



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 05:30 PM EDT

PDB ID : 3WFB / pdb_00003wfb
Title : Reduced cytochrome c-dependent nitric oxide reductase (cNOR) from *Pseudomonas aeruginosa* in complex with antibody fragment
Authors : Sato, N.; Ishii, S.; Hino, T.; Sugimoto, H.; Fukumori, Y.; Shiro, Y.; Tosha, T.
Deposited on : 2013-07-18
Resolution : 2.70 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	:	9.0.015 (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

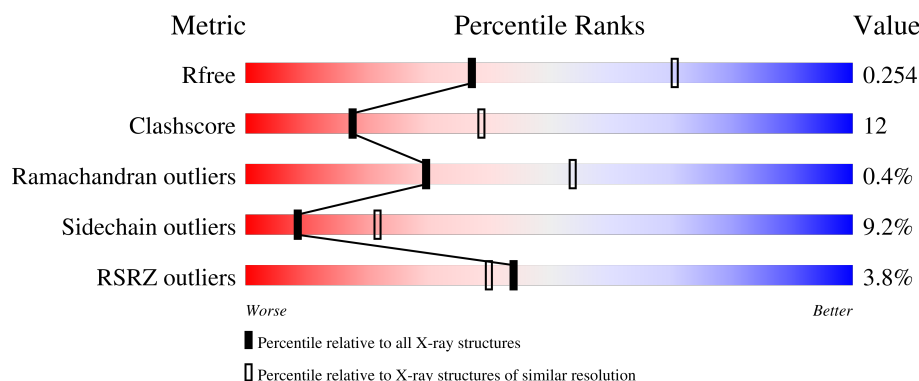
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	L	213	0% 75% 21% .
2	H	225	2% 75% 20% 5%
3	B	465	5% 67% 26% . .
4	C	146	5% 68% 25% . . .

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
9	HEC	C	201	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 8326 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 antibody fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1669	1047	277	338	7			

- Molecule 2 is a protein called antibody fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	225	Total	C	N	O	S	0	0	0
			1692	1065	280	338	9			

- Molecule 3 is a protein called Nitric oxide reductase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	449	Total	C	N	O	S	0	0	0
			3576	2416	563	572	25			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ARG	deletion	UNP Q59647

- Molecule 4 is a protein called Nitric oxide reductase subunit C.

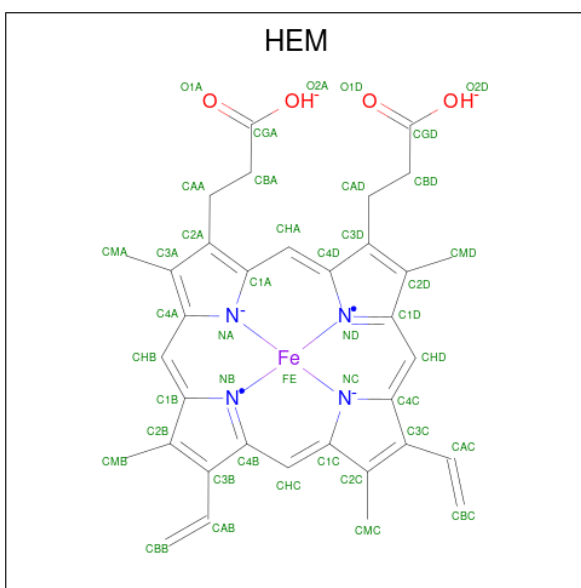
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	142	Total	C	N	O	S	0	0	0
			1123	720	195	202	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	100	LYS	ASN	conflict	UNP Q59646

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

$C_{34}H_{32}FeN_4O_4$).



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

- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Fe		
			1	1	0	0

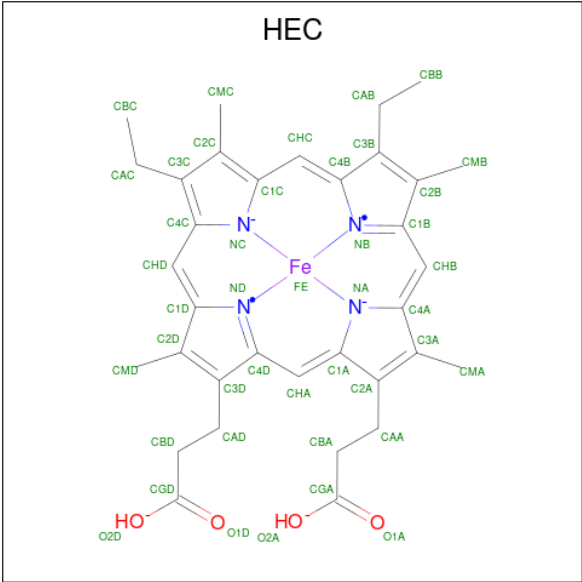
- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl		
			1	1	0	0

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Ca		
			1	1	0	0

- Molecule 9 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

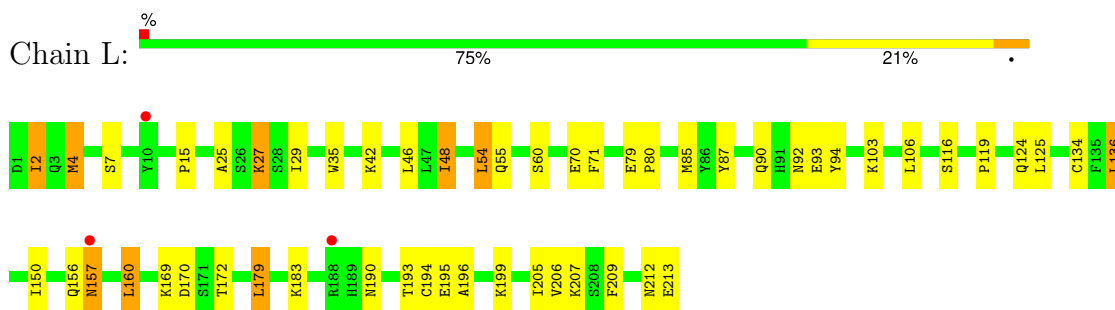
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	39	Total	O	0
			39	39	
10	H	42	Total	O	0
			42	42	
10	B	24	Total	O	0
			24	24	
10	C	29	Total	O	0
			29	29	

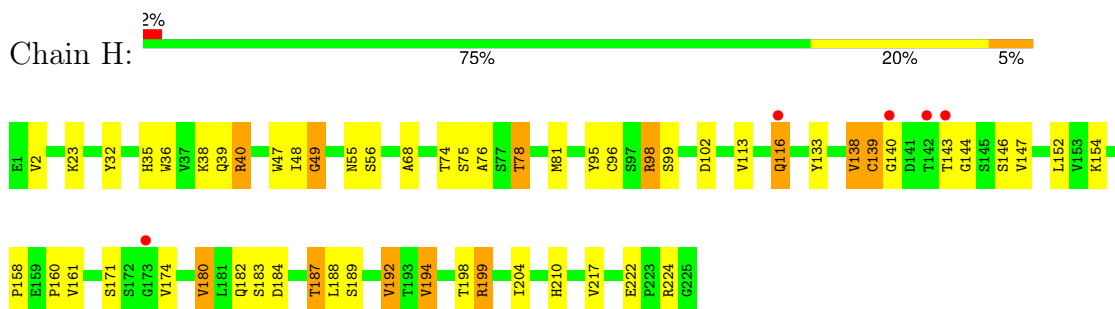
3 Residue-property plots [i](#)

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.

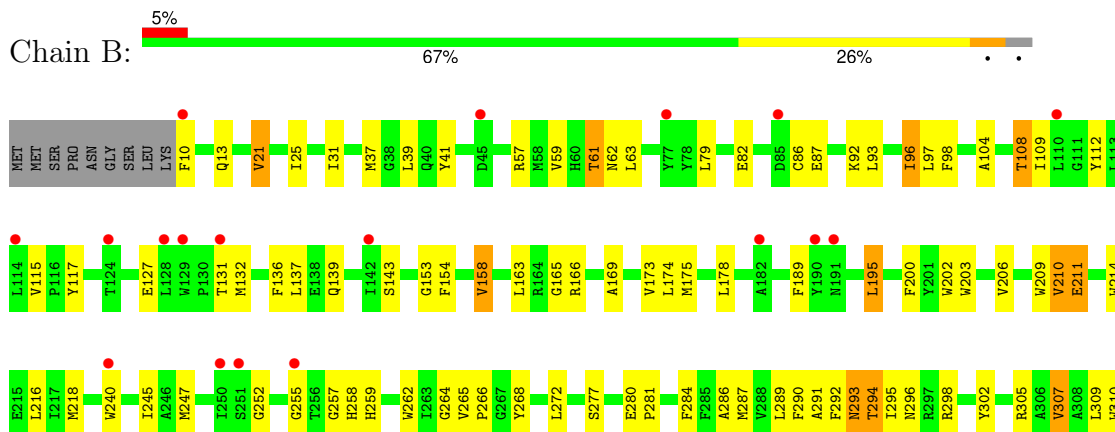
- Molecule 1: antibody fab fragment light chain

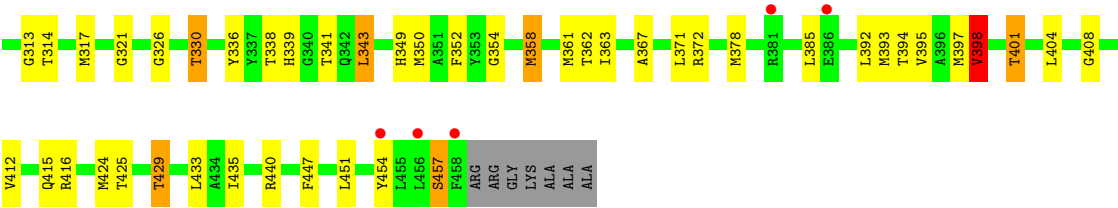


- Molecule 2: antibody fab fragment heavy chain

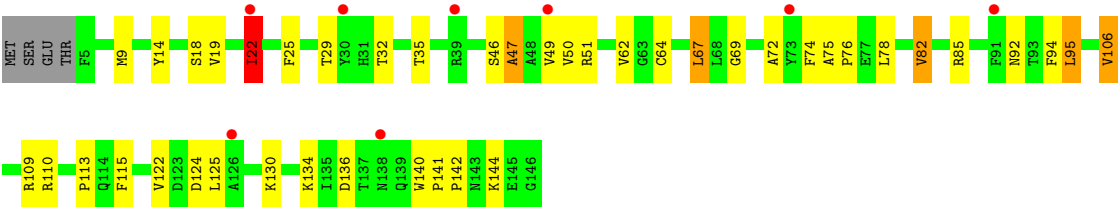


- Molecule 3: Nitric oxide reductase subunit B





● Molecule 4: Nitric oxide reductase subunit C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.76Å 110.64Å 193.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.07 – 2.70 41.07 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (41.07-2.70) 99.4 (41.07-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.202 , 0.250 0.204 , 0.254	Depositor DCC
R_{free} test set	2744 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8326	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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: CL, HEC, CA, FE, HEM

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	L	1.12	1/1709 (0.1%)	1.21	3/2317 (0.1%)
2	H	1.08	1/1735 (0.1%)	1.20	5/2367 (0.2%)
3	B	0.93	0/3693	1.13	9/5039 (0.2%)
4	C	0.86	1/1153 (0.1%)	1.07	2/1559 (0.1%)
All	All	1.00	3/8290 (0.0%)	1.15	19/11282 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	134	CYS	C-O	6.69	1.31	1.24
4	C	78	LEU	CA-C	5.05	1.59	1.52
2	H	49	GLY	N-CA	5.00	1.49	1.45

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	252	GLY	N-CA-C	6.91	120.51	112.50
3	B	166	ARG	N-CA-C	6.73	120.25	110.28
2	H	222	GLU	CA-C-N	5.66	125.98	119.93
2	H	222	GLU	C-N-CA	5.66	125.98	119.93
1	L	4	MET	CB-CG-SD	-5.65	95.74	112.70
3	B	313	GLY	N-CA-C	-5.65	105.95	112.73
3	B	302	TYR	CA-C-N	5.54	125.22	119.56
3	B	302	TYR	C-N-CA	5.54	125.22	119.56
3	B	307	VAL	CB-CA-C	-5.53	104.80	111.88
4	C	22	ILE	N-CA-CB	5.52	117.01	110.55
3	B	358	MET	N-CA-C	5.35	117.11	111.28
1	L	172	THR	N-CA-C	5.25	117.98	109.79
4	C	47	ALA	N-CA-C	-5.25	105.73	111.82
1	L	48	ILE	CB-CA-C	-5.21	101.38	110.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	41	TYR	N-CA-C	-5.21	105.50	111.07
2	H	39	GLN	N-CA-C	5.17	117.22	108.02
3	B	398	VAL	N-CA-CB	5.13	117.52	110.54
2	H	210	HIS	CA-C-N	5.06	124.55	119.19
2	H	210	HIS	C-N-CA	5.06	124.55	119.19

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1669	0	1606	38	1
2	H	1692	0	1647	40	0
3	B	3576	0	3619	103	1
4	C	1123	0	1091	26	0
5	B	86	0	60	21	0
6	B	1	0	0	0	0
7	B	1	0	0	1	0
8	B	1	0	0	0	0
9	C	43	0	30	2	0
10	B	24	0	0	1	0
10	C	29	0	0	0	0
10	H	42	0	0	1	0
10	L	39	0	0	1	0
All	All	8326	0	8053	201	1

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 12.

All (201) 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)
2:H:199:ARG:HH11	2:H:199:ARG:HG3	1.13	1.11
2:H:48:ILE:HG21	2:H:81:MET:HE1	1.48	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:199:ARG:HH11	2:H:199:ARG:CG	1.84	0.90
4:C:25:PHE:O	4:C:29:THR:HG23	1.78	0.84
4:C:32:THR:O	4:C:35:THR:HG22	1.79	0.83
2:H:199:ARG:HG3	2:H:199:ARG:NH1	1.81	0.83
5:B:801:HEM:HBB2	5:B:801:HEM:HHC	1.61	0.82
1:L:213:GLU:OE2	2:H:139:CYS:SG	2.42	0.77
2:H:48:ILE:HG21	2:H:81:MET:CE	2.14	0.77
3:B:317:MET:HE1	3:B:350:MET:HE2	1.67	0.76
5:B:802:HEM:HHC	5:B:802:HEM:HBB2	1.69	0.75
3:B:266:PRO:HD3	4:C:35:THR:HG21	1.69	0.74
1:L:70:GLU:HG3	10:L:324:HOH:O	1.86	0.73
3:B:321:GLY:CA	3:B:350:MET:HG2	2.19	0.73
1:L:157:ASN:OD1	1:L:157:ASN:N	2.22	0.72
3:B:350:MET:HB2	3:B:401:THR:HG21	1.69	0.72
3:B:104:ALA:O	3:B:108:THR:CG2	2.38	0.71
1:L:160:LEU:HD21	2:H:180:VAL:HG22	1.74	0.70
3:B:97:LEU:HD11	3:B:153:GLY:HA3	1.72	0.70
3:B:31:ILE:HD11	5:B:801:HEM:HMC3	1.73	0.70
2:H:183:SER:OG	2:H:184:ASP:N	2.23	0.69
3:B:284:PHE:HZ	5:B:802:HEM:HBB1	1.58	0.69
3:B:137:LEU:HA	3:B:139:GLN:NE2	2.08	0.67
1:L:124:GLN:HG3	2:H:133:TYR:CE2	2.29	0.67
3:B:424:MET:HB3	3:B:429:THR:HG22	1.75	0.67
3:B:79:LEU:HD11	3:B:174:LEU:HD12	1.77	0.66
3:B:321:GLY:HA3	3:B:350:MET:HG2	1.77	0.65
3:B:203:TRP:CE2	3:B:259:HIS:HB3	2.31	0.65
3:B:352:PHE:HB3	5:B:801:HEM:CBC	2.27	0.64
1:L:195:GLU:HG2	1:L:206:VAL:HG22	1.79	0.64
3:B:211:GLU:OE2	7:B:804:CL:CL	2.53	0.63
3:B:117:TYR:CZ	3:B:132:MET:HE2	2.33	0.63
3:B:57:ARG:NH2	5:B:801:HEM:HBD1	2.14	0.63
1:L:79:GLU:HG3	1:L:80:PRO:HD2	1.79	0.62
3:B:137:LEU:HA	3:B:139:GLN:HE22	1.63	0.62
3:B:59:VAL:O	3:B:63:LEU:HG	1.99	0.62
3:B:367:ALA:O	3:B:371:LEU:HB2	1.99	0.61
1:L:119:PRO:HD2	2:H:224:ARG:NH1	2.14	0.61
3:B:284:PHE:CZ	5:B:802:HEM:HBB1	2.35	0.61
3:B:104:ALA:O	3:B:108:THR:HG22	2.01	0.61
3:B:247:MET:HE1	3:B:286:ALA:HB2	1.83	0.61
3:B:290:PHE:O	3:B:294:THR:HG23	2.01	0.60
2:H:174:VAL:HG22	2:H:192:VAL:CG1	2.30	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:63:LEU:HD21	3:B:109:ILE:HG13	1.84	0.60
1:L:212:ASN:O	1:L:213:GLU:HB2	2.03	0.59
2:H:48:ILE:HD13	2:H:81:MET:HE1	1.84	0.59
3:B:361:MET:HE1	3:B:393:MET:HE1	1.83	0.59
3:B:31:ILE:HD12	5:B:801:HEM:HBB2	1.85	0.58
3:B:62:ASN:ND2	3:B:112:TYR:OH	2.36	0.58
1:L:136:LEU:CD1	1:L:196:ALA:HB2	2.34	0.57
2:H:116:GLN:O	2:H:116:GLN:HG2	2.04	0.57
1:L:156:GLN:HA	1:L:156:GLN:OE1	2.04	0.57
2:H:76:ALA:O	2:H:78:THR:HG22	2.05	0.57
3:B:169:ALA:O	3:B:173:VAL:HG23	2.04	0.56
3:B:247:MET:HE1	3:B:286:ALA:CB	2.36	0.56
3:B:31:ILE:HD11	5:B:801:HEM:CMC	2.36	0.55
3:B:265:VAL:HB	3:B:266:PRO:HD2	1.87	0.55
3:B:63:LEU:CD2	3:B:109:ILE:HG13	2.36	0.55
4:C:95:LEU:HD13	4:C:122:VAL:HG13	1.87	0.55
3:B:127:GLU:OE2	3:B:127:GLU:HA	2.05	0.55
4:C:92:ASN:OD1	4:C:130:LYS:HE2	2.07	0.55
3:B:104:ALA:O	3:B:108:THR:HG23	2.06	0.54
1:L:213:GLU:HA	1:L:213:GLU:OE1	2.08	0.54
3:B:350:MET:HE3	3:B:401:THR:HG21	1.91	0.53
2:H:55:ASN:O	2:H:56:SER:HB2	2.06	0.53
3:B:209:TRP:O	3:B:214:TRP:HB2	2.09	0.53
3:B:92:LYS:O	3:B:96:ILE:HG22	2.09	0.53
4:C:106:VAL:HG22	4:C:109:ARG:HB2	1.89	0.53
3:B:397:MET:O	3:B:401:THR:HG23	2.09	0.53
3:B:21:VAL:O	3:B:25:ILE:HG12	2.09	0.52
3:B:158:VAL:HG13	3:B:175:MET:SD	2.50	0.52
3:B:349:HIS:HD2	5:B:801:HEM:C4C	2.27	0.51
3:B:395:VAL:HA	3:B:398:VAL:HG13	1.90	0.51
5:B:801:HEM:HHD	5:B:801:HEM:HBC2	1.91	0.51
4:C:95:LEU:HD13	4:C:122:VAL:CG1	2.40	0.51
2:H:38:LYS:HE2	2:H:40:ARG:CD	2.41	0.51
2:H:199:ARG:CG	2:H:199:ARG:NH1	2.52	0.51
4:C:75:ALA:HB1	4:C:76:PRO:CD	2.41	0.51
1:L:94:TYR:CD1	1:L:94:TYR:C	2.89	0.51
3:B:317:MET:HB3	3:B:354:GLY:HA2	1.93	0.51
3:B:349:HIS:CD2	5:B:801:HEM:C4C	2.98	0.51
1:L:160:LEU:HD21	2:H:180:VAL:CG2	2.38	0.51
4:C:18:SER:O	4:C:22:ILE:HG12	2.10	0.51
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:202:TRP:CZ2	3:B:206:VAL:HG21	2.46	0.50
3:B:200:PHE:HD2	3:B:265:VAL:HG11	1.77	0.50
3:B:326:GLY:O	3:B:330:THR:HB	2.11	0.50
1:L:209:PHE:HB3	2:H:138:VAL:HG11	1.94	0.49
3:B:13:GLN:HE22	3:B:82:GLU:HG3	1.77	0.49
2:H:38:LYS:HE2	2:H:40:ARG:HD3	1.93	0.49
3:B:425:THR:O	3:B:429:THR:CG2	2.61	0.49
3:B:291:ALA:O	3:B:295:ILE:HD12	2.12	0.49
1:L:190:ASN:HD21	1:L:212:ASN:HD22	1.59	0.49
5:B:801:HEM:HHC	5:B:801:HEM:CBB	2.37	0.49
5:B:802:HEM:HHC	5:B:802:HEM:CBB	2.41	0.49
3:B:79:LEU:HD11	3:B:174:LEU:CD1	2.41	0.49
2:H:154:LYS:HA	2:H:187:THR:HB	1.94	0.49
3:B:206:VAL:O	3:B:210:VAL:HB	2.12	0.49
3:B:292:PHE:O	3:B:296:ASN:HB2	2.13	0.49
1:L:124:GLN:HG3	2:H:133:TYR:CZ	2.47	0.48
3:B:352:PHE:HB3	5:B:801:HEM:HBC2	1.95	0.48
1:L:29:ILE:HG21	1:L:90:GLN:CG	2.43	0.48
3:B:310:TRP:HB3	3:B:362:THR:OG1	2.14	0.48
2:H:76:ALA:O	2:H:78:THR:CG2	2.61	0.48
2:H:174:VAL:HG22	2:H:192:VAL:HG13	1.95	0.48
3:B:37:MET:SD	3:B:57:ARG:HA	2.53	0.48
3:B:10:PHE:HB3	3:B:87:GLU:OE1	2.14	0.48
3:B:174:LEU:CD2	3:B:178:LEU:HD11	2.44	0.48
1:L:125:LEU:HD22	1:L:183:LYS:HG3	1.95	0.48
3:B:98:PHE:CD1	3:B:98:PHE:C	2.92	0.48
3:B:394:THR:O	3:B:398:VAL:HG12	2.13	0.48
3:B:92:LYS:HG3	3:B:93:LEU:N	2.28	0.47
3:B:341:THR:HG23	3:B:416:ARG:NH1	2.29	0.47
1:L:2:ILE:CD1	1:L:25:ALA:HB1	2.45	0.47
3:B:93:LEU:HA	3:B:96:ILE:CG2	2.45	0.47
3:B:202:TRP:CH2	3:B:206:VAL:HG21	2.50	0.47
3:B:415:GLN:HB2	3:B:429:THR:HG21	1.97	0.47
5:B:801:HEM:HBB2	5:B:801:HEM:CHC	2.34	0.47
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.50	0.47
3:B:425:THR:O	3:B:429:THR:HG22	2.14	0.47
3:B:154:PHE:CZ	3:B:178:LEU:HD13	2.49	0.46
3:B:338:THR:HG22	3:B:412:VAL:HG21	1.97	0.46
4:C:113:PRO:HD3	9:C:201:HEC:HBC2	1.97	0.46
2:H:147:VAL:HG12	2:H:194:VAL:HG12	1.98	0.46
3:B:339:HIS:CD2	4:C:69:GLY:HA3	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:13:GLN:NE2	3:B:82:GLU:HG3	2.30	0.46
3:B:61:THR:HG23	3:B:136:PHE:HD1	1.80	0.46
2:H:147:VAL:CG1	2:H:194:VAL:HG12	2.46	0.46
2:H:194:VAL:HG13	2:H:198:THR:HB	1.97	0.46
3:B:372:ARG:HH11	3:B:378:MET:HE1	1.79	0.46
3:B:372:ARG:NH1	3:B:378:MET:HE1	2.31	0.46
1:L:29:ILE:HD11	1:L:71:PHE:CE1	2.51	0.46
1:L:212:ASN:OD1	1:L:213:GLU:N	2.49	0.45
3:B:393:MET:HE3	3:B:447:PHE:CZ	2.51	0.45
3:B:336:TYR:CE1	4:C:142:PRO:HG3	2.52	0.45
1:L:85:MET:HE2	1:L:103:LYS:HD2	1.97	0.45
1:L:54:LEU:HD11	1:L:60:SER:HA	1.99	0.45
3:B:280:GLU:N	3:B:281:PRO:CD	2.79	0.45
4:C:51:ARG:NH1	4:C:124:ASP:OD1	2.50	0.45
4:C:64:CYS:C	4:C:72:ALA:HB3	2.42	0.45
1:L:27:LYS:HE2	1:L:93:GLU:OE2	2.17	0.45
4:C:140:TRP:CG	4:C:141:PRO:HA	2.52	0.45
1:L:170:ASP:OD1	1:L:170:ASP:C	2.60	0.45
2:H:74:THR:O	2:H:75:SER:C	2.60	0.45
3:B:245:ILE:HD12	4:C:14:TYR:CE1	2.52	0.44
3:B:350:MET:HE3	3:B:401:THR:CG2	2.47	0.44
4:C:134:LYS:HB2	4:C:134:LYS:HE2	1.71	0.44
4:C:74:PHE:CE1	4:C:110:ARG:HD3	2.53	0.44
5:B:802:HEM:HBB2	5:B:802:HEM:CHC	2.38	0.44
3:B:349:HIS:HD2	5:B:801:HEM:NC	2.11	0.44
4:C:85:ARG:HG3	4:C:94:PHE:CE2	2.52	0.44
2:H:23:LYS:HG2	2:H:78:THR:HG22	2.00	0.44
3:B:258:HIS:ND1	3:B:277:SER:OG	2.50	0.44
1:L:29:ILE:HG21	1:L:90:GLN:HG3	2.00	0.44
3:B:31:ILE:HD12	5:B:801:HEM:CBB	2.48	0.44
1:L:90:GLN:OE1	1:L:92:ASN:N	2.48	0.43
3:B:264:GLY:HA2	4:C:136:ASP:O	2.18	0.43
1:L:15:PRO:HD3	1:L:106:LEU:HD11	2.00	0.43
3:B:218:MET:HG2	3:B:287:MET:HE1	2.00	0.43
1:L:212:ASN:CG	1:L:213:GLU:N	2.76	0.43
3:B:289:LEU:O	3:B:293:ASN:HB2	2.17	0.43
2:H:98:ARG:HD3	2:H:99:SER:O	2.18	0.43
3:B:163:LEU:HA	3:B:163:LEU:HD23	1.74	0.43
3:B:385:LEU:HB3	3:B:457:SER:HB3	2.01	0.43
3:B:108:THR:HB	3:B:143:SER:OG	2.18	0.43
2:H:35:HIS:O	2:H:96:CYS:HA	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:131:THR:HG21	3:B:189:PHE:HA	2.01	0.43
3:B:57:ARG:NH1	10:B:907:HOH:O	2.51	0.42
1:L:79:GLU:HG3	1:L:80:PRO:CD	2.49	0.42
3:B:218:MET:HE2	3:B:287:MET:HE1	2.00	0.42
2:H:68:ALA:HB1	2:H:81:MET:HE2	2.00	0.42
2:H:182:GLN:HG3	2:H:187:THR:CG2	2.49	0.42
3:B:305:ARG:HE	3:B:305:ARG:HB3	1.58	0.42
1:L:150:ILE:HD11	1:L:179:LEU:HD11	2.02	0.42
2:H:2:VAL:HG12	2:H:113:VAL:HG21	2.01	0.42
2:H:36:TRP:HA	2:H:95:TYR:O	2.20	0.42
3:B:352:PHE:HB3	5:B:801:HEM:HBC1	1.99	0.42
1:L:15:PRO:HD3	1:L:106:LEU:CD1	2.49	0.42
3:B:343:LEU:HD22	3:B:408:GLY:HA3	2.01	0.42
2:H:32:TYR:CZ	2:H:102:ASP:HB3	2.55	0.41
3:B:154:PHE:CE2	3:B:178:LEU:HD13	2.55	0.41
3:B:266:PRO:HG2	3:B:268:TYR:CZ	2.55	0.41
1:L:2:ILE:O	1:L:2:ILE:HG13	2.20	0.41
1:L:35:TRP:HA	1:L:87:TYR:O	2.19	0.41
3:B:31:ILE:CD1	5:B:801:HEM:HBB2	2.49	0.41
3:B:96:ILE:C	3:B:96:ILE:HD13	2.46	0.41
3:B:195:LEU:HD11	4:C:67:LEU:HD13	2.02	0.41
3:B:361:MET:HE2	3:B:454:TYR:CD2	2.56	0.41
1:L:193:THR:HG22	1:L:194:CYS:N	2.35	0.41
1:L:136:LEU:HD11	1:L:196:ALA:HB2	2.03	0.41
2:H:160:PRO:HA	10:H:317:HOH:O	2.21	0.41
1:L:205:ILE:HD13	1:L:205:ILE:HG21	1.86	0.41
3:B:255:GLY:C	3:B:257:GLY:N	2.76	0.41
4:C:46:SER:O	4:C:50:VAL:HG23	2.21	0.41
3:B:262:TRP:CZ2	3:B:336:TYR:HB2	2.56	0.41
2:H:2:VAL:CG1	2:H:113:VAL:HG21	2.51	0.40
4:C:115:PHE:CD2	9:C:201:HEC:HBB2	2.55	0.40
4:C:47:ALA:O	4:C:51:ARG:HB2	2.21	0.40
4:C:75:ALA:HB1	4:C:76:PRO:HD2	2.03	0.40
4:C:82:VAL:HG21	4:C:130:LYS:HG2	2.04	0.40
3:B:314:THR:OG1	3:B:358:MET:HB3	2.21	0.40

All (1) 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:L:157:ASN:ND2	3:B:165:GLY:O[2_554]	2.08	0.12

5.3 Torsion angles

5.3.1 Protein backbone

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	L	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
2	H	223/225 (99%)	208 (93%)	12 (5%)	3 (1%)	9	25
3	B	447/465 (96%)	427 (96%)	19 (4%)	1 (0%)	43	68
4	C	140/146 (96%)	135 (96%)	5 (4%)	0	100	100
All	All	1021/1049 (97%)	972 (95%)	45 (4%)	4 (0%)	30	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	457	SER
2	H	140	GLY
2	H	144	GLY
2	H	139	CYS

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	L	189/189 (100%)	172 (91%)	17 (9%)	9	23
2	H	192/192 (100%)	172 (90%)	20 (10%)	7	17
3	B	360/371 (97%)	329 (91%)	31 (9%)	10	25
4	C	116/120 (97%)	105 (90%)	11 (10%)	8	20
All	All	857/872 (98%)	778 (91%)	79 (9%)	8	22

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	ILE
1	L	4	MET
1	L	7	SER
1	L	27	LYS
1	L	42	LYS
1	L	46	LEU
1	L	48	ILE
1	L	54	LEU
1	L	55	GLN
1	L	116	SER
1	L	136	LEU
1	L	157	ASN
1	L	160	LEU
1	L	169	LYS
1	L	179	LEU
1	L	199	LYS
1	L	207	LYS
2	H	40	ARG
2	H	78	THR
2	H	98	ARG
2	H	116	GLN
2	H	138	VAL
2	H	143	THR
2	H	146	SER
2	H	152	LEU
2	H	158	PRO
2	H	161	VAL
2	H	171	SER
2	H	180	VAL
2	H	187	THR
2	H	188	LEU
2	H	189	SER
2	H	192	VAL
2	H	194	VAL
2	H	199	ARG
2	H	204	ILE
2	H	217	VAL
3	B	21	VAL
3	B	39	LEU
3	B	61	THR
3	B	86	CYS
3	B	96	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	108	THR
3	B	115	VAL
3	B	158	VAL
3	B	195	LEU
3	B	210	VAL
3	B	211	GLU
3	B	216	LEU
3	B	240	TRP
3	B	272	LEU
3	B	293	ASN
3	B	294	THR
3	B	298	ARG
3	B	307	VAL
3	B	309	LEU
3	B	330	THR
3	B	343	LEU
3	B	363	ILE
3	B	392	LEU
3	B	398	VAL
3	B	401	THR
3	B	404	LEU
3	B	429	THR
3	B	433	LEU
3	B	435	ILE
3	B	440	ARG
3	B	451	LEU
4	C	9	MET
4	C	19	VAL
4	C	22	ILE
4	C	49	VAL
4	C	62	VAL
4	C	67	LEU
4	C	82	VAL
4	C	95	LEU
4	C	106	VAL
4	C	125	LEU
4	C	144	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	212	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	13	GLN
3	B	62	ASN
3	B	139	GLN
3	B	411	GLN
3	B	415	GLN
4	C	41	ASN
4	C	105	ASN

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](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	HEC	C	201	4	50,50,50	1.78	7 (14%)	68,82,82	1.45	12 (17%)
5	HEM	B	802	8,3	50,50,50	1.88	11 (22%)	67,82,82	1.60	8 (11%)
5	HEM	B	801	8,3	50,50,50	1.87	10 (20%)	67,82,82	1.40	8 (11%)

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
9	HEC	C	201	4	1/1/3/7	5/14/54/54	-
5	HEM	B	802	8,3	-	5/14/54/54	-
5	HEM	B	801	8,3	-	7/14/54/54	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	201	HEC	C3D-C2D	8.06	1.54	1.36
5	B	802	HEM	C3D-C2D	7.57	1.53	1.36
5	B	801	HEM	C3D-C2D	6.40	1.50	1.36
5	B	802	HEM	FE-NB	4.87	2.09	1.94
5	B	801	HEM	FE-NB	4.84	2.09	1.94
9	C	201	HEC	FE-NB	4.81	2.09	1.94
5	B	801	HEM	CAC-C3C	3.58	1.56	1.47
5	B	802	HEM	CMC-C2C	3.28	1.57	1.50
5	B	801	HEM	FE-NC	3.10	2.05	1.95
5	B	801	HEM	CMB-C2B	3.06	1.57	1.50
9	C	201	HEC	FE-ND	3.00	2.04	1.94
9	C	201	HEC	FE-NA	2.98	2.05	1.95
9	C	201	HEC	CAC-C3C	2.92	1.58	1.51
5	B	802	HEM	CAC-C3C	2.89	1.55	1.47
5	B	801	HEM	C3B-C2B	-2.87	1.31	1.37
5	B	802	HEM	CAB-C3B	2.75	1.54	1.47
9	C	201	HEC	CMA-C3A	2.70	1.56	1.50
5	B	801	HEM	C1B-NB	-2.63	1.35	1.40
5	B	801	HEM	CAB-C3B	2.56	1.54	1.47
5	B	802	HEM	CMA-C3A	2.48	1.55	1.50
5	B	802	HEM	C3B-C2B	-2.44	1.32	1.37
5	B	802	HEM	CHB-C4A	-2.39	1.34	1.39
5	B	801	HEM	CMC-C2C	2.39	1.55	1.50
9	C	201	HEC	O1A-CGA	2.33	1.29	1.22
5	B	802	HEM	CMB-C2B	2.11	1.55	1.50
5	B	801	HEM	C4C-NC	-2.10	1.35	1.39
5	B	802	HEM	O1D-CGD	2.04	1.28	1.22
5	B	802	HEM	FE-NA	2.01	2.01	1.95

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	802	HEM	C4D-ND-C1D	5.49	111.71	105.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	802	HEM	CBA-CAA-C2A	-4.81	99.24	112.53
5	B	801	HEM	CMD-C2D-C1D	4.36	131.85	125.03
9	C	201	HEC	C1D-ND-C4D	3.83	109.74	105.21
5	B	801	HEM	C4D-ND-C1D	3.75	109.64	105.21
5	B	802	HEM	CHD-C1D-ND	3.71	128.41	124.42
5	B	802	HEM	CAA-CBA-CGA	-3.18	105.22	113.67
5	B	801	HEM	CMB-C2B-C1B	3.03	129.78	125.03
5	B	801	HEM	CAA-CBA-CGA	-3.02	105.65	113.67
5	B	802	HEM	CAD-C3D-C4D	3.01	129.94	124.70
9	C	201	HEC	C1D-C2D-C3D	-2.92	103.91	106.98
9	C	201	HEC	CBD-CAD-C3D	-2.81	104.78	112.53
5	B	802	HEM	CHC-C1C-NC	2.77	127.47	124.45
9	C	201	HEC	CHA-C1A-NA	2.75	127.45	124.45
5	B	801	HEM	CAD-C3D-C4D	2.67	129.35	124.70
9	C	201	HEC	CBC-CAC-C3C	2.64	119.58	112.42
9	C	201	HEC	C1C-C2C-C3C	2.50	109.68	106.82
9	C	201	HEC	O1D-CGD-CBD	-2.48	115.24	123.09
9	C	201	HEC	CHB-C1B-NB	2.38	126.99	124.42
9	C	201	HEC	O2D-CGD-CBD	2.36	121.45	114.00
5	B	801	HEM	CAC-C3C-C4C	2.33	130.38	124.82
5	B	802	HEM	O1A-CGA-CBA	-2.26	115.93	123.09
5	B	802	HEM	CBB-CAB-C3B	-2.17	116.69	127.53
9	C	201	HEC	CHC-C1C-NC	2.14	127.74	123.86
5	B	801	HEM	CHC-C1C-NC	2.14	126.78	124.45
9	C	201	HEC	CBA-CAA-C2A	-2.12	106.67	112.53
5	B	801	HEM	CAC-C3C-C2C	-2.08	121.66	128.43
9	C	201	HEC	CMC-C2C-C1C	-2.02	122.34	125.42

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	C	201	HEC	NA

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	201	HEC	C2C-C3C-CAC-CBC
9	C	201	HEC	C4C-C3C-CAC-CBC
5	B	801	HEM	C3D-CAD-CBD-CGD
5	B	801	HEM	C4D-C3D-CAD-CBD
5	B	801	HEM	C2D-C3D-CAD-CBD
9	C	201	HEC	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	802	HEM	C2C-C3C-CAC-CBC
9	C	201	HEC	C4B-C3B-CAB-CBB
5	B	802	HEM	C4C-C3C-CAC-CBC
5	B	802	HEM	CAA-CBA-CGA-O2A
5	B	801	HEM	CAD-CBD-CGD-O1D
9	C	201	HEC	C2D-C3D-CAD-CBD
5	B	802	HEM	CAA-CBA-CGA-O1A
5	B	801	HEM	CAD-CBD-CGD-O2D
5	B	801	HEM	CAA-CBA-CGA-O1A
5	B	802	HEM	CAD-CBD-CGD-O2D
5	B	801	HEM	CAA-CBA-CGA-O2A

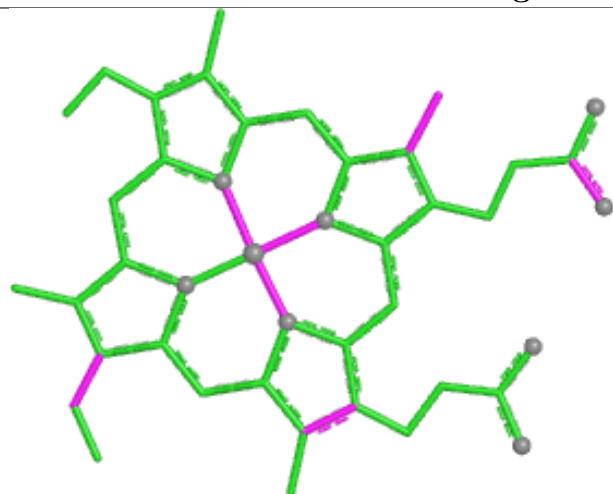
There are no ring outliers.

3 monomers are involved in 23 short contacts:

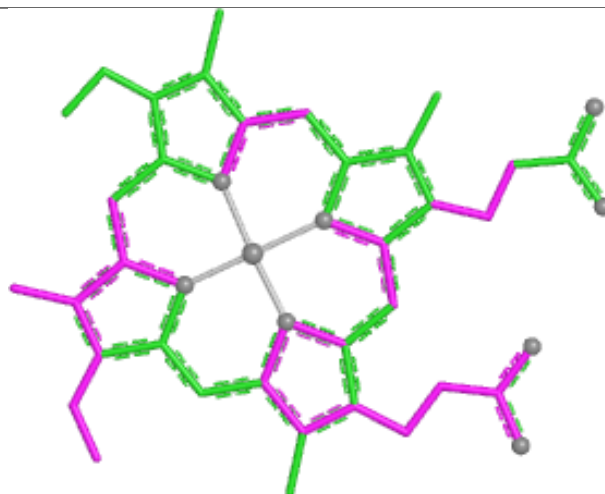
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	201	HEC	2	0
5	B	802	HEM	5	0
5	B	801	HEM	16	0

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.

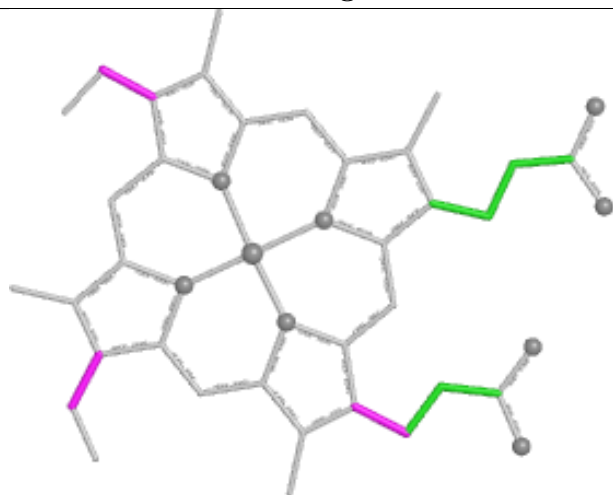
Ligand HEC C 201



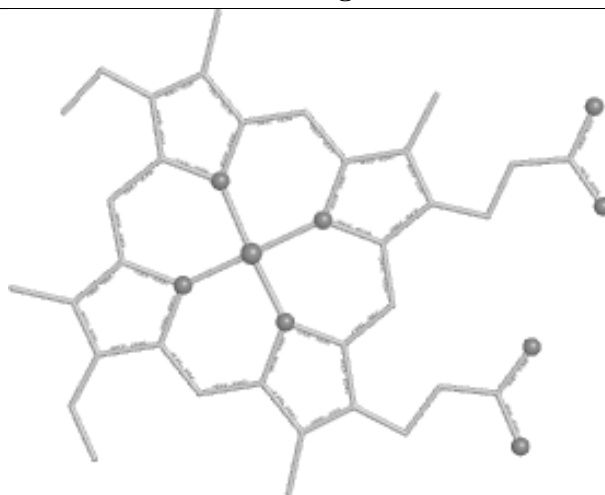
Bond lengths



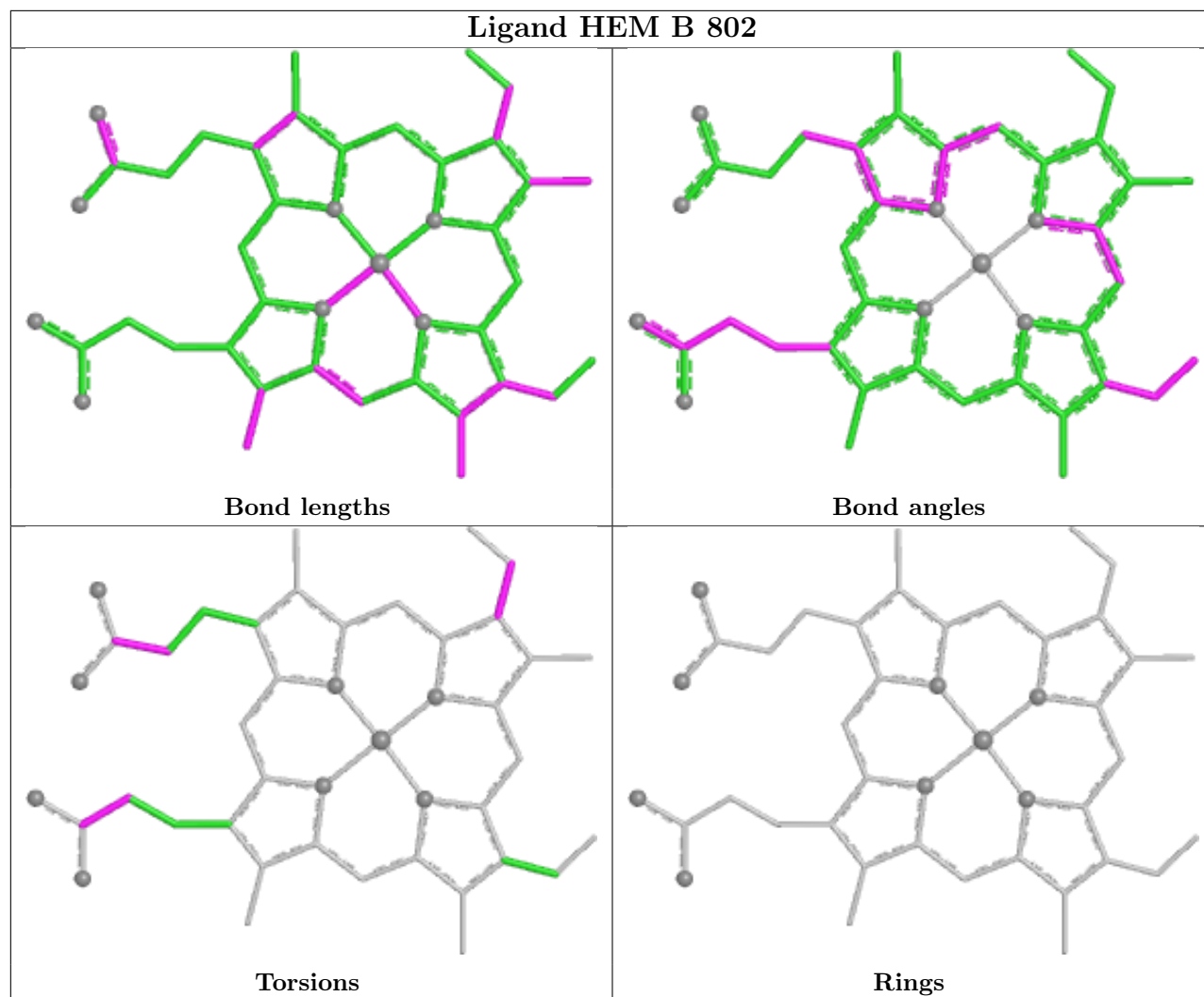
Bond angles

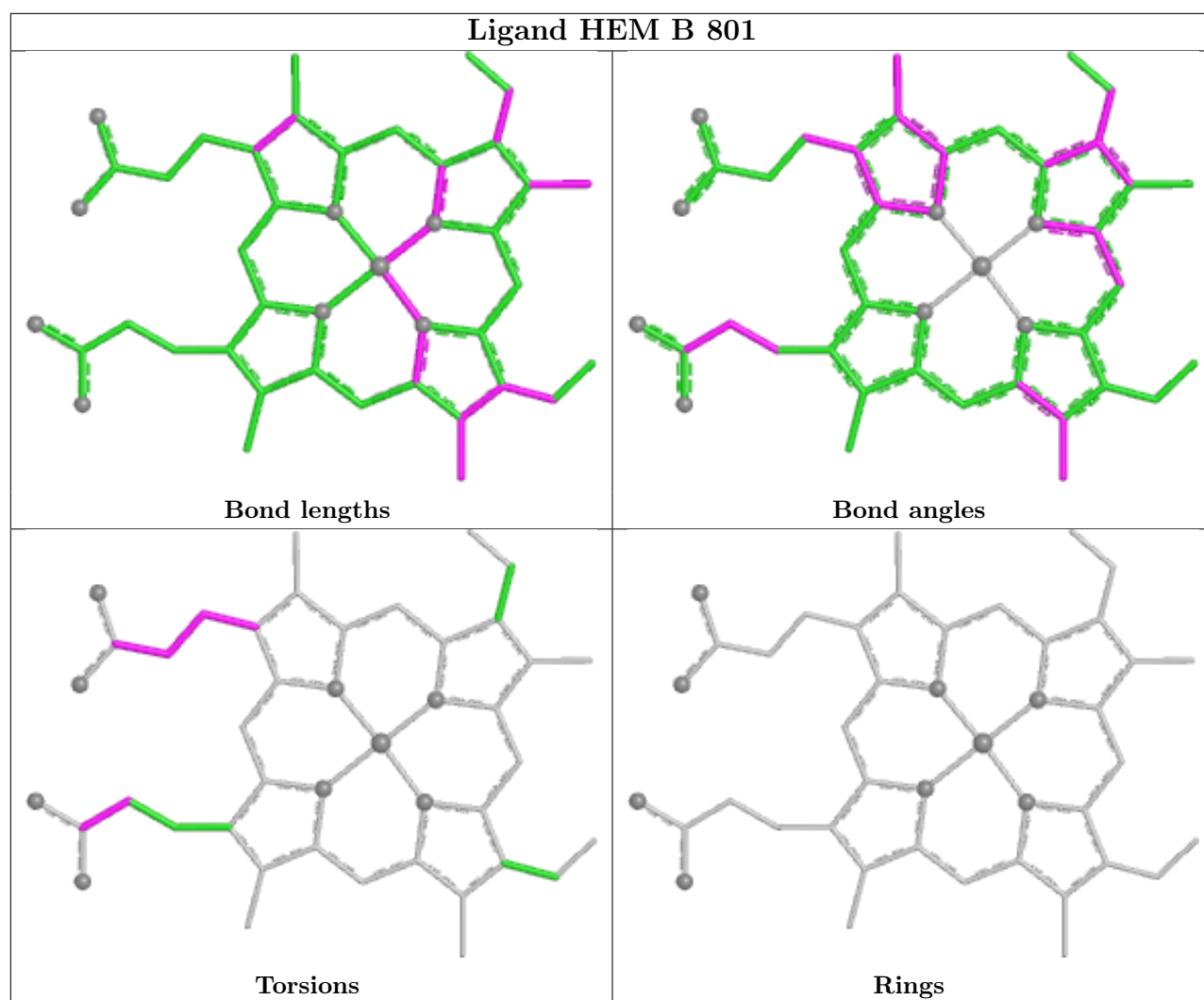


Torsions



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	L	213/213 (100%)	-0.22	3 (1%) 73 72	47, 62, 94, 150	0
2	H	225/225 (100%)	-0.10	5 (2%) 62 59	46, 62, 102, 201	0
3	B	449/465 (96%)	0.28	23 (5%) 33 29	54, 86, 127, 165	0
4	C	142/146 (97%)	0.24	8 (5%) 30 26	51, 85, 133, 156	0
All	All	1029/1049 (98%)	0.09	39 (3%) 44 40	46, 76, 126, 201	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	142	ILE	4.7
3	B	10	PHE	4.1
3	B	128	LEU	3.6
3	B	45	ASP	3.5
3	B	191	ASN	3.5
2	H	173	GLY	3.5
3	B	255	GLY	3.2
3	B	458	PHE	3.2
3	B	190	TYR	3.1
3	B	129	TRP	3.0
3	B	251	SER	2.9
2	H	140	GLY	2.9
3	B	182	ALA	2.9
1	L	10	TYR	2.9
4	C	126	ALA	2.8
2	H	116	GLN	2.7
4	C	138	ASN	2.7
3	B	381	ARG	2.6
4	C	91	PHE	2.5
4	C	73	TYR	2.4
3	B	454	TYR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	C	22	ILE	2.4
3	B	131	THR	2.3
1	L	188	ARG	2.3
2	H	142	THR	2.3
3	B	386	GLU	2.3
3	B	110	LEU	2.3
3	B	250	ILE	2.2
4	C	39	ARG	2.2
3	B	77	TYR	2.2
3	B	114	LEU	2.2
1	L	157	ASN	2.1
3	B	456	LEU	2.1
4	C	30	TYR	2.1
4	C	49	VAL	2.1
3	B	124	THR	2.0
3	B	85	ASP	2.0
2	H	143	THR	2.0
3	B	240	TRP	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.

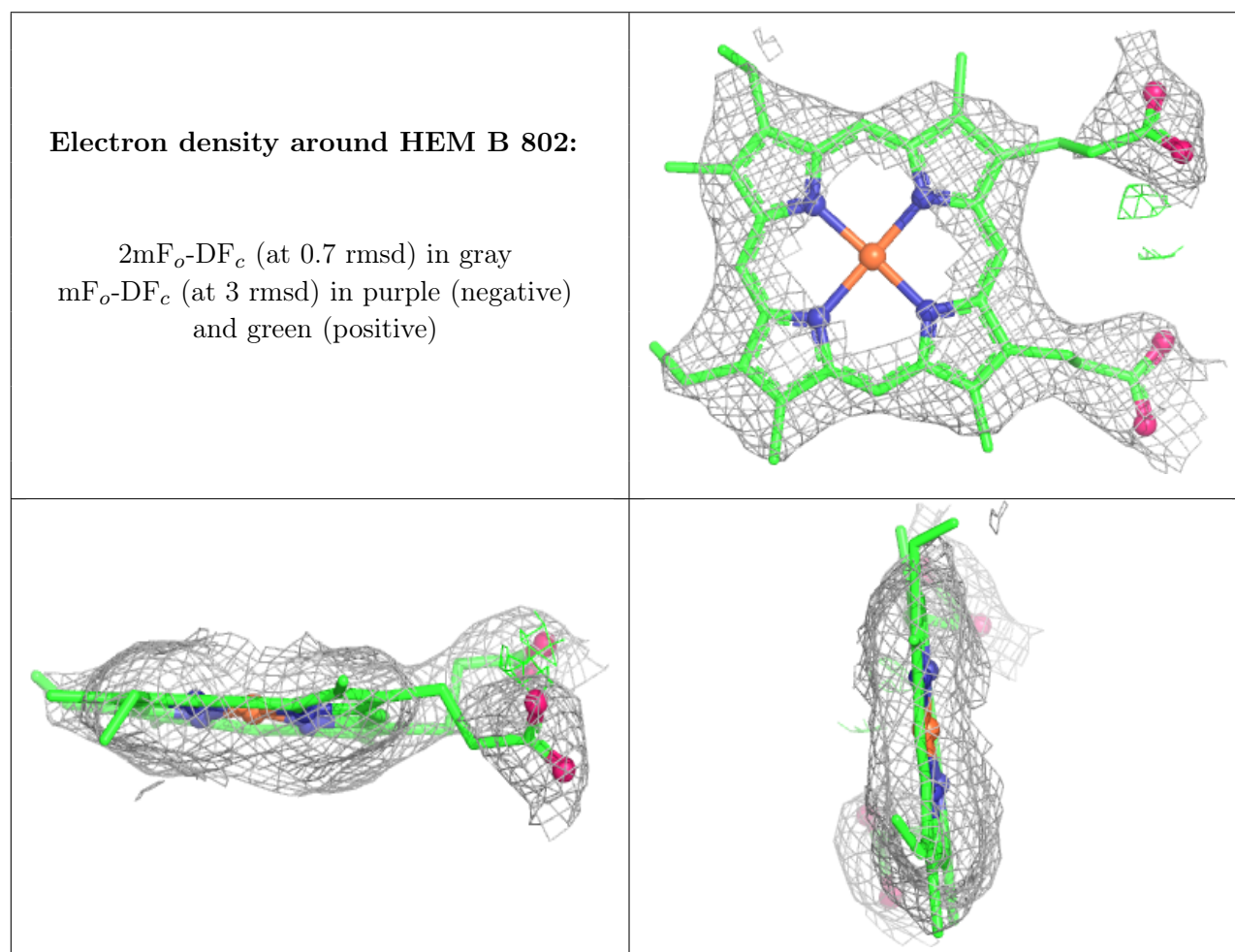
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CL	B	804	1/1	0.97	0.06	68,68,68,68	0
5	HEM	B	802	43/43	0.98	0.08	70,77,86,90	0
5	HEM	B	801	43/43	0.98	0.09	58,67,80,84	0
8	CA	B	805	1/1	0.99	0.05	73,73,73,73	0
9	HEC	C	201	43/43	0.99	0.07	54,61,66,68	0

Continued on next page...

Continued from previous page...

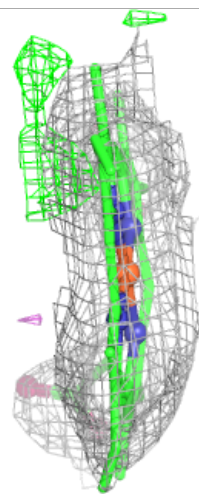
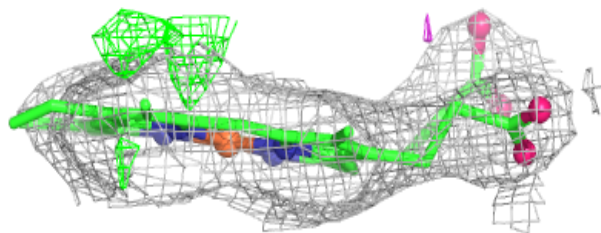
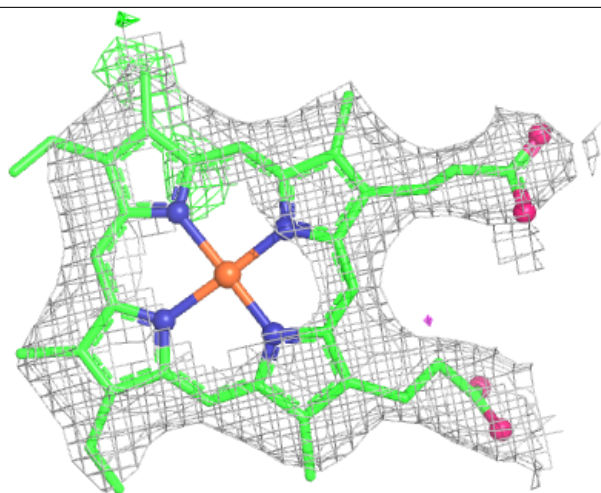
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	FE	B	803	1/1	1.00	0.03	74,74,74,74	0

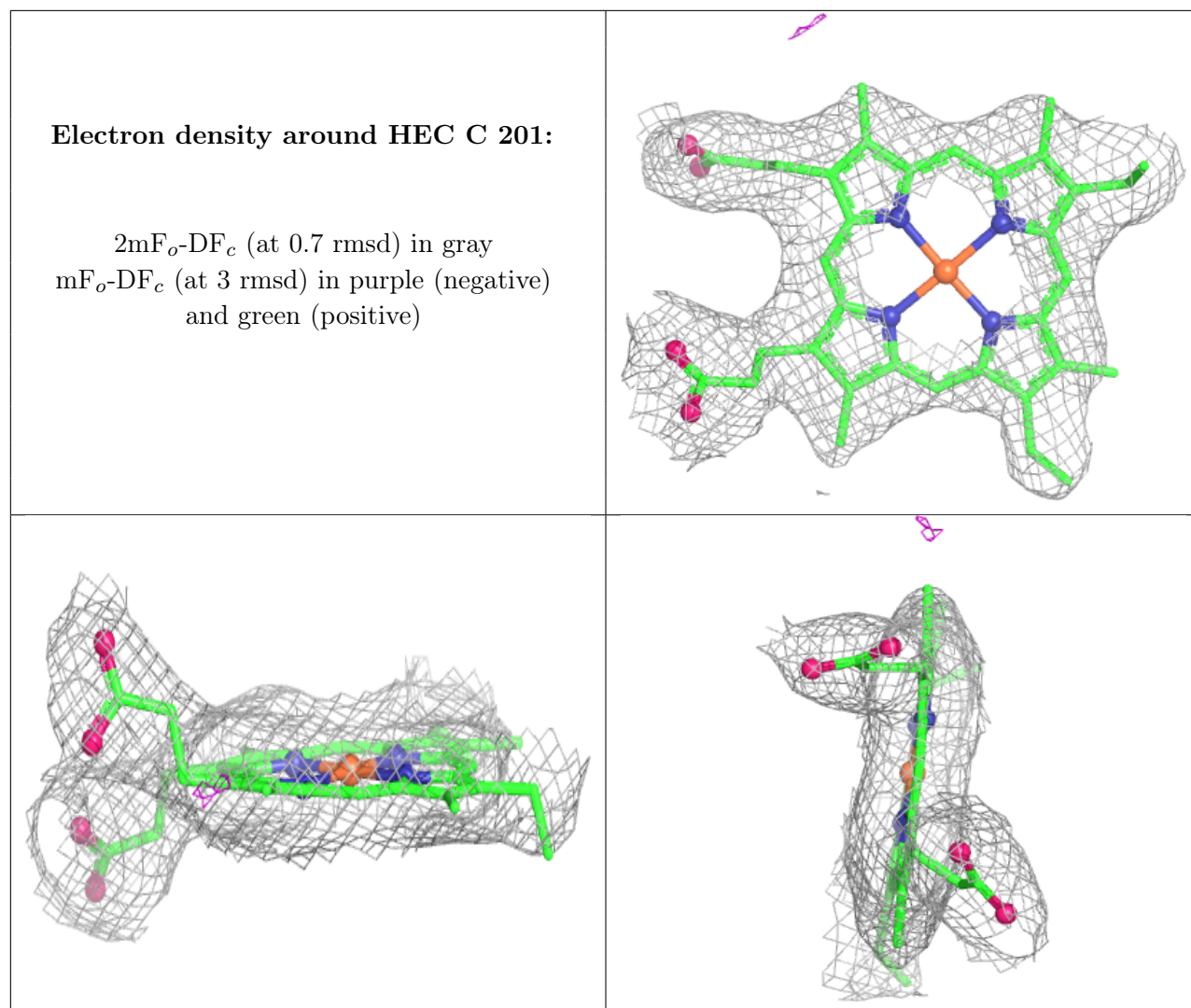
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around HEM B 801:

$2mF_o-DF_c$ (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.