WORLDWIDE wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 04:15 PM EDT

PDB ID	:	3GW9
Title	:	Crystal structure of sterol 14-alpha demethylase (CYP51) from Trypanosoma brucei bound to an inhibitor N-(1-(2,4-dichlorophenyl)-2-(1H-imidazol-1-yl)ethyl)-4-(5-phenyl-1,3,4-oxaziazol-2-yl)benzamide
Authors	:	Lepesheva, G.I.; Hargrove, T.Y.; Harp, J.; Wawrzak, Z.; Waterman, M.R.
Deposited on	:	2009-03-31
Resolution	:	1.87 Å(reported)

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

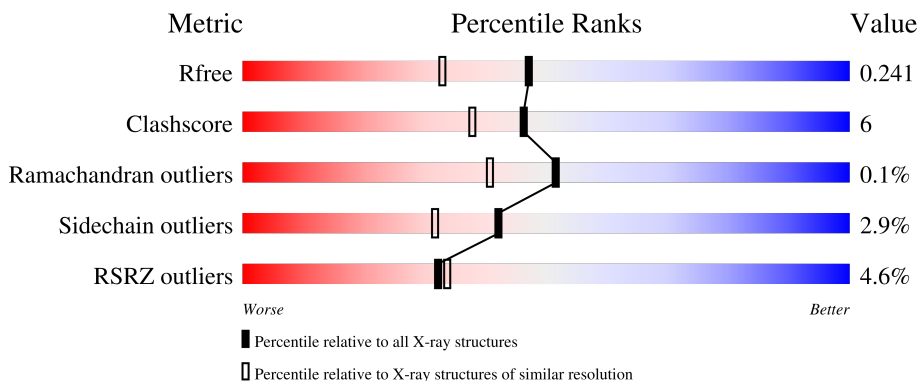|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.87 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	Percentile Ranks	Value
Rfree		0.241
Clashscore		6
Ramachandran outliers		0.1%
Sidechain outliers		2.9%
RSRZ outliers		4.6%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 <=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	450	4% / 85% / 15%
1	B	450	2% / 89% / 10% ·
1	C	450	4% / 88% / 11% ·
1	D	450	8% / 84% / 14% ·

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15276 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 STEROL 14ALPHA-DEMETHYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3575	2283	625	640	27			
1	B	449	Total	C	N	O	S	0	0	0
			3566	2277	623	639	27			
1	C	449	Total	C	N	O	S	0	0	0
			3566	2277	623	639	27			
1	D	449	Total	C	N	O	S	0	0	0
			3566	2277	623	639	27			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	LYS	ARG	engineered mutation	UNP Q385E8
A	29	GLY	PRO	engineered mutation	UNP Q385E8
A	30	LYS	THR	engineered mutation	UNP Q385E8
A	31	LEU	ASP	engineered mutation	UNP Q385E8
B	28	LYS	ARG	engineered mutation	UNP Q385E8
B	29	GLY	PRO	engineered mutation	UNP Q385E8
B	30	LYS	THR	engineered mutation	UNP Q385E8
B	31	LEU	ASP	engineered mutation	UNP Q385E8
C	28	LYS	ARG	engineered mutation	UNP Q385E8
C	29	GLY	PRO	engineered mutation	UNP Q385E8
C	30	LYS	THR	engineered mutation	UNP Q385E8
C	31	LEU	ASP	engineered mutation	UNP Q385E8
D	28	LYS	ARG	engineered mutation	UNP Q385E8
D	29	GLY	PRO	engineered mutation	UNP Q385E8
D	30	LYS	THR	engineered mutation	UNP Q385E8
D	31	LEU	ASP	engineered mutation	UNP Q385E8

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

HEM

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		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is N-[(1R)-1-(2,4-dichlorophenyl)-2-(1H-imidazol-1-yl)ethyl]-4-(5-phenyl-1,3,4-oxadiazol-2-yl)benzamide (three-letter code: VNI) (formula: $C_{26}H_{19}Cl_2N_5O_2$).

VNI

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 35	C 26	Cl 2	N 5	O 2	0	0
3	B	1	Total 35	C 26	Cl 2	N 5	O 2	0	0
3	C	1	Total 35	C 26	Cl 2	N 5	O 2	0	0
3	D	1	Total 35	C 26	Cl 2	N 5	O 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	149	Total 149	O 149	0	0
4	B	195	Total 195	O 195	0	0
4	C	219	Total 219	O 219	0	0
4	D	128	Total 128	O 128	0	0

3 Residue-property plots ⓘ

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.
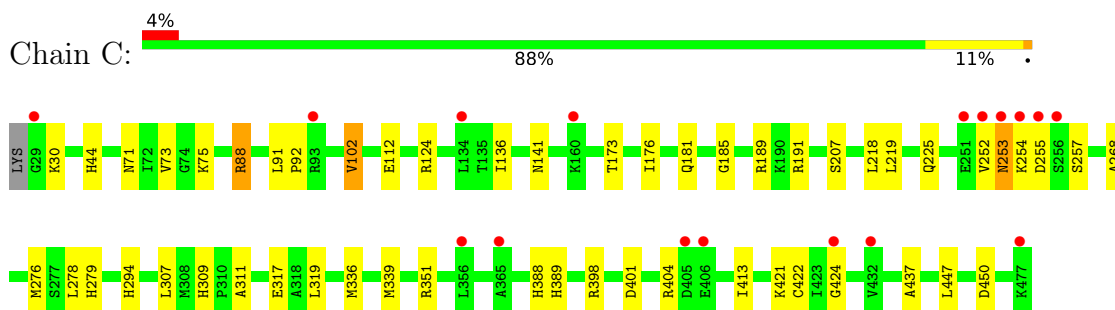
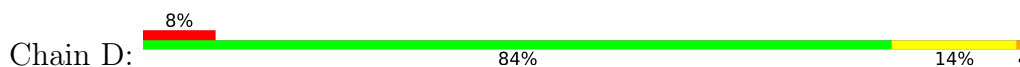• Molecule 1: STEROL 14ALPHA-DEMETHYLASE
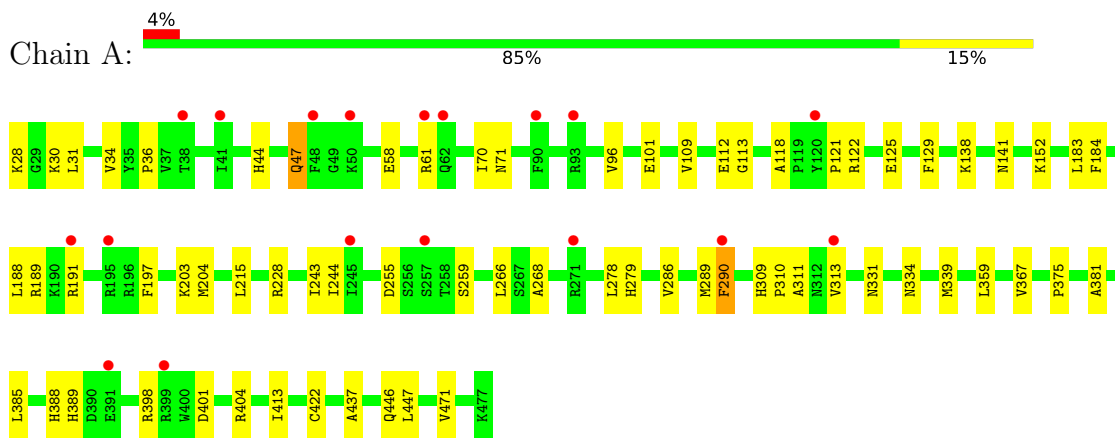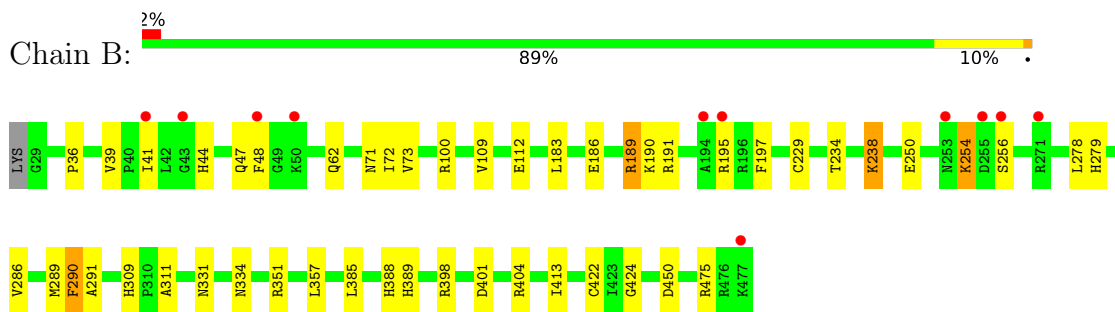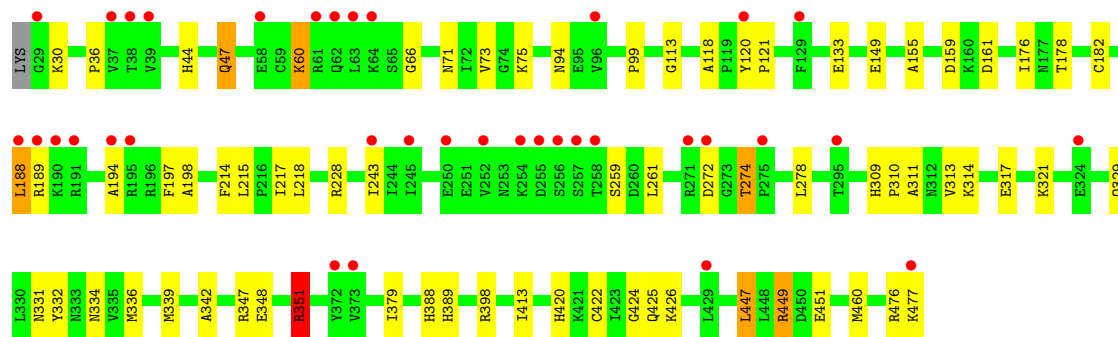
Chain A:

• Molecule 1: STEROL 14ALPHA-DEMETHYLASE

Chain B:

• Molecule 1: STEROL 14ALPHA-DEMETHYLASE

Chain C:

• Molecule 1: STEROL 14ALPHA-DEMETHYLASE

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.08Å 79.11Å 116.00Å 74.74° 79.13° 68.57°	Depositor
Resolution (Å)	37.48 – 1.87 37.46 – 1.87	Depositor EDS
% Data completeness (in resolution range)	97.0 (37.48-1.87) 97.0 (37.46-1.87)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.189 , 0.238 0.193 , 0.241	Depositor DCC
R_{free} test set	7635 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 44.1	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15276	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, VNI

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	0.79	0/3657	0.76	0/4944
1	B	0.78	1/3648 (0.0%)	0.77	2/4933 (0.0%)
1	C	0.87	0/3648	0.82	2/4933 (0.0%)
1	D	0.71	1/3648 (0.0%)	0.72	1/4933 (0.0%)
All	All	0.79	2/14601 (0.0%)	0.77	5/19743 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	182	CYS	CB-SG	-5.63	1.72	1.81
1	B	229	CYS	CB-SG	-5.29	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	189	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	C	124	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	C	124	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	351	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	189	ARG	NE-CZ-NH1	5.01	122.81	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	3575	0	3620	46	0
1	B	3566	0	3607	37	0
1	C	3566	0	3607	41	0
1	D	3566	0	3607	53	0
2	A	43	0	30	4	0
2	B	43	0	30	5	0
2	C	43	0	30	7	0
2	D	43	0	30	9	0
3	A	35	0	19	1	0
3	B	35	0	19	2	0
3	C	35	0	19	0	0
3	D	35	0	19	1	0
4	A	149	0	0	3	0
4	B	195	0	0	1	0
4	C	219	0	0	5	0
4	D	128	0	0	1	0
All	All	15276	0	14637	183	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 6.

All (183) 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:D:480:HEM:HMC2	2:D:480:HEM:HBC2	1.38	1.04
1:A:389:HIS:HE1	1:A:398:ARG:HH11	1.22	0.87
1:C:388:HIS:HE1	1:C:413:ILE:H	1.28	0.81
1:A:34:VAL:H	1:C:141:ASN:HD21	1.31	0.79
2:D:480:HEM:HBC2	2:D:480:HEM:CMC	2.11	0.78
1:A:389:HIS:CE1	1:A:398:ARG:HH11	2.02	0.78
1:B:44:HIS:HD2	1:B:71:ASN:H	1.31	0.78
1:D:75:LYS:HG2	1:D:379:ILE:HD12	1.68	0.75
2:A:480:HEM:HBC2	2:A:480:HEM:HMC2	1.68	0.75
1:B:388:HIS:HE1	1:B:413:ILE:H	1.32	0.74
1:A:47:GLN:HE21	1:A:47:GLN:H	1.36	0.73
2:C:480:HEM:HMC2	2:C:480:HEM:HBC2	1.70	0.73
1:D:449:ARG:HD3	1:D:451:GLU:O	1.90	0.71
1:D:347:ARG:HH22	1:D:425:GLN:NE2	1.89	0.70
1:D:388:HIS:HE1	1:D:413:ILE:H	1.40	0.70
1:D:389:HIS:CE1	1:D:398:ARG:HH11	2.09	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:HIS:HD2	1:D:71:ASN:H	1.39	0.70
1:A:388:HIS:HE1	1:A:413:ILE:H	1.37	0.69
1:A:191:ARG:HD2	1:A:243:ILE:CD1	2.22	0.69
1:B:389:HIS:CE1	1:B:398:ARG:HH11	2.14	0.66
1:D:310:PRO:O	1:D:313:VAL:HG13	1.96	0.65
2:A:480:HEM:HBC2	2:A:480:HEM:CMC	2.26	0.65
2:D:480:HEM:CMB	2:D:480:HEM:HBB2	2.26	0.65
2:D:480:HEM:HBB2	2:D:480:HEM:HMB2	1.78	0.65
1:B:389:HIS:HE1	1:B:398:ARG:HH11	1.45	0.64
1:C:44:HIS:HD2	1:C:71:ASN:H	1.46	0.64
1:C:102:VAL:HG13	4:C:628:HOH:O	1.95	0.64
1:C:253:ASN:HB3	1:C:255:ASP:O	1.98	0.64
2:C:480:HEM:HBC2	2:C:480:HEM:CMC	2.28	0.63
1:D:389:HIS:HE1	1:D:398:ARG:HD2	1.64	0.63
1:D:389:HIS:HE1	1:D:398:ARG:HH11	1.46	0.62
1:B:186:GLU:OE2	1:B:189:ARG:NH2	2.33	0.62
1:A:191:ARG:HD2	1:A:243:ILE:HD11	1.82	0.61
1:D:176:ILE:HD13	1:D:198:ALA:HB2	1.82	0.61
1:A:331:ASN:H	1:A:334:ASN:HD22	1.48	0.61
1:A:401:ASP:O	1:A:404:ARG:HG2	2.00	0.61
1:C:309:HIS:CD2	1:C:311:ALA:H	2.20	0.60
1:A:58:GLU:OE1	1:A:61:ARG:NH1	2.35	0.59
1:A:30:LYS:NZ	1:C:185:GLY:HA2	2.18	0.58
1:D:347:ARG:HH22	1:D:425:GLN:HE21	1.50	0.58
1:C:389:HIS:CE1	1:C:398:ARG:HH11	2.21	0.58
1:A:36:PRO:O	1:A:44:HIS:HE1	1.87	0.57
1:B:385:LEU:O	1:B:389:HIS:HD2	1.89	0.56
1:A:309:HIS:HD2	1:A:311:ALA:H	1.52	0.56
1:D:36:PRO:O	1:D:44:HIS:HE1	1.89	0.56
1:D:447:LEU:HD22	1:D:449:ARG:HG3	1.88	0.56
1:D:215:LEU:HD23	1:D:218:LEU:HD11	1.89	0.55
1:D:331:ASN:H	1:D:334:ASN:HD22	1.53	0.55
1:D:313:VAL:HG11	4:D:502:HOH:O	2.06	0.55
1:D:133:GLU:HG3	1:D:261:LEU:HD12	1.89	0.55
1:C:207:SER:O	1:C:225:GLN:HB3	2.07	0.55
1:C:424:GLY:HA3	2:C:480:HEM:C3C	2.41	0.55
1:C:112:GLU:O	1:C:279:HIS:HE1	1.89	0.54
1:C:389:HIS:HE1	1:C:398:ARG:HD2	1.72	0.54
1:A:31:LEU:HD22	1:A:375:PRO:HD3	1.90	0.54
1:D:460:MET:HG2	3:D:490:VNI:H17	1.90	0.54
1:B:48:PHE:CE2	3:B:490:VNI:H24	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:ARG:NH2	1:D:425:GLN:HE21	2.06	0.53
1:A:122:ARG:NH2	4:A:602:HOH:O	2.41	0.53
1:D:309:HIS:CD2	1:D:311:ALA:H	2.26	0.53
1:D:309:HIS:HD2	1:D:311:ALA:H	1.56	0.53
1:B:62:GLN:HE21	1:D:161:ASP:H	1.55	0.53
1:C:351:ARG:HA	1:C:388:HIS:CD2	2.43	0.53
1:B:109:VAL:CG1	1:B:286:VAL:HG11	2.39	0.52
1:A:44:HIS:HD2	1:A:71:ASN:H	1.56	0.52
1:C:401:ASP:O	1:C:404:ARG:HG2	2.10	0.52
1:D:348:GLU:OE1	1:D:351:ARG:HD3	2.10	0.52
1:A:422:CYS:HA	2:A:480:HEM:CHA	2.39	0.52
1:B:36:PRO:O	1:B:44:HIS:HE1	1.92	0.52
1:C:389:HIS:HE1	1:C:398:ARG:HH11	1.57	0.52
1:D:214:PHE:CE2	1:D:379:ILE:HD13	2.45	0.52
1:B:250:GLU:HB3	1:B:256:SER:HB3	1.91	0.52
1:C:91:LEU:N	1:C:92:PRO:CD	2.73	0.52
1:A:109:VAL:HG13	1:A:286:VAL:HG11	1.91	0.52
1:A:47:GLN:H	1:A:47:GLN:NE2	2.05	0.51
1:C:252:VAL:HG23	1:C:252:VAL:O	2.11	0.51
1:D:73:VAL:HG12	1:D:73:VAL:O	2.10	0.51
1:D:176:ILE:CD1	1:D:198:ALA:HB2	2.40	0.51
1:B:109:VAL:HG13	1:B:286:VAL:HG11	1.92	0.51
1:B:422:CYS:HA	2:B:480:HEM:CHA	2.41	0.51
1:C:268:ALA:HB3	1:C:276:MET:CE	2.41	0.51
1:A:446:GLN:O	1:A:471:VAL:HG13	2.10	0.51
1:B:424:GLY:HA3	2:B:480:HEM:C3C	2.46	0.51
1:B:286:VAL:O	1:B:290:PHE:HB2	2.09	0.50
1:D:189:ARG:NH2	1:D:194:ALA:HB2	2.26	0.50
1:B:234:THR:O	1:B:238:LYS:HD3	2.12	0.50
1:A:309:HIS:CD2	1:A:311:ALA:H	2.29	0.50
1:C:422:CYS:HB2	2:C:480:HEM:NA	2.27	0.50
1:C:309:HIS:HE1	1:C:450:ASP:O	1.94	0.50
1:B:331:ASN:H	1:B:334:ASN:HD22	1.59	0.50
1:A:244:ILE:HG12	1:A:266:LEU:HD11	1.93	0.49
1:A:101:GLU:HG3	4:A:657:HOH:O	2.11	0.49
1:A:331:ASN:H	1:A:334:ASN:ND2	2.09	0.49
1:D:120:TYR:HB2	1:D:121:PRO:HD3	1.95	0.48
1:B:62:GLN:NE2	1:D:161:ASP:H	2.10	0.48
1:D:388:HIS:CE1	1:D:413:ILE:H	2.25	0.48
2:D:480:HEM:HMB2	2:D:480:HEM:CBB	2.42	0.48
1:B:39:VAL:HG23	1:B:39:VAL:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:ARG:O	1:C:388:HIS:CD2	2.67	0.48
1:A:30:LYS:HE2	1:C:181:GLN:O	2.14	0.48
1:B:72:ILE:HG22	1:B:73:VAL:HG23	1.96	0.48
1:D:215:LEU:HD23	1:D:218:LEU:CD1	2.44	0.48
1:D:272:ASP:CB	1:D:274:THR:OG1	2.61	0.48
2:B:480:HEM:HBC2	2:B:480:HEM:HMC2	1.96	0.48
1:C:73:VAL:HG12	1:C:73:VAL:O	2.14	0.48
1:A:310:PRO:O	1:A:313:VAL:HG13	2.13	0.48
1:C:279:HIS:HD2	4:C:550:HOH:O	1.97	0.47
1:C:339:MET:HE1	1:C:437:ALA:HB2	1.96	0.47
1:C:421:LYS:HD3	4:C:25:HOH:O	2.14	0.47
1:B:357:LEU:HD22	1:B:385:LEU:HD22	1.97	0.47
1:D:272:ASP:HB3	1:D:274:THR:OG1	2.13	0.47
1:C:191:ARG:NH2	4:C:537:HOH:O	2.47	0.47
1:D:389:HIS:CE1	1:D:398:ARG:HD2	2.48	0.47
1:D:424:GLY:HA3	2:D:480:HEM:C3C	2.50	0.46
1:D:424:GLY:HA3	2:D:480:HEM:C2C	2.50	0.46
1:A:339:MET:HE3	1:A:437:ALA:HB2	1.97	0.46
1:D:60:LYS:HD3	1:D:66:GLY:HA2	1.97	0.46
1:C:173:THR:O	1:C:176:ILE:HG22	2.16	0.46
1:B:183:LEU:HD12	1:B:289:MET:CE	2.45	0.46
1:B:331:ASN:H	1:B:334:ASN:ND2	2.15	0.45
2:C:480:HEM:HMC2	2:C:480:HEM:CBC	2.44	0.45
1:D:314:LYS:HA	1:D:317:GLU:HG2	1.97	0.45
1:C:422:CYS:HA	2:C:480:HEM:CHA	2.46	0.45
1:A:112:GLU:O	1:A:279:HIS:HE1	1.99	0.45
1:D:47:GLN:HE21	1:D:47:GLN:H	1.65	0.45
1:A:47:GLN:HE21	1:A:47:GLN:N	2.11	0.45
1:A:129:PHE:CE2	1:A:268:ALA:HB1	2.52	0.44
1:A:34:VAL:H	1:C:141:ASN:ND2	2.07	0.44
1:A:121:PRO:O	1:A:125:GLU:HG3	2.17	0.44
1:B:44:HIS:CD2	1:B:71:ASN:H	2.22	0.44
1:A:113:GLY:O	1:A:118:ALA:HB2	2.18	0.44
1:B:401:ASP:O	1:B:404:ARG:HG2	2.17	0.44
1:C:218:LEU:HD21	1:D:218:LEU:HD11	1.99	0.44
1:B:238:LYS:CD	1:B:238:LYS:N	2.81	0.44
1:C:268:ALA:HB3	1:C:276:MET:HE2	1.99	0.44
1:D:331:ASN:H	1:D:334:ASN:ND2	2.15	0.44
1:D:422:CYS:HA	2:D:480:HEM:CHA	2.48	0.43
1:A:183:LEU:HD12	1:A:289:MET:CE	2.47	0.43
1:B:309:HIS:HE1	1:B:450:ASP:O	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:GLU:O	1:B:279:HIS:HE1	2.01	0.43
1:B:250:GLU:O	1:B:254:LYS:N	2.49	0.43
1:A:96:VAL:CG1	1:A:367:VAL:CG1	2.97	0.43
1:A:385:LEU:O	1:A:389:HIS:HD2	2.01	0.43
1:B:100:ARG:HD2	4:B:514:HOH:O	2.18	0.43
1:C:88:ARG:HA	1:C:88:ARG:HD2	1.83	0.43
1:C:336:MET:HE3	1:C:336:MET:HB2	1.82	0.43
1:D:113:GLY:O	1:D:118:ALA:HB2	2.19	0.43
2:D:480:HEM:CMC	2:D:480:HEM:CBC	2.91	0.42
1:A:183:LEU:HD12	1:A:289:MET:HE1	2.01	0.42
1:B:351:ARG:HA	1:B:388:HIS:CD2	2.54	0.42
1:B:309:HIS:CD2	1:B:311:ALA:H	2.38	0.42
1:C:254:LYS:O	1:C:257:SER:OG	2.30	0.42
1:A:109:VAL:HG22	1:A:204:MET:HB3	2.01	0.42
1:C:44:HIS:HD2	1:C:71:ASN:N	2.14	0.42
1:D:347:ARG:NH2	1:D:425:GLN:NE2	2.61	0.42
1:A:422:CYS:HA	2:A:480:HEM:C4D	2.55	0.42
1:D:36:PRO:O	1:D:44:HIS:CE1	2.72	0.42
1:D:332:TYR:CE1	1:D:336:MET:HG3	2.55	0.42
1:C:389:HIS:CE1	1:C:398:ARG:HD2	2.54	0.41
2:C:480:HEM:CMB	2:C:480:HEM:HBB2	2.49	0.41
1:C:294:HIS:HB2	4:C:554:HOH:O	2.20	0.41
1:A:70:ILE:HD13	1:A:70:ILE:HG21	1.85	0.41
1:B:291:ALA:HB1	3:B:490:VNI:C5	2.50	0.41
1:B:422:CYS:HA	2:B:480:HEM:C4D	2.54	0.41
1:A:290:PHE:HB3	3:A:490:VNI:CL2	2.57	0.41
1:B:309:HIS:HD2	1:B:311:ALA:H	1.69	0.41
1:C:307:LEU:HD13	1:C:319:LEU:HD22	2.03	0.41
1:D:476:ARG:O	1:D:477:LYS:C	2.58	0.41
1:C:309:HIS:HD2	1:C:311:ALA:H	1.66	0.41
1:D:149:GLU:HB2	1:D:178:THR:HG22	2.03	0.41
1:B:186:GLU:HG2	1:B:190:LYS:HE2	2.02	0.41
1:D:99:PRO:HG3	1:D:420:HIS:CE1	2.55	0.41
1:D:188:LEU:HD13	1:D:243:ILE:HD13	2.03	0.41
1:A:138:LYS:NZ	4:A:492:HOH:O	2.49	0.41
1:D:94:ASN:OD1	1:D:420:HIS:NE2	2.54	0.41
1:D:155:ALA:O	1:D:159:ASP:HB3	2.21	0.41
1:A:184:PHE:CD2	1:A:188:LEU:HD23	2.57	0.40
1:A:359:LEU:O	1:A:381:ALA:HA	2.21	0.40
1:C:181:GLN:OE1	1:C:189:ARG:NH1	2.55	0.40
1:A:203:LYS:HE3	1:A:228:ARG:HG2	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:GLY:HA3	2:B:480:HEM:C2C	2.56	0.40
1:D:339:MET:HE2	1:D:342:ALA:CB	2.51	0.40
1:A:184:PHE:O	1:A:189:ARG:NH1	2.43	0.40

There are no symmetry-related clashes.

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	A	448/450 (100%)	436 (97%)	12 (3%)	0	100	100
1	B	447/450 (99%)	432 (97%)	14 (3%)	1 (0%)	47	37
1	C	447/450 (99%)	435 (97%)	11 (2%)	1 (0%)	47	37
1	D	447/450 (99%)	438 (98%)	9 (2%)	0	100	100
All	All	1789/1800 (99%)	1741 (97%)	46 (3%)	2 (0%)	51	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	253	ASN
1	B	41	ILE

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	392/392 (100%)	381 (97%)	11 (3%)	43	33
1	B	391/392 (100%)	382 (98%)	9 (2%)	50	41
1	C	391/392 (100%)	382 (98%)	9 (2%)	50	41
1	D	391/392 (100%)	375 (96%)	16 (4%)	30	19
All	All	1565/1568 (100%)	1520 (97%)	45 (3%)	42	32

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	47	GLN
1	A	141	ASN
1	A	152	LYS
1	A	197	PHE
1	A	215	LEU
1	A	255	ASP
1	A	259	SER
1	A	278	LEU
1	A	290	PHE
1	A	447	LEU
1	B	47	GLN
1	B	191	ARG
1	B	195	ARG
1	B	197	PHE
1	B	238	LYS
1	B	254	LYS
1	B	278	LEU
1	B	290	PHE
1	B	475	ARG
1	C	30	LYS
1	C	75	LYS
1	C	88	ARG
1	C	102	VAL
1	C	136	ILE
1	C	219	LEU
1	C	278	LEU
1	C	317	GLU
1	C	447	LEU
1	D	30	LYS
1	D	47	GLN
1	D	60	LYS
1	D	188	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	197	PHE
1	D	217	ILE
1	D	228	ARG
1	D	259	SER
1	D	274	THR
1	D	278	LEU
1	D	321	LYS
1	D	329	GLN
1	D	351	ARG
1	D	426	LYS
1	D	447	LEU
1	D	449	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	47	GLN
1	A	279	HIS
1	A	309	HIS
1	A	334	ASN
1	A	388	HIS
1	A	389	HIS
1	A	446	GLN
1	B	44	HIS
1	B	47	GLN
1	B	62	GLN
1	B	94	ASN
1	B	157	ASN
1	B	279	HIS
1	B	309	HIS
1	B	334	ASN
1	B	388	HIS
1	B	389	HIS
1	C	44	HIS
1	C	141	ASN
1	C	279	HIS
1	C	309	HIS
1	C	329	GLN
1	C	333	ASN
1	C	334	ASN
1	C	388	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	389	HIS
1	D	44	HIS
1	D	47	GLN
1	D	253	ASN
1	D	279	HIS
1	D	309	HIS
1	D	334	ASN
1	D	388	HIS
1	D	389	HIS
1	D	425	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	VNI	D	490	2	31,39,39	1.13	1 (3%)	39,54,54	1.34	4 (10%)
2	HEM	B	480	1,3	41,50,50	1.80	9 (21%)	45,82,82	1.91	10 (22%)
3	VNI	A	490	2	31,39,39	1.21	2 (6%)	39,54,54	1.64	5 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
2	HEM	D	480	1,3	41,50,50	2.05	11 (26%)	45,82,82	1.67	11 (24%)
2	HEM	C	480	1,3	41,50,50	1.88	8 (19%)	45,82,82	1.93	12 (26%)
3	VNI	B	490	2	31,39,39	1.15	3 (9%)	39,54,54	1.85	8 (20%)
3	VNI	C	490	2	31,39,39	1.27	4 (12%)	39,54,54	2.08	13 (33%)
2	HEM	A	480	1,3	41,50,50	2.13	13 (31%)	45,82,82	2.14	15 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	VNI	D	490	2	-	2/16/24/24	0/5/5/5
2	HEM	B	480	1,3	-	0/12/54/54	-
3	VNI	A	490	2	-	5/16/24/24	0/5/5/5
2	HEM	D	480	1,3	-	2/12/54/54	-
2	HEM	C	480	1,3	-	0/12/54/54	-
3	VNI	B	490	2	-	3/16/24/24	0/5/5/5
3	VNI	C	490	2	-	2/16/24/24	0/5/5/5
2	HEM	A	480	1,3	-	0/12/54/54	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	480	HEM	C3C-C2C	-6.98	1.30	1.40
2	B	480	HEM	C3D-C2D	6.51	1.50	1.36
2	A	480	HEM	C3D-C2D	6.47	1.50	1.36
2	A	480	HEM	C3C-C2C	-5.96	1.32	1.40
2	D	480	HEM	C3D-C2D	5.83	1.49	1.36
2	C	480	HEM	C3C-C2C	-5.81	1.32	1.40
2	C	480	HEM	C3D-C2D	5.76	1.49	1.36
2	A	480	HEM	C3C-CAC	4.03	1.56	1.47
2	C	480	HEM	CAA-C2A	3.98	1.57	1.52
3	A	490	VNI	C7-C2	-3.64	1.46	1.52
2	D	480	HEM	C3B-C2B	-3.45	1.30	1.37
2	A	480	HEM	CMD-C2D	3.38	1.58	1.50
2	B	480	HEM	CAA-C2A	3.35	1.57	1.52
2	B	480	HEM	C3C-C2C	-3.27	1.35	1.40
2	D	480	HEM	FE-NB	-3.18	1.81	1.96
3	D	490	VNI	C7-C2	-3.10	1.47	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	480	HEM	CMC-C2C	3.09	1.58	1.51
3	B	490	VNI	C7-C2	-2.95	1.47	1.52
2	B	480	HEM	C3C-CAC	2.86	1.53	1.47
2	D	480	HEM	O2D-CGD	-2.85	1.21	1.30
2	A	480	HEM	CAA-C2A	2.84	1.56	1.52
2	B	480	HEM	CMC-C2C	2.78	1.58	1.51
2	D	480	HEM	C1A-CHA	-2.70	1.33	1.41
2	B	480	HEM	C1B-NB	-2.53	1.35	1.40
2	C	480	HEM	CMB-C2B	2.53	1.56	1.50
3	B	490	VNI	C3-N2	-2.44	1.45	1.48
2	D	480	HEM	C4A-CHB	-2.43	1.34	1.41
2	B	480	HEM	C1A-NA	2.42	1.41	1.36
2	D	480	HEM	O2A-CGA	-2.41	1.22	1.30
2	D	480	HEM	CHD-C1D	-2.37	1.34	1.41
2	A	480	HEM	CMA-C3A	2.37	1.56	1.51
2	D	480	HEM	C2A-C3A	-2.35	1.30	1.37
2	C	480	HEM	CAB-C3B	2.35	1.53	1.47
2	A	480	HEM	O2A-CGA	-2.34	1.22	1.30
3	B	490	VNI	N4-N5	2.33	1.42	1.37
3	C	490	VNI	C15-C16	-2.33	1.36	1.41
2	C	480	HEM	C3C-CAC	2.29	1.52	1.47
2	A	480	HEM	CMB-C2B	2.25	1.55	1.50
2	C	480	HEM	C3B-C2B	-2.22	1.32	1.37
3	C	490	VNI	C7-C2	-2.20	1.48	1.52
2	B	480	HEM	CAB-C3B	2.19	1.53	1.47
3	C	490	VNI	C12-CL2	2.19	1.78	1.73
2	A	480	HEM	C1A-CHA	-2.16	1.35	1.41
2	C	480	HEM	CMC-C2C	2.12	1.56	1.51
3	A	490	VNI	C12-CL2	2.12	1.78	1.73
2	D	480	HEM	C4A-NA	-2.08	1.31	1.36
2	A	480	HEM	C3B-C4B	-2.05	1.40	1.44
2	A	480	HEM	C4A-CHB	-2.04	1.35	1.41
3	C	490	VNI	C15-C14	2.02	1.40	1.36
2	B	480	HEM	CMD-C2D	2.02	1.55	1.50
2	A	480	HEM	CAB-C3B	2.01	1.52	1.47

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	490	VNI	C3-C2-N1	-8.18	96.18	110.45
3	C	490	VNI	C3-C2-N1	-6.75	98.67	110.45
3	A	490	VNI	C3-C2-N1	-6.38	99.32	110.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	480	HEM	CHC-C4B-NB	5.47	130.37	124.43
3	D	490	VNI	C3-C2-N1	-5.39	101.05	110.45
2	A	480	HEM	CAD-C3D-C4D	5.13	133.62	124.66
2	B	480	HEM	C4D-ND-C1D	4.86	110.09	105.07
2	B	480	HEM	C2C-C3C-C4C	4.41	109.98	106.90
2	B	480	HEM	CHC-C4B-NB	4.36	129.17	124.43
2	A	480	HEM	CMC-C2C-C3C	4.33	132.78	124.68
3	C	490	VNI	C2-C3-N2	4.29	117.80	112.25
2	C	480	HEM	C4D-ND-C1D	4.25	109.46	105.07
2	B	480	HEM	CMA-C3A-C4A	-4.18	122.03	128.46
2	D	480	HEM	CAD-C3D-C4D	4.09	131.81	124.66
2	C	480	HEM	CMA-C3A-C4A	-4.08	122.20	128.46
2	A	480	HEM	CMA-C3A-C4A	-3.91	122.46	128.46
2	A	480	HEM	CAD-C3D-C2D	-3.90	120.61	127.88
2	A	480	HEM	CMD-C2D-C1D	3.87	130.94	125.04
2	C	480	HEM	C2C-C3C-C4C	3.87	109.60	106.90
2	A	480	HEM	CHD-C1D-ND	3.85	128.62	124.43
2	A	480	HEM	C4B-C3B-C2B	3.71	110.06	107.11
3	C	490	VNI	C11-C10-CL1	-3.67	114.57	119.15
3	C	490	VNI	C12-C7-C2	-3.54	117.18	121.71
2	D	480	HEM	C1B-NB-C4B	-3.32	101.64	105.07
2	A	480	HEM	C2C-C3C-C4C	3.29	109.19	106.90
2	D	480	HEM	CMC-C2C-C3C	3.26	130.77	124.68
3	C	490	VNI	C8-C7-C12	3.19	119.98	116.81
2	B	480	HEM	CAD-C3D-C4D	3.08	130.03	124.66
3	C	490	VNI	C7-C2-N1	3.06	117.63	111.47
3	C	490	VNI	C13-C1-N1	-3.00	111.31	117.06
3	B	490	VNI	C2-N1-C1	-2.88	118.63	122.34
2	A	480	HEM	CHC-C4B-NB	2.88	127.56	124.43
2	C	480	HEM	C4B-C3B-C2B	2.83	109.36	107.11
2	C	480	HEM	CAD-C3D-C4D	2.79	129.53	124.66
2	A	480	HEM	C4D-ND-C1D	2.79	107.95	105.07
2	C	480	HEM	CHC-C4B-C3B	-2.76	120.35	124.57
2	D	480	HEM	O2D-CGD-CBD	2.75	122.85	114.03
3	A	490	VNI	C12-C7-C2	-2.67	118.28	121.71
3	A	490	VNI	C13-C1-N1	-2.66	111.97	117.06
2	B	480	HEM	CMD-C2D-C1D	2.65	129.08	125.04
2	A	480	HEM	O2D-CGD-CBD	2.64	122.51	114.03
2	C	480	HEM	CBA-CAA-C2A	-2.64	108.12	112.62
2	D	480	HEM	CMA-C3A-C4A	-2.63	124.43	128.46
2	D	480	HEM	C2C-C3C-C4C	2.62	108.73	106.90
2	A	480	HEM	CHD-C1D-C2D	-2.61	120.90	124.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	490	VNI	C9-C10-CL1	2.60	123.41	119.35
2	B	480	HEM	C4A-C3A-C2A	2.58	108.79	107.00
3	C	490	VNI	C15-C16-C17	2.53	120.90	118.65
2	A	480	HEM	CMA-C3A-C2A	2.53	129.71	124.94
3	C	490	VNI	C7-C12-CL2	2.52	123.02	120.41
2	C	480	HEM	CMA-C3A-C2A	2.52	129.69	124.94
2	C	480	HEM	O2D-CGD-CBD	2.52	122.12	114.03
3	D	490	VNI	C7-C12-CL2	-2.50	117.83	120.41
3	B	490	VNI	C15-C16-C17	2.46	120.83	118.65
2	D	480	HEM	C4D-C3D-C2D	-2.42	103.38	106.90
3	A	490	VNI	C18-C13-C1	-2.38	112.90	120.62
2	A	480	HEM	CMB-C2B-C1B	2.33	128.58	125.04
2	A	480	HEM	O1D-CGD-CBD	-2.33	115.61	123.08
3	C	490	VNI	C15-C14-C13	-2.30	118.19	120.79
2	D	480	HEM	CMD-C2D-C1D	2.26	128.48	125.04
2	B	480	HEM	CAD-CBD-CGD	-2.24	108.78	113.60
3	C	490	VNI	O1-C1-N1	2.20	126.50	122.45
2	B	480	HEM	CMA-C3A-C2A	2.20	129.09	124.94
3	D	490	VNI	C12-C7-C2	-2.19	118.90	121.71
2	D	480	HEM	C2B-C1B-NB	2.17	112.41	109.84
3	D	490	VNI	C8-C7-C12	2.14	118.94	116.81
3	B	490	VNI	C12-C7-C2	-2.13	118.99	121.71
3	B	490	VNI	C15-C14-C13	-2.12	118.40	120.79
2	C	480	HEM	CHD-C1D-ND	2.11	126.73	124.43
2	D	480	HEM	C3D-C4D-ND	2.10	112.50	110.17
2	C	480	HEM	O1D-CGD-CBD	-2.09	116.38	123.08
3	A	490	VNI	C26-C21-C22	2.08	120.49	118.65
3	B	490	VNI	C4-N2-C6	2.07	110.24	108.21
2	D	480	HEM	CHD-C1D-ND	2.06	126.67	124.43
3	B	490	VNI	C18-C13-C14	2.06	121.53	118.59
3	C	490	VNI	C26-C21-C22	2.02	120.44	118.65
2	B	480	HEM	C4B-C3B-C2B	2.02	108.72	107.11
3	B	490	VNI	C11-C12-CL2	-2.01	115.25	118.49

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	490	VNI	N1-C1-C13-C18
3	A	490	VNI	N1-C1-C13-C18
3	C	490	VNI	N1-C1-C13-C18
3	B	490	VNI	O1-C1-C13-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	490	VNI	N1-C1-C13-C14
3	A	490	VNI	C3-C2-C7-C8
3	D	490	VNI	C3-C2-C7-C8
3	C	490	VNI	O1-C1-C13-C18
2	D	480	HEM	CAD-CBD-CGD-O2D
3	A	490	VNI	O1-C1-C13-C18
2	D	480	HEM	CAD-CBD-CGD-O1D
3	A	490	VNI	N1-C1-C13-C14
3	A	490	VNI	C7-C2-N1-C1
3	D	490	VNI	C7-C2-N1-C1

There are no ring outliers.

7 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	490	VNI	1	0
2	B	480	HEM	5	0
3	A	490	VNI	1	0
2	D	480	HEM	9	0
2	C	480	HEM	7	0
3	B	490	VNI	2	0
2	A	480	HEM	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand VNI D 490

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 480

Bond lengths

Bond angles

Torsions

Rings

Ligand VNI A 490

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM D 480

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 480

Bond lengths

Bond angles

Torsions

Rings

Ligand VNI B 490

Bond lengths

Bond angles

Torsions

Rings

Ligand VNI C 490

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 480

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	450/450 (100%)	0.25	18 (4%)	38	39	22, 35, 51, 61	0
1	B	449/450 (99%)	0.11	11 (2%)	59	60	21, 32, 45, 57	0
1	C	449/450 (99%)	0.13	17 (3%)	40	42	20, 30, 42, 61	0
1	D	449/450 (99%)	0.40	36 (8%)	12	13	23, 38, 61, 71	0
All	All	1797/1800 (99%)	0.22	82 (4%)	32	34	20, 33, 52, 71	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	29	GLY	7.5
1	B	256	SER	6.7
1	B	255	ASP	5.7
1	D	257	SER	5.3
1	C	255	ASP	5.1
1	D	194	ALA	4.9
1	C	253	ASN	4.6
1	D	243	ILE	4.4
1	D	256	SER	4.4
1	C	256	SER	4.0
1	D	61	ARG	3.9
1	D	62	GLN	3.9
1	C	29	GLY	3.8
1	C	477	LYS	3.6
1	C	252	VAL	3.6
1	C	405	ASP	3.6
1	D	191	ARG	3.4
1	C	254	LYS	3.4
1	A	50	LYS	3.4
1	B	41	ILE	3.3
1	B	195	ARG	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	64	LYS	3.2
1	A	257	SER	3.1
1	A	93	ARG	3.1
1	D	477	LYS	3.0
1	D	37	VAL	3.0
1	D	120	TYR	2.8
1	A	195	ARG	2.8
1	D	373	VAL	2.8
1	A	61	ARG	2.8
1	C	251	GLU	2.8
1	B	271	ARG	2.7
1	D	39	VAL	2.7
1	C	93	ARG	2.7
1	D	255	ASP	2.7
1	D	250	GLU	2.7
1	A	271	ARG	2.6
1	D	38	THR	2.6
1	B	253	ASN	2.6
1	D	429	LEU	2.6
1	D	195	ARG	2.6
1	D	271	ARG	2.6
1	A	313	VAL	2.6
1	D	129	PHE	2.5
1	A	399	ARG	2.5
1	B	194	ALA	2.5
1	B	43	GLY	2.5
1	C	424	GLY	2.5
1	A	191	ARG	2.5
1	D	272	ASP	2.5
1	D	63	LEU	2.5
1	A	62	GLN	2.5
1	D	190	LYS	2.4
1	A	120	TYR	2.4
1	D	258	THR	2.4
1	D	189	ARG	2.4
1	C	365	ALA	2.4
1	D	295	THR	2.3
1	A	41	ILE	2.3
1	D	254	LYS	2.3
1	A	245	ILE	2.3
1	D	96	VAL	2.3
1	A	38	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	290	PHE	2.3
1	C	160	LYS	2.2
1	B	48	PHE	2.2
1	C	134	LEU	2.2
1	D	58	GLU	2.2
1	D	324	GLU	2.2
1	D	372	TYR	2.1
1	D	252	VAL	2.1
1	B	477	LYS	2.1
1	C	406	GLU	2.1
1	A	90	PHE	2.1
1	A	391	GLU	2.1
1	D	275	PRO	2.1
1	C	432	VAL	2.0
1	C	356	LEU	2.0
1	D	188	LEU	2.0
1	A	48	PHE	2.0
1	D	245	ILE	2.0
1	B	50	LYS	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 monosaccharides 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
3	VNI	A	490	35/35	0.93	0.15	21,31,50,50	0
3	VNI	B	490	35/35	0.93	0.13	23,32,53,53	0
3	VNI	D	490	35/35	0.93	0.12	23,31,45,45	0
3	VNI	C	490	35/35	0.95	0.14	20,25,40,43	0

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	D	480	43/43	0.96	0.16	24,28,37,42	0
2	HEM	C	480	43/43	0.98	0.14	16,20,26,30	0
2	HEM	A	480	43/43	0.98	0.20	16,22,28,33	0
2	HEM	B	480	43/43	0.98	0.18	19,22,25,30	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 VNI A 490:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
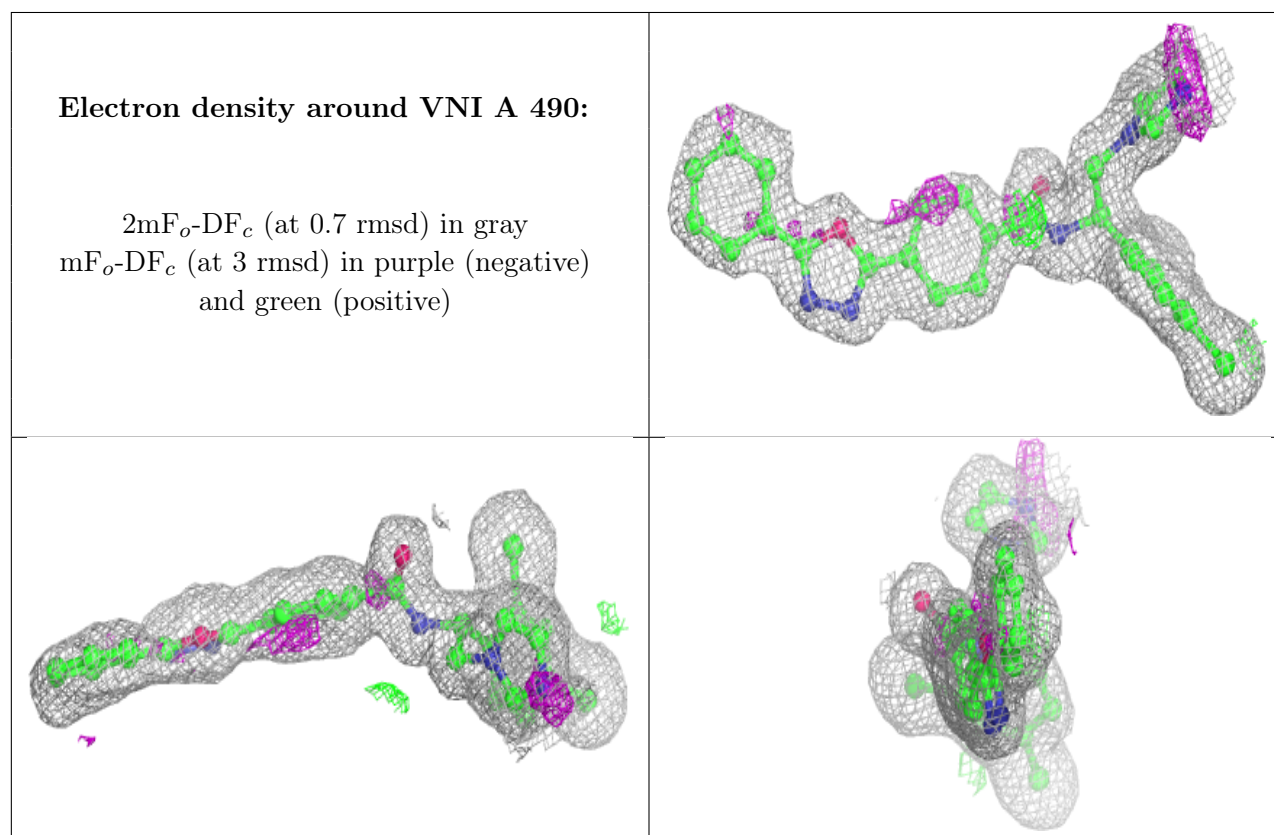
Electron density around VNI B 490:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
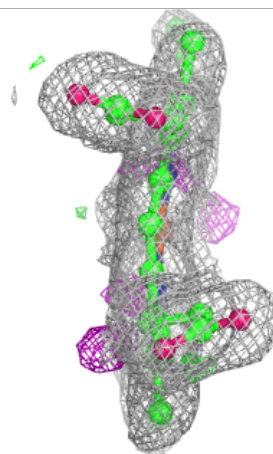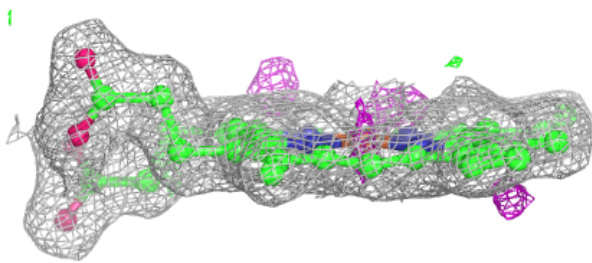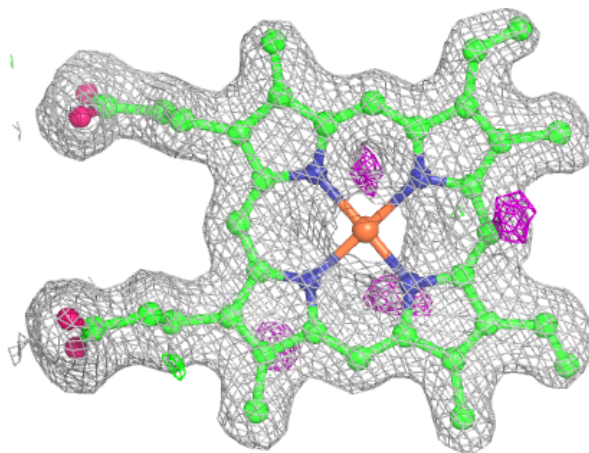and green (positive)
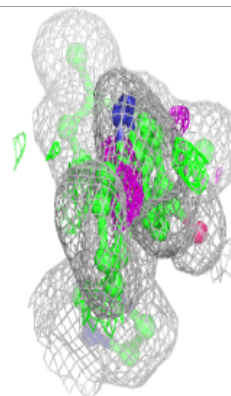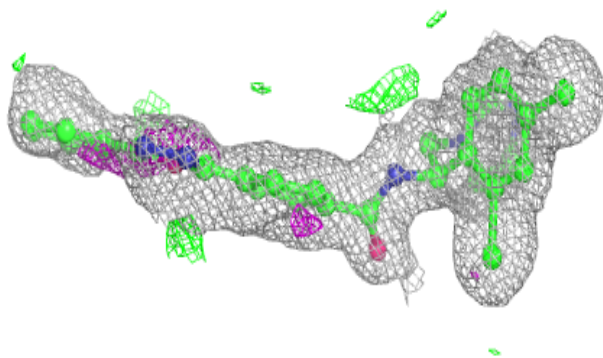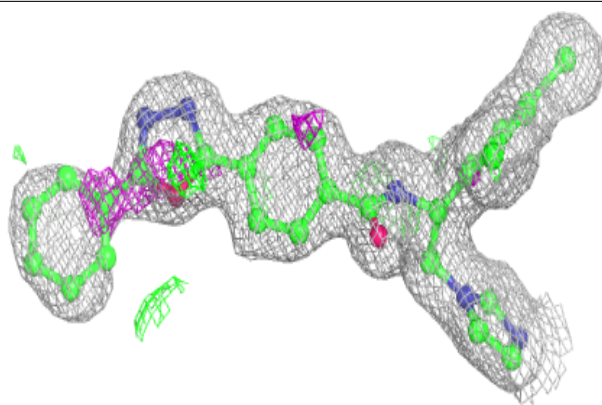
Electron density around VNI D 490:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
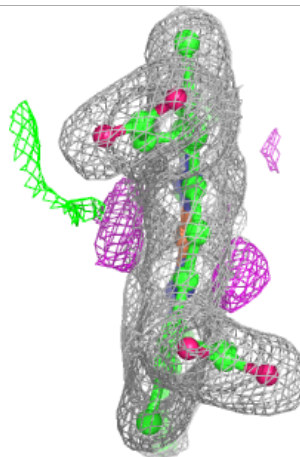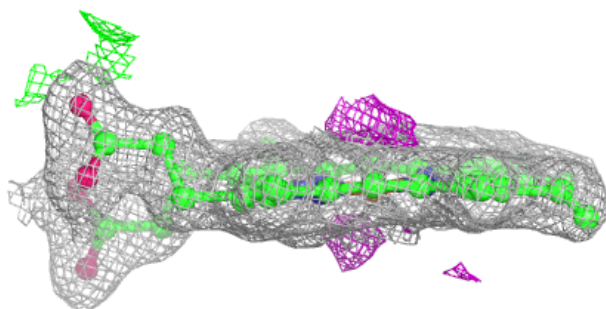mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
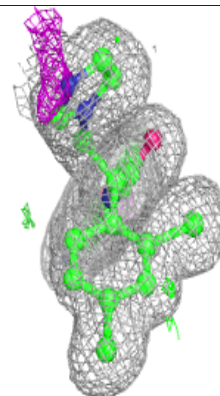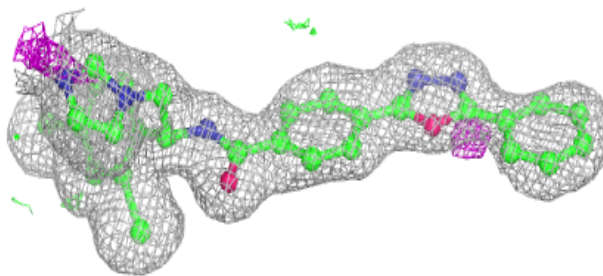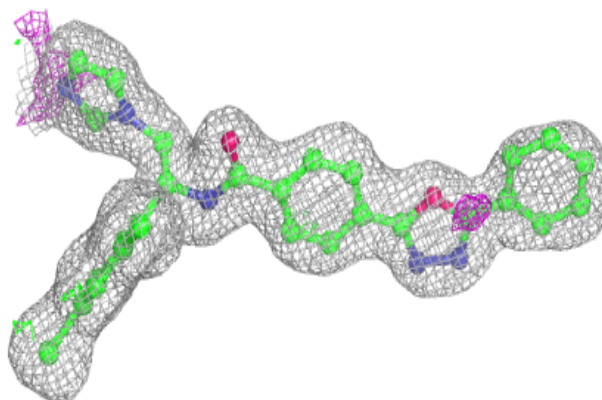
Electron density around VNI C 490:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
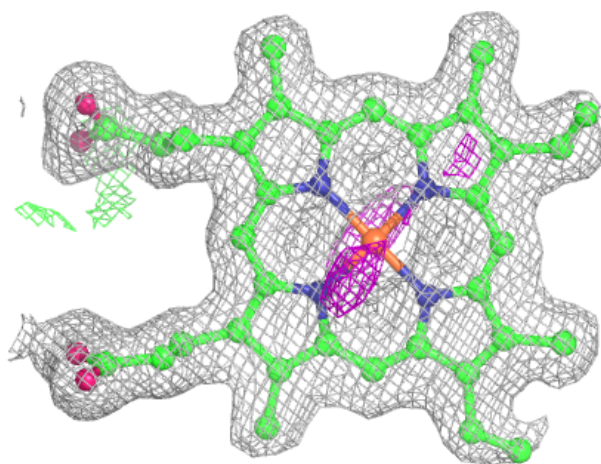and green (positive)
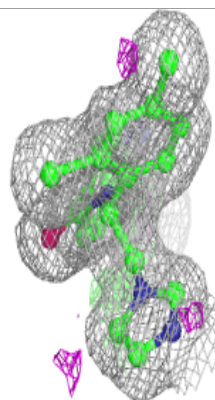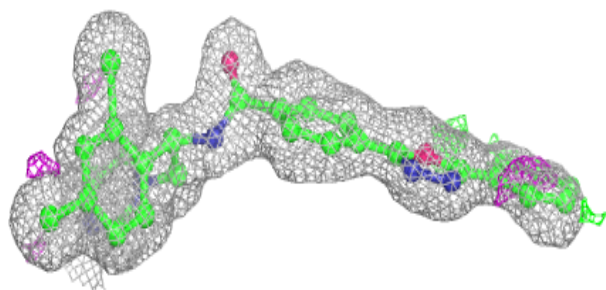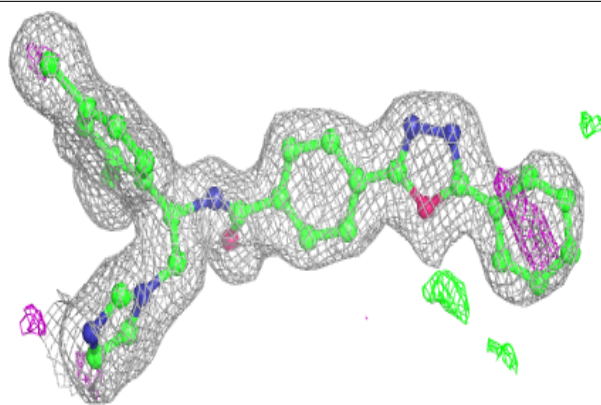
Electron density around HEM D 480:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
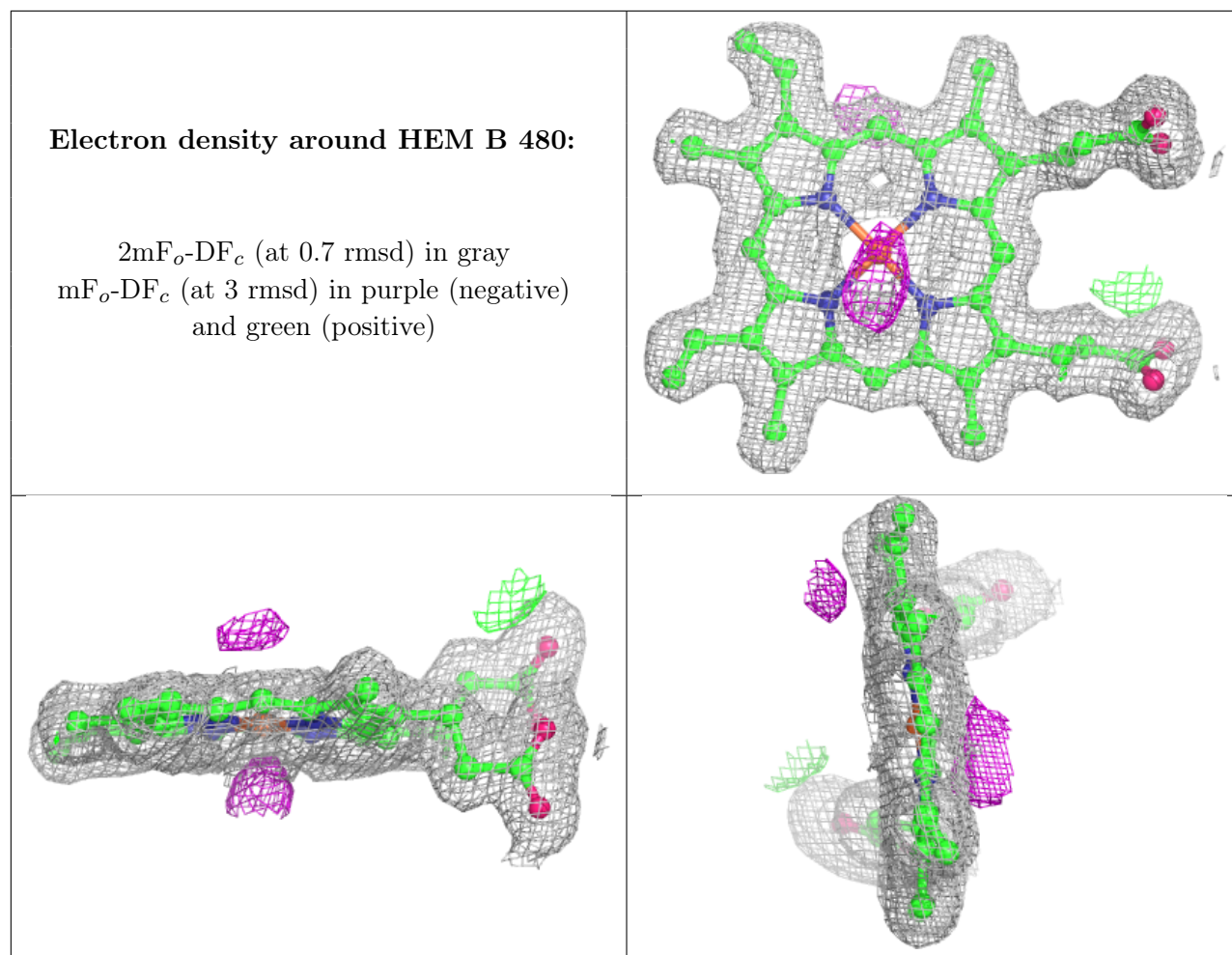and green (positive)
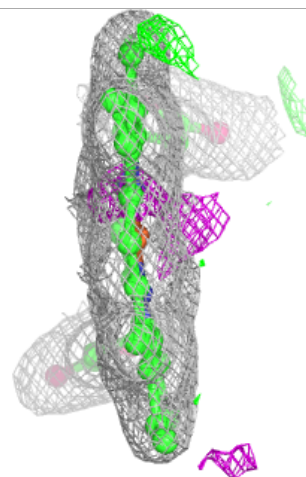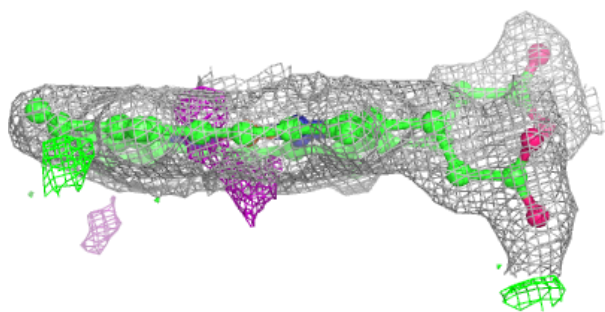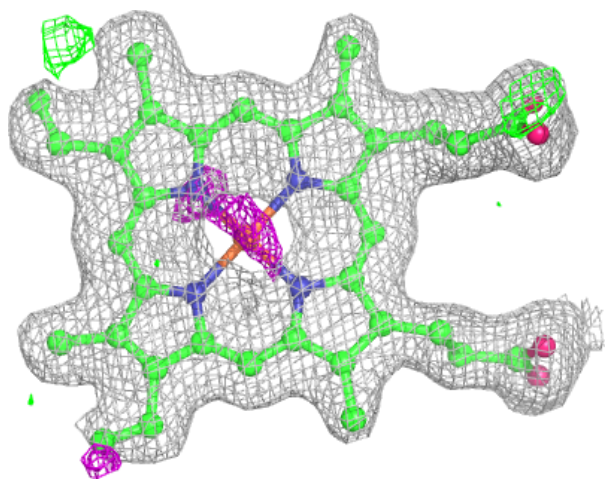
Electron density around HEM C 480:

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

Electron density around HEM A 480:

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

Electron density around HEM B 480:

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

6.5 Other polymers (i)

There are no such residues in this entry.