



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:00 PM UTC

PDB ID : 4WG2 / pdb_00004wg2
Title : P411BM3-CIS T438S I263F regioselective C-H amination catalyst
Authors : Hyster, T.K.; Farwell, C.C.; Buller, A.R.; McIntosh, J.A.; Arnold, F.H.
Deposited on : 2014-09-17
Resolution : 2.66 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

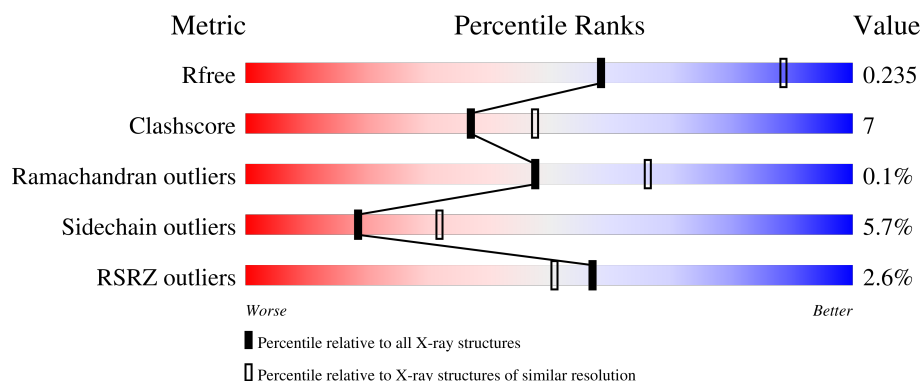
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	469	% 79% 18% ..
1	B	469	3% 83% 11% ..
1	C	469	3% 80% 17% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10947 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 Bifunctional P-450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3621	2313	615	677	16			
1	B	451	Total	C	N	O	S	0	0	0
			3533	2261	599	657	16			
1	C	460	Total	C	N	O	S	0	0	0
			3583	2290	602	675	16			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	ALA	VAL	engineered mutation	UNP P14779
A	87	VAL	PHE	engineered mutation	UNP P14779
A	142	SER	PRO	engineered mutation	UNP P14779
A	175	ILE	THR	engineered mutation	UNP P14779
A	184	VAL	ALA	engineered mutation	UNP P14779
A	226	ARG	SER	engineered mutation	UNP P14779
A	236	GLN	HIS	engineered mutation	UNP P14779
A	252	GLY	GLU	engineered mutation	UNP P14779
A	263	PHE	ILE	engineered mutation	UNP P14779
A	268	ALA	THR	engineered mutation	UNP P14779
A	290	VAL	ALA	engineered mutation	UNP P14779
A	353	VAL	LEU	engineered mutation	UNP P14779
A	366	VAL	ILE	engineered mutation	UNP P14779
A	400	SER	CYS	engineered mutation	UNP P14779
A	438	SER	THR	engineered mutation	UNP P14779
A	442	LYS	GLU	engineered mutation	UNP P14779
A	464	HIS	-	expression tag	UNP P14779
A	465	HIS	-	expression tag	UNP P14779
A	466	HIS	-	expression tag	UNP P14779
A	467	HIS	-	expression tag	UNP P14779
A	468	HIS	-	expression tag	UNP P14779
A	469	HIS	-	expression tag	UNP P14779
B	78	ALA	VAL	engineered mutation	UNP P14779

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	87	VAL	PHE	engineered mutation	UNP P14779
B	142	SER	PRO	engineered mutation	UNP P14779
B	175	ILE	THR	engineered mutation	UNP P14779
B	184	VAL	ALA	engineered mutation	UNP P14779
B	226	ARG	SER	engineered mutation	UNP P14779
B	236	GLN	HIS	engineered mutation	UNP P14779
B	252	GLY	GLU	engineered mutation	UNP P14779
B	263	PHE	ILE	engineered mutation	UNP P14779
B	268	ALA	THR	engineered mutation	UNP P14779
B	290	VAL	ALA	engineered mutation	UNP P14779
B	353	VAL	LEU	engineered mutation	UNP P14779
B	366	VAL	ILE	engineered mutation	UNP P14779
B	400	SER	CYS	engineered mutation	UNP P14779
B	438	SER	THR	engineered mutation	UNP P14779
B	442	LYS	GLU	engineered mutation	UNP P14779
B	464	HIS	-	expression tag	UNP P14779
B	465	HIS	-	expression tag	UNP P14779
B	466	HIS	-	expression tag	UNP P14779
B	467	HIS	-	expression tag	UNP P14779
B	468	HIS	-	expression tag	UNP P14779
B	469	HIS	-	expression tag	UNP P14779
C	78	ALA	VAL	engineered mutation	UNP P14779
C	87	VAL	PHE	engineered mutation	UNP P14779
C	142	SER	PRO	engineered mutation	UNP P14779
C	175	ILE	THR	engineered mutation	UNP P14779
C	184	VAL	ALA	engineered mutation	UNP P14779
C	226	ARG	SER	engineered mutation	UNP P14779
C	236	GLN	HIS	engineered mutation	UNP P14779
C	252	GLY	GLU	engineered mutation	UNP P14779
C	263	PHE	ILE	engineered mutation	UNP P14779
C	268	ALA	THR	engineered mutation	UNP P14779
C	290	VAL	ALA	engineered mutation	UNP P14779
C	353	VAL	LEU	engineered mutation	UNP P14779
C	366	VAL	ILE	engineered mutation	UNP P14779
C	400	SER	CYS	engineered mutation	UNP P14779
C	438	SER	THR	engineered mutation	UNP P14779
C	442	LYS	GLU	engineered mutation	UNP P14779
C	464	HIS	-	expression tag	UNP P14779
C	465	HIS	-	expression tag	UNP P14779
C	466	HIS	-	expression tag	UNP P14779
C	467	HIS	-	expression tag	UNP P14779
C	468	HIS	-	expression tag	UNP P14779

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	469	HIS	-	expression tag	UNP P14779

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

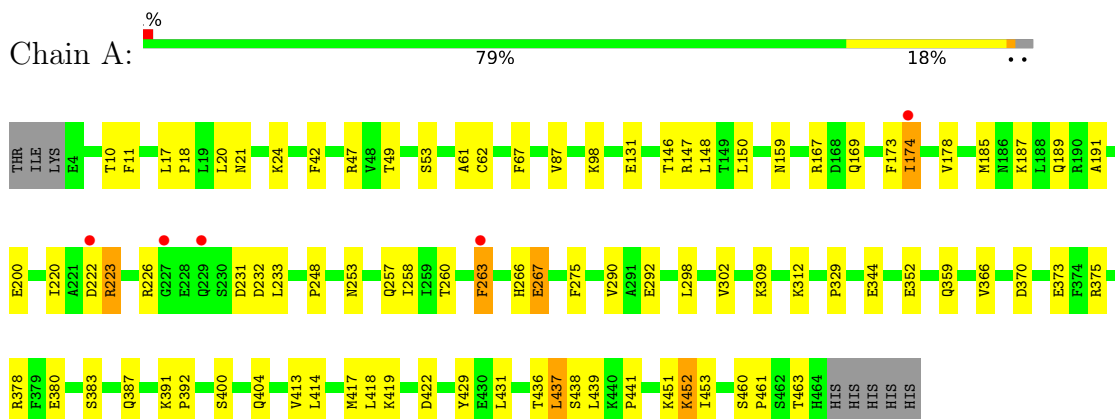
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	22	Total	O	0	0
			22	22		
4	C	20	Total	O	0	0
			20	20		

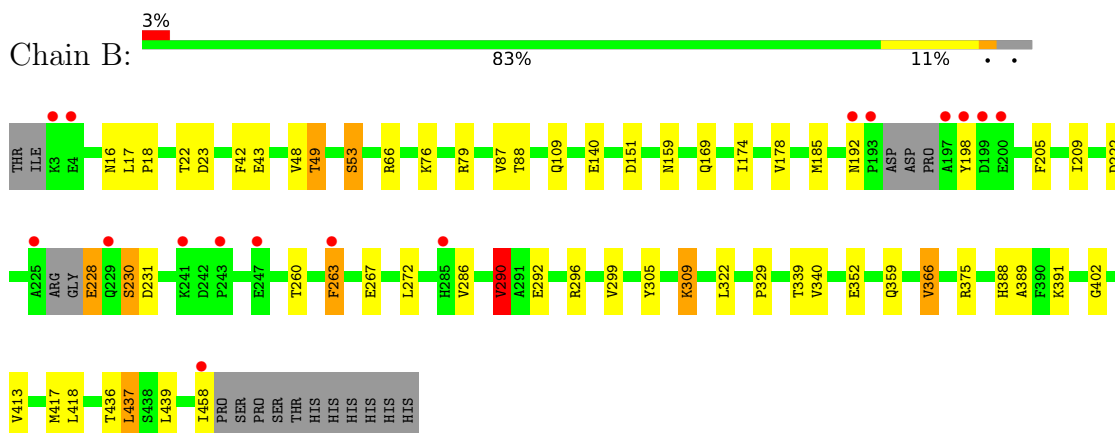
3 Residue-property plots [i](#)

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.

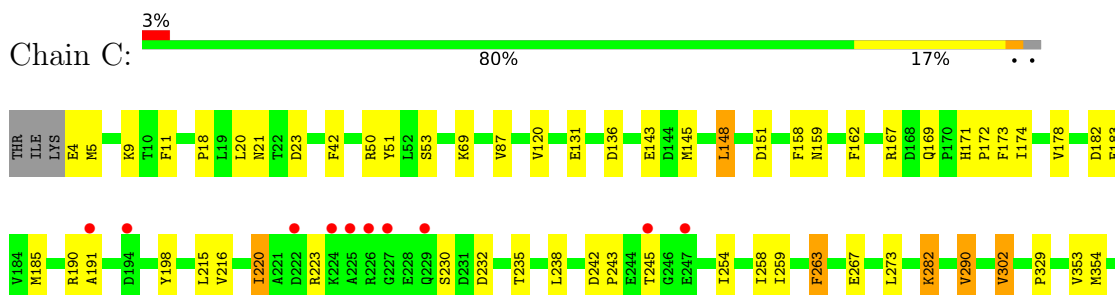
- Molecule 1: Bifunctional P-450/NADPH-P450 reductase



- Molecule 1: Bifunctional P-450/NADPH-P450 reductase



- Molecule 1: Bifunctional P-450/NADPH-P450 reductase





HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	206.90Å 206.90Å 119.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.66 40.00 – 2.66	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-2.66) 99.9 (40.00-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.197 , 0.235 0.201 , 0.235	Depositor DCC
R_{free} test set	3794 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10947	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: SO4, 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	A	0.83	0/3707	0.90	4/5030 (0.1%)
1	B	0.79	0/3613	0.88	3/4900 (0.1%)
1	C	0.80	0/3668	0.86	2/4984 (0.0%)
All	All	0.81	0/10988	0.88	9/14914 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	GLN	CA-C-N	7.46	127.50	119.89
1	A	169	GLN	C-N-CA	7.46	127.50	119.89
1	B	290	VAL	CB-CA-C	-7.12	102.52	112.14
1	C	385	ILE	CB-CA-C	-6.94	104.49	110.94
1	A	453	ILE	CA-C-N	-5.69	114.40	120.03
1	A	453	ILE	C-N-CA	-5.69	114.40	120.03
1	B	169	GLN	CA-C-N	-5.63	114.46	120.03
1	B	169	GLN	C-N-CA	-5.63	114.46	120.03
1	C	290	VAL	CB-CA-C	-5.41	104.93	112.02

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	3621	0	3513	53	0
1	B	3533	0	3420	33	0
1	C	3583	0	3445	58	0
2	A	10	0	0	1	0
2	C	5	0	0	0	0
3	A	43	0	30	4	0
3	B	43	0	30	3	0
3	C	43	0	30	6	0
4	A	24	0	0	0	0
4	B	22	0	0	0	0
4	C	20	0	0	0	0
All	All	10947	0	10468	152	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 7.

All (152) 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:C:185:MET:HE3	1:C:437:LEU:HD12	1.32	1.06
1:C:185:MET:HE3	1:C:437:LEU:CD1	2.03	0.89
1:A:185:MET:HA	1:A:185:MET:HE2	1.56	0.88
1:A:185:MET:HE3	1:A:437:LEU:HD12	1.63	0.81
1:A:185:MET:HE3	1:A:437:LEU:CD1	2.11	0.81
1:A:413:VAL:HG12	1:A:417:MET:HE2	1.64	0.79
1:B:192:ASN:O	1:B:198:TYR:CE2	2.37	0.77
3:A:603:HEM:HMC1	3:A:603:HEM:HBC2	1.66	0.76
3:C:602:HEM:HBB2	3:C:602:HEM:HMB1	1.69	0.75
1:C:413:VAL:HG12	1:C:417:MET:CE	2.20	0.71
1:B:413:VAL:HG12	1:B:417:MET:CE	2.23	0.69
1:B:413:VAL:HG12	1:B:417:MET:HE2	1.74	0.68
1:A:370:ASP:HB3	1:A:378:ARG:HH22	1.58	0.68
1:C:370:ASP:OD2	1:C:375:ARG:NH1	2.25	0.68
1:C:131:GLU:OE2	1:C:460:SER:HB2	1.95	0.66
1:A:167:ARG:HH11	1:A:167:ARG:HG2	1.61	0.64
1:A:62:CYS:SG	1:A:391:LYS:HE3	2.38	0.64
1:B:185:MET:HE3	1:B:437:LEU:HD12	1.79	0.63
1:A:185:MET:CE	1:A:437:LEU:HD12	2.27	0.63
1:A:223:ARG:NH2	1:A:232:ASP:OD1	2.26	0.63
1:B:185:MET:HE3	1:B:437:LEU:CD1	2.29	0.62
1:B:290:VAL:HB	1:B:418:LEU:HD13	1.82	0.61
1:C:391:LYS:NZ	1:C:395:ASN:OD1	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:VAL:O	1:A:417:MET:HG3	2.01	0.60
1:C:9:LYS:HD3	1:C:11:PHE:CZ	2.36	0.60
1:C:185:MET:HE2	1:C:185:MET:HA	1.83	0.60
1:A:373:GLU:OE2	1:A:375:ARG:HD3	2.01	0.60
1:C:413:VAL:HG12	1:C:417:MET:HE2	1.82	0.60
1:C:370:ASP:HB3	1:C:378:ARG:HH12	1.63	0.60
1:C:183:GLU:OE2	1:C:190:ARG:NH1	2.30	0.60
1:C:436:THR:O	1:C:437:LEU:HB2	2.02	0.60
1:C:11:PHE:CD1	1:C:18:PRO:HG2	2.37	0.60
1:A:174:ILE:O	1:A:178:VAL:HG23	2.03	0.59
1:C:413:VAL:HG12	1:C:417:MET:HE3	1.83	0.59
1:A:223:ARG:HH22	1:A:232:ASP:CG	2.11	0.58
3:C:602:HEM:HBC2	3:C:602:HEM:HMC2	1.83	0.58
1:C:426:HIS:CD2	1:C:447:LYS:HE3	2.40	0.57
1:A:460:SER:O	1:A:463:THR:HG22	2.03	0.57
1:C:375:ARG:O	1:C:378:ARG:HG3	2.05	0.57
1:C:120:VAL:HG11	1:C:302:VAL:CG2	2.35	0.56
1:A:21:ASN:ND2	1:A:189:GLN:HB3	2.21	0.56
1:B:109:GLN:OE1	1:B:305:TYR:OH	2.17	0.56
1:C:174:ILE:O	1:C:178:VAL:HG23	2.06	0.56
1:C:173:PHE:CD2	1:C:215:LEU:HD22	2.41	0.55
1:C:5:MET:SD	1:C:50:ARG:HG2	2.47	0.55
1:A:150:LEU:HD22	1:A:174:ILE:CG1	2.36	0.55
1:A:11:PHE:CD1	1:A:18:PRO:HG2	2.41	0.55
1:A:20:LEU:HG	1:A:42:PHE:CZ	2.42	0.55
1:A:49:THR:HG22	1:A:352:GLU:OE1	2.07	0.54
1:C:402:GLY:HA3	3:C:602:HEM:C3C	2.43	0.54
1:A:167:ARG:HG2	1:A:167:ARG:NH1	2.23	0.53
3:C:602:HEM:HBB2	3:C:602:HEM:CMB	2.37	0.53
1:C:69:LYS:HE2	3:C:602:HEM:O2A	2.08	0.53
1:A:253:ASN:O	1:A:257:GLN:HG2	2.09	0.53
1:A:414:LEU:HA	1:A:417:MET:HE3	1.91	0.52
1:A:275:PHE:CE2	1:A:441:PRO:HD3	2.45	0.52
1:C:282:LYS:NZ	1:C:429:TYR:O	2.43	0.52
1:A:222:ASP:O	1:A:226:ARG:HB2	2.09	0.52
1:B:49:THR:HG22	1:B:352:GLU:CB	2.40	0.51
1:C:120:VAL:HG11	1:C:302:VAL:HG21	1.92	0.51
1:C:290:VAL:CG1	1:C:418:LEU:HD13	2.41	0.51
1:C:429:TYR:CE2	1:C:431:LEU:HA	2.46	0.51
1:A:329:PRO:HG3	1:A:439:LEU:HG	1.94	0.50
1:B:366:VAL:HG11	1:B:389:ALA:HB1	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:THR:HG22	1:B:352:GLU:HB2	1.94	0.50
1:C:173:PHE:CD2	1:C:215:LEU:CD2	2.94	0.50
1:C:216:VAL:HG21	1:C:259:ILE:HG13	1.94	0.50
3:A:603:HEM:HBC2	3:A:603:HEM:CMC	2.40	0.50
3:B:500:HEM:HBB2	3:B:500:HEM:HMB2	1.93	0.49
1:C:223:ARG:HH22	1:C:232:ASP:CG	2.21	0.49
1:A:290:VAL:CG1	1:A:418:LEU:HD13	2.42	0.49
1:B:366:VAL:HG11	1:B:389:ALA:CB	2.42	0.49
1:B:388:HIS:ND1	1:B:391:LYS:HE3	2.27	0.49
1:C:329:PRO:HG3	1:C:439:LEU:HG	1.93	0.49
1:C:290:VAL:CG1	1:C:418:LEU:CD1	2.91	0.48
1:A:87:VAL:HG23	1:A:260:THR:CG2	2.44	0.48
1:B:53:SER:HB3	1:B:359:GLN:HB3	1.94	0.48
3:C:602:HEM:HBC2	3:C:602:HEM:CMC	2.44	0.48
1:A:17:LEU:N	1:A:18:PRO:HD2	2.29	0.48
1:C:190:ARG:HD2	1:C:198:TYR:CE2	2.48	0.48
1:A:263:PHE:C	1:A:263:PHE:CD1	2.92	0.48
1:C:366:VAL:HG11	1:C:389:ALA:CB	2.44	0.48
1:A:400:SER:HB2	3:A:603:HEM:NA	2.29	0.47
1:A:222:ASP:O	1:A:226:ARG:CB	2.63	0.47
1:B:185:MET:HA	1:B:185:MET:HE2	1.96	0.47
1:C:238:LEU:HD23	1:C:254:ILE:HD13	1.95	0.47
3:B:500:HEM:HMC2	3:B:500:HEM:HBC2	1.97	0.47
1:B:76:LYS:O	1:B:79:ARG:HB2	2.14	0.46
1:B:292:GLU:OE2	1:B:296:ARG:NH1	2.47	0.46
1:C:143:GLU:OE1	1:C:143:GLU:N	2.47	0.46
1:C:290:VAL:HG11	1:C:418:LEU:CD1	2.44	0.46
1:B:263:PHE:C	1:B:263:PHE:CD1	2.93	0.46
1:A:131:GLU:HB3	1:A:461:PRO:HD2	1.98	0.46
1:B:413:VAL:HG12	1:B:417:MET:HE3	1.96	0.46
1:B:436:THR:O	1:B:436:THR:OG1	2.31	0.45
1:A:220:ILE:HD11	1:A:258:ILE:HD12	1.97	0.45
1:C:23:ASP:OD1	1:C:23:ASP:N	2.48	0.45
1:A:98:LYS:NZ	1:A:248:PRO:O	2.41	0.45
1:B:413:VAL:CG1	1:B:417:MET:HE2	2.45	0.45
1:A:53:SER:HB3	1:A:359:GLN:HB3	1.98	0.45
1:A:404:GLN:NE2	2:A:601:SO4:O3	2.48	0.45
1:A:20:LEU:HG	1:A:42:PHE:HZ	1.82	0.45
1:A:223:ARG:NH2	1:A:232:ASP:CG	2.73	0.45
1:A:298:LEU:O	1:A:419:LYS:HE3	2.17	0.45
1:C:242:ASP:OD1	1:C:243:PRO:HD2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ASP:HB3	1:A:378:ARG:NH2	2.31	0.44
1:A:146:THR:O	1:A:147:ARG:C	2.60	0.44
1:B:109:GLN:OE1	1:B:309:LYS:HE3	2.17	0.44
1:C:145:MET:SD	1:C:273:LEU:HB3	2.58	0.44
1:B:329:PRO:HG3	1:B:439:LEU:HG	2.00	0.44
1:B:205:PHE:O	1:B:209:ILE:HG13	2.18	0.44
1:C:20:LEU:HG	1:C:42:PHE:CZ	2.53	0.44
1:C:53:SER:HB3	1:C:359:GLN:HB3	1.99	0.44
1:A:429:TYR:CE2	1:A:431:LEU:HA	2.52	0.44
1:C:51:TYR:CE1	1:C:354:MET:HG2	2.53	0.43
1:A:290:VAL:HG12	1:A:418:LEU:HD13	2.00	0.43
1:C:216:VAL:O	1:C:220:ILE:HG12	2.19	0.43
1:C:242:ASP:HB3	1:C:245:THR:OG1	2.18	0.43
1:C:158:PHE:CE1	1:C:258:ILE:HG12	2.53	0.43
1:A:233:LEU:HD23	1:A:233:LEU:HA	1.88	0.43
1:C:162:PHE:O	1:C:167:ARG:NH1	2.50	0.43
1:A:61:ALA:HA	1:A:67:PHE:CD2	2.54	0.43
1:C:69:LYS:NZ	1:C:87:VAL:O	2.52	0.43
1:C:232:ASP:O	1:C:235:THR:HB	2.19	0.43
3:A:603:HEM:HMB2	3:A:603:HEM:HBB2	2.01	0.43
1:C:4:GLU:HG2	1:C:5:MET:H	1.84	0.43
1:A:266:HIS:CG	1:A:267:GLU:N	2.86	0.42
1:B:272:LEU:HD13	1:B:322:LEU:HG	2.00	0.42
1:A:173:PHE:CD1	1:A:173:PHE:C	2.96	0.42
1:A:436:THR:O	1:A:437:LEU:HB2	2.19	0.42
1:C:171:HIS:CG	1:C:172:PRO:HD2	2.53	0.42
1:A:391:LYS:N	1:A:392:PRO:CD	2.83	0.42
1:B:402:GLY:HA3	3:B:500:HEM:C3C	2.54	0.42
1:C:263:PHE:CD1	1:C:263:PHE:C	2.97	0.42
1:B:87:VAL:HG23	1:B:260:THR:CG2	2.50	0.42
1:B:174:ILE:O	1:B:178:VAL:HG23	2.19	0.42
1:B:286:VAL:O	1:B:290:VAL:HG23	2.20	0.42
1:C:148:LEU:HD21	1:C:413:VAL:HG21	2.02	0.41
1:C:190:ARG:HD2	1:C:198:TYR:CD2	2.55	0.41
1:A:150:LEU:HD22	1:A:174:ILE:HG13	2.03	0.41
1:B:228:GLU:OE1	1:B:230:SER:O	2.39	0.41
1:C:363:ASP:C	1:C:363:ASP:OD1	2.64	0.41
1:A:267:GLU:HG2	1:A:438:SER:HB2	2.02	0.41
1:A:451:LYS:C	1:A:452:LYS:HG2	2.46	0.41
1:B:16:ASN:HB2	1:B:43:GLU:O	2.20	0.41
1:C:69:LYS:HB2	1:C:398:ARG:HG3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ARG:NH1	1:C:171:HIS:HD2	2.19	0.41
1:B:16:ASN:HB3	1:B:42:PHE:CE1	2.55	0.40
1:B:17:LEU:N	1:B:18:PRO:CD	2.84	0.40
1:A:191:ALA:HB3	1:C:191:ALA:HB1	2.03	0.40
1:B:66:ARG:NH2	1:B:340:VAL:O	2.54	0.40
1:C:391:LYS:N	1:C:392:PRO:CD	2.85	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	459/469 (98%)	441 (96%)	18 (4%)	0	100	100
1	B	445/469 (95%)	432 (97%)	13 (3%)	0	100	100
1	C	458/469 (98%)	440 (96%)	17 (4%)	1 (0%)	43	60
All	All	1362/1407 (97%)	1313 (96%)	48 (4%)	1 (0%)	48	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	461	PRO

5.3.2 Protein sidechains [i](#)

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	383/410 (93%)	359 (94%)	24 (6%)	16	29
1	B	370/410 (90%)	347 (94%)	23 (6%)	16	29
1	C	376/410 (92%)	359 (96%)	17 (4%)	24	42
All	All	1129/1230 (92%)	1065 (94%)	64 (6%)	18	32

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	24	LYS
1	A	47	ARG
1	A	148	LEU
1	A	159	ASN
1	A	174	ILE
1	A	187	LYS
1	A	200	GLU
1	A	223	ARG
1	A	231	ASP
1	A	263	PHE
1	A	267	GLU
1	A	292	GLU
1	A	302	VAL
1	A	309	LYS
1	A	312	LYS
1	A	344	GLU
1	A	366	VAL
1	A	380	GLU
1	A	383	SER
1	A	387	GLN
1	A	422	ASP
1	A	437	LEU
1	A	452	LYS
1	B	22	THR
1	B	23	ASP
1	B	48	VAL
1	B	49	THR
1	B	53	SER
1	B	88	THR
1	B	140	GLU
1	B	151	ASP
1	B	159	ASN
1	B	222	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	228	GLU
1	B	230	SER
1	B	231	ASP
1	B	263	PHE
1	B	267	GLU
1	B	290	VAL
1	B	299	VAL
1	B	309	LYS
1	B	339	THR
1	B	366	VAL
1	B	375	ARG
1	B	437	LEU
1	B	458	ILE
1	C	21	ASN
1	C	136	ASP
1	C	148	LEU
1	C	151	ASP
1	C	159	ASN
1	C	169	GLN
1	C	182	ASP
1	C	220	ILE
1	C	230	SER
1	C	263	PHE
1	C	267	GLU
1	C	282	LYS
1	C	302	VAL
1	C	353	VAL
1	C	434	LYS
1	C	437	LEU
1	C	460	SER

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	21	ASN
1	A	70	ASN
1	A	134	ASN
1	A	359	GLN
1	B	92	HIS
1	B	128	GLN
1	C	70	ASN
1	C	125	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	206	GLN
1	C	359	GLN
1	C	428	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](#)

6 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	$\# Z > 2$
2	SO4	C	601	-	4,4,4	0.45	0	6,6,6	0.24	0
2	SO4	A	602	-	4,4,4	0.48	0	6,6,6	0.97	0
3	HEM	C	602	1	50,50,50	1.78	11 (22%)	67,82,82	1.73	15 (22%)
3	HEM	B	500	1	50,50,50	1.75	10 (20%)	67,82,82	1.62	13 (19%)
2	SO4	A	601	-	4,4,4	0.31	0	6,6,6	0.48	0
3	HEM	A	603	1	50,50,50	1.71	13 (26%)	67,82,82	1.70	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
3	HEM	B	500	1	-	2/14/54/54	-
3	HEM	A	603	1	-	2/14/54/54	-
3	HEM	C	602	1	-	2/14/54/54	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	HEM	C1B-NB	-5.32	1.31	1.40
3	C	602	HEM	C1B-NB	-4.83	1.31	1.40
3	A	603	HEM	FE-NB	4.54	2.08	1.94
3	B	500	HEM	FE-NB	4.12	2.07	1.94
3	B	500	HEM	FE-NC	4.12	2.08	1.95
3	C	602	HEM	FE-NB	3.84	2.06	1.94
3	A	603	HEM	C1C-NC	-3.63	1.32	1.39
3	A	603	HEM	FE-NC	3.54	2.06	1.95
3	C	602	HEM	C4D-ND	-3.48	1.34	1.40
3	B	500	HEM	C1C-C2C	-3.47	1.38	1.45
3	C	602	HEM	FE-NC	3.29	2.06	1.95
3	C	602	HEM	C4B-NB	-3.25	1.32	1.38
3	B	500	HEM	C1C-NC	-3.18	1.33	1.39
3	C	602	HEM	C1C-C2C	-3.10	1.39	1.45
3	A	603	HEM	C4B-NB	-3.00	1.33	1.38
3	A	603	HEM	C1D-ND	-2.93	1.33	1.38
3	B	500	HEM	C4B-NB	-2.90	1.33	1.38
3	A	603	HEM	C4C-NC	-2.89	1.34	1.39
3	C	602	HEM	C4C-NC	-2.86	1.34	1.39
3	A	603	HEM	C1C-C2C	-2.81	1.39	1.45
3	B	500	HEM	C4D-ND	-2.77	1.35	1.40
3	C	602	HEM	C1D-ND	-2.76	1.33	1.38
3	C	602	HEM	C1C-NC	-2.68	1.34	1.39
3	A	603	HEM	C1B-NB	-2.65	1.35	1.40
3	C	602	HEM	C3C-C4C	-2.57	1.41	1.46
3	A	603	HEM	C3C-C4C	-2.51	1.41	1.46
3	B	500	HEM	C3C-C4C	-2.50	1.41	1.46
3	B	500	HEM	C1D-ND	-2.42	1.34	1.38
3	A	603	HEM	C4D-ND	-2.40	1.36	1.40
3	C	602	HEM	C4A-NA	-2.34	1.35	1.39
3	A	603	HEM	FE-ND	-2.27	1.87	1.94
3	A	603	HEM	FE-NA	2.09	2.02	1.95
3	B	500	HEM	C4A-NA	-2.06	1.35	1.39
3	A	603	HEM	C3B-C4B	2.01	1.48	1.44

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	HEM	CHC-C4B-NB	5.39	130.22	124.42
3	B	500	HEM	CHC-C4B-NB	5.01	129.82	124.42
3	C	602	HEM	C1B-NB-C4B	4.54	110.58	105.21
3	A	603	HEM	CHA-C4D-ND	4.53	129.97	124.37
3	A	603	HEM	C1B-NB-C4B	4.42	110.44	105.21
3	B	500	HEM	C1B-NB-C4B	4.39	110.41	105.21
3	A	603	HEM	CHC-C4B-NB	4.25	129.00	124.42
3	B	500	HEM	CHD-C1D-ND	4.03	128.76	124.42
3	C	602	HEM	CHD-C1D-ND	3.97	128.70	124.42
3	C	602	HEM	CHD-C1D-C2D	-3.66	119.25	125.03
3	A	603	HEM	CHB-C1B-NB	3.50	128.70	124.37
3	C	602	HEM	CHA-C4D-ND	3.36	128.52	124.37
3	C	602	HEM	CHB-C1B-NB	3.32	128.48	124.37
3	C	602	HEM	CHD-C4C-NC	3.27	128.01	124.45
3	A	603	HEM	CHD-C1D-ND	3.22	127.89	124.42
3	A	603	HEM	CHA-C4D-C3D	-3.21	119.31	125.23
3	B	500	HEM	CHA-C4D-ND	3.19	128.31	124.37
3	B	500	HEM	CHD-C1D-C2D	-3.17	120.02	125.03
3	B	500	HEM	CHD-C4C-NC	3.02	127.74	124.45
3	B	500	HEM	C4B-C3B-C2B	-2.83	104.68	107.28
3	A	603	HEM	CMD-C2D-C1D	2.69	129.24	125.03
3	A	603	HEM	C1A-CHA-C4D	-2.62	120.09	126.25
3	C	602	HEM	C3B-C4B-NB	-2.61	107.59	109.47
3	A	603	HEM	C3B-C4B-NB	-2.60	107.60	109.47
3	B	500	HEM	CHB-C1B-NB	2.59	127.58	124.37
3	A	603	HEM	O2D-CGD-CBD	2.52	121.97	114.00
3	C	602	HEM	O2D-CGD-CBD	2.42	121.65	114.00
3	C	602	HEM	CHA-C4D-C3D	-2.37	120.85	125.23
3	C	602	HEM	C4B-C3B-C2B	-2.37	105.10	107.28
3	B	500	HEM	CHA-C4D-C3D	-2.34	120.92	125.23
3	A	603	HEM	CHD-C1D-C2D	-2.33	121.35	125.03
3	B	500	HEM	O2D-CGD-CBD	2.33	121.36	114.00
3	A	603	HEM	CHD-C4C-NC	2.29	126.95	124.45
3	A	603	HEM	CAD-C3D-C4D	2.29	128.69	124.70
3	C	602	HEM	C4C-NC-C1C	2.24	109.48	105.82
3	C	602	HEM	O1D-CGD-CBD	-2.24	115.98	123.09
3	B	500	HEM	C3B-C4B-NB	-2.24	107.86	109.47
3	A	603	HEM	O2D-CGD-O1D	-2.22	117.62	123.33
3	A	603	HEM	C4C-NC-C1C	2.21	109.42	105.82
3	B	500	HEM	C1A-CHA-C4D	-2.21	121.06	126.25
3	B	500	HEM	CAD-C3D-C4D	2.13	128.41	124.70
3	C	602	HEM	C1A-CHA-C4D	-2.06	121.40	126.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	HEM	CMD-C2D-C1D	2.03	128.21	125.03

There are no chirality outliers.

All (6) torsion outliers are listed below:

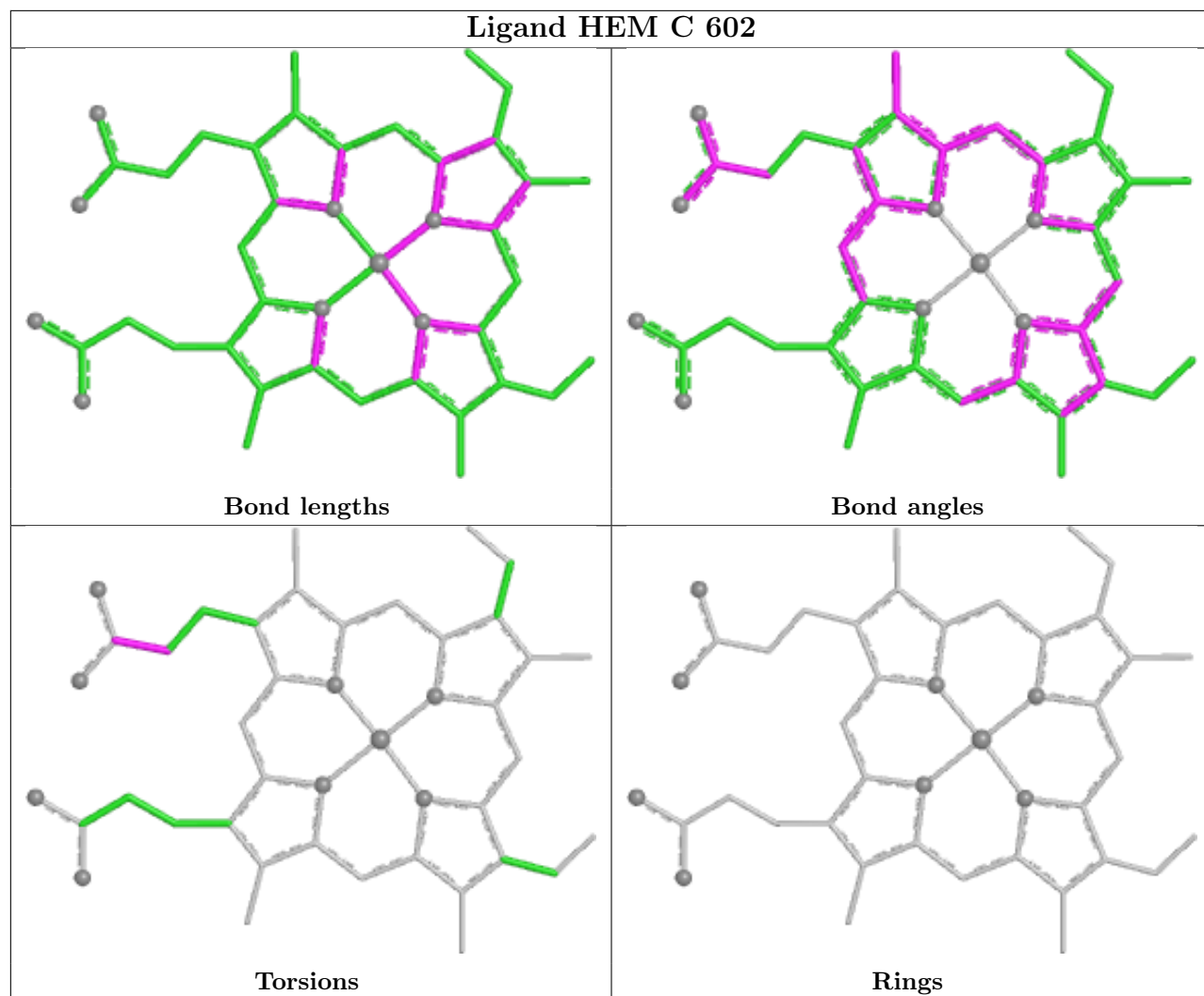
Mol	Chain	Res	Type	Atoms
3	C	602	HEM	CAD-CBD-CGD-O1D
3	A	603	HEM	CAD-CBD-CGD-O2D
3	A	603	HEM	CAD-CBD-CGD-O1D
3	C	602	HEM	CAD-CBD-CGD-O2D
3	B	500	HEM	CAD-CBD-CGD-O2D
3	B	500	HEM	CAD-CBD-CGD-O1D

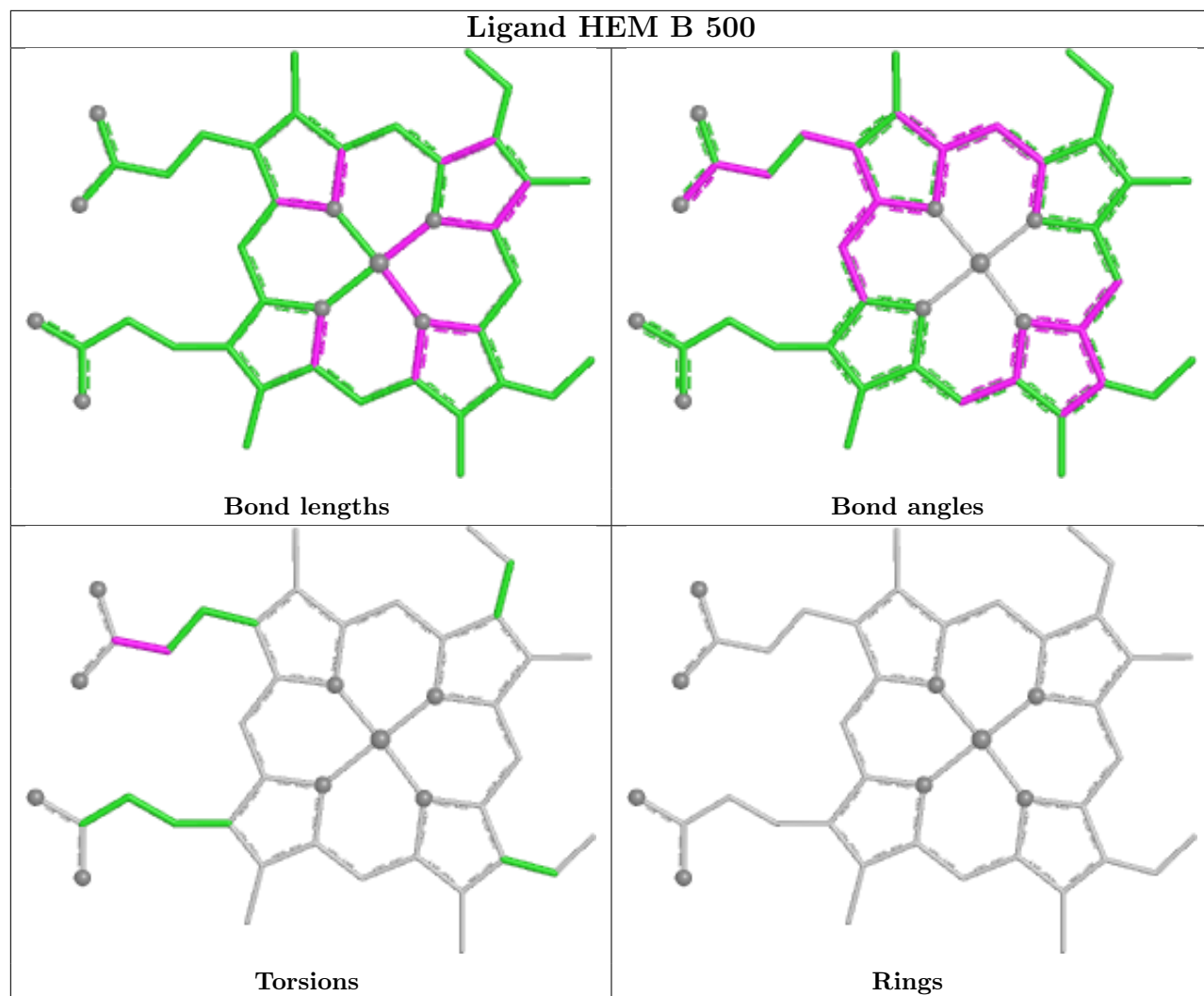
There are no ring outliers.

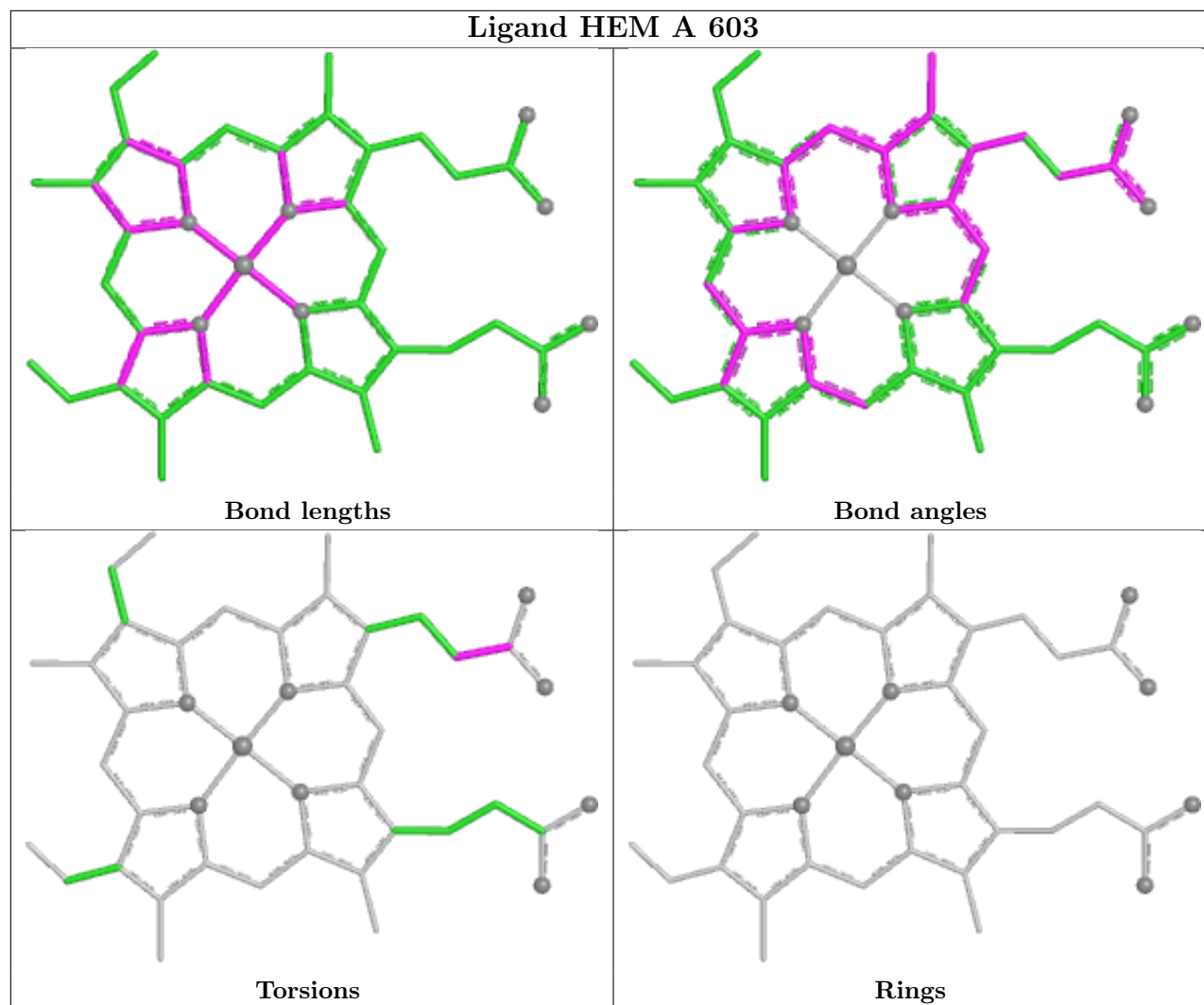
4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	HEM	6	0
3	B	500	HEM	3	0
2	A	601	SO4	1	0
3	A	603	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	461/469 (98%)	-0.28	5 (1%) 78 75	32, 49, 82, 118	0
1	B	451/469 (96%)	-0.09	16 (3%) 47 38	31, 54, 90, 122	0
1	C	460/469 (98%)	-0.10	14 (3%) 52 45	36, 56, 89, 121	0
All	All	1372/1407 (97%)	-0.16	35 (2%) 57 51	31, 54, 87, 122	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	197	ALA	6.7
1	B	458	ILE	5.0
1	B	193	PRO	4.6
1	C	227	GLY	4.2
1	B	199	ASP	4.1
1	C	229	GLN	3.9
1	B	229	GLN	3.7
1	B	198	TYR	3.5
1	A	222	ASP	3.2
1	C	226	ARG	3.2
1	C	224	LYS	3.1
1	B	225	ALA	3.1
1	B	263	PHE	3.0
1	C	457	GLY	2.9
1	B	3	LYS	2.9
1	C	461	PRO	2.9
1	C	194	ASP	2.9
1	A	263	PHE	2.9
1	A	229	GLN	2.8
1	A	227	GLY	2.7
1	C	191	ALA	2.5
1	B	247	GLU	2.4
1	B	243	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	200	GLU	2.4
1	C	247	GLU	2.4
1	B	4	GLU	2.4
1	C	222	ASP	2.3
1	C	245	THR	2.2
1	C	225	ALA	2.2
1	C	387	GLN	2.2
1	C	381	ASN	2.1
1	B	285	HIS	2.1
1	A	174	ILE	2.1
1	B	192	ASN	2.0
1	B	241	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](#)

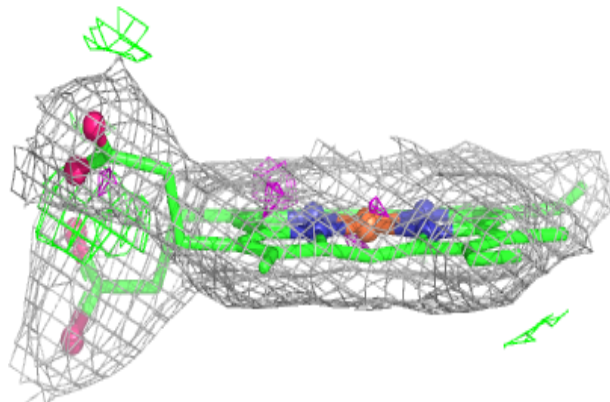
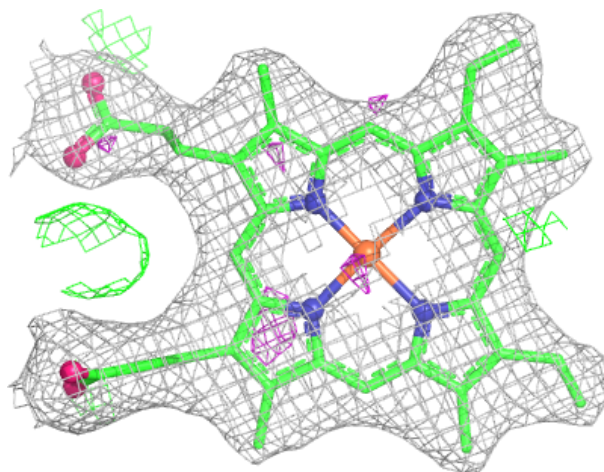
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	602	5/5	0.92	0.10	70,71,73,81	0
2	SO4	C	601	5/5	0.94	0.10	79,80,85,88	5
2	SO4	A	601	5/5	0.98	0.07	41,42,44,51	0
3	HEM	A	603	43/43	0.98	0.06	30,34,37,40	0
3	HEM	B	500	43/43	0.98	0.06	38,43,46,49	0
3	HEM	C	602	43/43	0.98	0.06	29,35,45,49	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.

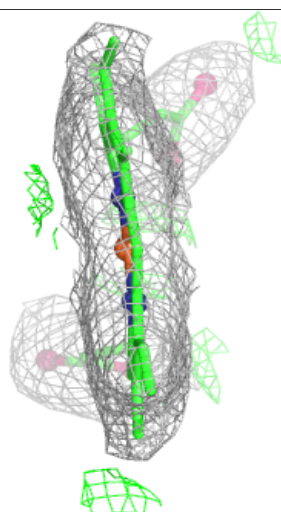
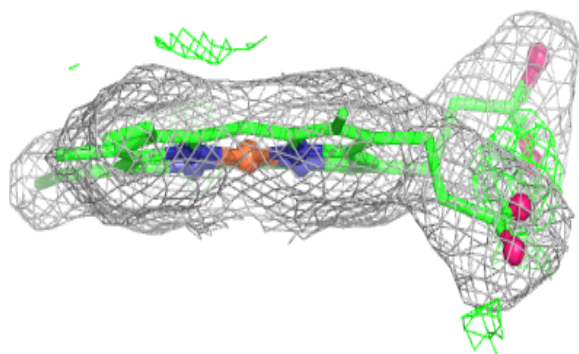
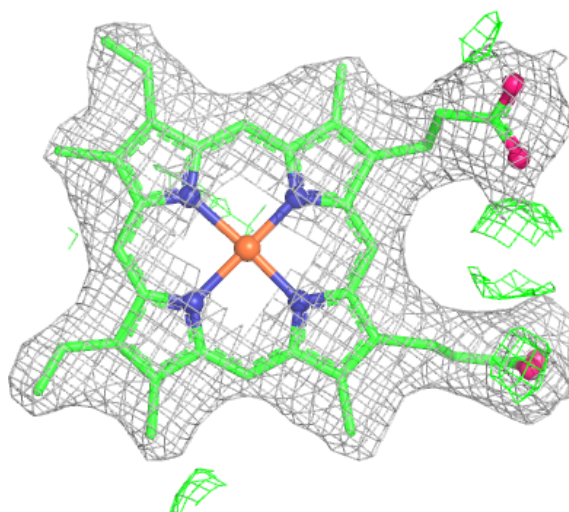
Electron density around HEM A 603:

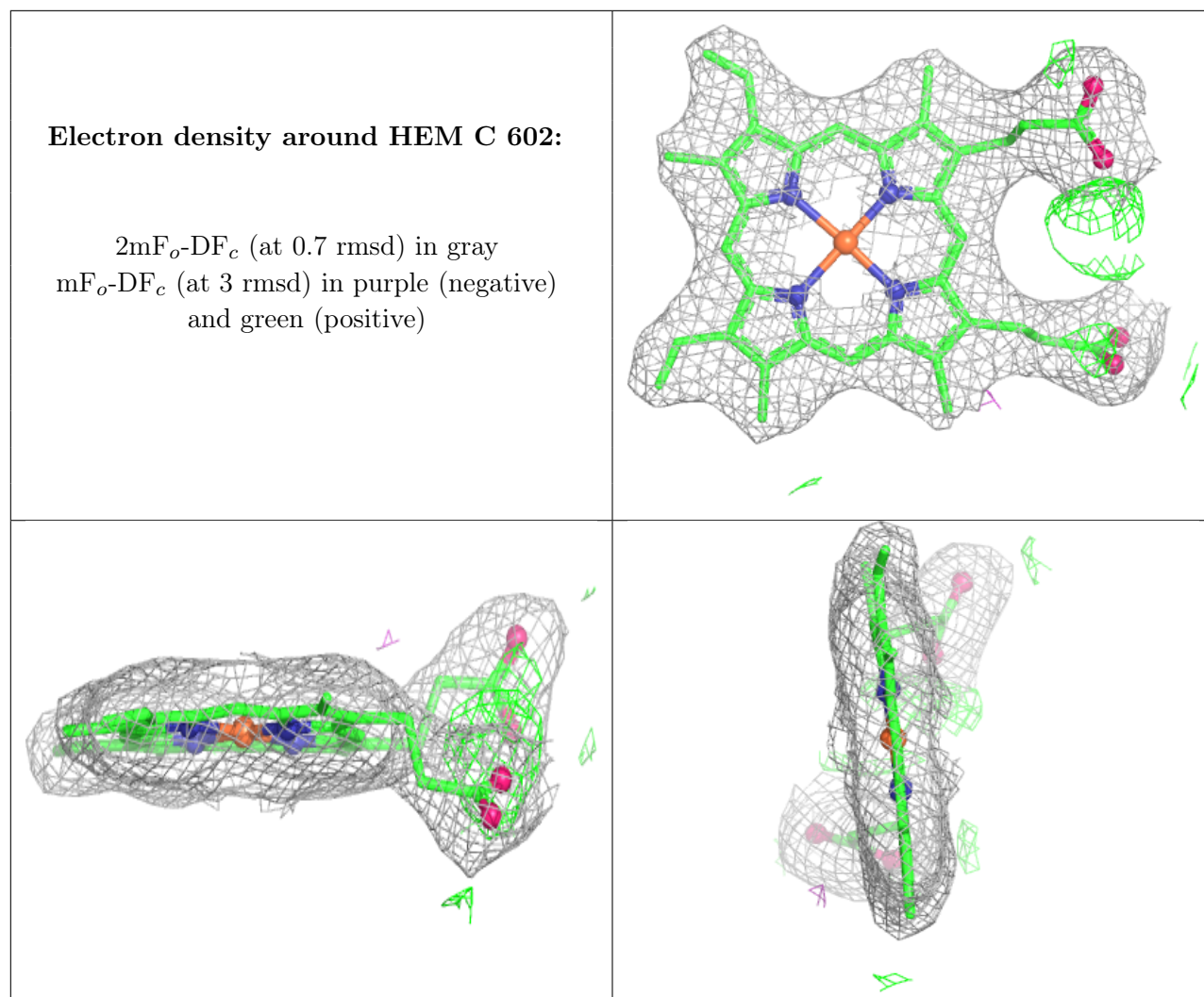
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 500:

$2mF_o-DF_c$ (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.