB2	2.23	0.52
1:A:412:ASP:HB3	1:A:439:GLY:HA2	1.92	0.51
1:A:366:LEU:HG	1:A:382:THR:HG22	1.93	0.51
1:A:197:TYR:O	1:A:198:ALA:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:GLY:HA2	1:B:199:VAL:HG22	1.93	0.51
1:A:438:LEU:HG	1:A:471:ALA:HB2	1.94	0.51
1:B:106:MET:HB2	2:B:601:HEC:C4D	2.41	0.51
1:A:297:GLU:N	1:A:298:PRO:HD3	2.26	0.50
1:B:222:MET:HE2	1:B:233:VAL:HG23	1.92	0.50
1:B:295:HIS:CE1	1:B:297:GLU:HG2	2.47	0.50
1:A:200:HIS:HE1	3:A:602:DHE:NC	2.07	0.50
1:B:280:LYS:NZ	1:B:282:GLN:HE22	2.10	0.50
1:B:86:THR:CG2	1:B:128:LEU:HA	2.41	0.50
1:B:309:ARG:HB3	1:B:310:PRO:HD2	1.92	0.49
1:B:308:TYR:CE1	1:B:354:ARG:HB2	2.47	0.49
2:A:601:HEC:HMC1	2:A:601:HEC:HBC3	1.92	0.49
1:B:146:TRP:CZ2	1:B:277:GLU:HB2	2.47	0.49
1:B:304:LEU:HD11	1:B:348:GLY:HA2	1.94	0.49
3:B:602:DHE:HMD1	3:B:602:DHE:HBD2	1.95	0.49
1:A:389:PRO:HB3	1:A:406:THR:HB	1.94	0.48
1:B:557:PHE:HZ	3:B:602:DHE:HAD1	1.77	0.48
5:B:621:SO4:O3	5:B:621:SO4:O4	2.31	0.48
1:B:116:SER:O	1:B:117:ALA:C	2.51	0.48
1:B:236:ILE:HG12	1:B:237:LYS:N	2.29	0.48
1:B:515:THR:HB	1:B:537:LYS:HE2	1.94	0.48
1:B:112:SER:OG	1:B:114:GLU:HB2	2.14	0.48
1:A:508:GLY:HA2	1:A:518:TRP:O	2.13	0.47
1:B:375:LYS:HB3	1:B:375:LYS:NZ	2.29	0.47
1:B:142:MET:CE	1:B:281:ILE:HD12	2.45	0.47
1:A:108:ASN:HD22	1:A:111:THR:CG2	2.10	0.47
1:B:342:ARG:O	1:B:343:PHE:HB2	2.14	0.47
1:B:195:THR:OG1	1:B:199:VAL:HG13	2.14	0.47
1:B:495:TRP:HZ3	1:B:534:VAL:HG22	1.79	0.47
1:A:245:ILE:HA	1:A:259:ILE:O	2.15	0.46
1:B:102:SER:HB2	1:B:103:PRO:HD2	1.96	0.46
1:A:292:GLN:HB2	1:B:139:MET:HB2	1.97	0.46
1:A:243:ARG:HH21	3:A:602:DHE:CBB	2.27	0.46
1:B:176:ALA:O	1:B:178:GLN:HG3	2.16	0.46
1:B:166:GLU:HB3	1:B:560:TYR:HB2	1.98	0.46
1:A:380:GLU:HG3	1:A:429:TRP:O	2.14	0.46
1:A:426:ASP:O	1:A:430:LYS:HD2	2.16	0.46
1:B:295:HIS:HE1	1:B:297:GLU:HG2	1.80	0.46
1:A:155:ARG:HB3	1:A:156:PRO:CD	2.46	0.45
1:B:304:LEU:HD13	6:B:2119:HOH:O	2.16	0.45
1:A:167:ASN:ND2	1:A:511:ASN:HB2	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ALA:HB1	1:B:216:ARG:HB2	1.98	0.45
1:A:427:ASN:HB3	1:A:432:LEU:HD11	1.99	0.45
1:B:109:TRP:HE3	1:B:114:GLU:HB3	1.81	0.45
1:B:253:TRP:CE3	1:B:256:LYS:HG2	2.52	0.45
1:B:289:TYR:CZ	1:B:290:ASP:HB3	2.52	0.45
1:B:175:ASP:HB3	1:B:525:LYS:HD2	1.99	0.45
1:B:98:ILE:HB	1:B:120:VAL:HG13	1.99	0.44
1:A:264:TRP:HA	1:A:265:PRO:C	2.36	0.44
1:B:222:MET:CE	1:B:233:VAL:HG23	2.48	0.44
1:B:453:TYR:HB3	1:B:472:VAL:CG1	2.47	0.44
1:A:218:GLY:HA2	1:A:242:ALA:HB3	2.00	0.44
1:B:86:THR:HG23	1:B:128:LEU:HA	1.99	0.44
1:B:341:GLU:OE1	1:B:363:ARG:NH1	2.41	0.43
1:B:484:ASP:HB3	6:B:2095:HOH:O	2.16	0.43
1:A:222:MET:CE	1:A:276:LEU:HG	2.47	0.43
1:B:222:MET:CE	1:B:234:ALA:HB3	2.48	0.43
1:B:236:ILE:HG12	1:B:237:LYS:H	1.82	0.43
1:B:71:VAL:HG22	1:B:241:GLU:OE2	2.19	0.43
1:B:264:TRP:HA	1:B:265:PRO:C	2.38	0.43
1:B:280:LYS:NZ	1:B:282:GLN:NE2	2.66	0.43
1:B:280:LYS:HG3	1:B:282:GLN:HE21	1.83	0.43
1:B:508:GLY:HA2	1:B:518:TRP:O	2.18	0.43
1:B:59:LYS:O	1:B:63:GLU:HG3	2.18	0.43
1:A:243:ARG:HG3	3:A:602:DHE:HHB	1.99	0.43
1:A:271:MET:HE1	1:A:276:LEU:HD22	2.01	0.43
1:A:222:MET:HE3	1:A:276:LEU:HG	2.01	0.43
1:A:74:LYS:HD2	5:A:621:SO4:O3	2.19	0.43
1:B:535:ASP:OD1	1:B:537:LYS:NZ	2.51	0.43
1:A:109:TRP:NE1	2:A:601:HEC:HBB2	2.34	0.43
1:A:438:LEU:HB3	1:A:466:ILE:HG23	2.01	0.43
1:A:61:TYR:CD1	1:A:65:CYS:HB2	2.53	0.43
1:B:275:THR:O	1:B:276:LEU:HB2	2.18	0.43
1:B:479:THR:OG1	1:B:480:GLY:N	2.52	0.43
1:A:495:TRP:HZ3	1:A:534:VAL:HG22	1.84	0.43
1:A:523:ASN:O	1:A:552:THR:HG22	2.19	0.43
1:A:106:MET:HB2	2:A:601:HEC:C4D	2.49	0.42
1:B:367:VAL:HG22	1:B:379:ILE:HG12	2.01	0.42
1:B:438:LEU:HG	1:B:471:ALA:HB2	2.01	0.42
5:B:621:SO4:O2	5:B:621:SO4:O4	2.37	0.42
1:B:264:TRP:CD2	1:B:265:PRO:HA	2.54	0.42
1:B:473:PHE:CD2	1:B:485:PRO:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:621:SO4:O2	5:B:621:SO4:O3	2.37	0.42
1:B:130:ASP:HA	1:B:131:PRO:HD3	1.87	0.42
1:A:280:LYS:HE2	1:A:282:GLN:HE22	1.85	0.42
1:A:397:HIS:CD2	1:A:478:MET:HE1	2.53	0.42
5:B:621:SO4:O2	5:B:621:SO4:O1	2.38	0.42
1:A:83:PRO:HG3	1:A:130:ASP:HA	2.00	0.42
1:B:50:SER:H	1:B:53:GLN:HE21	1.68	0.42
1:A:304:LEU:HD21	1:A:348:GLY:HA2	2.02	0.42
1:B:139:MET:O	1:B:143:ARG:HG3	2.19	0.41
1:A:453:TYR:HA	1:A:473:PHE:O	2.20	0.41
1:B:491:PRO:HB2	1:B:494:GLU:HB3	2.02	0.41
1:B:297:GLU:N	1:B:298:PRO:HD3	2.34	0.41
1:A:243:ARG:NE	3:A:602:DHE:O2B	2.42	0.41
1:B:54:TYR:OH	1:B:132:ALA:HB2	2.20	0.41
1:A:442:SER:HA	1:A:458:ALA:HA	2.02	0.41
1:B:109:TRP:CE3	1:B:114:GLU:HB3	2.56	0.41
1:B:253:TRP:HE3	1:B:256:LYS:HG2	1.86	0.41
1:A:453:TYR:HB3	1:A:472:VAL:CG1	2.51	0.41
1:B:264:TRP:CG	1:B:265:PRO:HA	2.56	0.41
1:A:361:ASN:O	1:A:386:THR:HA	2.21	0.41
1:B:133:ALA:HA	1:B:134:PRO:HD3	1.95	0.41
1:B:108:ASN:HB2	1:B:111:THR:OG1	2.20	0.40
1:A:130:ASP:HA	1:A:131:PRO:HD3	1.95	0.40
1:B:289:TYR:CG	1:B:290:ASP:N	2.89	0.40
1:B:106:MET:HB2	2:B:601:HEC:C1D	2.51	0.40
1:B:280:LYS:HZ3	1:B:282:GLN:HE22	1.69	0.40
1:B:444:PHE:CE1	3:B:602:DHE:HBD1	2.57	0.40
5:B:621:SO4:O1	5:B:621:SO4:O3	2.40	0.40

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	518/567 (91%)	490 (95%)	27 (5%)	1 (0%)	47	62
1	B	517/567 (91%)	491 (95%)	24 (5%)	2 (0%)	34	48
All	All	1035/1134 (91%)	981 (95%)	51 (5%)	3 (0%)	41	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	507	GLN
1	B	507	GLN
1	B	174	ARG

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	432/469 (92%)	419 (97%)	13 (3%)	41	61
1	B	432/469 (92%)	418 (97%)	14 (3%)	39	59
All	All	864/938 (92%)	837 (97%)	27 (3%)	40	60

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	71	VAL
1	A	88	ASP
1	A	97	PHE
1	A	102	SER
1	A	111	THR
1	A	122	LEU
1	A	213	VAL
1	A	227	MET
1	A	377	VAL
1	A	406	THR
1	A	499	THR
1	A	500	GLU

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Mol	Chain	Res	Type
1	B	77	THR
1	B	86	THR
1	B	97	PHE
1	B	114	GLU
1	B	144	GLU
1	B	161	ASN
1	B	174	ARG
1	B	199	VAL
1	B	256	LYS
1	B	297	GLU
1	B	304	LEU
1	B	375	LYS
1	B	430	LYS
1	B	537	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	282	GLN
1	A	452	GLN
1	A	527	GLN
1	A	561	ASN
1	B	53	GLN
1	B	158	GLN
1	B	161	ASN
1	B	178	GLN
1	B	282	GLN
1	B	424	HIS
1	B	452	GLN
1	B	527	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

9 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
4	CYN	A	603	3	0,1,1	0.00	-	-		
2	HEC	A	601	1	26,50,50	2.31	7 (26%)	18,82,82	2.24	8 (44%)
5	SO4	A	621	-	4,4,4	0.63	0	6,6,6	0.30	0
4	CYN	B	603	3	0,1,1	0.00	-	-		
5	SO4	B	622	-	4,4,4	0.64	0	6,6,6	0.32	0
2	HEC	B	601	1	26,50,50	2.39	5 (19%)	18,82,82	2.22	10 (55%)
3	DHE	A	602	1,4	38,56,56	8.02	27 (71%)	37,94,94	4.34	26 (70%)
3	DHE	B	602	1,4	38,56,56	7.75	28 (73%)	37,94,94	3.92	20 (54%)

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	HEC	A	601	1	-	0/6/54/54	-
3	DHE	A	602	1,4	-	3/12/108/108	-
2	HEC	B	601	1	-	0/6/54/54	-
3	DHE	B	602	1,4	-	4/12/108/108	-

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	DHE	OMB-C2B	18.84	1.53	1.21
3	A	602	DHE	OMC-C2C	18.84	1.53	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	DHE	OMC-C2C	18.62	1.53	1.21
3	B	602	DHE	OMB-C2B	18.61	1.53	1.21
3	A	602	DHE	C3B-C2B	-16.13	1.33	1.52
3	A	602	DHE	C3C-C2C	-15.59	1.33	1.52
3	B	602	DHE	C3C-C2C	-15.24	1.34	1.52
3	B	602	DHE	C3B-C2B	-14.40	1.35	1.52
3	A	602	DHE	CHA-C4D	-13.29	1.37	1.51
3	A	602	DHE	CHA-C1A	-13.23	1.37	1.51
3	B	602	DHE	CHA-C4D	-12.75	1.38	1.51
3	B	602	DHE	CHA-C1A	-12.51	1.38	1.51
3	A	602	DHE	C4B-NB	-11.19	1.38	1.49
3	A	602	DHE	C4C-NC	-11.12	1.38	1.49
3	B	602	DHE	C4B-NB	-11.11	1.38	1.49
3	B	602	DHE	C4C-NC	-10.93	1.38	1.49
3	A	602	DHE	CHB-C1B	-8.55	1.38	1.53
3	A	602	DHE	C1B-NB	-8.33	1.38	1.49
3	B	602	DHE	C1B-NB	-8.14	1.38	1.49
3	B	602	DHE	C1C-NC	-8.14	1.38	1.49
3	B	602	DHE	CHB-C1B	-7.81	1.39	1.53
3	A	602	DHE	C1C-NC	-7.68	1.39	1.49
3	A	602	DHE	C3B-C4B	-7.37	1.44	1.55
3	A	602	DHE	C3C-C4C	-7.10	1.45	1.55
2	A	601	HEC	C3C-C2C	-7.04	1.33	1.40
2	B	601	HEC	C3C-C2C	-6.98	1.33	1.40
3	B	602	DHE	C3B-C4B	-6.75	1.45	1.55
2	B	601	HEC	C3B-C2B	-6.50	1.34	1.40
3	B	602	DHE	C3C-C4C	-6.36	1.46	1.55
3	B	602	DHE	CHD-C4C	-6.31	1.37	1.54
3	A	602	DHE	CHD-C4C	-6.28	1.37	1.54
3	A	602	DHE	CHC-C4B	-6.10	1.37	1.52
3	B	602	DHE	CHC-C4B	-6.05	1.38	1.52
3	A	602	DHE	CHB-C4A	-5.71	1.37	1.51
2	A	601	HEC	C3B-C2B	-5.68	1.34	1.40
3	A	602	DHE	C4A-C3A	5.61	1.45	1.38
3	A	602	DHE	C1D-C2D	5.43	1.45	1.38
3	B	602	DHE	CHD-C1D	-5.37	1.38	1.51
3	A	602	DHE	C4D-C3D	5.30	1.45	1.38
3	B	602	DHE	C1D-C2D	5.22	1.45	1.38
3	B	602	DHE	CHB-C4A	-5.19	1.38	1.51
3	B	602	DHE	C4D-C3D	5.03	1.45	1.38
3	A	602	DHE	C1A-C2A	5.02	1.45	1.38
3	A	602	DHE	CHD-C1D	-4.88	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	DHE	C4A-C3A	4.79	1.44	1.38
3	B	602	DHE	C1A-C2A	4.58	1.44	1.38
3	B	602	DHE	C1B-C2B	-4.00	1.44	1.50
3	B	602	DHE	CHC-C1C	-3.93	1.38	1.53
3	A	602	DHE	C1C-C2C	-3.83	1.44	1.50
3	A	602	DHE	CHC-C1C	-3.69	1.39	1.53
3	A	602	DHE	C1B-C2B	-3.52	1.44	1.50
2	B	601	HEC	CBC-CAC	-3.38	1.36	1.49
2	A	601	HEC	CBC-CAC	-3.36	1.36	1.49
3	B	602	DHE	C1C-C2C	-3.36	1.45	1.50
2	B	601	HEC	CBB-CAB	-3.04	1.38	1.49
3	A	602	DHE	CAB-C3B	-3.02	1.51	1.56
3	B	602	DHE	CAA-C2A	2.87	1.56	1.52
2	A	601	HEC	CBB-CAB	-2.85	1.38	1.49
3	B	602	DHE	CAB-C3B	-2.74	1.51	1.56
3	B	602	DHE	CAC-C3C	-2.65	1.51	1.56
2	A	601	HEC	CAD-C3D	2.56	1.55	1.52
2	B	601	HEC	CAD-C3D	2.49	1.55	1.52
3	A	602	DHE	CAA-C2A	2.13	1.55	1.52
3	A	602	DHE	CAC-C3C	-2.08	1.52	1.56
2	A	601	HEC	CAA-C2A	2.07	1.55	1.52
2	A	601	HEC	CMD-C2D	2.06	1.55	1.51
3	B	602	DHE	CAD-C3D	2.05	1.55	1.52

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	DHE	CHC-C1C-NC	11.53	125.27	110.94
3	B	602	DHE	CHC-C1C-NC	10.84	124.41	110.94
3	A	602	DHE	CAA-C2A-C1A	-9.64	120.52	127.30
3	A	602	DHE	CHB-C1B-NB	8.30	126.41	110.75
3	A	602	DHE	C4B-C3B-C2B	8.10	108.54	100.71
3	B	602	DHE	CHB-C1B-NB	7.83	125.51	110.75
3	A	602	DHE	C4C-C3C-C2C	7.63	108.08	100.71
3	B	602	DHE	CAA-C2A-C1A	-7.47	122.05	127.30
3	B	602	DHE	C4B-C3B-C2B	6.87	107.35	100.71
3	B	602	DHE	C4C-C3C-C2C	6.43	106.93	100.71
3	A	602	DHE	C4D-CHA-C1A	5.67	126.71	112.87
3	B	602	DHE	CAD-C3D-C4D	-5.52	123.42	127.30
3	B	602	DHE	C4D-CHA-C1A	5.48	126.24	112.87
3	B	602	DHE	C3C-C4C-NC	5.46	109.48	104.67
3	A	602	DHE	CAD-C3D-C4D	-5.21	123.64	127.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	DHE	CHC-C4B-C3B	4.63	127.43	118.34
2	A	601	HEC	CAD-CBD-CGD	4.61	120.41	112.67
3	A	602	DHE	CHC-C4B-C3B	4.49	127.14	118.34
3	A	602	DHE	CGB-C3B-CAB	4.47	118.12	110.77
3	A	602	DHE	C3C-C4C-NC	4.41	108.56	104.67
3	A	602	DHE	CHA-C1A-C2A	-4.31	124.47	129.68
3	B	602	DHE	C1C-CHC-C4B	3.77	127.22	116.16
3	B	602	DHE	CHB-C1B-C2B	3.73	125.47	114.47
3	B	602	DHE	CAA-CBA-CGA	3.69	118.86	112.67
2	A	601	HEC	CMB-C2B-C3B	3.65	130.12	125.82
3	B	602	DHE	CHC-C1C-C2C	3.64	126.06	114.70
3	A	602	DHE	C3B-C4B-NB	3.59	107.83	104.67
3	A	602	DHE	CHC-C1C-C2C	3.54	125.74	114.70
3	A	602	DHE	CHB-C1B-C2B	3.51	124.81	114.47
3	A	602	DHE	C1C-CHC-C4B	3.48	126.37	116.16
3	B	602	DHE	CHA-C1A-C2A	-3.43	125.54	129.68
2	A	601	HEC	CMB-C2B-C1B	-3.39	123.25	128.46
3	B	602	DHE	CHD-C1D-C2D	-3.22	123.87	129.45
2	B	601	HEC	C4C-C3C-C2C	3.00	109.60	106.35
3	A	602	DHE	OMB-C2B-C3B	2.98	129.71	125.59
3	B	602	DHE	CHA-C4D-C3D	-2.97	126.09	129.68
2	B	601	HEC	CMB-C2B-C1B	-2.94	123.94	128.46
3	A	602	DHE	OMC-C2C-C3C	2.94	129.66	125.59
3	A	602	DHE	CHA-C4D-C3D	-2.91	126.17	129.68
2	B	601	HEC	CAA-CBA-CGA	2.90	117.54	112.67
3	A	602	DHE	CMD-C2D-C3D	2.85	130.31	124.94
2	B	601	HEC	CAD-CBD-CGD	2.80	117.37	112.67
3	B	602	DHE	OMB-C2B-C3B	2.79	129.45	125.59
3	A	602	DHE	CAA-CBA-CGA	2.78	117.33	112.67
2	B	601	HEC	CMB-C2B-C3B	2.76	129.07	125.82
2	B	601	HEC	CMC-C2C-C3C	2.74	129.04	125.82
3	A	602	DHE	CGC-C3C-C2C	-2.70	99.65	106.42
2	B	601	HEC	CMD-C2D-C1D	-2.59	124.49	128.46
2	A	601	HEC	CMA-C3A-C2A	2.57	129.79	124.94
2	A	601	HEC	CMC-C2C-C1C	-2.56	124.52	128.46
2	B	601	HEC	CMC-C2C-C1C	-2.55	124.55	128.46
3	A	602	DHE	CAD-CBD-CGD	2.53	116.92	112.67
2	B	601	HEC	CMA-C3A-C2A	2.50	129.66	124.94
2	A	601	HEC	CMD-C2D-C1D	-2.47	124.67	128.46
3	B	602	DHE	CAD-CBD-CGD	2.45	116.79	112.67
2	B	601	HEC	C4B-C3B-C2B	2.42	108.96	106.35
3	B	602	DHE	C3B-C4B-NB	2.40	106.79	104.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	DHE	CGB-C3B-C2B	-2.36	100.50	106.42
2	A	601	HEC	CAA-CBA-CGA	2.33	116.59	112.67
3	A	602	DHE	CHD-C1D-C2D	-2.32	125.43	129.45
2	A	601	HEC	CMC-C2C-C3C	2.28	128.50	125.82
3	A	602	DHE	CGC-C3C-CAC	-2.25	107.06	110.77
3	B	602	DHE	OMC-C2C-C3C	2.06	128.44	125.59
3	A	602	DHE	CBD-CAD-C3D	2.04	116.24	112.49

There are no chirality outliers.

All (7) torsion outliers are listed below:

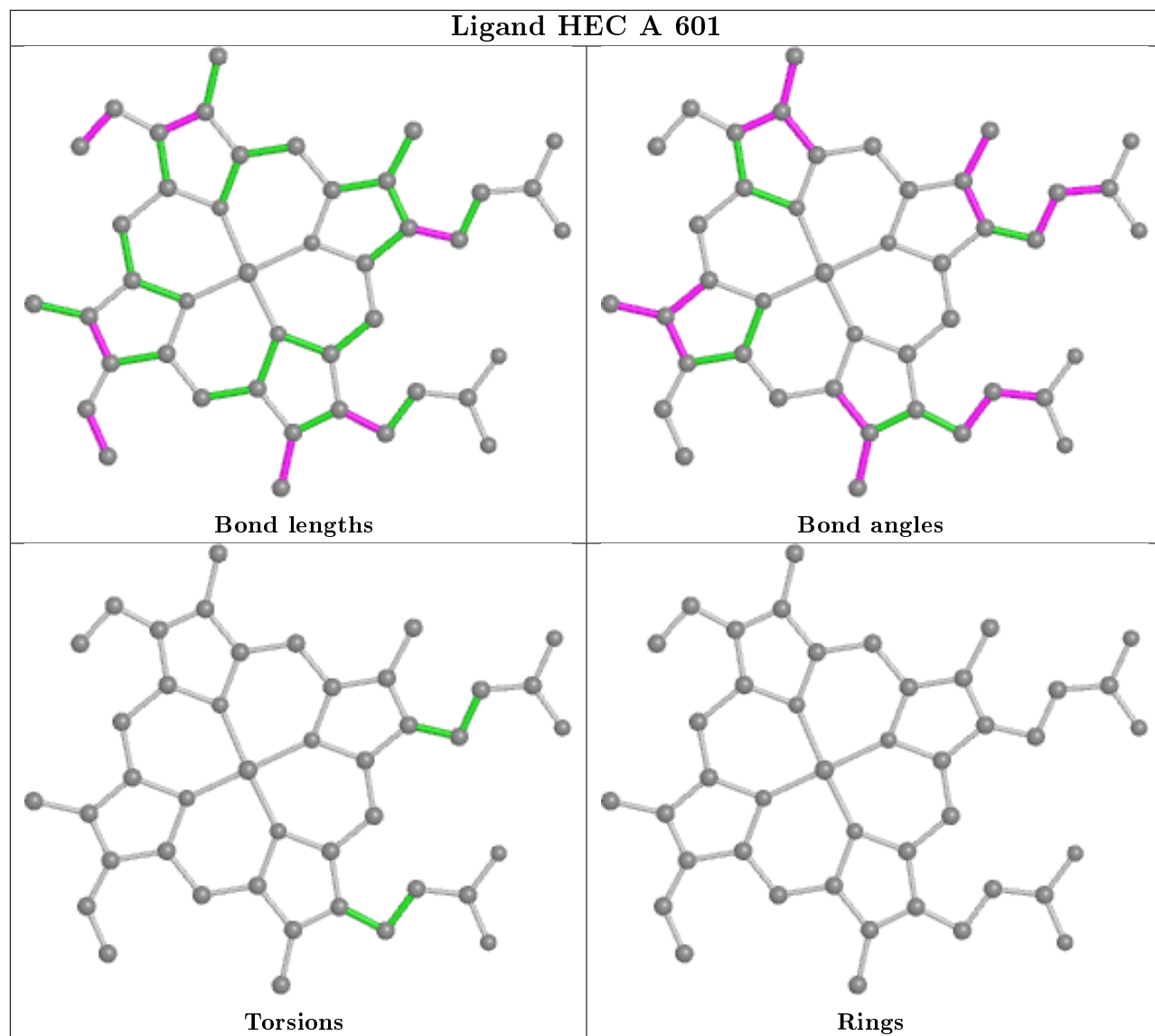
Mol	Chain	Res	Type	Atoms
3	A	602	DHE	C2D-C3D-CAD-CBD
3	A	602	DHE	C4D-C3D-CAD-CBD
3	B	602	DHE	C2D-C3D-CAD-CBD
3	B	602	DHE	C4D-C3D-CAD-CBD
3	B	602	DHE	CGC-C3C-CAC-CBC
3	A	602	DHE	C4B-C3B-CAB-CBB
3	B	602	DHE	CGB-C3B-CAB-CBB

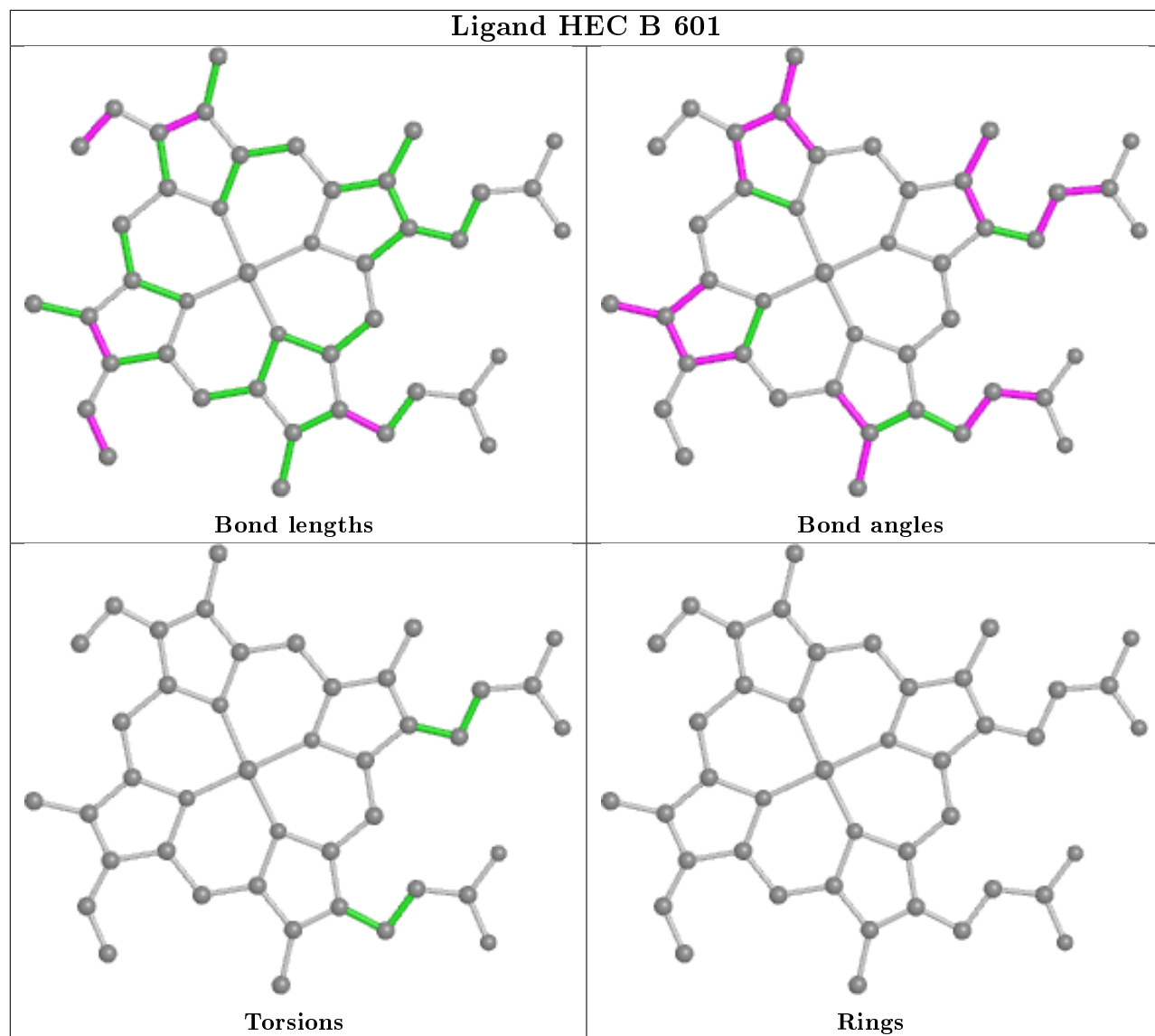
There are no ring outliers.

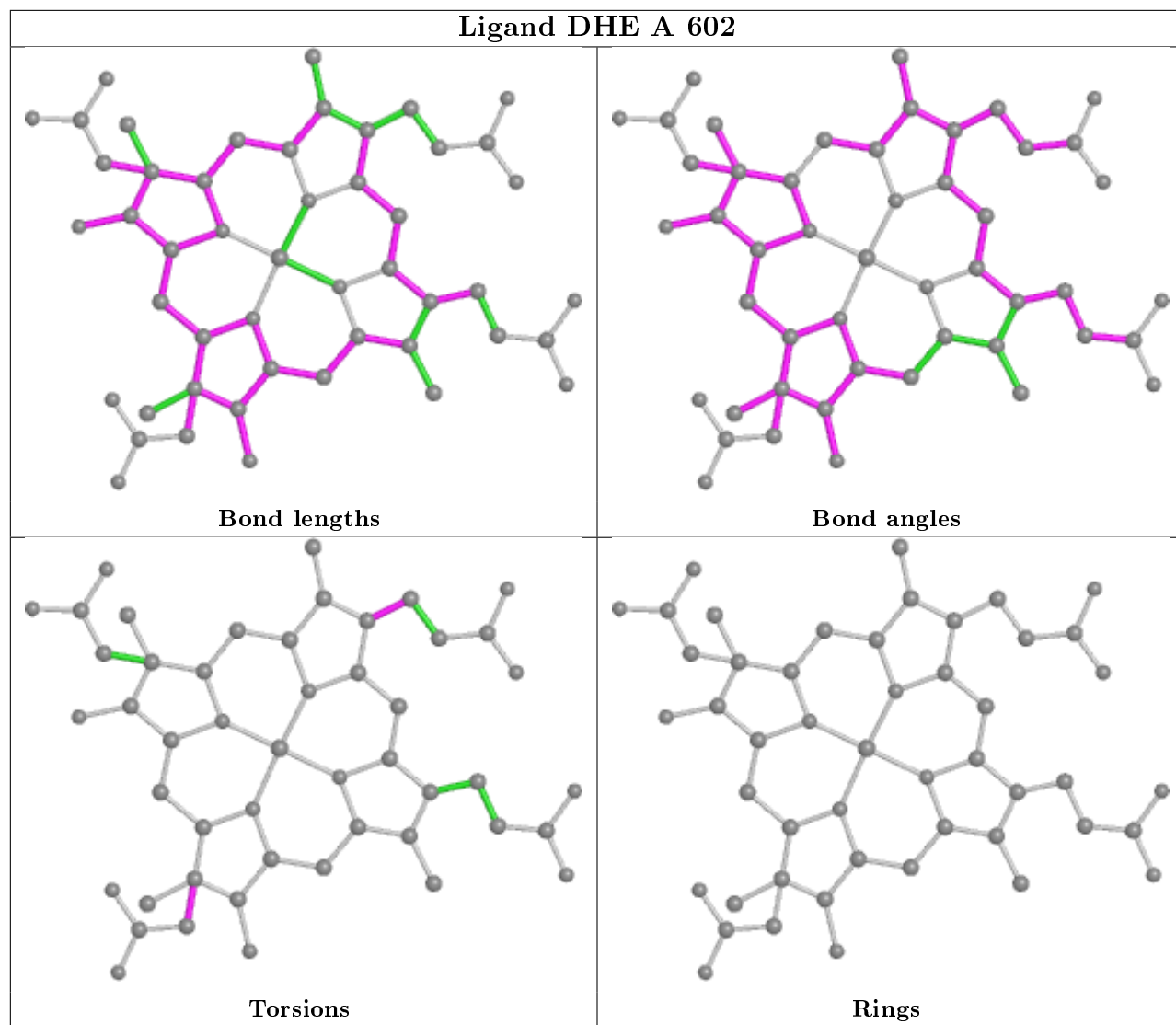
5 monomers are involved in 17 short contacts:

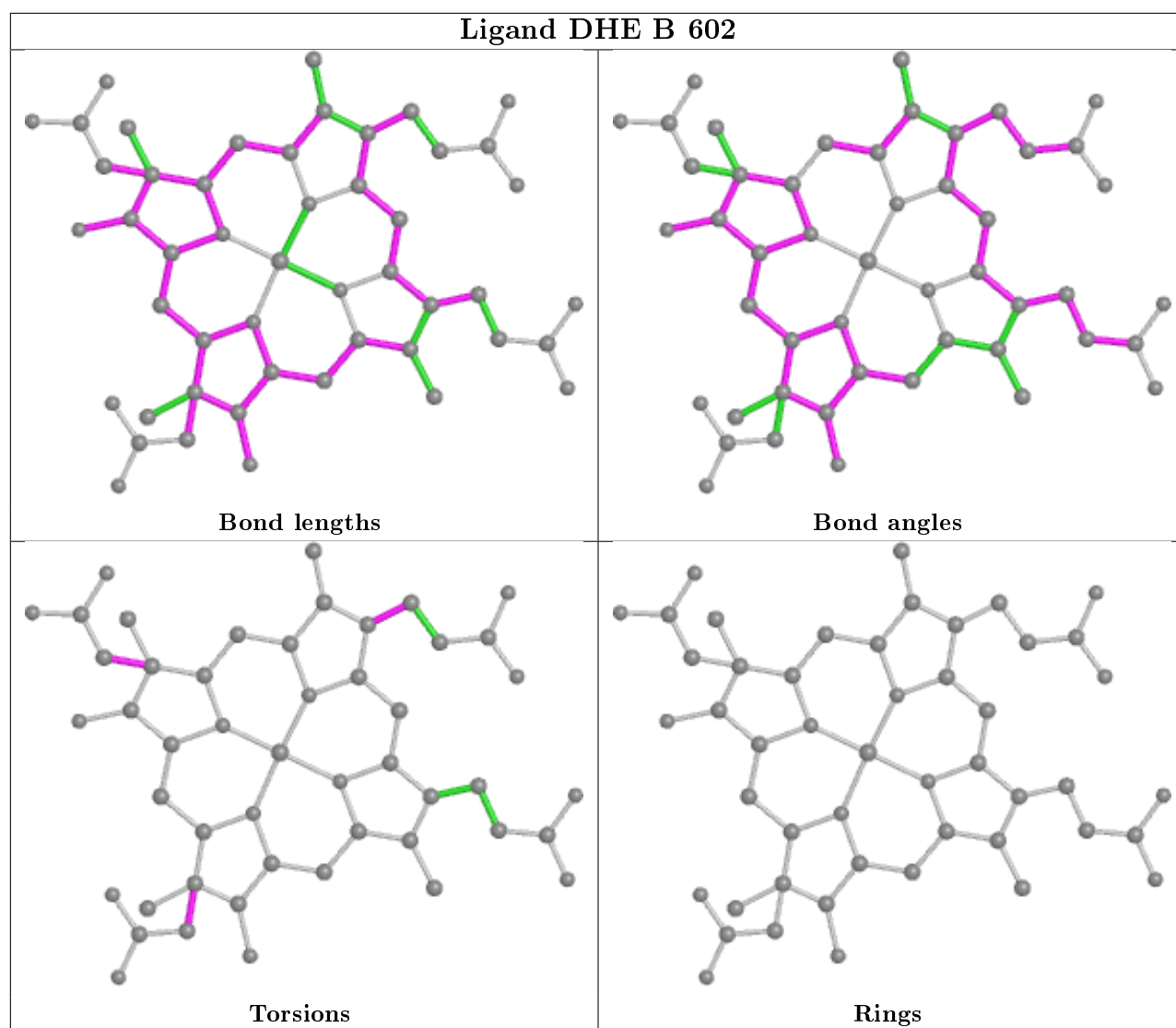
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEC	4	0
5	A	621	SO4	1	0
2	B	601	HEC	4	0
3	A	602	DHE	5	0
3	B	602	DHE	3	0

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.









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, 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	520/567 (91%)	-0.23	11 (2%) 63 61	32, 43, 61, 81	0
1	B	519/567 (91%)	-0.14	12 (2%) 60 58	30, 43, 64, 87	0
All	All	1039/1134 (91%)	-0.18	23 (2%) 62 60	30, 43, 62, 87	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	482	GLY	7.6
1	B	483	SER	6.7
1	A	48	ALA	4.1
1	A	482	GLY	4.0
1	B	484	ASP	4.0
1	A	500	GLU	3.5
1	A	502	GLN	3.0
1	A	127	LEU	3.0
1	B	116	SER	2.9
1	B	49	LEU	2.8
1	A	481	ASP	2.8
1	A	483	SER	2.4
1	B	228	LYS	2.4
1	A	153	GLU	2.4
1	B	87	ARG	2.3
1	B	481	ASP	2.3
1	B	162	ASP	2.2
1	A	499	THR	2.2
1	A	55	ASN	2.2
1	A	526	ASP	2.2
1	B	113	GLY	2.2
1	B	127	LEU	2.1
1	B	117	ALA	2.0

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 carbohydrates in this entry.

6.4 Ligands ⓘ

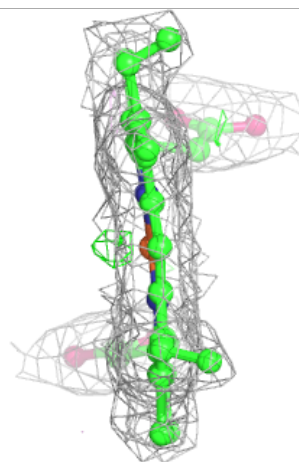
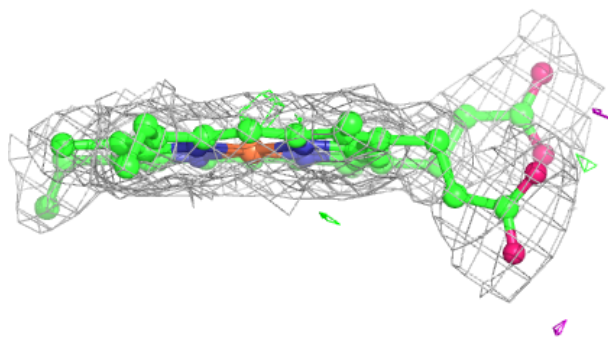
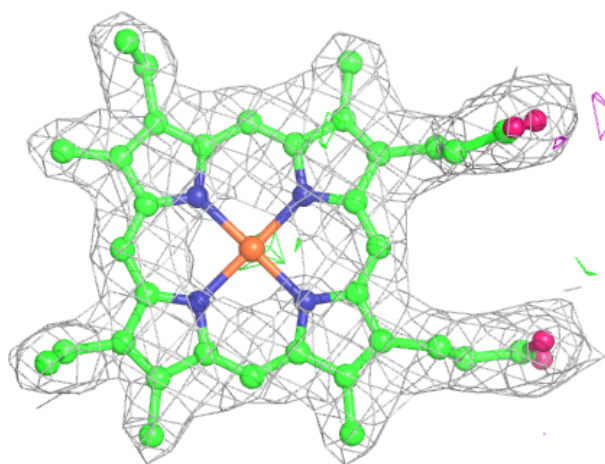
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	B	621	4/5	0.92	0.34	51,54,55,56	0
5	SO4	B	622	5/5	0.94	0.15	65,66,67,67	0
5	SO4	A	621	5/5	0.95	0.33	79,79,80,80	0
2	HEC	B	601	43/43	0.95	0.14	36,40,42,42	0
3	DHE	A	602	49/49	0.95	0.12	35,39,42,46	0
2	HEC	A	601	43/43	0.96	0.12	28,31,36,39	0
3	DHE	B	602	49/49	0.97	0.11	31,35,38,42	0
4	CYN	A	603	2/2	0.98	0.10	30,30,30,31	0
4	CYN	B	603	2/2	0.98	0.12	34,34,34,36	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.

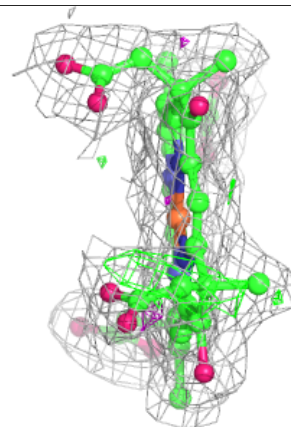
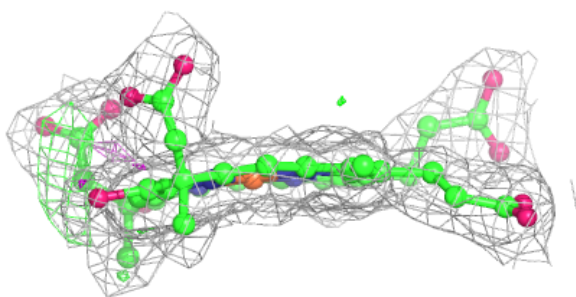
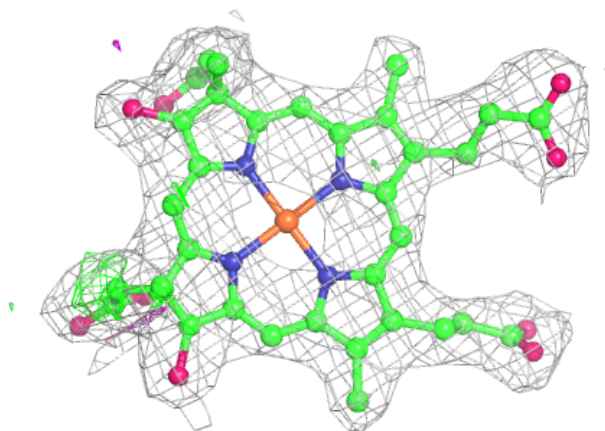
Electron density around HEC B 601:

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



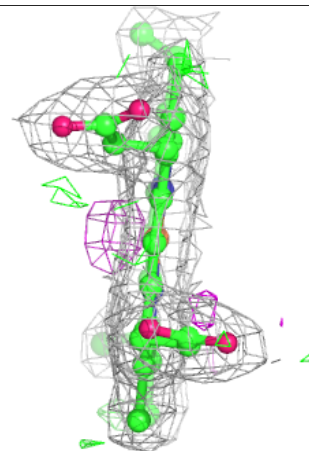
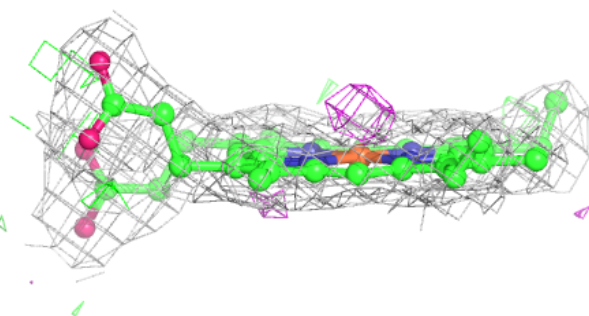
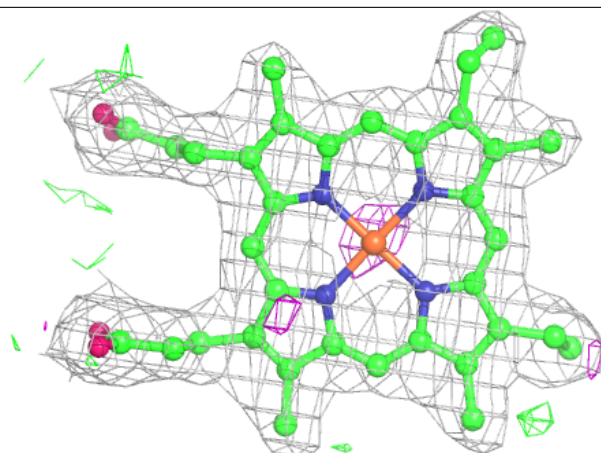
Electron density around DHE A 602:

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

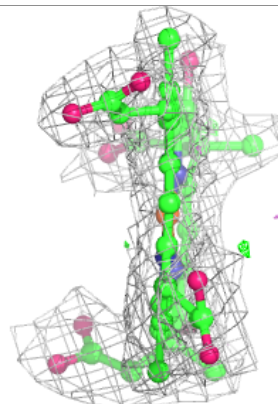
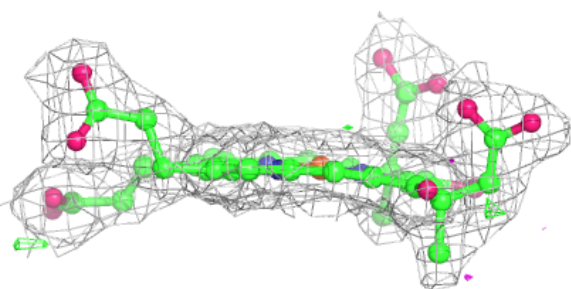
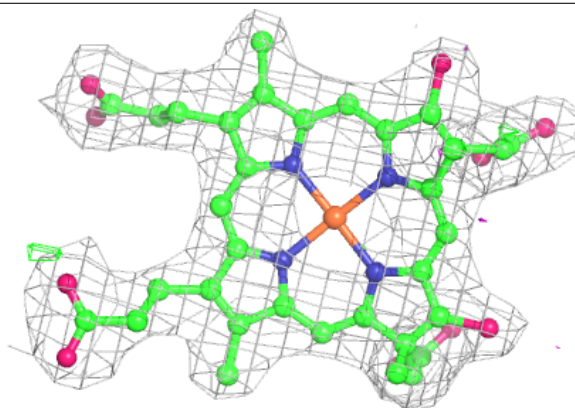


Electron density around HEC A 601:

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

**Electron density around DHE 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.