



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:53 AM UTC

PDB ID : 1H9Y / pdb_00001h9y
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 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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

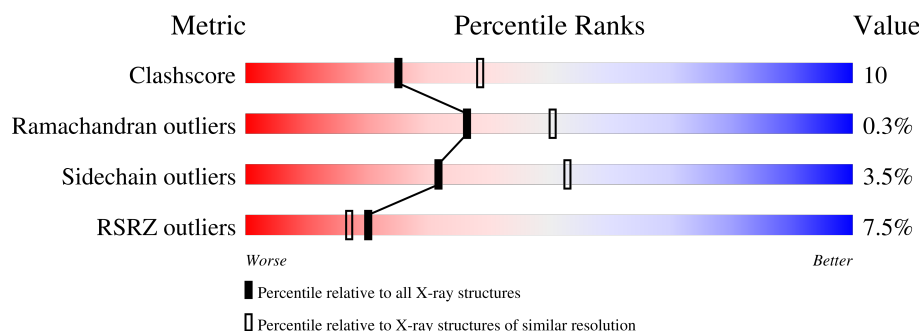
1 Overall quality at a glance

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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	567	5% 72% 17% 8%
1	B	567	9% 67% 22% 8%

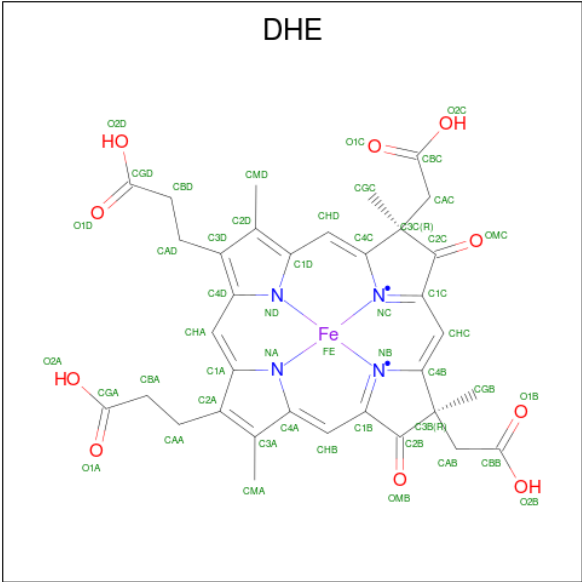
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DHE	A	602	X	-	-	-
3	DHE	B	602	X	-	-	-

Continued on next page...

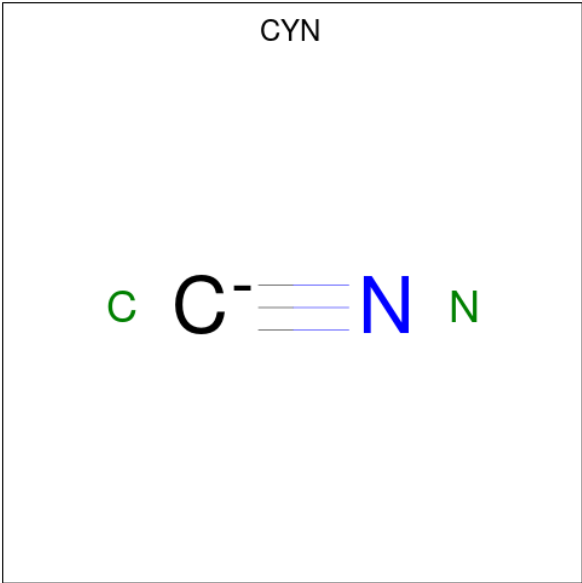
Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	B	621	-	-	X	-



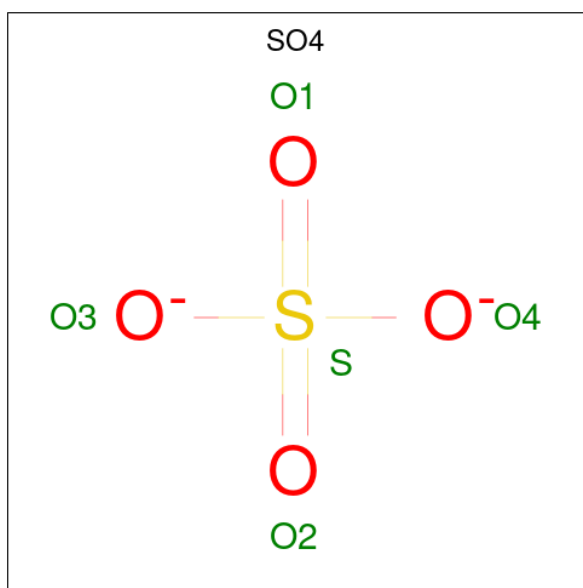
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			49	34	1	4	10		
3	B	1	Total	C	Fe	N	O	0	0
			49	34	1	4	10		

- Molecule 4 is CYANIDE ION (CCD ID: 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 (CCD ID: SO4) (formula: O₄S).



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

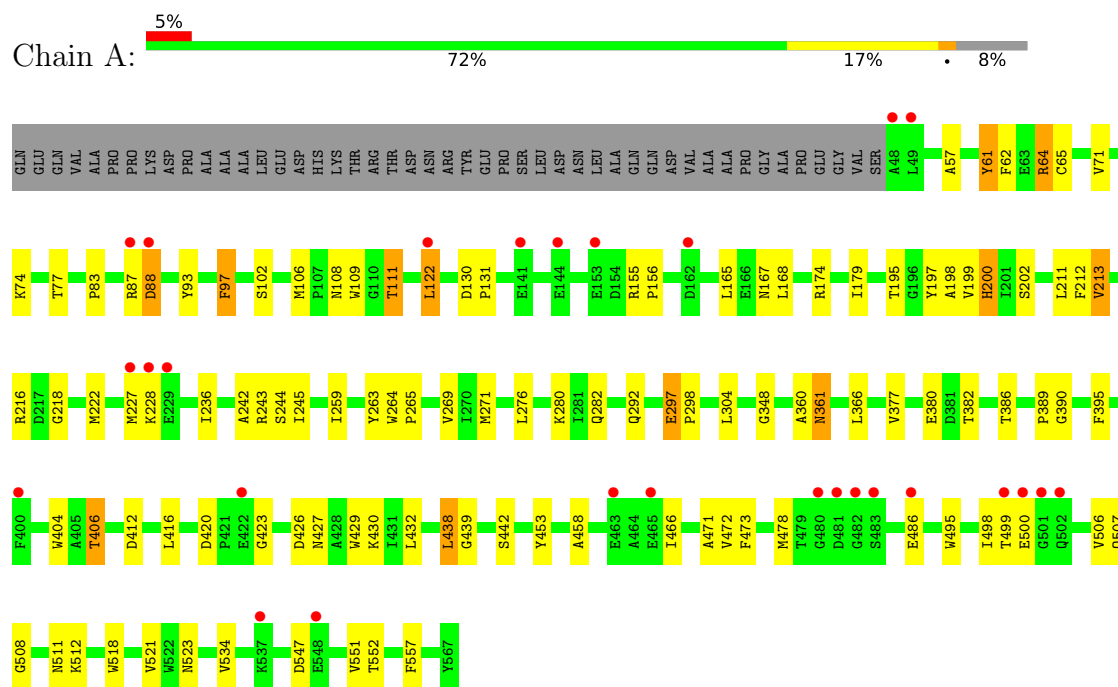
- Molecule 6 is water.

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

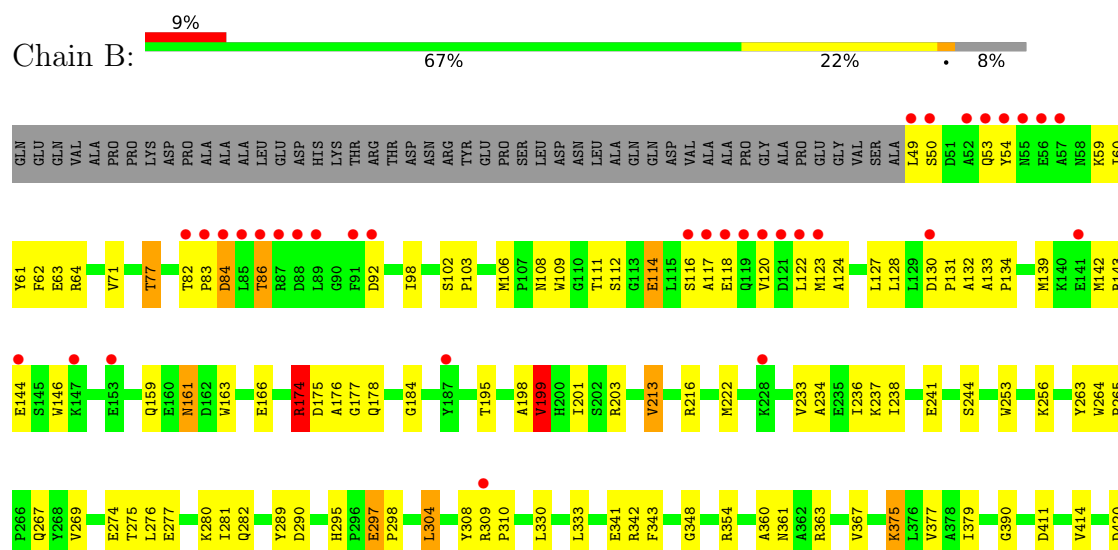
3 Residue-property plots [i](#)

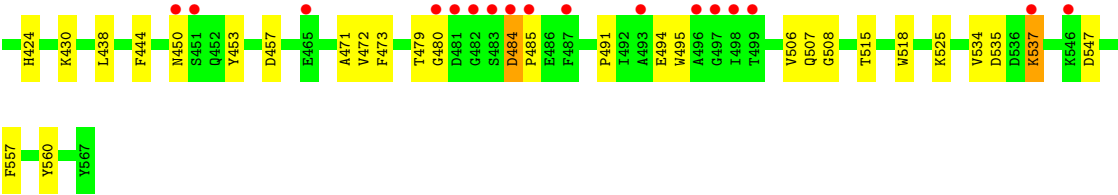
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CYTOCHROME CD1 NITRITE REDUCTASE



• Molecule 1: CYTOCHROME CD1 NITRITE REDUCTASE





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 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.40) 97.5 (20.00-2.40)	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)	0.38 , 31.7	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: SO4, DHE, HEC, CYN

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	0.52	0/4156	1.39	25/5651 (0.4%)
1	B	0.54	0/4151	1.41	27/5644 (0.5%)
All	All	0.53	0/8307	1.40	52/11295 (0.5%)

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	484	ASP	CA-CB-CG	14.85	127.45	112.60
1	B	174	ARG	CD-NE-CZ	11.89	141.05	124.40
1	B	92	ASP	CA-CB-CG	-11.65	100.95	112.60
1	B	199	VAL	CB-CA-C	-8.46	97.42	111.29
1	A	62	PHE	CA-CB-CG	-7.91	105.89	113.80
1	B	62	PHE	CA-CB-CG	-7.78	106.02	113.80
1	A	547	ASP	CA-CB-CG	7.53	120.12	112.60
1	A	361	ASN	N-CA-C	7.21	120.05	111.33
1	B	390	GLY	N-CA-C	-7.20	97.61	110.86
1	B	238	ILE	N-CA-C	7.13	118.99	112.43
1	B	62	PHE	N-CA-C	7.05	118.97	111.28
1	B	244	SER	N-CA-C	6.79	120.53	109.59
1	A	97	PHE	CA-CB-CG	-6.70	107.10	113.80
1	B	118	GLU	N-CA-C	6.62	120.95	112.34
1	A	269	VAL	CB-CA-C	-6.46	100.54	110.50
1	A	263	TYR	N-CA-C	-6.42	104.49	112.90
1	A	390	GLY	N-CA-C	-6.39	100.38	111.50
1	A	174	ARG	N-CA-C	6.31	118.71	111.02
1	B	361	ASN	N-CA-C	6.16	118.50	111.11
1	B	333	LEU	N-CA-C	6.15	118.01	109.15
1	A	557	PHE	CA-CB-CG	-6.14	107.66	113.80
1	A	64	ARG	CD-NE-CZ	6.04	132.86	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	450	ASN	CA-CB-CG	-5.94	106.66	112.60
1	B	263	TYR	N-CA-C	-5.94	104.38	111.69
1	A	360	ALA	N-CA-C	-5.88	97.61	108.24
1	B	361	ASN	CA-CB-CG	5.87	118.47	112.60
1	A	420	ASP	CA-CB-CG	5.77	118.37	112.60
1	B	184	GLY	N-CA-C	5.68	120.92	114.67
1	A	438	LEU	N-CA-C	5.67	117.14	111.07
1	A	77	THR	N-CA-C	-5.62	105.53	112.90
1	A	506	VAL	N-CA-C	5.62	115.76	108.35
1	B	84	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	395	PHE	CA-CB-CG	5.60	119.40	113.80
1	B	77	THR	N-CA-C	-5.59	104.81	111.69
1	A	88	ASP	CA-CB-CG	-5.51	107.09	112.60
1	B	77	THR	CB-CA-C	5.47	120.71	110.70
1	B	124	ALA	N-CA-C	-5.46	104.18	112.04
1	A	404	TRP	CA-CB-CG	5.46	123.97	113.60
1	B	411	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	506	VAL	N-CA-C	5.37	116.39	108.45
1	B	360	ALA	N-CA-C	-5.34	98.57	108.24
1	A	244	SER	N-CA-C	5.27	117.82	109.50
1	B	414	VAL	CA-C-O	-5.21	114.92	120.39
1	A	87	ARG	NE-CZ-NH2	-5.20	114.52	119.20
1	A	390	GLY	CA-C-O	-5.08	115.27	121.68
1	B	457	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	61	TYR	CA-CB-CG	-5.04	104.82	113.90
1	A	297	GLU	N-CA-C	5.04	116.81	109.30
1	B	267	GLN	O-C-N	5.03	128.44	123.46
1	B	547	ASP	CA-CB-CG	5.01	117.61	112.60
1	A	200	HIS	CE1-NE2-CD2	-5.01	103.99	109.00
1	A	423	GLY	O-C-N	-5.01	116.40	122.71

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	63	0
1	B	4051	0	3908	90	0
2	A	43	0	30	3	0
2	B	43	0	30	4	0
3	A	49	0	28	5	0
3	B	49	0	28	2	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	158	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 10.

All (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: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
1:B:222:MET:HE2	1:B:234:ALA:HB3	1.52	0.92
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:A:222:MET:HE3	1:A:276:LEU:HG	1.58	0.83
1:B:159:GLN:HE21	1:B:161:ASN:ND2	1.79	0.81
1:B:222:MET:HE3	1:B:233:VAL:HG23	1.66	0.77
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: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:B:537:LYS:HZ2	1:B:537:LYS:H	1.40	0.69
1:A:167:ASN:HD22	1:A:512:LYS:H	1.44	0.66
1:A:271:MET:HE2	1:A:276:LEU:HD22	1.78	0.66
1:B:109:TRP:CE2	2:B:601:HEC:HBB2	2.31	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LYS:HE2	1:A:282:GLN:NE2	2.14	0.62
1:A:236:ILE:HG21	1:A:271:MET:HE3	1.81	0.62
1:B:49:LEU:HD22	1:B:122:LEU:HD23	1.82	0.62
1:B:537:LYS:H	1:B:537:LYS:NZ	1.97	0.61
1:A:416:LEU:HD11	1:A:478:MET:HE1	1.82	0.61
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
1:A:236:ILE:HG21	1:A:271:MET:CE	2.34	0.58
1:A:155:ARG:HB3	1:A:156:PRO:HD2	1.86	0.57
1:B:222:MET:HE2	1:B:234:ALA:CB	2.29	0.56
1:B:280:LYS:HE3	1:B:330:LEU:O	2.06	0.56
1:B:222:MET:HE1	1:B:274:GLU:O	2.06	0.55
1:B:82:THR:O	1:B:86:THR:HB	2.07	0.54
1:A:57:ALA:HB2	1:A:122:LEU:HD22	1.90	0.53
1:B:142:MET:HE1	1:B:281:ILE:HD12	1.89	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:B:116:SER:O	1:B:117:ALA:C	2.51	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:B:177:GLY:HA2	1:B:199:VAL:HG22	1.93	0.51
1:A:197:TYR:O	1:A:198:ALA:HB3	2.11	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: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:86:THR:CG2	1:B:128:LEU:HA	2.41	0.50
1:B:280:LYS:NZ	1:B:282:GLN:HE22	2.10	0.50
1:B:308:TYR:CE1	1:B:354:ARG:HB2	2.47	0.49
1:B:309:ARG:HB3	1:B:310:PRO:HD2	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
1:A:264:TRP:HA	1:A:265:PRO:C	2.36	0.48
1:A:389:PRO:HB3	1:A:406:THR:HB	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:264:TRP:HA	1:B:265:PRO:C	2.38	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:A:292:GLN:HB2	1:B:139:MET:HB2	1.97	0.46
1:B:102:SER:HB2	1:B:103:PRO:HD2	1.96	0.46
1:A:243:ARG:HH21	3:A:602:DHE:CBB	2.27	0.46
3:A:602:DHE:HMD3	3:A:602:DHE:HBD2	1.98	0.46
1:B:166:GLU:HB3	1:B:560:TYR:HB2	1.98	0.46
1:B:176:ALA:O	1:B:178:GLN:HG3	2.16	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:222:MET:HE3	1:B:233:VAL:CG2	2.41	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
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:175:ASP:HB3	1:B:525:LYS:HD2	1.99	0.45
1:B:289:TYR:CZ	1:B:290:ASP:HB3	2.52	0.45
1:A:212:PHE:CE2	1:A:222:MET:HE2	2.52	0.45
1:B:98:ILE:HB	1:B:120:VAL:HG13	1.99	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:B:61:TYR:HB2	1:B:123:MET:HE1	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:VAL:HG22	1:B:241:GLU:OE2	2.19	0.43
1:B:236:ILE:HG12	1:B:237:LYS:H	1.82	0.43
1:B:59:LYS:O	1:B:63:GLU:HG3	2.18	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:A:243:ARG:HG3	3:A:602:DHE:HHB	1.99	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:61:TYR:CD1	1:A:65:CYS:HB2	2.53	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:B:275:THR:O	1:B:276:LEU:HB2	2.18	0.43
1:A:198:ALA:O	1:A:199:VAL:C	2.62	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:O4	5:B:621:SO4:O2	2.37	0.42
1:B:264:TRP:CD2	1:B:265:PRO:HA	2.54	0.42
1:B:280:LYS:HZ3	1:B:282:GLN:HE22	1.67	0.42
1:B:473:PHE:CD2	1:B:485:PRO:HB2	2.54	0.42
5:B:621:SO4:O3	5:B:621:SO4:O2	2.37	0.42
1:B:130:ASP:HA	1:B:131:PRO:HD3	1.87	0.42
1:A:271:MET:HE2	1:A:276:LEU:CD2	2.48	0.42
1:A:280:LYS:HE2	1:A:282:GLN:HE22	1.85	0.42
1:B:479:THR:OG1	1:B:480:GLY:N	2.52	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:83:PRO:O	1:B:84:ASP:C	2.63	0.41
1:B:297:GLU:N	1:B:298:PRO:HD3	2.34	0.41
1:A:93:TYR:CD1	1:A:93:TYR:C	2.98	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:MET:HE3	1:A:276:LEU:CG	2.40	0.41
1:A:453:TYR:HB3	1:A:472:VAL:CG1	2.51	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: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:A:551:VAL:O	1:A:552:THR:C	2.62	0.40
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:106:MET:HB2	2:B:601:HEC:C1D	2.51	0.40
1:B:444:PHE:CE1	3:B:602:DHE:HBD1	2.57	0.40
5:B:621:SO4:O3	5:B:621:SO4:O1	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%)	43	58
1	B	517/567 (91%)	491 (95%)	24 (5%)	2 (0%)	30	43
All	All	1035/1134 (91%)	981 (95%)	51 (5%)	3 (0%)	36	50

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%)	417 (96%)	15 (4%)	32	53
1	B	432/469 (92%)	417 (96%)	15 (4%)	32	53
All	All	864/938 (92%)	834 (96%)	30 (4%)	32	53

All (30) 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	228	LYS
1	A	377	VAL
1	A	406	THR
1	A	486	GLU
1	A	499	THR
1	A	500	GLU
1	B	77	THR
1	B	86	THR
1	B	114	GLU
1	B	144	GLU
1	B	161	ASN
1	B	174	ARG
1	B	199	VAL
1	B	213	VAL
1	B	269	VAL
1	B	297	GLU
1	B	304	LEU
1	B	375	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	377	VAL
1	B	430	LYS
1	B	537	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	282	GLN
1	A	450	ASN
1	A	561	ASN
1	B	53	GLN
1	B	158	GLN
1	B	161	ASN
1	B	221	ASN
1	B	282	GLN
1	B	424	HIS
1	B	527	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 oligosaccharides 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
3	DHE	A	602	1,4	52,56,56	4.51	11 (21%)	68,94,94	3.25	21 (30%)
5	SO4	A	621	-	4,4,4	0.71	0	6,6,6	0.31	0
4	CYN	B	603	3	1,1,1	0.25	0	-		
4	CYN	A	603	3	1,1,1	0.25	0	-		
5	SO4	B	622	-	4,4,4	0.71	0	6,6,6	0.34	0
2	HEC	B	601	1	46,50,50	1.97	10 (21%)	58,82,82	1.78	5 (8%)
2	HEC	A	601	1	46,50,50	1.99	8 (17%)	58,82,82	1.65	5 (8%)
3	DHE	B	602	1,4	52,56,56	4.38	9 (17%)	68,94,94	2.82	15 (22%)

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	B	601	1	-	5/14/54/54	-
3	DHE	A	602	1,4	1/1/15/19	7/20/108/108	-
2	HEC	A	601	1	-	6/14/54/54	-
3	DHE	B	602	1,4	1/1/15/19	8/20/108/108	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	DHE	OMB-C2B	18.15	1.53	1.22
3	A	602	DHE	OMC-C2C	18.15	1.53	1.22
3	B	602	DHE	OMC-C2C	17.93	1.53	1.22
3	B	602	DHE	OMB-C2B	17.92	1.53	1.22
3	A	602	DHE	C3B-C2B	-11.35	1.33	1.52
3	A	602	DHE	C3C-C2C	-10.97	1.33	1.52
3	B	602	DHE	C3C-C2C	-10.72	1.34	1.52
3	B	602	DHE	C3B-C2B	-10.14	1.35	1.52
2	A	601	HEC	CAC-C3C	7.37	1.58	1.35
2	B	601	HEC	CAC-C3C	7.34	1.58	1.35
2	B	601	HEC	CAB-C3B	7.11	1.58	1.35
2	A	601	HEC	CAB-C3B	6.79	1.57	1.35
3	A	602	DHE	CAC-CBC	-6.16	1.32	1.50
3	A	602	DHE	CAB-CBB	-6.14	1.32	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	DHE	CAC-CBC	-5.88	1.32	1.50
3	B	602	DHE	CAB-CBB	-5.85	1.33	1.50
2	B	601	HEC	CBC-CAC	-3.42	1.36	1.49
2	A	601	HEC	CBC-CAC	-3.40	1.36	1.49
2	B	601	HEC	CBB-CAB	-3.08	1.38	1.49
3	B	602	DHE	FE-NC	2.97	2.04	1.94
2	A	601	HEC	CBB-CAB	-2.89	1.38	1.49
3	A	602	DHE	FE-NC	2.84	2.03	1.94
2	A	601	HEC	CMD-C2D	2.51	1.55	1.50
2	A	601	HEC	CMC-C2C	2.42	1.55	1.50
2	B	601	HEC	CMD-C2D	2.30	1.55	1.50
2	A	601	HEC	C3C-C2C	-2.30	1.33	1.41
3	A	602	DHE	FE-NB	2.30	2.02	1.94
3	B	602	DHE	C1B-C2B	-2.29	1.44	1.47
2	B	601	HEC	C3C-C2C	-2.28	1.33	1.41
3	A	602	DHE	FE-NA	2.21	2.02	1.95
3	B	602	DHE	FE-ND	2.18	2.02	1.95
2	A	601	HEC	CMA-C3A	2.18	1.55	1.50
3	A	602	DHE	CMD-C2D	2.15	1.55	1.50
3	A	602	DHE	C1C-C2C	-2.13	1.44	1.47
2	B	601	HEC	C3B-C2B	-2.13	1.34	1.41
2	B	601	HEC	CMB-C2B	2.05	1.55	1.50
2	B	601	HEC	CMA-C3A	2.02	1.54	1.50
2	B	601	HEC	CMC-C2C	2.00	1.54	1.50

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	DHE	C2B-C3B-C4B	15.43	108.54	100.35
3	A	602	DHE	C2C-C3C-C4C	14.57	108.08	100.35
3	B	602	DHE	C2B-C3B-C4B	13.19	107.35	100.35
3	B	602	DHE	C2C-C3C-C4C	12.40	106.93	100.35
2	A	601	HEC	CBB-CAB-C3B	-8.12	111.21	127.43
2	B	601	HEC	CBB-CAB-C3B	-7.67	112.11	127.43
2	B	601	HEC	CBC-CAC-C3C	-7.62	112.21	127.43
2	A	601	HEC	CBC-CAC-C3C	-6.03	115.38	127.43
3	A	602	DHE	C3C-C4C-CHD	5.74	127.55	122.44
3	B	602	DHE	C3B-C4B-CHC	5.61	127.43	122.44
3	A	602	DHE	C3B-C4B-CHC	5.29	127.14	122.44
3	A	602	DHE	CAB-C3B-C2B	4.30	117.02	112.22
3	B	602	DHE	O2B-CBB-O1B	-4.24	112.44	123.33
3	A	602	DHE	CGC-C3C-C2C	-3.96	99.65	109.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	DHE	CGB-C3B-C2B	-3.62	100.50	109.38
3	A	602	DHE	OMB-C2B-C1B	-3.59	122.62	126.49
3	A	602	DHE	OMC-C2C-C1C	-3.58	122.64	126.49
3	B	602	DHE	O2C-CBC-CAC	3.56	125.64	114.35
3	B	602	DHE	O2B-CBB-CAB	3.55	125.61	114.35
3	B	602	DHE	O2C-CBC-O1C	-3.53	114.25	123.33
3	B	602	DHE	CHC-C1C-C2C	3.43	126.06	122.21
3	A	602	DHE	OMB-C2B-C3B	3.21	129.71	125.93
3	B	602	DHE	OMB-C2B-C1B	-3.21	123.03	126.49
3	A	602	DHE	OMC-C2C-C3C	3.16	129.66	125.93
3	A	602	DHE	CHC-C1C-C2C	3.14	125.74	122.21
2	B	601	HEC	O1D-CGD-CBD	-3.09	113.29	123.09
3	B	602	DHE	OMB-C2B-C3B	2.99	129.45	125.93
3	B	602	DHE	CHB-C1B-C2B	2.91	125.47	122.21
3	A	602	DHE	CGB-C3B-C4B	-2.74	99.33	109.93
3	B	602	DHE	OMC-C2C-C1C	-2.71	123.57	126.49
3	B	602	DHE	C3C-C4C-CHD	2.68	124.83	122.44
3	A	602	DHE	O2C-CBC-CAC	2.65	122.74	114.35
3	A	602	DHE	O2C-CBC-O1C	-2.61	116.61	123.33
2	A	601	HEC	CAD-CBD-CGD	2.54	120.41	113.67
3	A	602	DHE	CMD-C2D-C1D	-2.39	121.78	125.42
3	A	602	DHE	CHB-C1B-C2B	2.32	124.81	122.21
3	A	602	DHE	CAC-C3C-C2C	2.31	114.79	112.22
3	B	602	DHE	CAC-C3C-C2C	2.27	114.74	112.22
3	A	602	DHE	O2B-CBB-CAB	2.25	121.47	114.35
2	A	601	HEC	O1D-CGD-CBD	-2.24	115.98	123.09
3	A	602	DHE	CMD-C2D-C3D	2.21	130.31	125.62
2	B	601	HEC	CHC-C4B-NB	2.18	126.83	124.45
3	B	602	DHE	OMC-C2C-C3C	2.13	128.44	125.93
3	A	602	DHE	CAA-C2A-C1A	-2.13	120.52	124.85
2	B	601	HEC	O1A-CGA-CBA	-2.11	116.39	123.09
2	A	601	HEC	O1A-CGA-CBA	-2.04	116.61	123.09

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	602	DHE	NA
3	B	602	DHE	NA

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	HEC	C2C-C3C-CAC-CBC
2	A	601	HEC	C4C-C3C-CAC-CBC
2	B	601	HEC	C2C-C3C-CAC-CBC
2	B	601	HEC	C4C-C3C-CAC-CBC
3	A	602	DHE	C4B-C3B-CAB-CBB
3	A	602	DHE	C2D-C3D-CAD-CBD
3	A	602	DHE	C4D-C3D-CAD-CBD
3	B	602	DHE	C3B-CAB-CBB-O1B
3	B	602	DHE	C2D-C3D-CAD-CBD
3	A	602	DHE	C3B-CAB-CBB-O2B
3	A	602	DHE	C3B-CAB-CBB-O1B
3	A	602	DHE	C3C-CAC-CBC-O2C
3	B	602	DHE	C3B-CAB-CBB-O2B
3	B	602	DHE	C3C-CAC-CBC-O1C
3	B	602	DHE	C3C-CAC-CBC-O2C
2	A	601	HEC	C4B-C3B-CAB-CBB
2	B	601	HEC	C4B-C3B-CAB-CBB
2	A	601	HEC	C2B-C3B-CAB-CBB
2	B	601	HEC	C2B-C3B-CAB-CBB
3	A	602	DHE	C3C-CAC-CBC-O1C
3	B	602	DHE	C4D-C3D-CAD-CBD
2	A	601	HEC	CAA-CBA-CGA-O2A
2	A	601	HEC	CAA-CBA-CGA-O1A
3	B	602	DHE	CAD-CBD-CGD-O1D
3	B	602	DHE	CAD-CBD-CGD-O2D
2	B	601	HEC	CAA-CBA-CGA-O2A

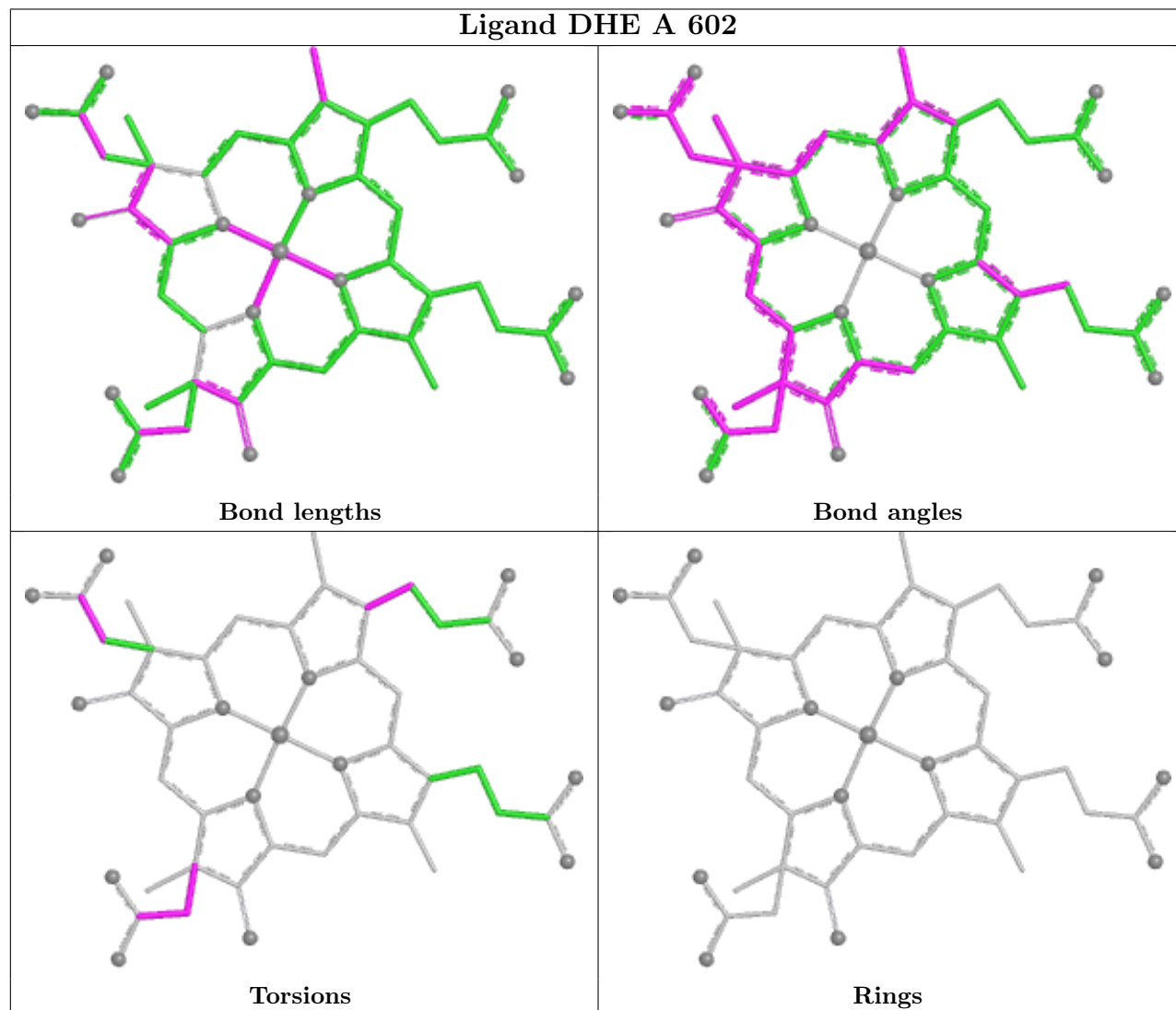
There are no ring outliers.

5 monomers are involved in 15 short contacts:

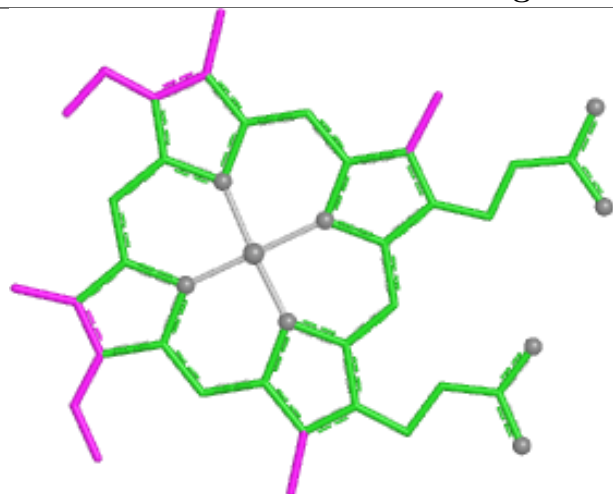
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	DHE	5	0
5	A	621	SO4	1	0
2	B	601	HEC	4	0
2	A	601	HEC	3	0
3	B	602	DHE	2	0

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 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

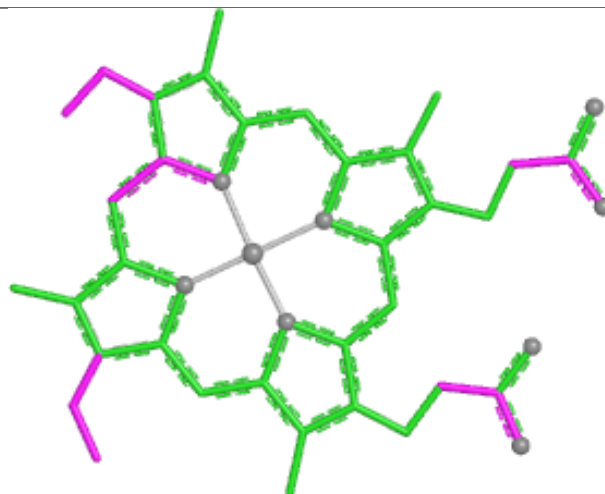
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



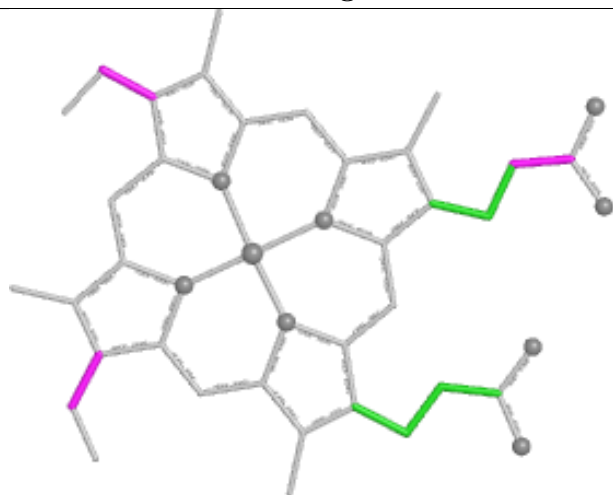
Ligand HEC B 601



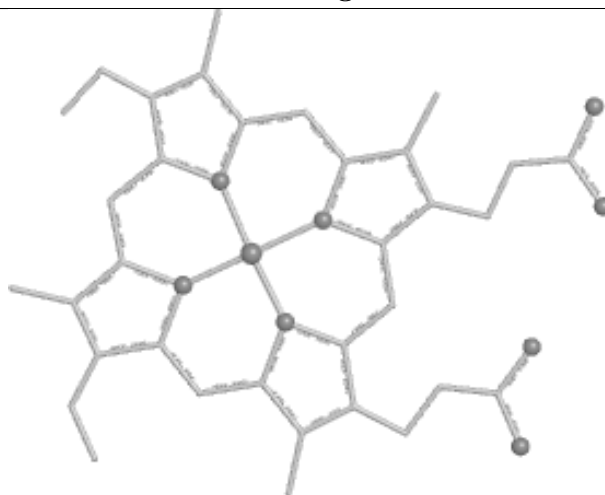
Bond lengths



Bond angles

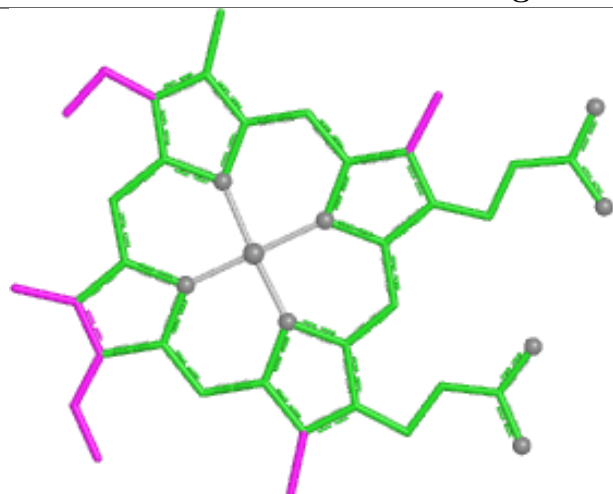


Torsions

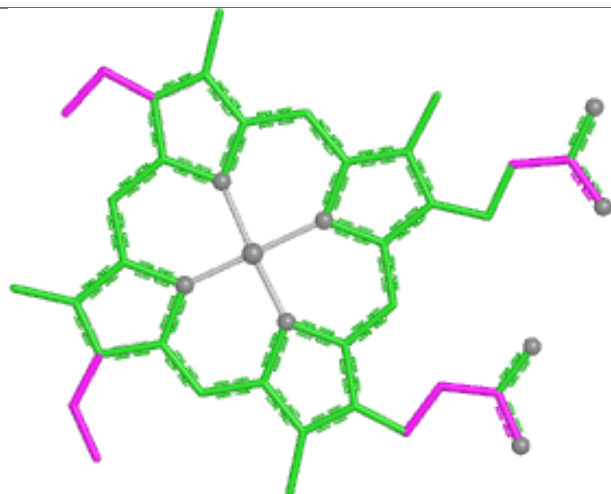


Rings

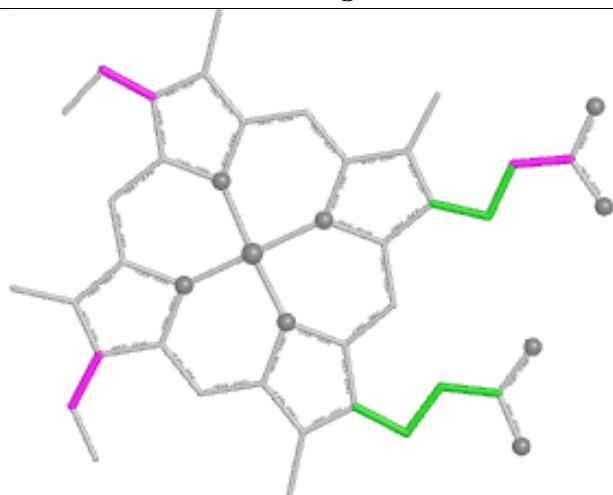
Ligand HEC A 601



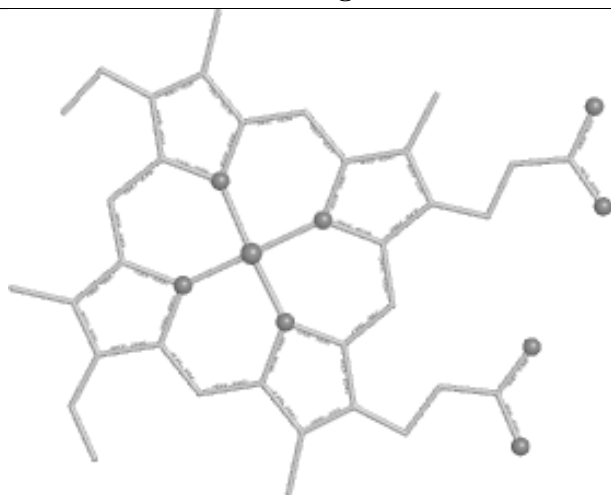
Bond lengths



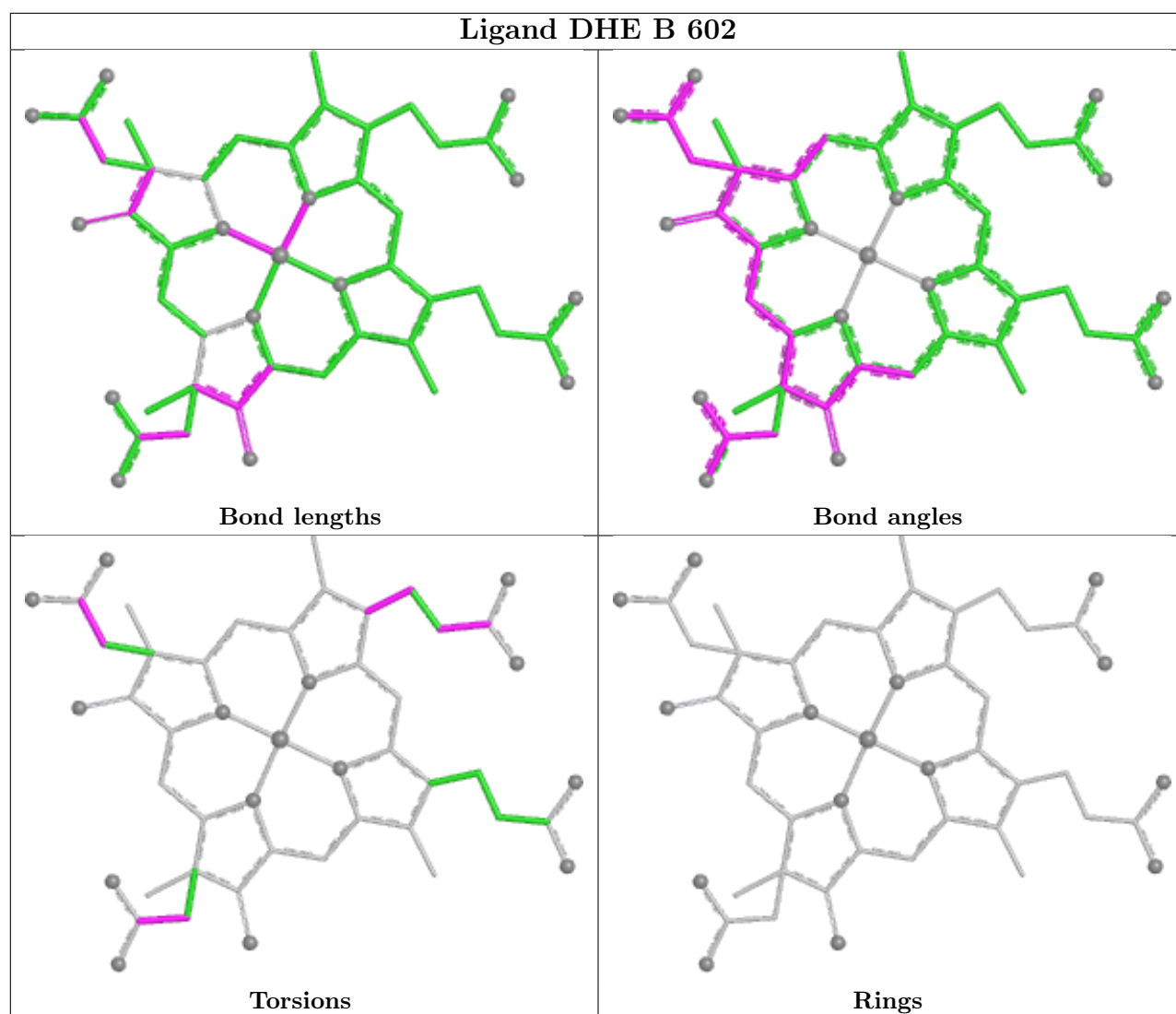
Bond angles



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, 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%)	0.27	27 (5%)	33 29	32, 43, 61, 81	0
1	B	519/567 (91%)	0.44	51 (9%)	13 10	30, 43, 64, 87	0
All	All	1039/1134 (91%)	0.35	78 (7%)	20 17	30, 43, 62, 87	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	482	GLY	11.3
1	A	48	ALA	7.1
1	B	484	ASP	6.5
1	B	483	SER	6.4
1	B	480	GLY	6.4
1	B	49	LEU	5.7
1	A	500	GLU	5.2
1	B	84	ASP	5.0
1	A	480	GLY	5.0
1	A	502	GLN	4.9
1	B	54	TYR	4.7
1	B	497	GLY	4.5
1	B	116	SER	4.5
1	B	499	THR	4.2
1	B	498	ILE	4.1
1	B	451	SER	4.1
1	A	153	GLU	4.0
1	B	91	PHE	4.0
1	B	87	ARG	3.5
1	B	117	ALA	3.5
1	B	120	VAL	3.5
1	A	499	THR	3.4
1	A	87	ARG	3.4
1	B	130	ASP	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	57	ALA	3.2
1	B	144	GLU	3.2
1	A	548	GLU	3.2
1	B	450	ASN	3.1
1	B	119	GLN	3.1
1	B	52	ALA	3.1
1	A	144	GLU	3.0
1	B	118	GLU	3.0
1	B	53	GLN	3.0
1	B	121	ASP	2.9
1	B	123	MET	2.9
1	A	481	ASP	2.8
1	B	141	GLU	2.8
1	B	481	ASP	2.8
1	B	147	LYS	2.7
1	A	483	SER	2.7
1	B	50	SER	2.7
1	B	122	LEU	2.6
1	B	153	GLU	2.6
1	A	501	GLY	2.6
1	B	82	THR	2.6
1	B	86	THR	2.6
1	A	122	LEU	2.5
1	A	88	ASP	2.5
1	A	141	GLU	2.4
1	B	496	ALA	2.4
1	B	83	PRO	2.4
1	B	228	LYS	2.4
1	B	88	ASP	2.4
1	B	187	TYR	2.4
1	B	465	GLU	2.4
1	B	85	LEU	2.4
1	B	493	ALA	2.4
1	A	229	GLU	2.4
1	A	486	GLU	2.4
1	A	465	GLU	2.3
1	A	482	GLY	2.3
1	A	49	LEU	2.3
1	A	537	LYS	2.3
1	A	463	GLU	2.3
1	B	537	LYS	2.2
1	B	56	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	309	ARG	2.2
1	B	546	LYS	2.2
1	A	162	ASP	2.2
1	B	92	ASP	2.2
1	A	400	PHE	2.2
1	B	55	ASN	2.2
1	B	89	LEU	2.2
1	A	422	GLU	2.2
1	B	487	PHE	2.2
1	B	485	PRO	2.1
1	A	227	MET	2.1
1	A	228	LYS	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 oligosaccharides in this entry.

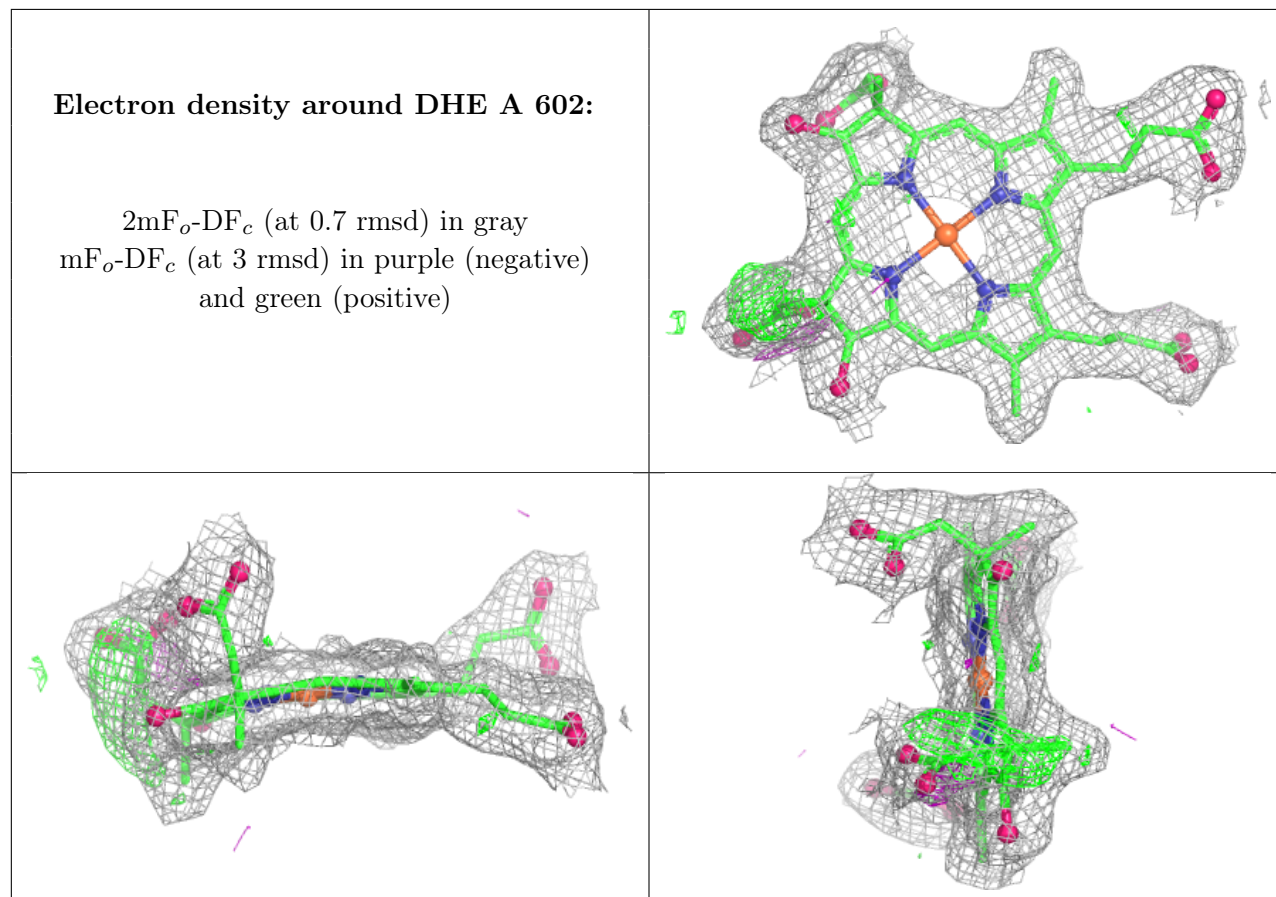
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	B	621	4/5	0.80	0.38	51,54,55,56	0
5	SO4	A	621	5/5	0.91	0.27	79,79,80,80	0
5	SO4	B	622	5/5	0.91	0.14	65,66,67,67	0
3	DHE	A	602	49/49	0.95	0.10	35,39,42,46	0
4	CYN	A	603	2/2	0.97	0.07	30,30,30,31	0
3	DHE	B	602	49/49	0.97	0.08	31,35,38,42	0
2	HEC	B	601	43/43	0.98	0.08	36,40,42,42	0
2	HEC	A	601	43/43	0.98	0.07	28,31,36,39	0
4	CYN	B	603	2/2	0.98	0.06	34,34,34,36	0

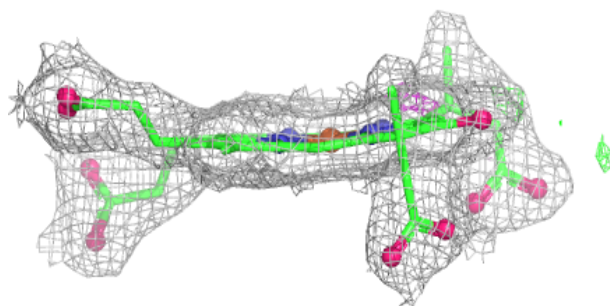
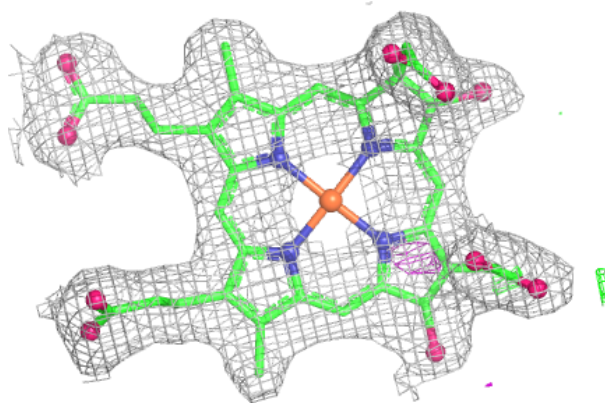
The following is a graphical depiction of the model fit to experimental electron density of all

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.



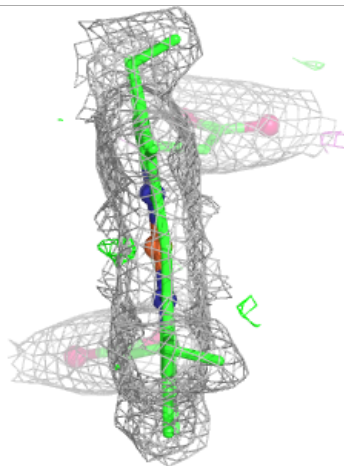
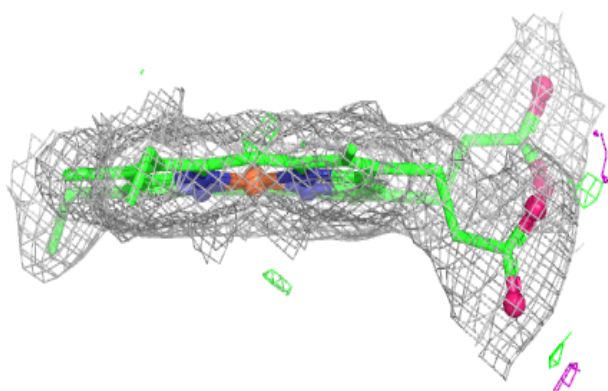
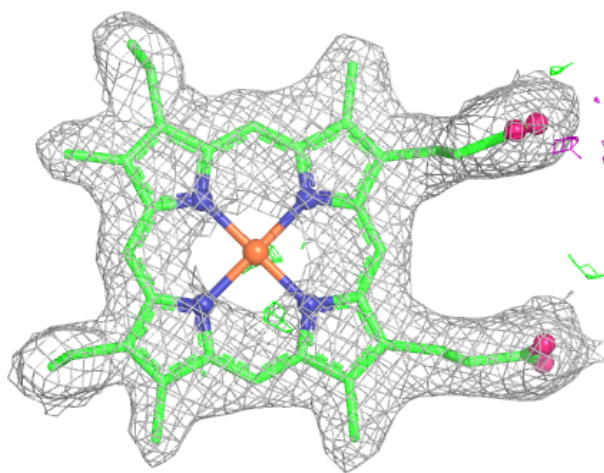
Electron density around DHE B 602:

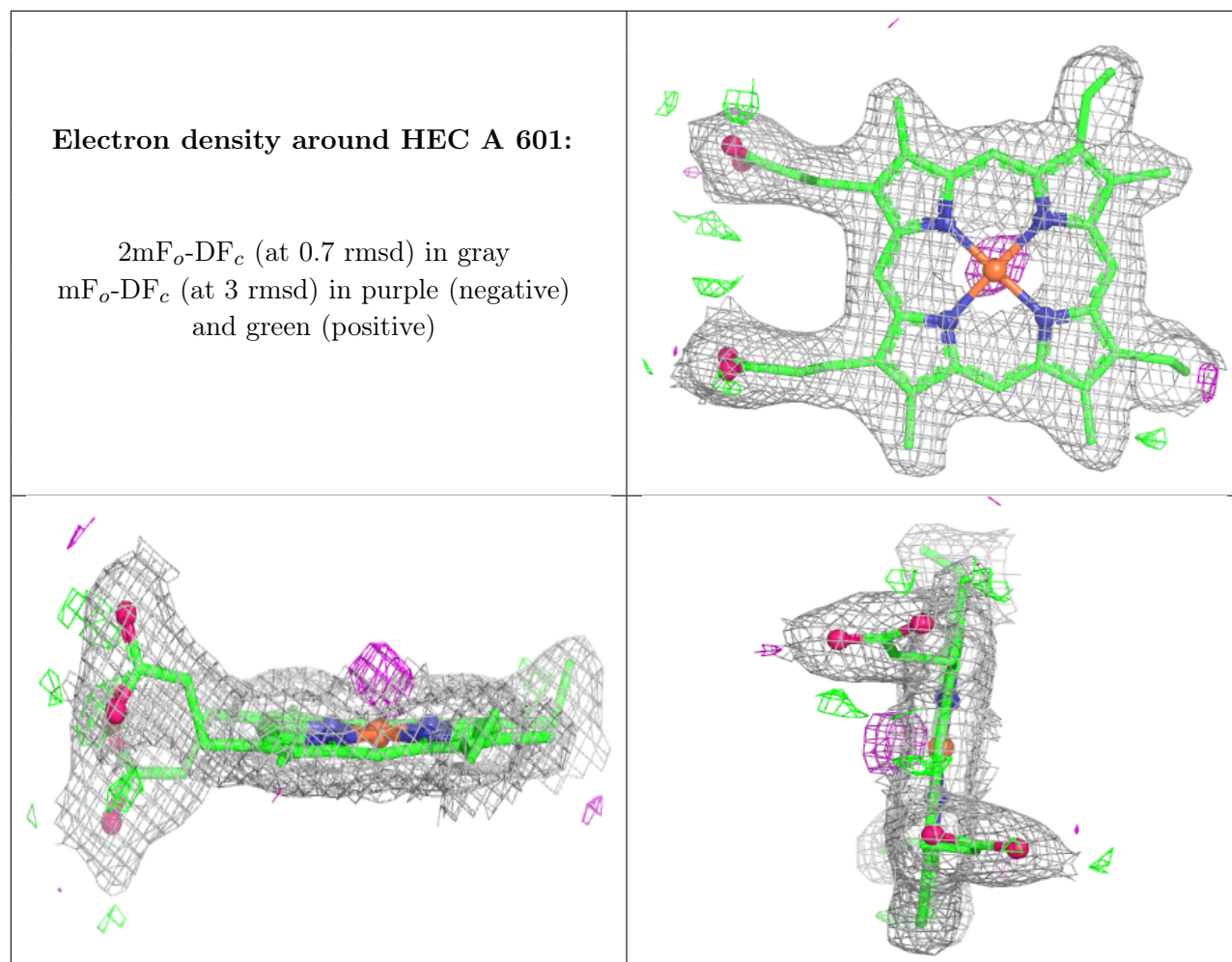
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.