



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2026 – 02:02 pm BST

PDB ID : 9IFD / pdb_00009ifd
Title : OleP triple mutant F84Q/S240A/V291G in complex with LCA
Authors : Montemiglio, L.C.; Costanzo, A.; Fata, F.; Freda, I.; Demitri, N.; Savino, C.; Vallone, B.; Bulfaro, G.; Lardieri, A.
Deposited on : 2025-02-18
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:

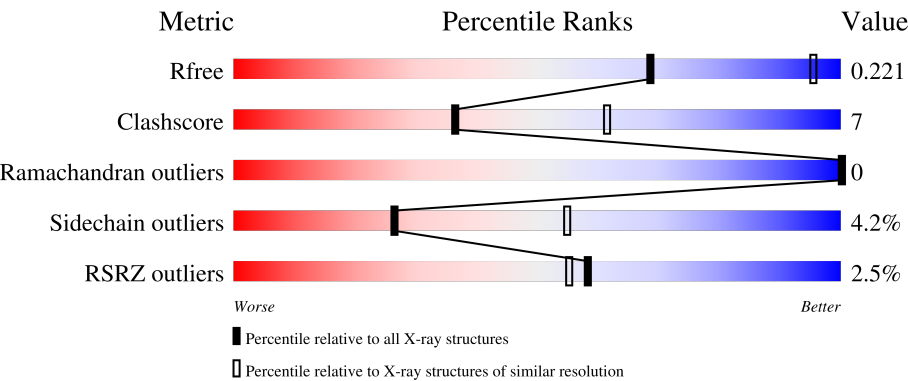
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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	A	410	2% 78% 17% ..
1	B	410	% 80% 15% ..
1	C	410	% 76% 19% ..
1	D	410	2% 78% 16% ..
1	E	410	4% 78% 17% ..

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Mol	Chain	Length	Quality of chain
1	F	410	 5% 83% 13% . .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	FMT	A	512	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19375 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome P-450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3098	1946	557	582	13			
1	B	401	Total	C	N	O	S	0	0	0
			3109	1953	559	584	13			
1	C	396	Total	C	N	O	S	0	1	0
			3087	1939	555	579	14			
1	D	396	Total	C	N	O	S	0	0	0
			3079	1934	554	578	13			
1	E	394	Total	C	N	O	S	0	2	0
			3078	1935	553	577	13			
1	F	396	Total	C	N	O	S	0	0	0
			3079	1934	554	578	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q59819
A	-1	SER	-	expression tag	UNP Q59819
A	0	HIS	-	expression tag	UNP Q59819
A	84	GLN	PHE	engineered mutation	UNP Q59819
A	240	ALA	SER	engineered mutation	UNP Q59819
A	291	GLY	VAL	engineered mutation	UNP Q59819
B	-2	GLY	-	expression tag	UNP Q59819
B	-1	SER	-	expression tag	UNP Q59819
B	0	HIS	-	expression tag	UNP Q59819
B	84	GLN	PHE	engineered mutation	UNP Q59819
B	240	ALA	SER	engineered mutation	UNP Q59819
B	291	GLY	VAL	engineered mutation	UNP Q59819
C	-2	GLY	-	expression tag	UNP Q59819
C	-1	SER	-	expression tag	UNP Q59819
C	0	HIS	-	expression tag	UNP Q59819
C	84	GLN	PHE	engineered mutation	UNP Q59819
C	240	ALA	SER	engineered mutation	UNP Q59819

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Chain	Residue	Modelled	Actual	Comment	Reference
C	291	GLY	VAL	engineered mutation	UNP Q59819
D	-2	GLY	-	expression tag	UNP Q59819
D	-1	SER	-	expression tag	UNP Q59819
D	0	HIS	-	expression tag	UNP Q59819
D	84	GLN	PHE	engineered mutation	UNP Q59819
D	240	ALA	SER	engineered mutation	UNP Q59819
D	291	GLY	VAL	engineered mutation	UNP Q59819
E	-2	GLY	-	expression tag	UNP Q59819
E	-1	SER	-	expression tag	UNP Q59819
E	0	HIS	-	expression tag	UNP Q59819
E	84	GLN	PHE	engineered mutation	UNP Q59819
E	240	ALA	SER	engineered mutation	UNP Q59819
E	291	GLY	VAL	engineered mutation	UNP Q59819
F	-2	GLY	-	expression tag	UNP Q59819
F	-1	SER	-	expression tag	UNP Q59819
F	0	HIS	-	expression tag	UNP Q59819
F	84	GLN	PHE	engineered mutation	UNP Q59819
F	240	ALA	SER	engineered mutation	UNP Q59819
F	291	GLY	VAL	engineered mutation	UNP Q59819

- # HEM

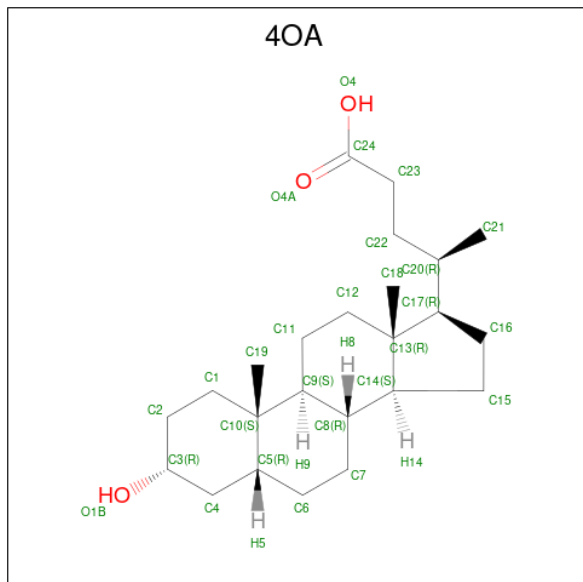
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	F	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 3 is (3beta,5beta,14beta,17alpha)-3-hydroxycholan-24-oic acid (CCD ID: 4OA)
(formula: C₂₄H₄₀O₃).

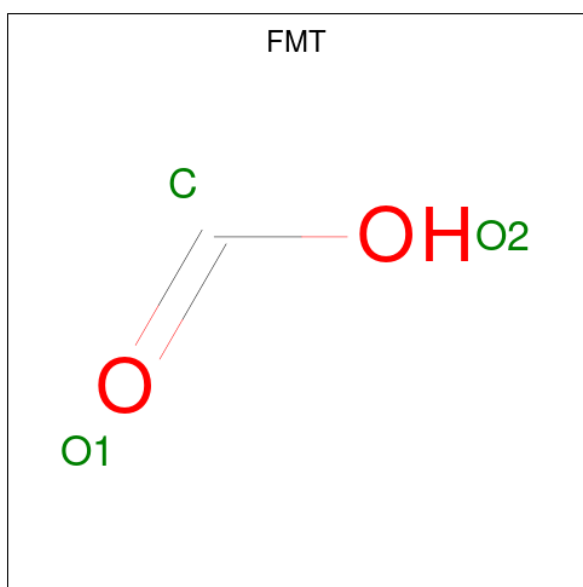


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O		
			27	24	3		
3	B	1	Total	C	O		
			27	24	3		
3	C	1	Total	C	O		
			27	24	3		
3	D	1	Total	C	O		
			27	24	3		
3	E	1	Total	C	O		
			27	24	3		
3	F	1	Total	C	O		
			27	24	3		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		
4	D	1	Total	Na	0	0
			1	1		

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		
5	D	1	Total	C	O	0	0
			3	1	2		
5	D	1	Total	C	O	0	0
			3	1	2		
5	D	1	Total	C	O	0	0
			3	1	2		
5	D	1	Total	C	O	0	0
			3	1	2		
5	D	1	Total	C	O	0	0
			3	1	2		
5	D	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 3 1 2	0	0
5	E	1	Total C O 3 1 2	0	0
5	E	1	Total C O 3 1 2	0	0
5	E	1	Total C O 3 1 2	0	0
5	F	1	Total C O 3 1 2	0	0
5	F	1	Total C O 3 1 2	0	0

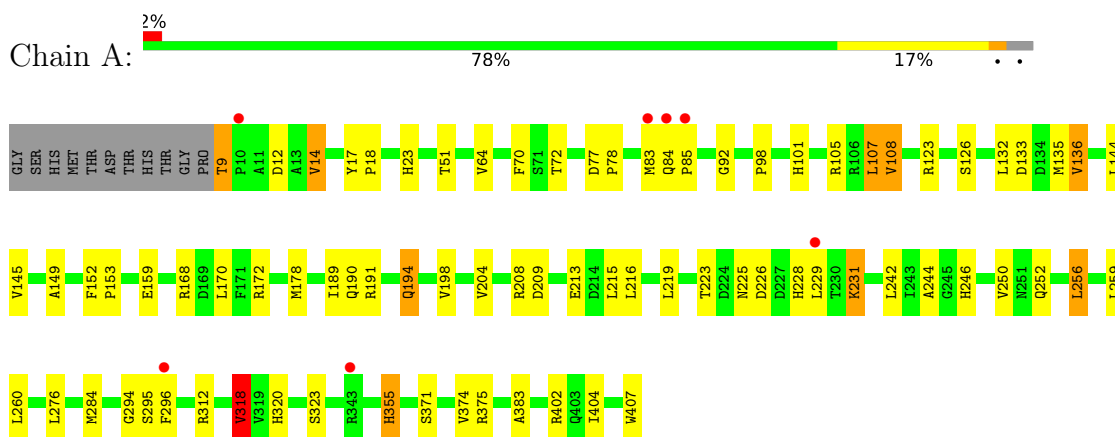
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	61	Total O 61 61	0	0
6	B	58	Total O 58 58	0	0
6	C	53	Total O 53 53	0	0
6	D	41	Total O 41 41	0	0
6	E	16	Total O 16 16	0	0
6	F	27	Total O 27 27	0	0

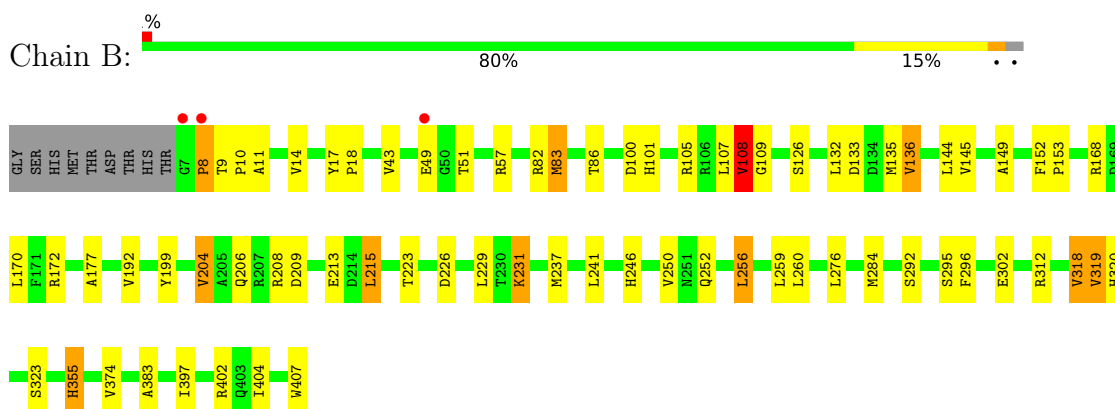
3 Residue-property plots

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.

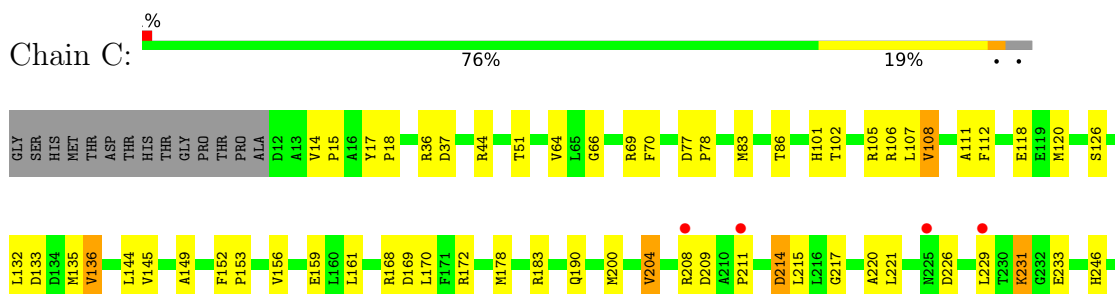
• Molecule 1: Cytochrome P-450



• Molecule 1: Cytochrome P-450

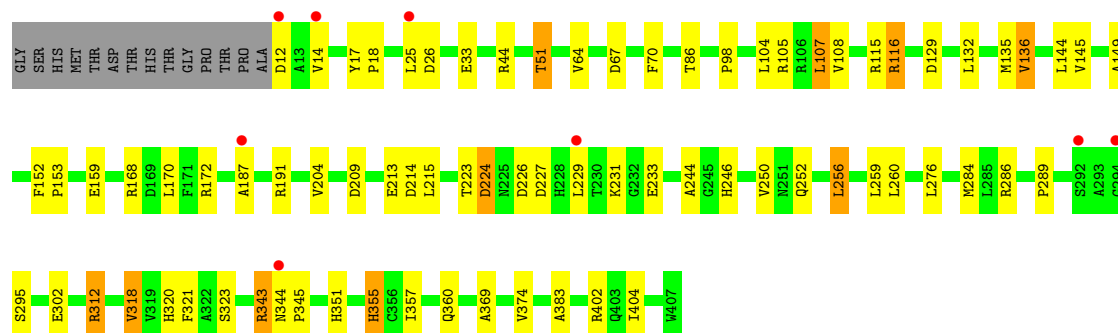
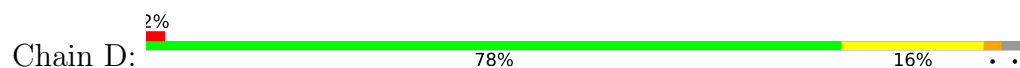


• Molecule 1: Cytochrome P-450

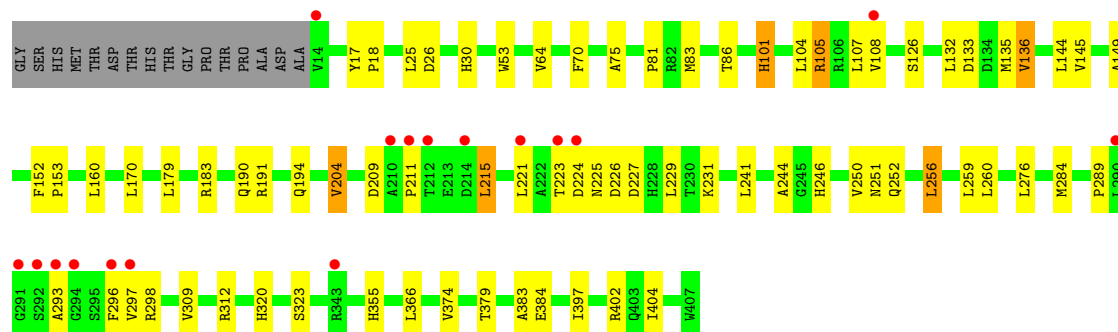
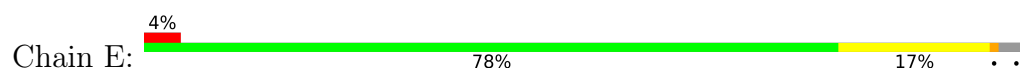




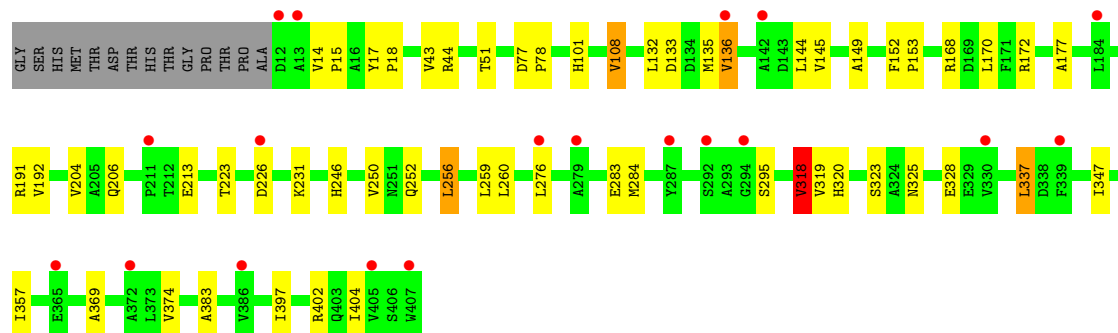
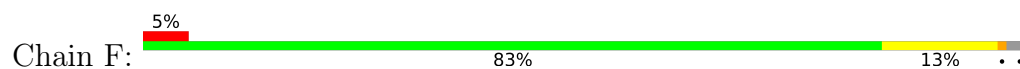
• Molecule 1: Cytochrome P-450



• Molecule 1: Cytochrome P-450



• Molecule 1: Cytochrome P-450



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	248.04Å 106.59Å 163.73Å 90.00° 131.27° 90.00°	Depositor
Resolution (Å)	53.74 – 2.70 53.74 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (53.74-2.70) 98.6 (53.74-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.187 , 0.219 0.194 , 0.221	Depositor DCC
R_{free} test set	5947 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19375	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6357e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4OA, HEM, FMT, NA

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	1.18	5/3165 (0.2%)	1.52	16/4314 (0.4%)
1	B	1.20	5/3177 (0.2%)	1.56	15/4331 (0.3%)
1	C	1.21	6/3153 (0.2%)	1.53	18/4295 (0.4%)
1	D	1.14	1/3145 (0.0%)	1.49	13/4285 (0.3%)
1	E	1.11	3/3150 (0.1%)	1.49	13/4292 (0.3%)
1	F	1.15	3/3145 (0.1%)	1.53	10/4285 (0.2%)
All	All	1.17	23/18935 (0.1%)	1.52	85/25802 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
1	E	0	1
All	All	0	3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	101	HIS	CE1-NE2	8.65	1.41	1.32
1	B	101	HIS	CE1-NE2	7.58	1.40	1.32
1	F	101	HIS	CE1-NE2	7.50	1.40	1.32
1	C	66	GLY	C-O	-6.88	1.16	1.23
1	B	355	HIS	C-O	-6.34	1.16	1.23
1	B	83	MET	C-O	6.13	1.31	1.24
1	A	355	HIS	C-O	-6.09	1.16	1.23
1	F	318	VAL	C-O	-5.95	1.17	1.24
1	A	23	HIS	CE1-NE2	5.93	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	318	VAL	C-O	-5.91	1.17	1.24
1	B	319	VAL	C-O	-5.78	1.17	1.24
1	E	355	HIS	CE1-NE2	5.69	1.38	1.32
1	E	101	HIS	CE1-NE2	5.63	1.38	1.32
1	C	355	HIS	CE1-NE2	5.42	1.38	1.32
1	F	319	VAL	C-O	-5.41	1.17	1.24
1	D	355	HIS	C-O	-5.36	1.17	1.23
1	C	200	MET	C-O	-5.30	1.17	1.24
1	E	225	ASN	C-O	5.29	1.30	1.24
1	B	8	PRO	CA-CB	5.21	1.58	1.53
1	A	178	MET	CG-SD	-5.15	1.67	1.80
1	A	9	THR	N-CA	5.09	1.55	1.46
1	C	15	PRO	C-O	-5.04	1.18	1.23
1	C	112	PHE	C-O	5.01	1.31	1.24

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	SER	N-CA-C	-9.45	100.96	111.07
1	B	209	ASP	CA-CB-CG	8.43	121.03	112.60
1	E	209	ASP	CA-CB-CG	8.39	120.99	112.60
1	F	328	GLU	CB-CG-CD	7.04	124.56	112.60
1	A	194	GLN	CB-CG-CD	6.63	123.87	112.60
1	B	109	GLY	CA-C-O	-6.43	114.12	120.75
1	F	213	GLU	CB-CA-C	6.41	121.80	112.05
1	C	211	PRO	CA-C-N	6.25	129.17	120.29
1	C	211	PRO	C-N-CA	6.25	129.17	120.29
1	A	407	TRP	CA-C-O	-6.22	110.23	120.80
1	B	292	SER	CB-CA-C	6.20	120.62	110.88
1	E	227	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	213	GLU	CB-CA-C	6.16	121.41	112.05
1	B	276	LEU	CA-C-N	6.14	125.24	120.33
1	B	276	LEU	C-N-CA	6.14	125.24	120.33
1	C	276	LEU	CA-C-N	6.08	125.19	120.33
1	C	276	LEU	C-N-CA	6.08	125.19	120.33
1	D	213	GLU	CB-CA-C	6.00	121.17	112.05
1	E	231	LYS	CA-C-N	5.87	126.45	119.94
1	E	231	LYS	C-N-CA	5.87	126.45	119.94
1	A	98	PRO	CB-CA-C	5.85	116.89	111.39
1	D	276	LEU	CA-C-N	5.85	125.01	120.33
1	D	276	LEU	C-N-CA	5.85	125.01	120.33
1	E	276	LEU	CA-C-N	5.82	124.98	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	276	LEU	C-N-CA	5.82	124.98	120.33
1	A	276	LEU	CA-C-N	5.73	124.92	120.33
1	A	276	LEU	C-N-CA	5.73	124.92	120.33
1	B	133	ASP	CA-CB-CG	5.73	118.33	112.60
1	E	227	ASP	CB-CA-C	-5.66	99.16	110.42
1	E	133	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	133	ASP	CA-CB-CG	5.55	118.16	112.60
1	E	204	VAL	CA-C-O	-5.54	114.98	120.85
1	C	108	VAL	CA-C-N	5.51	125.94	119.94
1	C	108	VAL	C-N-CA	5.51	125.94	119.94
1	D	209	ASP	CA-C-N	5.49	127.93	122.00
1	D	209	ASP	C-N-CA	5.49	127.93	122.00
1	B	108	VAL	CA-C-N	5.49	126.07	119.98
1	B	108	VAL	C-N-CA	5.49	126.07	119.98
1	C	133	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	108	VAL	N-CA-CB	-5.45	105.84	112.33
1	F	108	VAL	CA-C-N	5.45	126.03	119.98
1	F	108	VAL	C-N-CA	5.45	126.03	119.98
1	C	369	ALA	CA-C-O	-5.42	115.13	120.82
1	B	51	THR	CB-CA-C	5.41	121.01	110.30
1	E	204	VAL	N-CA-CB	5.40	118.69	110.58
1	B	209	ASP	CA-C-N	5.40	127.83	122.00
1	B	209	ASP	C-N-CA	5.40	127.83	122.00
1	D	116	ARG	CB-CG-CD	5.38	123.68	111.30
1	F	51	THR	CB-CA-C	5.36	120.77	109.79
1	C	108	VAL	N-CA-CB	-5.32	106.00	112.33
1	C	51	THR	CB-CA-C	5.31	120.68	109.79
1	C	159	GLU	CB-CG-CD	5.31	121.63	112.60
1	F	369	ALA	CA-C-O	-5.31	115.42	121.00
1	E	224	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	51	THR	CB-CA-C	5.30	120.65	109.79
1	F	133	ASP	CA-CB-CG	5.29	117.89	112.60
1	C	51	THR	N-CA-CB	-5.29	102.35	111.55
1	B	204	VAL	N-CA-CB	5.26	118.47	110.58
1	C	51	THR	CA-CB-OG1	-5.25	101.72	109.60
1	A	231	LYS	CA-C-N	5.24	125.75	119.94
1	A	231	LYS	C-N-CA	5.24	125.75	119.94
1	C	204	VAL	CA-C-O	-5.24	114.81	120.47
1	C	231	LYS	CA-C-N	5.22	125.73	119.94
1	C	231	LYS	C-N-CA	5.22	125.73	119.94
1	B	14	VAL	N-CA-CB	-5.21	108.24	111.83
1	D	51	THR	CB-CA-C	5.20	120.44	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	ALA	CA-C-N	5.17	125.82	120.03
1	A	244	ALA	C-N-CA	5.17	125.82	120.03
1	C	169	ASP	CA-CB-CG	5.16	117.76	112.60
1	F	226	ASP	CA-C-O	-5.16	115.13	120.70
1	D	159	GLU	CB-CG-CD	5.16	121.37	112.60
1	E	244	ALA	CA-C-N	5.15	125.80	120.03
1	E	244	ALA	C-N-CA	5.15	125.80	120.03
1	D	369	ALA	CA-C-O	-5.15	115.59	121.00
1	D	244	ALA	CA-C-N	5.14	125.79	120.03
1	D	244	ALA	C-N-CA	5.14	125.79	120.03
1	D	51	THR	N-CA-CB	-5.14	102.61	111.55
1	F	276	LEU	CA-C-N	5.13	124.44	120.33
1	F	276	LEU	C-N-CA	5.13	124.44	120.33
1	B	213	GLU	CB-CA-C	5.11	119.81	112.05
1	A	108	VAL	CA-C-N	5.09	125.60	120.00
1	A	108	VAL	C-N-CA	5.09	125.60	120.00
1	C	214	ASP	CB-CA-C	-5.08	99.33	109.33
1	D	33	GLU	CB-CG-CD	5.04	121.16	112.60
1	A	51	THR	N-CA-CB	-5.02	102.81	111.55

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	312	ARG	Sidechain
1	D	312	ARG	Sidechain
1	E	105	ARG	Sidechain

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	A	3098	0	3072	49	0
1	B	3109	0	3082	44	0
1	C	3087	0	3061	46	0
1	D	3079	0	3053	46	0
1	E	3078	0	3058	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3079	0	3053	30	0
2	A	43	0	30	4	0
2	B	43	0	30	4	0
2	C	43	0	30	3	0
2	D	43	0	30	5	0
2	E	43	0	30	6	0
2	F	43	0	30	2	0
3	A	27	0	39	0	0
3	B	27	0	39	2	0
3	C	27	0	39	0	0
3	D	27	0	39	1	0
3	E	27	0	39	1	0
3	F	27	0	39	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	60	0	20	3	0
5	B	27	0	9	0	0
5	C	36	0	12	0	0
5	D	24	0	8	1	0
5	E	12	0	4	0	0
5	F	6	0	2	0	0
6	A	61	0	0	1	0
6	B	58	0	0	3	0
6	C	53	0	0	2	0
6	D	41	0	0	1	0
6	E	16	0	0	0	0
6	F	27	0	0	1	0
All	All	19375	0	18848	273	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 (273) 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:C:501:HEM:HMC1	2:C:501:HEM:HBC2	1.59	0.85
1:E:211:PRO:HG3	1:E:221:LEU:HD11	1.63	0.81
1:C:208:ARG:HG2	1:C:220:ALA:HB1	1.66	0.77
1:E:108:VAL:HG13	1:E:215:LEU:HD21	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASN:O	1:A:226:ASP:OD1	2.05	0.74
1:B:9:THR:HG22	1:D:360:GLN:HE22	1.53	0.74
1:A:371:SER:OG	1:A:375:ARG:NH2	2.20	0.74
1:A:105:ARG:NH2	1:A:355:HIS:O	2.21	0.74
1:D:105:ARG:NH2	1:D:355:HIS:O	2.21	0.73
1:B:105:ARG:NH2	1:B:355:HIS:O	2.22	0.72
2:D:501:HEM:HMC1	2:D:501:HEM:HBC2	1.72	0.72
1:B:108:VAL:HG22	1:B:215:LEU:CD2	2.20	0.72
1:A:84:GLN:HB3	6:A:649:HOH:O	1.91	0.71
1:F:325:ASN:HD21	1:F:347:ILE:H	1.39	0.70
1:D:320:HIS:HD2	1:D:323:SER:H	1.40	0.69
1:F:44:ARG:HD2	6:F:618:HOH:O	1.90	0.69
1:C:320:HIS:HD2	1:C:323:SER:H	1.41	0.69
1:C:105:ARG:NH2	1:C:355:HIS:O	2.24	0.69
1:A:320:HIS:HD2	1:A:323:SER:H	1.42	0.68
1:F:320:HIS:HD2	1:F:323:SER:H	1.42	0.67
2:E:501:HEM:HMB1	2:E:501:HEM:HBB2	1.75	0.67
1:E:320:HIS:HD2	1:E:323:SER:H	1.42	0.67
1:C:295:SER:HB3	1:C:321:PHE:CE2	2.30	0.67
1:A:295:SER:H	1:A:318:VAL:HG23	1.60	0.66
1:F:223:THR:HG21	1:F:231:LYS:HZ1	1.61	0.66
1:E:226:ASP:OD2	1:E:229:LEU:HB2	1.95	0.66
1:E:108:VAL:HG13	1:E:215:LEU:CD2	2.25	0.65
1:B:320:HIS:HD2	1:B:323:SER:H	1.42	0.65
1:F:260:LEU:HG	1:F:284:MET:HE1	1.79	0.64
1:E:260:LEU:HG	1:E:284:MET:HE1	1.81	0.63
1:A:260:LEU:HG	1:A:284:MET:HE1	1.81	0.63
2:B:501:HEM:HMB1	2:B:501:HEM:HBB2	1.80	0.63
1:E:18:PRO:HD3	1:E:83:MET:HE1	1.82	0.62
1:C:260:LEU:HG	1:C:284:MET:HE1	1.80	0.62
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.81	0.62
1:B:260:LEU:HG	1:B:284:MET:HE1	1.81	0.61
1:E:296:PHE:HB3	1:E:298:ARG:NH1	2.15	0.61
1:E:108:VAL:HG11	1:E:241:LEU:HD11	1.83	0.61
1:B:168:ARG:HG2	1:B:172:ARG:HG3	1.83	0.61
1:F:168:ARG:HG2	1:F:172:ARG:HG3	1.81	0.60
1:E:18:PRO:HG3	1:E:293:ALA:HA	1.83	0.60
1:B:295:SER:H	1:B:318:VAL:HG23	1.66	0.59
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.84	0.59
1:F:223:THR:HG21	1:F:231:LYS:NZ	2.17	0.59
1:B:108:VAL:HG22	1:B:215:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ARG:HD3	1:C:302:GLU:OE1	2.04	0.58
1:B:246:HIS:O	1:B:250:VAL:HG23	2.03	0.58
1:C:326:ARG:NH1	6:C:601:HOH:O	2.28	0.58
1:D:260:LEU:HG	1:D:284:MET:HE1	1.83	0.58
1:D:168:ARG:HG2	1:D:172:ARG:HG3	1.86	0.58
1:E:251:ASN:ND2	1:E:397:ILE:HD12	2.19	0.57
1:A:168:ARG:HG2	1:A:172:ARG:HG3	1.85	0.57
1:C:18:PRO:HD3	1:C:83:MET:HE1	1.85	0.57
1:E:101:HIS:CE1	1:E:105:ARG:HD2	2.39	0.57
1:C:256:LEU:HD22	1:C:284:MET:HB3	1.87	0.57
2:C:501:HEM:HBC2	2:C:501:HEM:CMC	2.32	0.56
1:B:108:VAL:HG22	1:B:215:LEU:HD22	1.88	0.56
1:C:168:ARG:HG2	1:C:172:ARG:HG3	1.87	0.56
1:A:256:LEU:HD22	1:A:284:MET:HB3	1.88	0.56
1:E:160:LEU:HG	1:E:215:LEU:HD12	1.87	0.56
1:B:208:ARG:HH21	1:B:223:THR:HG21	1.71	0.55
1:D:295:SER:HB3	1:D:321:PHE:CE2	2.41	0.55
1:B:18:PRO:HD3	1:B:83:MET:HE1	1.89	0.55
1:B:383:ALA:HB3	1:B:404:ILE:HG22	1.88	0.55
1:D:246:HIS:O	1:D:250:VAL:HG23	2.06	0.55
1:E:191:ARG:NH2	1:E:194[B]:GLN:OE1	2.40	0.55
1:F:191:ARG:HA	1:F:191:ARG:NE	2.21	0.55
1:A:14:VAL:CG2	1:C:118:GLU:HG2	2.36	0.55
1:A:14:VAL:HG23	1:C:118:GLU:HG2	1.89	0.55
1:F:283:GLU:HG3	1:F:337:LEU:HD23	1.89	0.55
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	1.89	0.54
1:C:295:SER:HB3	1:C:321:PHE:HE2	1.70	0.54
1:A:383:ALA:HB3	1:A:404:ILE:HG22	1.88	0.54
1:D:104:LEU:HB2	1:D:229:LEU:HD22	1.89	0.54
1:D:259:LEU:HB2	1:D:284:MET:CE	2.37	0.54
1:A:246:HIS:O	1:A:250:VAL:HG23	2.07	0.54
1:E:383:ALA:HB3	1:E:404:ILE:HG22	1.89	0.54
1:B:256:LEU:HD22	1:B:284:MET:HB3	1.89	0.54
1:D:256:LEU:HD22	1:D:284:MET:HB3	1.90	0.54
1:F:383:ALA:HB3	1:F:404:ILE:HG22	1.91	0.53
2:A:501:HEM:HBB2	2:A:501:HEM:CMB	2.38	0.53
1:A:208:ARG:HD3	1:D:302:GLU:HG3	1.90	0.53
1:C:259:LEU:HB2	1:C:284:MET:CE	2.39	0.53
1:D:383:ALA:HB3	1:D:404:ILE:HG22	1.90	0.53
1:A:231:LYS:HE2	1:D:67:ASP:OD2	2.07	0.53
1:A:72:THR:HB	1:A:296:PHE:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ASP:HB2	6:B:621:HOH:O	2.08	0.53
1:D:14:VAL:HG23	1:D:44:ARG:HB2	1.90	0.52
1:C:383:ALA:HB3	1:C:404:ILE:HG22	1.91	0.52
1:D:25:LEU:HB3	1:D:289:PRO:HD2	1.91	0.52
1:E:402:ARG:HD3	1:E:404:ILE:HG13	1.92	0.52
1:A:259:LEU:HB2	1:A:284:MET:CE	2.39	0.52
1:B:259:LEU:HB2	1:B:284:MET:CE	2.40	0.52
1:E:256:LEU:HD22	1:E:284:MET:HB3	1.91	0.52
1:D:286:ARG:HD3	1:D:344:ASN:OD1	2.10	0.52
1:E:75:ALA:HB2	1:E:297:VAL:O	2.10	0.52
1:E:259:LEU:HB2	1:E:284:MET:CE	2.40	0.51
1:F:132:LEU:O	1:F:136:VAL:HG13	2.10	0.51
1:B:208:ARG:NH1	1:C:69:ARG:HG3	2.24	0.51
1:F:256:LEU:HD22	1:F:284:MET:HB3	1.91	0.51
1:A:191:ARG:HH22	5:A:512:FMT:C	2.24	0.51
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.41	0.50
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.94	0.50
1:C:132:LEU:O	1:C:136:VAL:HG13	2.12	0.50
2:E:501:HEM:C4A	3:E:502:4OA:H6	2.47	0.50
2:E:501:HEM:HBC2	2:E:501:HEM:HMC2	1.94	0.50
1:A:132:LEU:O	1:A:136:VAL:HG13	2.12	0.50
1:E:246:HIS:O	1:E:250:VAL:HG23	2.11	0.50
1:B:8:PRO:HB2	1:B:11:ALA:HB3	1.93	0.49
1:F:259:LEU:HB2	1:F:284:MET:CE	2.42	0.49
1:B:57:ARG:NE	6:B:601:HOH:O	2.44	0.49
5:A:512:FMT:H	1:D:351:HIS:CD2	2.47	0.49
2:D:501:HEM:HBC2	2:D:501:HEM:CMC	2.42	0.49
1:F:246:HIS:O	1:F:250:VAL:HG23	2.13	0.49
1:A:84:GLN:HE21	1:A:189:ILE:HD13	1.78	0.49
1:C:295:SER:H	1:C:318:VAL:HG23	1.77	0.49
1:B:132:LEU:O	1:B:136:VAL:HG13	2.12	0.48
1:A:84:GLN:HE21	1:A:189:ILE:HG21	1.78	0.48
1:B:82:ARG:HD3	6:B:606:HOH:O	2.13	0.48
1:D:226:ASP:OD1	1:D:227:ASP:N	2.44	0.48
1:D:132:LEU:O	1:D:136:VAL:HG13	2.13	0.48
2:F:501:HEM:HMB1	2:F:501:HEM:HBB2	1.96	0.48
1:C:246:HIS:O	1:C:250:VAL:HG23	2.14	0.48
1:E:132:LEU:O	1:E:136:VAL:HG13	2.13	0.48
1:A:92:GLY:HA3	5:A:516:FMT:C	2.44	0.48
1:A:123:ARG:NH1	1:A:159:GLU:HG3	2.28	0.48
1:E:25:LEU:HB3	1:E:289:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:MET:HE1	1:B:144:LEU:HD13	1.96	0.47
1:C:402:ARG:HD3	1:C:404:ILE:HG13	1.95	0.47
1:A:402:ARG:HD3	1:A:404:ILE:HG13	1.96	0.47
1:E:108:VAL:O	1:E:108:VAL:HG12	2.14	0.47
1:B:223:THR:HG23	1:B:231:LYS:HG3	1.96	0.47
1:C:170:LEU:HD23	1:C:170:LEU:C	2.39	0.47
1:A:72:THR:HB	1:A:296:PHE:HE1	1.80	0.47
1:C:111:ALA:HB3	1:C:215:LEU:HD21	1.95	0.47
1:E:170:LEU:HD23	1:E:170:LEU:C	2.40	0.47
1:C:111:ALA:CB	1:C:215:LEU:HD21	2.45	0.47
1:F:145:VAL:HA	1:F:149:ALA:HB3	1.96	0.47
1:A:123:ARG:HH12	1:A:159:GLU:HG3	1.80	0.47
1:F:402:ARG:HD3	1:F:404:ILE:HG13	1.96	0.47
1:E:83:MET:CE	1:E:293:ALA:HB1	2.45	0.46
1:E:104:LEU:O	1:E:107:LEU:HB2	2.15	0.46
1:B:177:ALA:HB3	1:B:192:VAL:HG11	1.97	0.46
1:C:17:TYR:CZ	1:C:293:ALA:HB1	2.51	0.46
1:B:312:ARG:NH2	1:D:129:ASP:OD1	2.49	0.46
1:C:320:HIS:HD2	1:C:323:SER:N	2.12	0.46
1:D:343:ARG:HG3	1:D:345:PRO:HD3	1.95	0.46
1:E:179:LEU:HD13	1:E:397:ILE:HD13	1.96	0.46
1:D:223:THR:HG23	1:D:231:LYS:HG3	1.97	0.46
1:E:152:PHE:HB3	1:E:153:PRO:HD3	1.97	0.46
1:A:17:TYR:CD1	1:A:18:PRO:HA	2.50	0.46
1:F:295:SER:H	1:F:318:VAL:HG23	1.79	0.46
1:C:36:ARG:HG3	1:C:37:ASP:CG	2.41	0.46
1:E:17:TYR:CD1	1:E:18:PRO:HA	2.50	0.46
1:F:14:VAL:HB	1:F:15:PRO:HD2	1.98	0.46
1:F:152:PHE:HB3	1:F:153:PRO:HD3	1.98	0.46
1:C:145:VAL:HA	1:C:149:ALA:HB3	1.98	0.45
1:E:179:LEU:CD1	1:E:397:ILE:HD13	2.46	0.45
1:A:145:VAL:HA	1:A:149:ALA:HB3	1.99	0.45
1:B:402:ARG:HD3	1:B:404:ILE:HG13	1.97	0.45
1:D:145:VAL:HA	1:D:149:ALA:HB3	1.97	0.45
1:F:17:TYR:CD1	1:F:18:PRO:HA	2.51	0.45
1:F:325:ASN:ND2	1:F:347:ILE:H	2.12	0.45
1:A:152:PHE:HB3	1:A:153:PRO:HD3	1.98	0.45
1:C:208:ARG:HG2	1:C:220:ALA:CB	2.42	0.45
1:E:81:PRO:O	1:E:297:VAL:HG21	2.17	0.45
1:A:215:LEU:HD23	1:A:215:LEU:HA	1.77	0.45
1:B:252:GLN:OE1	1:B:252:GLN:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:HIS:O	1:E:105:ARG:HG3	2.16	0.45
1:C:36:ARG:HG3	1:C:37:ASP:OD1	2.16	0.45
1:E:101:HIS:CE1	1:E:105:ARG:CD	2.99	0.45
1:A:9:THR:HB	1:A:12:ASP:HB2	1.98	0.45
1:A:252:GLN:OE1	1:A:252:GLN:HA	2.17	0.45
1:E:83:MET:HE2	1:E:293:ALA:HB1	1.98	0.45
1:E:145:VAL:HA	1:E:149:ALA:HB3	1.99	0.45
1:E:252:GLN:HA	1:E:252:GLN:OE1	2.17	0.45
1:A:135:MET:HE1	1:A:144:LEU:HD13	1.99	0.45
1:B:17:TYR:CD1	1:B:18:PRO:HA	2.52	0.45
2:B:501:HEM:C4A	3:B:502:4OA:H6	2.52	0.45
1:C:252:GLN:HA	1:C:252:GLN:OE1	2.17	0.45
1:B:152:PHE:HB3	1:B:153:PRO:HD3	1.99	0.44
1:B:199:TYR:HB2	1:C:102:THR:HG21	1.98	0.44
1:D:135:MET:HE1	1:D:144:LEU:HD13	1.99	0.44
1:B:170:LEU:C	1:B:170:LEU:HD23	2.42	0.44
1:B:407:TRP:CD1	1:B:407:TRP:C	2.96	0.44
1:C:135:MET:HE1	1:C:144:LEU:HD13	1.99	0.44
1:F:283:GLU:HG3	1:F:337:LEU:CD2	2.47	0.44
1:F:252:GLN:OE1	1:F:252:GLN:HA	2.17	0.44
1:C:44:ARG:HD2	6:C:641:HOH:O	2.18	0.44
1:D:229:LEU:HA	1:D:233:GLU:OE1	2.17	0.44
1:D:256:LEU:O	1:D:284:MET:HE1	2.18	0.44
1:D:402:ARG:HD3	1:D:404:ILE:HG13	1.99	0.44
2:E:501:HEM:HBB2	2:E:501:HEM:CMB	2.46	0.44
1:A:191:ARG:NH2	1:A:194:GLN:HB2	2.32	0.43
1:D:17:TYR:CD1	1:D:18:PRO:HA	2.52	0.43
1:D:170:LEU:C	1:D:170:LEU:HD23	2.43	0.43
1:A:83:MET:SD	1:A:294:GLY:HA3	2.58	0.43
1:B:9:THR:HB	1:B:10:PRO:HD3	2.00	0.43
1:C:17:TYR:CD1	1:C:18:PRO:HA	2.53	0.43
1:D:295:SER:H	1:D:318:VAL:HG23	1.82	0.43
1:A:107:LEU:HD22	1:A:229:LEU:HD13	2.00	0.43
1:A:223:THR:HG23	1:A:231:LYS:HG3	1.99	0.43
1:B:145:VAL:HA	1:B:149:ALA:HB3	2.00	0.43
1:A:101:HIS:CE1	1:A:105:ARG:HD2	2.53	0.43
1:E:256:LEU:O	1:E:284:MET:HE1	2.19	0.43
1:D:320:HIS:HD2	1:D:323:SER:N	2.11	0.43
1:F:170:LEU:C	1:F:170:LEU:HD23	2.43	0.43
1:A:198:VAL:CG1	1:D:98:PRO:HG3	2.49	0.43
1:D:343:ARG:HE	1:D:344:ASN:H	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:501:HEM:HMC2	2:F:501:HEM:HBC2	2.01	0.43
1:A:320:HIS:HD2	1:A:323:SER:N	2.12	0.43
1:A:170:LEU:C	1:A:170:LEU:HD23	2.44	0.42
1:D:104:LEU:O	1:D:107:LEU:HB2	2.19	0.42
1:C:120[B]:MET:HE1	1:C:156:VAL:HG13	2.01	0.42
1:C:229:LEU:HA	1:C:233:GLU:OE1	2.19	0.42
1:D:152:PHE:HB3	1:D:153:PRO:HD3	2.01	0.42
1:B:295:SER:HB3	1:B:319:VAL:O	2.20	0.42
1:B:17:TYR:HB2	1:B:43:VAL:HB	2.02	0.42
1:B:208:ARG:NH2	1:B:223:THR:HG21	2.33	0.42
1:A:64:VAL:HA	1:A:70:PHE:CD2	2.54	0.42
1:C:217:GLY:O	1:C:221:LEU:HG	2.19	0.42
1:D:187:ALA:O	1:D:191:ARG:HG3	2.20	0.42
1:E:135:MET:HE1	1:E:144:LEU:HD13	2.02	0.42
1:A:216:LEU:HD23	1:A:219:LEU:HD12	2.02	0.42
1:D:214:ASP:HA	5:D:509:FMT:C	2.49	0.42
1:E:18:PRO:HG3	1:E:293:ALA:CB	2.50	0.42
1:E:384:GLU:CD	1:E:402:ARG:HH11	2.28	0.42
1:F:17:TYR:HB2	1:F:43:VAL:HB	2.02	0.42
1:B:295:SER:O	1:B:296:PHE:C	2.62	0.41
1:A:84:GLN:HG3	1:A:85:PRO:HD2	2.01	0.41
1:F:135:MET:HE1	1:F:144:LEU:HD13	2.02	0.41
1:A:84:GLN:NE2	1:A:189:ILE:HG21	2.35	0.41
1:A:77:ASP:HA	1:A:78:PRO:HD3	1.93	0.41
1:D:12:ASP:HB3	1:D:14:VAL:HG22	2.03	0.41
1:D:252:GLN:OE1	1:D:252:GLN:HA	2.19	0.41
1:C:152:PHE:HB3	1:C:153:PRO:HD3	2.02	0.41
1:C:161:LEU:O	1:C:214:ASP:HB3	2.20	0.41
2:D:501:HEM:HBB2	2:D:501:HEM:CMB	2.49	0.41
1:F:177:ALA:HB3	1:F:192:VAL:HG11	2.03	0.41
1:D:115:ARG:HG2	6:D:626:HOH:O	2.20	0.41
1:D:224:ASP:OD1	1:D:224:ASP:N	2.54	0.41
3:B:502:4OA:H21A	3:B:502:4OA:H18B	2.03	0.41
1:C:64:VAL:HA	1:C:70:PHE:CD2	2.55	0.41
2:D:501:HEM:C4A	3:D:502:4OA:H6	2.55	0.41
2:E:501:HEM:HBC2	2:E:501:HEM:CMC	2.49	0.41
1:C:77:ASP:HA	1:C:78:PRO:HD3	1.95	0.41
1:E:53:TRP:CH2	1:E:309:VAL:HG21	2.56	0.41
1:E:64:VAL:HA	1:E:70:PHE:CD2	2.56	0.41
1:F:77:ASP:HA	1:F:78:PRO:HD3	1.94	0.41
1:D:104:LEU:HA	1:D:229:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:366:LEU:HD11	2:E:501:HEM:HBB1	2.02	0.41
1:B:320:HIS:HD2	1:B:323:SER:N	2.12	0.41
1:C:256:LEU:O	1:C:284:MET:HE1	2.20	0.41
1:C:384:GLU:CD	1:C:402:ARG:HH11	2.28	0.41
1:A:84:GLN:NE2	1:A:189:ILE:HD13	2.36	0.40
1:A:256:LEU:O	1:A:284:MET:HE1	2.21	0.40
1:D:215:LEU:HD23	1:D:215:LEU:HA	1.59	0.40
3:F:502:4OA:H12	3:F:502:4OA:H21A	2.04	0.40
1:B:237:MET:HE2	1:B:241:LEU:HG	2.03	0.40
1:B:256:LEU:O	1:B:284:MET:HE1	2.21	0.40
1:D:12:ASP:CB	1:D:44:ARG:HH12	2.34	0.40
1:D:14:VAL:HG11	1:D:51:THR:OG1	2.22	0.40
1:B:226:ASP:OD2	1:B:229:LEU:HB2	2.21	0.40
2:B:501:HEM:HBB2	2:B:501:HEM:CMB	2.48	0.40
1:C:226:ASP:OD2	1:C:226:ASP:N	2.54	0.40
1:C:357:ILE:HG22	2:C:501:HEM:C2D	2.55	0.40
1:E:17:TYR:HA	1:E:18:PRO:C	2.46	0.40
1:A:242:LEU:O	1:A:246:HIS:HD2	2.04	0.40
1:B:17:TYR:HA	1:B:18:PRO:C	2.47	0.40
1:C:135:MET:HE1	1:C:144:LEU:CD1	2.52	0.40
1:D:64:VAL:HA	1:D:70:PHE:CD2	2.56	0.40
1:F:320:HIS:HD2	1:F:323:SER:N	2.13	0.40
1:F:256:LEU:O	1:F:284:MET:HE1	2.22	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	397/410 (97%)	383 (96%)	14 (4%)	0	100	100
1	B	399/410 (97%)	388 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	395/410 (96%)	381 (96%)	14 (4%)	0	100	100
1	D	394/410 (96%)	382 (97%)	12 (3%)	0	100	100
1	E	394/410 (96%)	377 (96%)	17 (4%)	0	100	100
1	F	394/410 (96%)	383 (97%)	11 (3%)	0	100	100
All	All	2373/2460 (96%)	2294 (97%)	79 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	332/341 (97%)	319 (96%)	13 (4%)	28	57
1	B	333/341 (98%)	318 (96%)	15 (4%)	24	52
1	C	331/341 (97%)	313 (95%)	18 (5%)	20	45
1	D	330/341 (97%)	316 (96%)	14 (4%)	26	55
1	E	331/341 (97%)	317 (96%)	14 (4%)	26	55
1	F	330/341 (97%)	320 (97%)	10 (3%)	36	66
All	All	1987/2046 (97%)	1903 (96%)	84 (4%)	26	55

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	107	LEU
1	A	108	VAL
1	A	126	SER
1	A	136	VAL
1	A	190	GLN
1	A	204	VAL
1	A	209	ASP
1	A	228	HIS

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Mol	Chain	Res	Type
1	A	256	LEU
1	A	312	ARG
1	A	318	VAL
1	A	374	VAL
1	B	49	GLU
1	B	86	THR
1	B	107	LEU
1	B	108	VAL
1	B	126	SER
1	B	136	VAL
1	B	204	VAL
1	B	206	GLN
1	B	215	LEU
1	B	231	LYS
1	B	256	LEU
1	B	302	GLU
1	B	318	VAL
1	B	374	VAL
1	B	397	ILE
1	C	14	VAL
1	C	86	THR
1	C	106	ARG
1	C	107	LEU
1	C	108	VAL
1	C	126	SER
1	C	136	VAL
1	C	178	MET
1	C	183	ARG
1	C	190	GLN
1	C	204	VAL
1	C	209	ASP
1	C	231	LYS
1	C	256	LEU
1	C	302	GLU
1	C	318	VAL
1	C	374	VAL
1	C	397	ILE
1	D	26	ASP
1	D	86	THR
1	D	107	LEU
1	D	108	VAL
1	D	116	ARG

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Mol	Chain	Res	Type
1	D	136	VAL
1	D	204	VAL
1	D	224	ASP
1	D	256	LEU
1	D	312	ARG
1	D	318	VAL
1	D	343	ARG
1	D	357	ILE
1	D	374	VAL
1	E	26	ASP
1	E	30	HIS
1	E	86	THR
1	E	126	SER
1	E	136	VAL
1	E	183	ARG
1	E	190	GLN
1	E	204	VAL
1	E	215	LEU
1	E	223	THR
1	E	256	LEU
1	E	312	ARG
1	E	374	VAL
1	E	379	THR
1	F	108	VAL
1	F	136	VAL
1	F	204	VAL
1	F	206	GLN
1	F	256	LEU
1	F	318	VAL
1	F	337	LEU
1	F	357	ILE
1	F	374	VAL
1	F	397	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	101	HIS
1	A	246	HIS
1	A	258	HIS
1	A	355	HIS

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Mol	Chain	Res	Type
1	B	194	GLN
1	B	206	GLN
1	B	246	HIS
1	C	236	ASN
1	C	246	HIS
1	C	258	HIS
1	C	351	HIS
1	D	246	HIS
1	D	258	HIS
1	D	351	HIS
1	D	355	HIS
1	D	360	GLN
1	E	96	GLN
1	E	236	ASN
1	E	246	HIS
1	E	258	HIS
1	E	360	GLN
1	E	393	GLN
1	F	246	HIS
1	F	258	HIS
1	F	325	ASN
1	F	351	HIS
1	F	360	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 71 ligands modelled in this entry, 4 are monoatomic - leaving 67 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	$\# Z > 2$
5	FMT	B	510	-	2,2,2	0.46	0	1,1,1	0.04	0
5	FMT	A	512	-	2,2,2	0.50	0	1,1,1	0.05	0
5	FMT	E	504	-	2,2,2	0.41	0	1,1,1	0.10	0
3	4OA	D	502	-	30,30,30	0.54	0	47,47,47	0.66	0
5	FMT	A	511	-	2,2,2	0.33	0	1,1,1	0.19	0
5	FMT	C	507	-	2,2,2	0.67	0	1,1,1	0.11	0
5	FMT	A	516	-	2,2,2	0.43	0	1,1,1	0.03	0
5	FMT	A	515	-	2,2,2	0.33	0	1,1,1	0.16	0
5	FMT	C	506	-	2,2,2	0.56	0	1,1,1	0.03	0
5	FMT	E	505	-	2,2,2	0.34	0	1,1,1	0.19	0
3	4OA	A	502	-	30,30,30	0.50	0	47,47,47	0.80	0
5	FMT	A	523	-	2,2,2	0.41	0	1,1,1	0.10	0
5	FMT	A	520	-	2,2,2	0.44	0	1,1,1	0.08	0
5	FMT	B	508	-	2,2,2	0.43	0	1,1,1	0.04	0
5	FMT	A	509	-	2,2,2	0.56	0	1,1,1	0.06	0
5	FMT	E	506	-	2,2,2	0.55	0	1,1,1	0.04	0
2	HEM	A	501	1	50,50,50	1.60	10 (20%)	66,82,82	1.82	12 (18%)
5	FMT	B	511	-	2,2,2	0.24	0	1,1,1	0.24	0
5	FMT	C	514	-	2,2,2	0.35	0	1,1,1	0.07	0
5	FMT	D	504	-	2,2,2	0.28	0	1,1,1	0.20	0
5	FMT	A	507	-	2,2,2	0.38	0	1,1,1	0.10	0
5	FMT	D	508	-	2,2,2	0.36	0	1,1,1	0.16	0
5	FMT	D	505	-	2,2,2	0.29	0	1,1,1	0.17	0
3	4OA	B	502	-	30,30,30	0.57	0	47,47,47	0.82	0
5	FMT	A	519	-	2,2,2	0.74	0	1,1,1	0.07	0
2	HEM	C	501	1	50,50,50	1.65	13 (26%)	66,82,82	1.98	16 (24%)
5	FMT	A	508	-	2,2,2	0.40	0	1,1,1	0.15	0
5	FMT	B	509	-	2,2,2	0.34	0	1,1,1	0.18	0
5	FMT	C	512	-	2,2,2	0.45	0	1,1,1	0.07	0
5	FMT	D	511	-	2,2,2	0.35	0	1,1,1	0.15	0
5	FMT	C	511	-	2,2,2	0.42	0	1,1,1	0.12	0
5	FMT	C	515	-	2,2,2	0.45	0	1,1,1	0.09	0
5	FMT	B	506	-	2,2,2	0.37	0	1,1,1	0.14	0
5	FMT	C	504	-	2,2,2	0.32	0	1,1,1	0.17	0
5	FMT	A	505	-	2,2,2	0.40	0	1,1,1	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	D	501	1	50,50,50	1.85	13 (26%)	66,82,82	1.77	17 (25%)
5	FMT	A	513	-	2,2,2	0.52	0	1,1,1	0.03	0
5	FMT	D	506	-	2,2,2	0.65	0	1,1,1	0.01	0
5	FMT	A	522	-	2,2,2	0.53	0	1,1,1	0.05	0
5	FMT	B	507	-	2,2,2	0.40	0	1,1,1	0.10	0
5	FMT	D	510	-	2,2,2	0.32	0	1,1,1	0.14	0
5	FMT	C	510	-	2,2,2	0.43	0	1,1,1	0.05	0
5	FMT	A	521	-	2,2,2	0.46	0	1,1,1	0.13	0
5	FMT	D	507	-	2,2,2	0.46	0	1,1,1	0.05	0
5	FMT	E	503	-	2,2,2	0.59	0	1,1,1	0.01	0
5	FMT	A	504	-	2,2,2	0.36	0	1,1,1	0.13	0
5	FMT	A	506	-	2,2,2	0.38	0	1,1,1	0.11	0
3	4OA	C	502	-	30,30,30	0.51	0	47,47,47	0.78	0
5	FMT	B	504	-	2,2,2	0.39	0	1,1,1	0.10	0
2	HEM	E	501	1	50,50,50	1.62	8 (16%)	66,82,82	1.65	18 (27%)
5	FMT	B	512	-	2,2,2	0.38	0	1,1,1	0.14	0
5	FMT	D	509	-	2,2,2	0.42	0	1,1,1	0.02	0
5	FMT	C	505	-	2,2,2	0.91	0	1,1,1	0.24	0
3	4OA	E	502	-	30,30,30	0.53	0	47,47,47	0.79	2 (4%)
5	FMT	F	504	-	2,2,2	0.39	0	1,1,1	0.18	0
5	FMT	A	514	-	2,2,2	0.77	0	1,1,1	0.20	0
5	FMT	B	505	-	2,2,2	0.37	0	1,1,1	0.17	0
5	FMT	C	508	-	2,2,2	0.45	0	1,1,1	0.08	0
2	HEM	F	501	1	50,50,50	1.57	8 (16%)	66,82,82	1.79	11 (16%)
2	HEM	B	501	1	50,50,50	1.65	11 (22%)	66,82,82	1.64	13 (19%)
5	FMT	A	518	-	2,2,2	0.63	0	1,1,1	0.04	0
5	FMT	C	509	-	2,2,2	0.35	0	1,1,1	0.15	0
5	FMT	A	510	-	2,2,2	0.60	0	1,1,1	0.01	0
5	FMT	F	503	-	2,2,2	0.83	0	1,1,1	0.17	0
5	FMT	C	513	-	2,2,2	0.29	0	1,1,1	0.21	0
5	FMT	A	517	-	2,2,2	0.26	0	1,1,1	0.18	0
3	4OA	F	502	-	30,30,30	0.51	0	47,47,47	0.80	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	D	501	1	-	0/14/54/54	-
3	4OA	E	502	-	-	1/9/67/67	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	4OA	B	502	-	-	2/9/67/67	0/4/4/4
2	HEM	C	501	1	-	0/14/54/54	-
3	4OA	D	502	-	-	0/9/67/67	0/4/4/4
2	HEM	F	501	1	-	0/14/54/54	-
2	HEM	B	501	1	-	0/14/54/54	-
3	4OA	A	502	-	-	0/9/67/67	0/4/4/4
3	4OA	C	502	-	-	0/9/67/67	0/4/4/4
3	4OA	F	502	-	-	0/9/67/67	0/4/4/4
2	HEM	A	501	1	-	0/14/54/54	-
2	HEM	E	501	1	-	0/14/54/54	-

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	HEM	FE-NB	5.68	2.12	1.94
2	D	501	HEM	C1B-NB	-5.01	1.31	1.40
2	A	501	HEM	C4B-NB	-4.49	1.29	1.38
2	E	501	HEM	FE-NC	4.44	2.10	1.95
2	D	501	HEM	C4D-ND	-4.23	1.33	1.40
2	C	501	HEM	FE-NB	4.20	2.07	1.94
2	A	501	HEM	FE-NB	4.17	2.07	1.94
2	C	501	HEM	C4D-ND	-3.97	1.33	1.40
2	C	501	HEM	FE-NC	3.94	2.08	1.95
2	F	501	HEM	FE-NC	3.74	2.07	1.95
2	B	501	HEM	C4B-NB	-3.71	1.31	1.38
2	D	501	HEM	C4B-NB	-3.65	1.31	1.38
2	A	501	HEM	C4D-ND	-3.54	1.34	1.40
2	B	501	HEM	C1B-NB	-3.49	1.34	1.40
2	D	501	HEM	FE-NC	3.47	2.06	1.95
2	F	501	HEM	C1B-NB	-3.44	1.34	1.40
2	F	501	HEM	FE-NB	3.34	2.05	1.94
2	C	501	HEM	C1D-ND	-3.33	1.31	1.38
2	A	501	HEM	C1C-NC	-3.31	1.33	1.39
2	C	501	HEM	CHB-C1B	3.27	1.45	1.38
2	B	501	HEM	C1D-ND	-3.20	1.32	1.38
2	D	501	HEM	FE-NB	3.20	2.04	1.94
2	D	501	HEM	FE-ND	-3.17	1.84	1.94
2	F	501	HEM	C4B-NB	-3.11	1.32	1.38
2	B	501	HEM	FE-NB	3.10	2.04	1.94
2	F	501	HEM	C1C-NC	-3.10	1.33	1.39
2	A	501	HEM	FE-NC	3.06	2.05	1.95
2	F	501	HEM	C3C-C4C	-3.06	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C1C-C2C	-2.99	1.39	1.45
2	D	501	HEM	C1D-ND	-2.93	1.32	1.38
2	B	501	HEM	C1C-NC	-2.91	1.34	1.39
2	F	501	HEM	C4D-ND	-2.89	1.35	1.40
2	D	501	HEM	C1C-C2C	-2.85	1.39	1.45
2	B	501	HEM	FE-NC	2.82	2.04	1.95
2	D	501	HEM	C1C-NC	-2.75	1.34	1.39
2	B	501	HEM	FE-ND	-2.74	1.86	1.94
2	E	501	HEM	C1A-C2A	-2.68	1.39	1.44
2	C	501	HEM	C1C-C2C	-2.67	1.40	1.45
2	E	501	HEM	C1B-NB	-2.66	1.35	1.40
2	B	501	HEM	C4D-ND	-2.62	1.35	1.40
2	D	501	HEM	C4A-NA	-2.60	1.34	1.39
2	C	501	HEM	C4B-NB	-2.56	1.33	1.38
2	A	501	HEM	C1D-ND	-2.54	1.33	1.38
2	E	501	HEM	C1C-C2C	-2.47	1.40	1.45
2	D	501	HEM	C3C-C4C	-2.44	1.41	1.46
2	B	501	HEM	C3C-C4C	-2.42	1.41	1.46
2	E	501	HEM	C4B-NB	-2.34	1.34	1.38
2	F	501	HEM	C1C-C2C	-2.33	1.40	1.45
2	B	501	HEM	C3D-C2D	-2.28	1.31	1.36
2	A	501	HEM	C1C-C2C	-2.27	1.40	1.45
2	C	501	HEM	C3C-C4C	-2.27	1.42	1.46
2	A	501	HEM	C3D-C2D	-2.20	1.32	1.36
2	A	501	HEM	C1B-C2B	-2.19	1.40	1.44
2	C	501	HEM	C3D-C2D	-2.17	1.32	1.36
2	E	501	HEM	C4D-ND	-2.15	1.36	1.40
2	D	501	HEM	C4C-NC	-2.14	1.35	1.39
2	C	501	HEM	FE-ND	-2.13	1.88	1.94
2	D	501	HEM	C3D-C2D	-2.11	1.32	1.36
2	C	501	HEM	C2A-C3A	-2.07	1.33	1.38
2	E	501	HEM	C1C-NC	-2.05	1.35	1.39
2	C	501	HEM	C1C-NC	-2.03	1.35	1.39
2	A	501	HEM	C1B-NB	-2.03	1.36	1.40
2	C	501	HEM	FE-NA	2.03	2.02	1.95

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	HEM	C1B-NB-C4B	6.31	111.59	105.07
2	F	501	HEM	CHC-C4B-NB	6.23	131.19	124.42
2	C	501	HEM	CHC-C4B-NB	6.22	131.17	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CHC-C4B-NB	5.96	130.90	124.42
2	B	501	HEM	CHC-C4B-NB	5.53	130.43	124.42
2	C	501	HEM	C1B-NB-C4B	5.25	110.50	105.07
2	D	501	HEM	CHC-C4B-NB	5.24	130.11	124.42
2	A	501	HEM	C1B-NB-C4B	4.99	110.23	105.07
2	E	501	HEM	CHC-C4B-NB	4.58	129.40	124.42
2	D	501	HEM	CHD-C1D-ND	4.30	129.09	124.42
2	C	501	HEM	CHD-C1D-ND	4.01	128.78	124.42
2	A	501	HEM	CMD-C2D-C1D	3.91	130.99	125.04
2	D	501	HEM	CHD-C1D-C2D	-3.75	119.12	124.98
2	C	501	HEM	CHA-C4D-ND	3.71	128.94	124.37
2	B	501	HEM	CHD-C1D-ND	3.62	128.35	124.42
2	B	501	HEM	C1B-NB-C4B	3.57	108.76	105.07
2	C	501	HEM	CHD-C1D-C2D	-3.43	119.62	124.98
2	F	501	HEM	CHB-C1B-NB	3.38	128.54	124.37
2	D	501	HEM	C1B-NB-C4B	3.31	108.49	105.07
2	F	501	HEM	CHD-C1D-C2D	-3.28	119.86	124.98
2	B	501	HEM	CHA-C4D-ND	3.18	128.30	124.37
2	E	501	HEM	CMD-C2D-C1D	3.14	129.82	125.04
2	C	501	HEM	CHB-C1B-NB	3.13	128.23	124.37
2	A	501	HEM	CHA-C4D-ND	3.08	128.18	124.37
2	C	501	HEM	CMD-C2D-C1D	3.06	129.70	125.04
2	A	501	HEM	C4C-NC-C1C	3.06	108.34	105.35
2	D	501	HEM	CHA-C4D-ND	3.06	128.15	124.37
2	E	501	HEM	CBD-CAD-C3D	-3.03	104.20	112.63
2	B	501	HEM	C4C-NC-C1C	3.02	108.31	105.35
2	E	501	HEM	C1B-NB-C4B	3.02	108.19	105.07
2	D	501	HEM	C4B-C3B-C2B	-3.02	104.72	107.11
2	B	501	HEM	CAD-C3D-C4D	3.01	129.93	124.66
2	A	501	HEM	C4A-C3A-C2A	3.01	110.35	106.83
2	C	501	HEM	CHA-C4D-C3D	-3.00	119.69	125.33
2	C	501	HEM	C4A-C3A-C2A	2.99	110.33	106.83
2	F	501	HEM	CHD-C4C-NC	2.95	127.63	124.44
2	A	501	HEM	CHA-C4D-C3D	-2.95	119.80	125.33
2	F	501	HEM	CHD-C1D-ND	2.92	127.59	124.42
2	B	501	HEM	CHD-C1D-C2D	-2.88	120.49	124.98
2	C	501	HEM	CAD-C3D-C4D	2.85	129.64	124.66
3	F	502	4OA	C22-C23-C24	2.78	119.89	112.51
2	B	501	HEM	CHB-C1B-NB	2.76	127.78	124.37
2	E	501	HEM	CHA-C1A-NA	2.72	128.86	123.85
2	B	501	HEM	O2D-CGD-O1D	-2.72	116.52	123.30
2	D	501	HEM	O2D-CGD-CBD	2.71	122.74	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	HEM	C4A-NA-C1A	2.70	108.00	105.35
2	D	501	HEM	CHC-C4B-C3B	-2.69	119.33	125.13
2	C	501	HEM	CMA-C3A-C4A	2.69	129.47	125.37
2	E	501	HEM	C4C-NC-C1C	2.65	107.94	105.35
2	F	501	HEM	CHA-C4D-ND	2.65	127.64	124.37
2	D	501	HEM	CMA-C3A-C4A	2.60	129.34	125.37
2	F	501	HEM	C4C-NC-C1C	2.59	107.89	105.35
2	E	501	HEM	CHA-C4D-ND	2.55	127.52	124.37
2	B	501	HEM	CAA-C2A-C1A	2.55	129.91	124.89
2	C	501	HEM	CMA-C3A-C2A	-2.50	120.20	125.61
2	F	501	HEM	CMD-C2D-C1D	2.50	128.84	125.04
2	C	501	HEM	C2B-C1B-NB	-2.50	106.88	109.84
2	E	501	HEM	CHD-C1D-ND	2.48	127.11	124.42
2	D	501	HEM	CAD-C3D-C4D	2.48	128.99	124.66
2	D	501	HEM	CHA-C4D-C3D	-2.46	120.71	125.33
3	E	502	4OA	C22-C23-C24	2.43	118.95	112.51
2	C	501	HEM	CHC-C4B-C3B	-2.40	119.97	125.13
2	D	501	HEM	O2A-CGA-O1A	-2.37	117.40	123.30
2	A	501	HEM	CHB-C1B-NB	2.32	127.23	124.37
2	C	501	HEM	O2A-CGA-CBA	2.32	121.47	114.03
2	E	501	HEM	CAD-C3D-C4D	2.28	128.64	124.66
2	E	501	HEM	C1A-CHA-C4D	-2.27	120.94	126.34
2	E	501	HEM	C3C-C2C-C1C	-2.27	104.91	107.08
2	D	501	HEM	C1A-CHA-C4D	-2.27	120.96	126.34
2	A	501	HEM	C4A-CHB-C1B	-2.27	120.96	126.34
2	E	501	HEM	CHD-C4C-NC	2.25	126.87	124.44
2	E	501	HEM	CAA-CBA-CGA	-2.24	108.79	113.60
2	D	501	HEM	CHB-C1B-NB	2.22	127.11	124.37
2	B	501	HEM	CHA-C4D-C3D	-2.22	121.17	125.33
2	F	501	HEM	C2D-C1D-ND	2.20	112.52	109.88
2	B	501	HEM	C1A-CHA-C4D	-2.17	121.19	126.34
2	D	501	HEM	O2A-CGA-CBA	2.15	120.93	114.03
2	A	501	HEM	CBA-CAA-C2A	2.14	118.58	112.63
2	E	501	HEM	C4C-C3C-C2C	2.14	108.51	106.75
2	D	501	HEM	C3C-C2C-C1C	-2.13	105.04	107.08
2	E	501	HEM	C4B-C3B-C2B	-2.12	105.43	107.11
2	A	501	HEM	CHA-C1A-NA	2.12	127.74	123.85
2	F	501	HEM	CAD-C3D-C4D	2.11	128.34	124.66
2	C	501	HEM	CAB-C3B-C2B	2.09	135.50	128.60
2	B	501	HEM	CHC-C4B-C3B	-2.07	120.67	125.13
2	A	501	HEM	C1A-CHA-C4D	-2.04	121.50	126.34
2	D	501	HEM	CAA-CBA-CGA	-2.02	109.26	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	HEM	O2D-CGD-CBD	2.01	120.50	114.03
2	E	501	HEM	CHA-C4D-C3D	-2.00	121.57	125.33
3	E	502	4OA	C4-C5-C10	2.00	114.78	112.66

There are no chirality outliers.

All (3) torsion outliers are listed below:

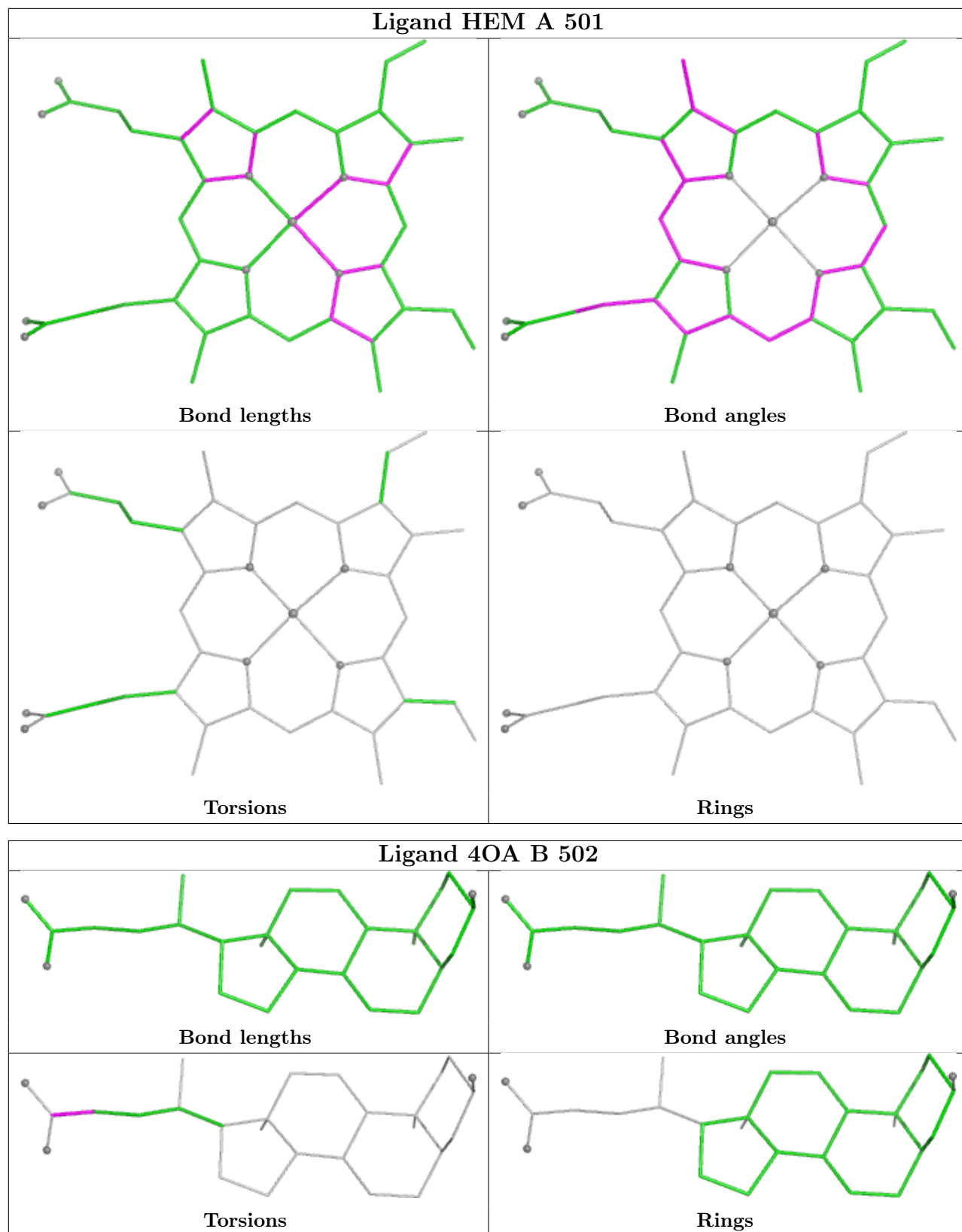
Mol	Chain	Res	Type	Atoms
3	E	502	4OA	C20-C22-C23-C24
3	B	502	4OA	C22-C23-C24-O4
3	B	502	4OA	C22-C23-C24-O4A

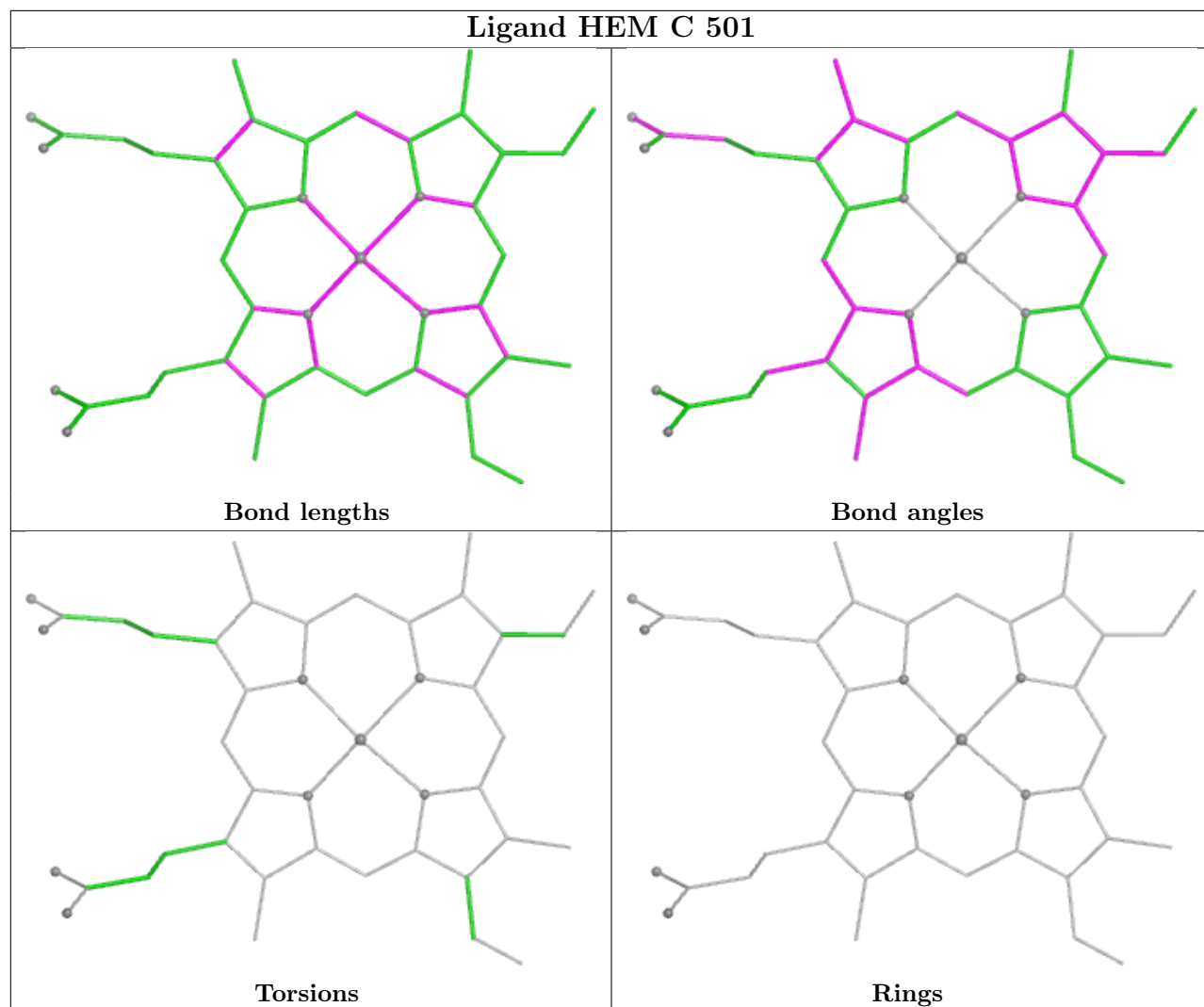
There are no ring outliers.

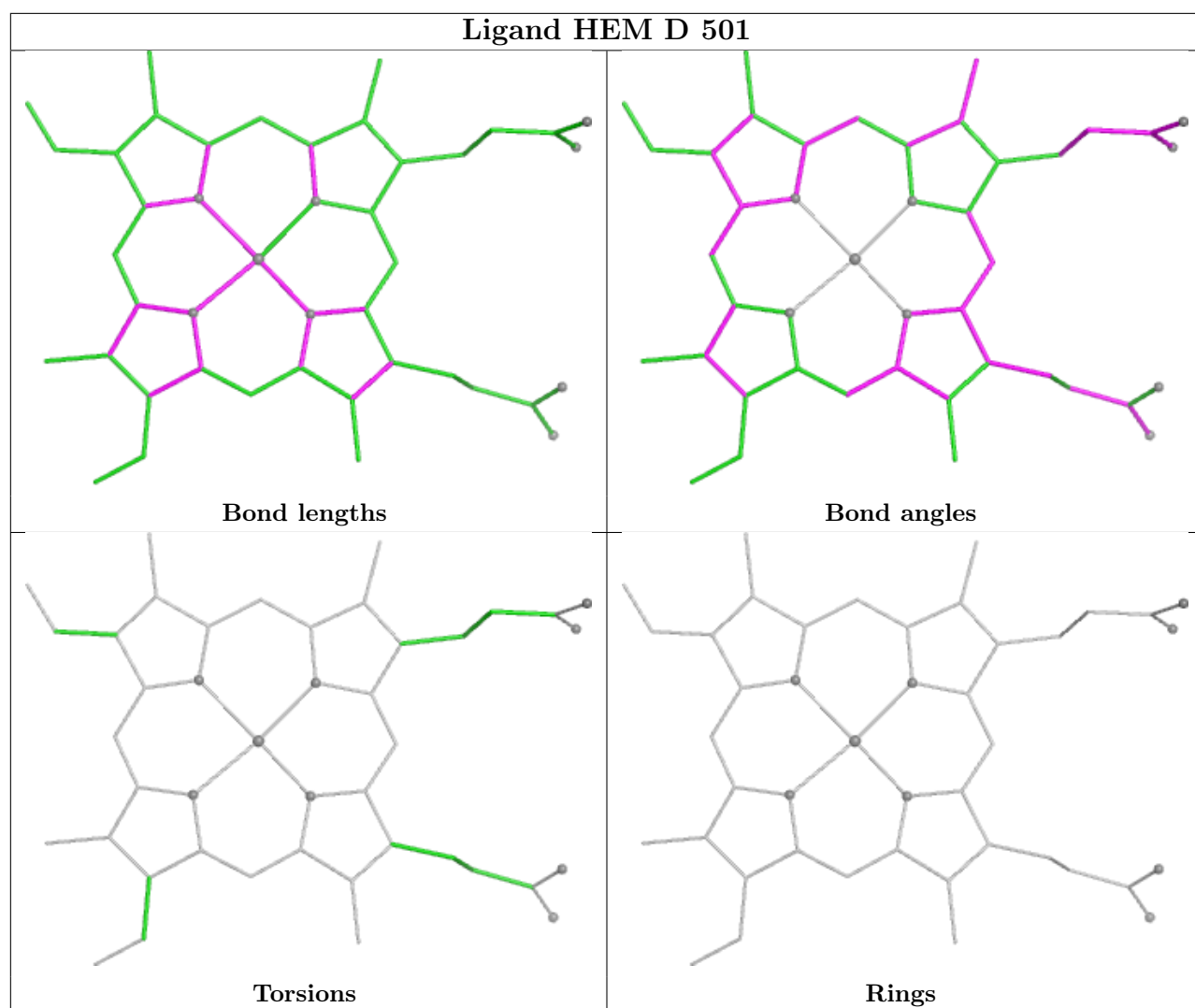
13 monomers are involved in 30 short contacts:

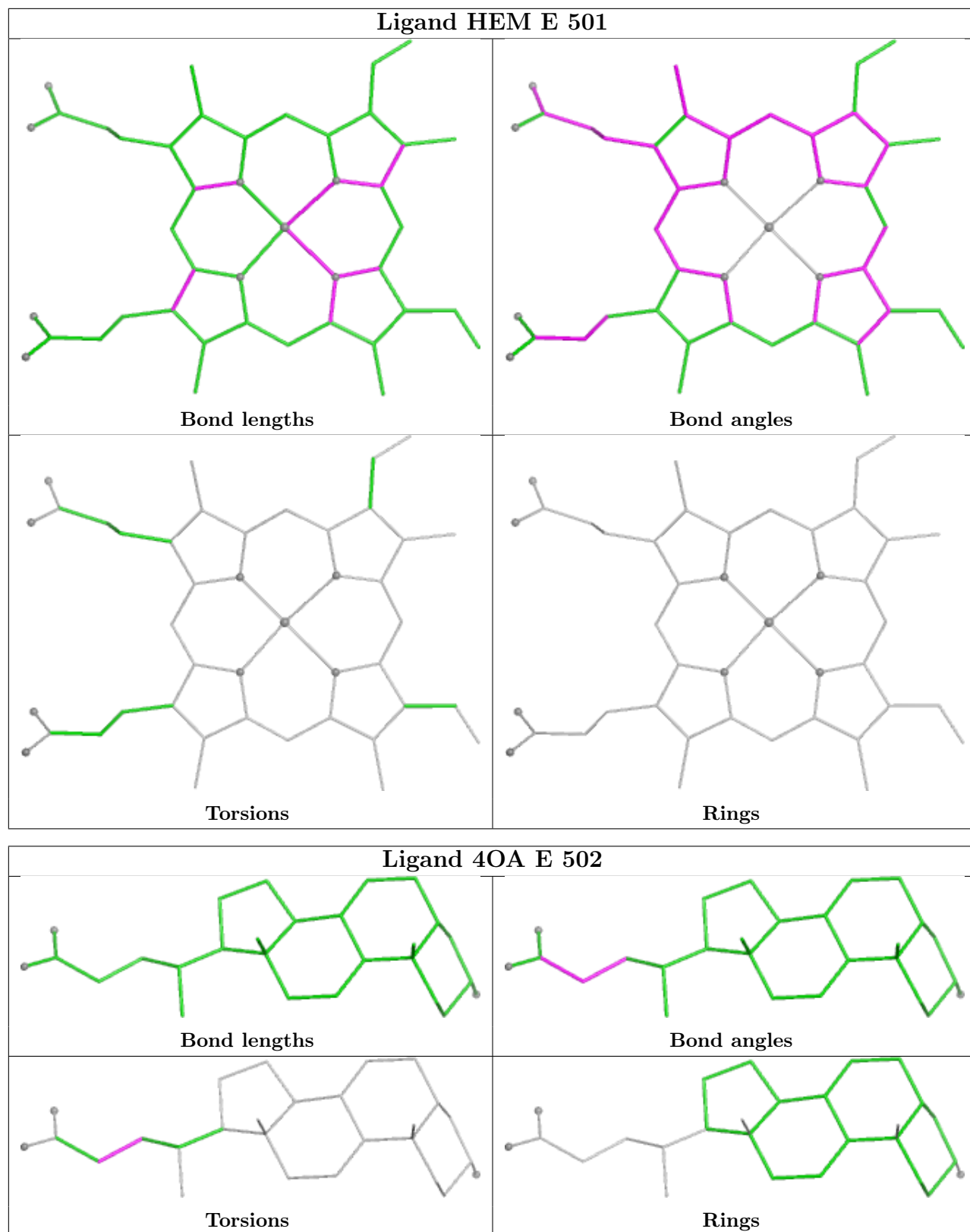
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	512	FMT	2	0
3	D	502	4OA	1	0
5	A	516	FMT	1	0
2	A	501	HEM	4	0
3	B	502	4OA	2	0
2	C	501	HEM	3	0
2	D	501	HEM	5	0
2	E	501	HEM	6	0
5	D	509	FMT	1	0
3	E	502	4OA	1	0
2	F	501	HEM	2	0
2	B	501	HEM	4	0
3	F	502	4OA	1	0

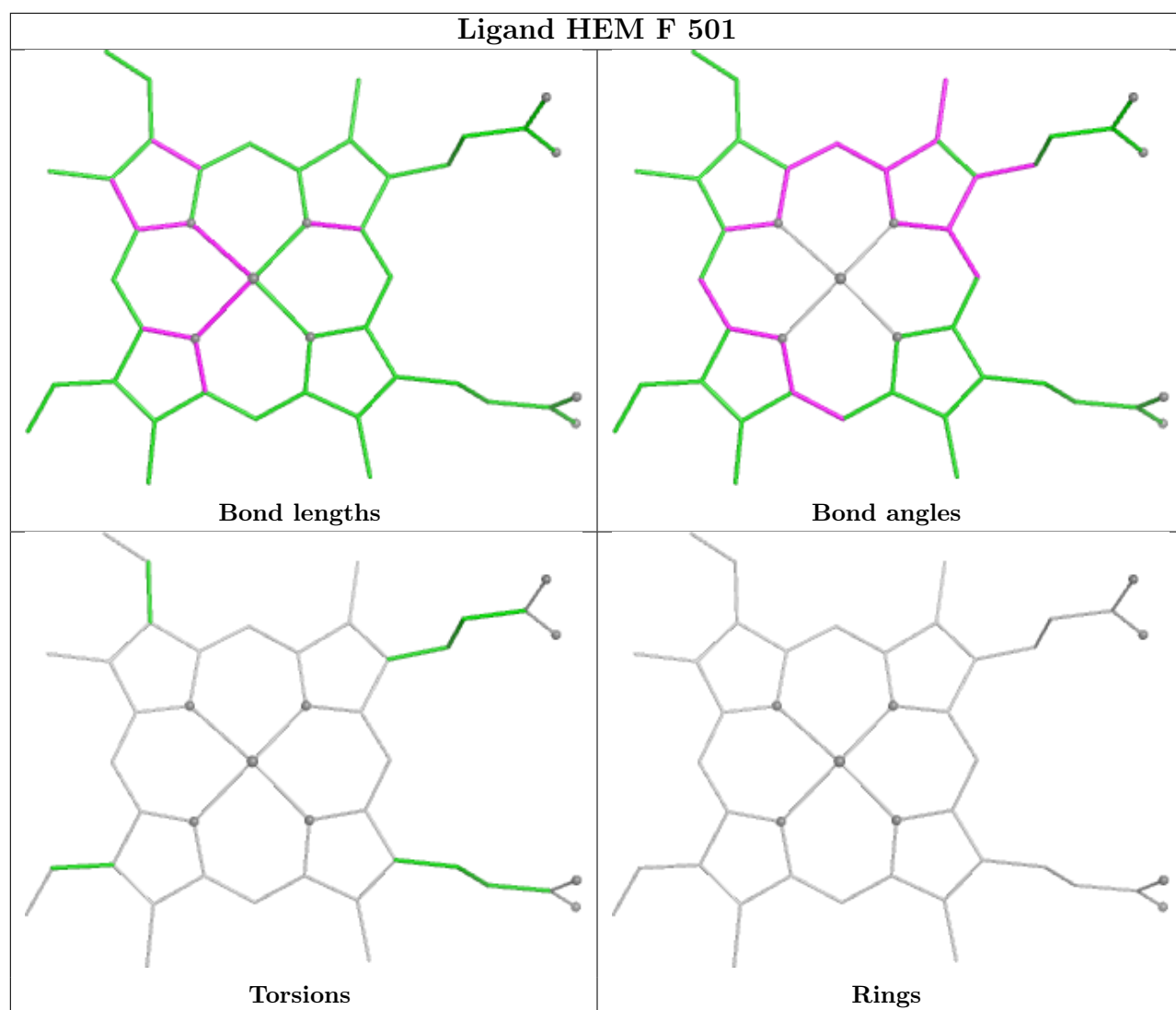
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

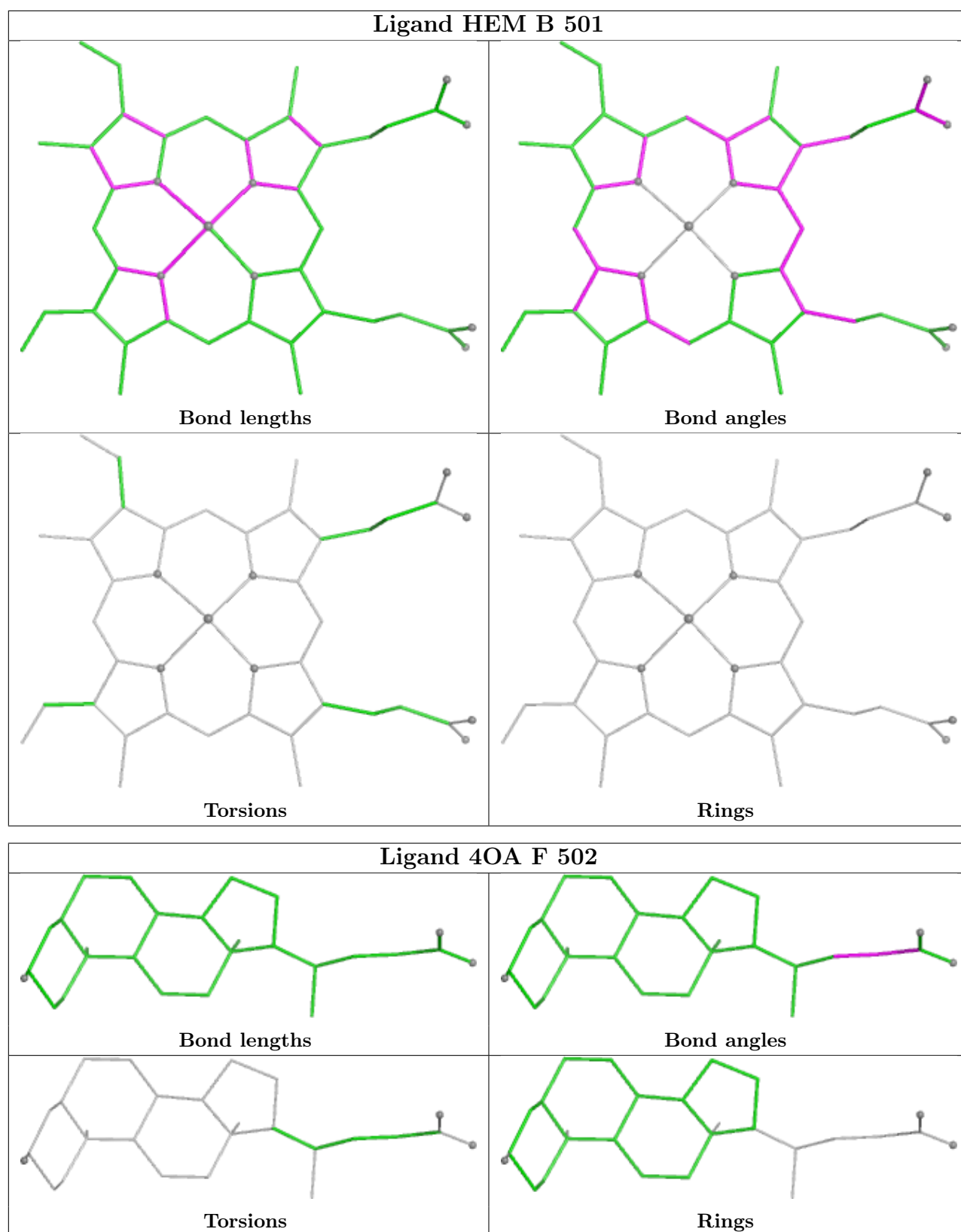












5.7 Other polymers ⓘ

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	399/410 (97%)	-0.17	7 (1%) 67 65	35, 55, 80, 121	0
1	B	401/410 (97%)	-0.15	3 (0%) 84 83	40, 59, 83, 115	0
1	C	396/410 (96%)	-0.15	6 (1%) 72 70	25, 55, 85, 128	1 (0%)
1	D	396/410 (96%)	-0.06	8 (2%) 65 62	37, 62, 86, 121	0
1	E	394/410 (96%)	0.39	17 (4%) 40 36	39, 74, 104, 126	2 (0%)
1	F	396/410 (96%)	0.52	19 (4%) 35 32	50, 81, 123, 135	0
All	All	2382/2460 (96%)	0.06	60 (2%) 58 55	25, 64, 104, 135	3 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	293	ALA	6.5
1	F	294	GLY	5.4
1	E	211	PRO	4.5
1	E	291	GLY	4.2
1	E	294	GLY	4.2
1	F	226	ASP	3.9
1	B	8	PRO	3.8
1	E	292	SER	3.6
1	A	296	PHE	3.5
1	C	293	ALA	3.5
1	F	142	ALA	3.4
1	E	296	PHE	3.4
1	D	14	VAL	3.2
1	D	12	ASP	3.2
1	E	212	THR	3.2
1	E	108	VAL	3.2
1	F	276	LEU	3.1
1	F	292	SER	3.1
1	E	210	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	13	ALA	3.1
1	E	343	ARG	3.1
1	E	297	VAL	3.1
1	D	292	SER	2.9
1	C	294	GLY	2.9
1	D	294	GLY	2.9
1	D	187	ALA	2.8
1	C	208	ARG	2.7
1	D	344	ASN	2.7
1	B	7	GLY	2.6
1	A	343	ARG	2.6
1	A	10	PRO	2.6
1	F	407	TRP	2.6
1	A	85	PRO	2.6
1	E	224	ASP	2.5
1	F	405	VAL	2.5
1	F	339	PHE	2.5
1	E	290	LEU	2.5
1	F	386	VAL	2.5
1	A	83	MET	2.5
1	F	330	VAL	2.4
1	D	229	LEU	2.4
1	E	221	LEU	2.3
1	F	365	GLU	2.3
1	C	229	LEU	2.3
1	C	211	PRO	2.3
1	D	25	LEU	2.2
1	E	14	VAL	2.2
1	F	211	PRO	2.2
1	F	372	ALA	2.2
1	E	223	THR	2.2
1	F	287	TYR	2.2
1	F	279	ALA	2.1
1	A	84	GLN	2.1
1	F	184	LEU	2.1
1	A	229	LEU	2.1
1	F	12	ASP	2.1
1	B	49	GLU	2.0
1	E	214	ASP	2.0
1	C	225	ASN	2.0
1	F	136	VAL	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
5	FMT	C	506	3/3	0.53	0.18	77,77,92,98	0
5	FMT	A	504	3/3	0.55	0.12	80,80,84,87	0
5	FMT	B	505	3/3	0.58	0.12	86,86,86,95	0
5	FMT	D	511	3/3	0.58	0.18	79,79,88,88	0
5	FMT	D	510	3/3	0.63	0.15	78,78,86,87	0
5	FMT	C	511	3/3	0.67	0.20	82,82,86,94	0
5	FMT	B	506	3/3	0.71	0.10	77,77,85,89	0
5	FMT	D	506	3/3	0.71	0.21	69,69,71,84	0
5	FMT	D	508	3/3	0.74	0.15	80,80,82,86	0
5	FMT	A	508	3/3	0.75	0.14	71,71,77,83	0
5	FMT	A	517	3/3	0.76	0.12	79,79,88,91	0
5	FMT	D	505	3/3	0.76	0.09	81,81,82,89	0
5	FMT	E	505	3/3	0.76	0.12	84,84,84,89	0
5	FMT	A	519	3/3	0.77	0.28	68,68,76,82	0
5	FMT	D	509	3/3	0.79	0.11	78,78,82,86	0
5	FMT	A	505	3/3	0.79	0.14	74,74,81,86	0
5	FMT	B	511	3/3	0.80	0.13	73,73,80,81	0
5	FMT	B	504	3/3	0.80	0.12	82,82,83,91	0
5	FMT	C	504	3/3	0.81	0.17	73,73,74,83	0
5	FMT	A	522	3/3	0.81	0.14	72,72,78,88	0
5	FMT	A	511	3/3	0.82	0.10	66,66,73,78	0
5	FMT	F	504	3/3	0.82	0.12	74,74,77,78	0
5	FMT	A	515	3/3	0.84	0.18	81,81,87,87	0
5	FMT	B	509	3/3	0.84	0.19	75,75,75,75	0
5	FMT	C	512	3/3	0.84	0.12	68,68,77,82	0
5	FMT	D	504	3/3	0.84	0.14	71,71,72,74	0
5	FMT	C	508	3/3	0.85	0.17	70,70,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FMT	A	520	3/3	0.85	0.11	71,71,72,80	0
5	FMT	A	514	3/3	0.85	0.23	65,65,68,78	0
5	FMT	E	506	3/3	0.85	0.16	77,77,81,88	0
5	FMT	F	503	3/3	0.85	0.22	61,61,67,75	0
4	NA	D	503	1/1	0.85	0.19	70,70,70,70	0
4	NA	C	503	1/1	0.86	0.17	69,69,69,69	0
5	FMT	A	510	3/3	0.86	0.20	68,68,72,81	0
5	FMT	B	512	3/3	0.86	0.11	70,70,80,82	0
5	FMT	E	504	3/3	0.86	0.08	80,80,89,91	0
5	FMT	C	509	3/3	0.87	0.13	68,68,78,79	0
4	NA	A	503	1/1	0.87	0.19	70,70,70,70	0
5	FMT	B	507	3/3	0.87	0.13	73,73,74,82	0
5	FMT	C	513	3/3	0.87	0.10	74,74,76,82	0
5	FMT	D	507	3/3	0.88	0.19	70,70,78,85	0
5	FMT	A	516	3/3	0.88	0.24	65,65,82,87	0
5	FMT	E	503	3/3	0.88	0.12	62,62,67,71	0
5	FMT	A	518	3/3	0.88	0.32	63,63,67,76	0
5	FMT	C	507	3/3	0.89	0.20	66,66,73,79	0
5	FMT	A	523	3/3	0.89	0.13	76,76,78,82	0
5	FMT	A	507	3/3	0.89	0.09	83,83,83,88	0
5	FMT	B	508	3/3	0.89	0.22	66,66,70,79	0
5	FMT	A	506	3/3	0.89	0.13	70,70,72,76	0
5	FMT	A	513	3/3	0.90	0.20	67,67,72,77	0
5	FMT	A	512	3/3	0.90	0.16	78,78,86,91	0
5	FMT	A	509	3/3	0.91	0.09	58,58,72,73	0
5	FMT	C	505	3/3	0.92	0.20	57,57,61,75	0
5	FMT	A	521	3/3	0.92	0.12	74,74,77,83	0
5	FMT	C	510	3/3	0.92	0.13	72,72,76,82	0
4	NA	B	503	1/1	0.92	0.13	62,62,62,62	0
5	FMT	C	515	3/3	0.93	0.13	77,77,80,87	0
3	4OA	B	502	27/27	0.94	0.14	49,55,69,71	0
5	FMT	B	510	3/3	0.94	0.17	70,70,87,89	0
5	FMT	C	514	3/3	0.94	0.16	78,78,87,89	0
3	4OA	F	502	27/27	0.95	0.12	61,67,76,81	0
3	4OA	E	502	27/27	0.95	0.12	59,65,80,82	0
3	4OA	C	502	27/27	0.96	0.12	44,48,60,62	0
3	4OA	D	502	27/27	0.96	0.12	48,57,82,84	0
3	4OA	A	502	27/27	0.96	0.12	44,50,64,68	0
2	HEM	E	501	43/43	0.97	0.07	43,53,58,61	0
2	HEM	C	501	43/43	0.98	0.06	31,38,45,50	0
2	HEM	A	501	43/43	0.98	0.06	31,36,42,50	0
2	HEM	F	501	43/43	0.98	0.08	45,55,72,94	0

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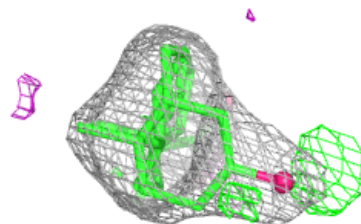
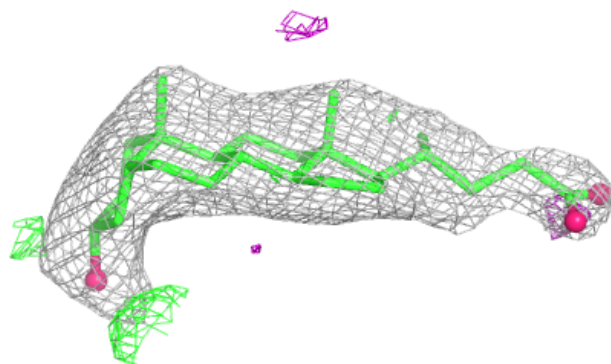
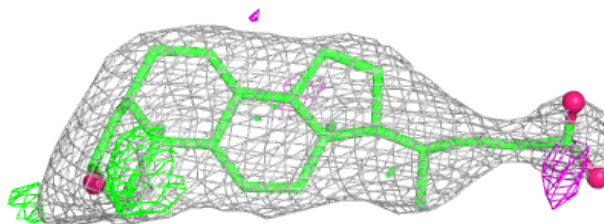
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	B	501	43/43	0.98	0.07	34,39,50,57	0
2	HEM	D	501	43/43	0.99	0.06	31,38,47,49	0

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.

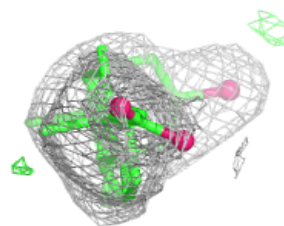
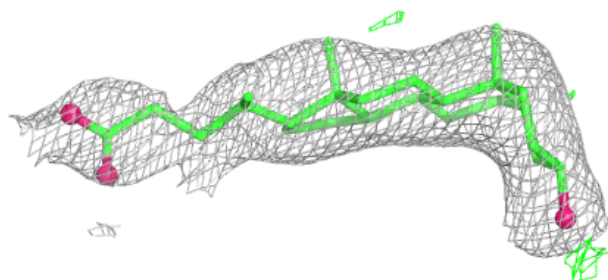
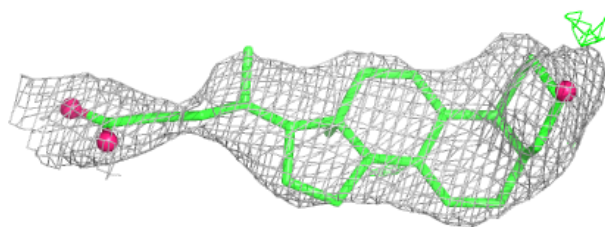
Electron density around 4OA B 502:

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

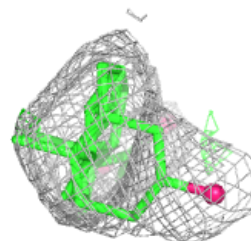
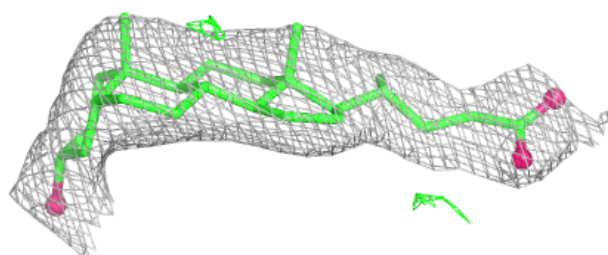
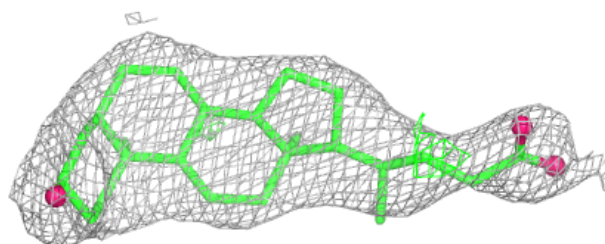


Electron density around 4OA F 502:

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

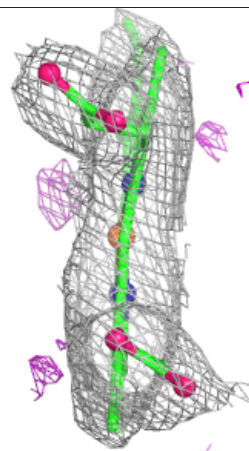
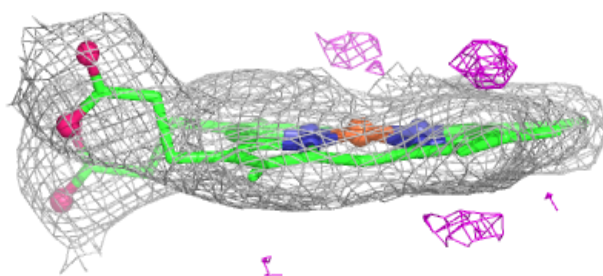
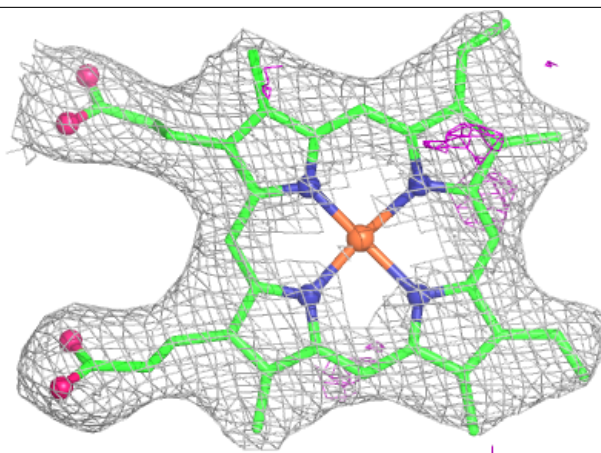
**Electron density around 4OA E 502:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



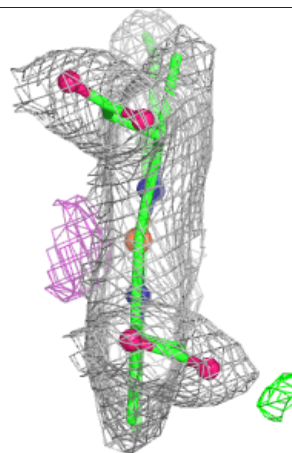
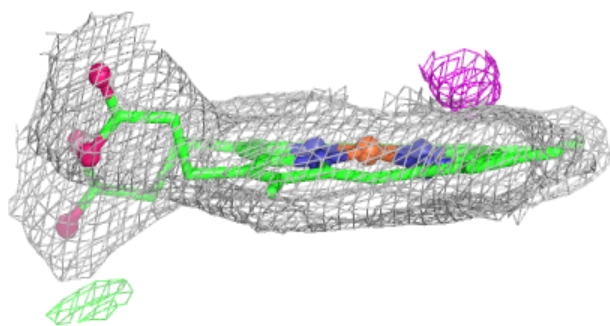
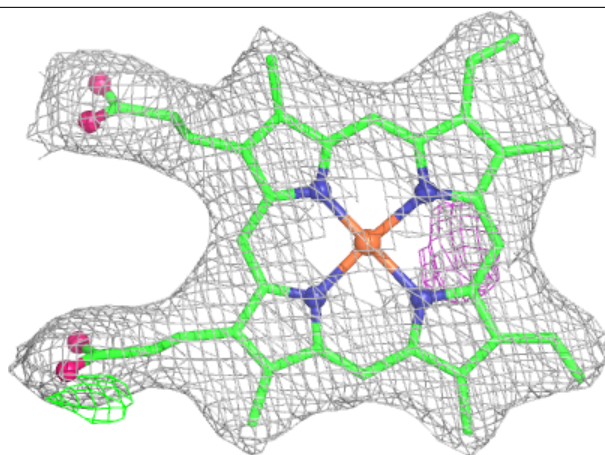
Electron density around HEM E 501:

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



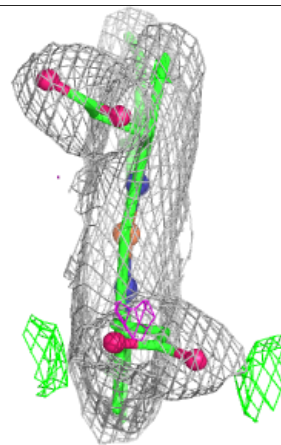
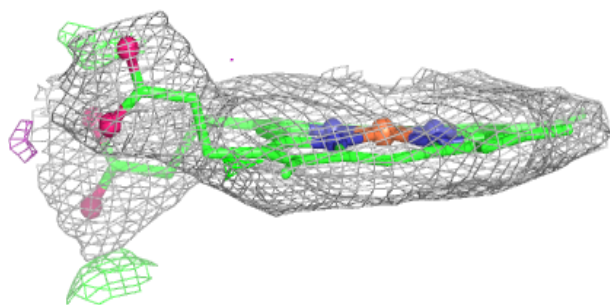
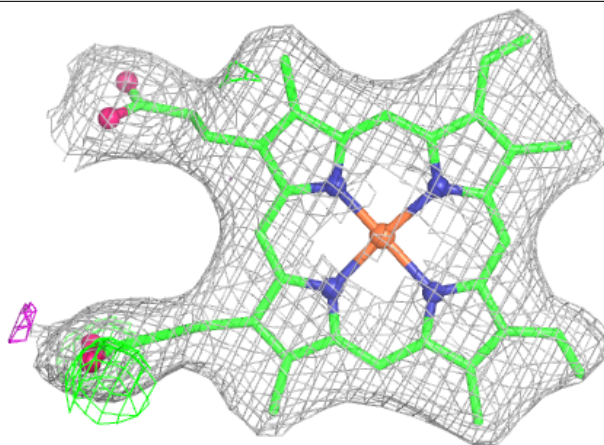
Electron density around HEM C 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



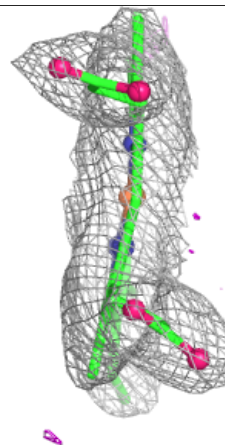
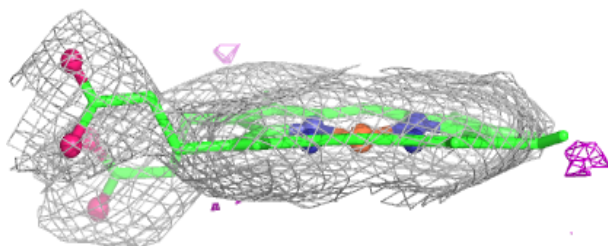
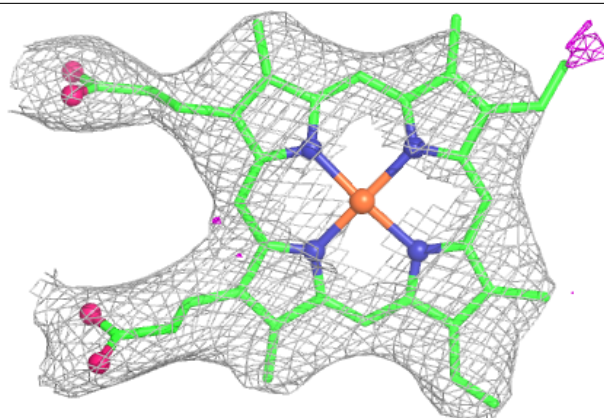
Electron density around HEM A 501:

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



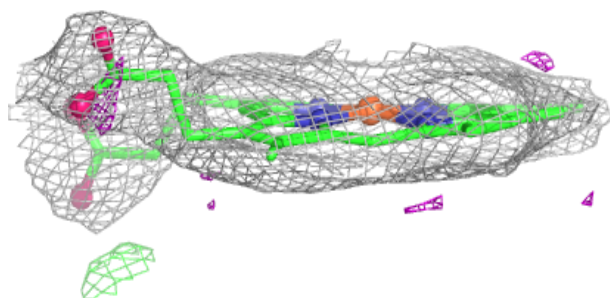
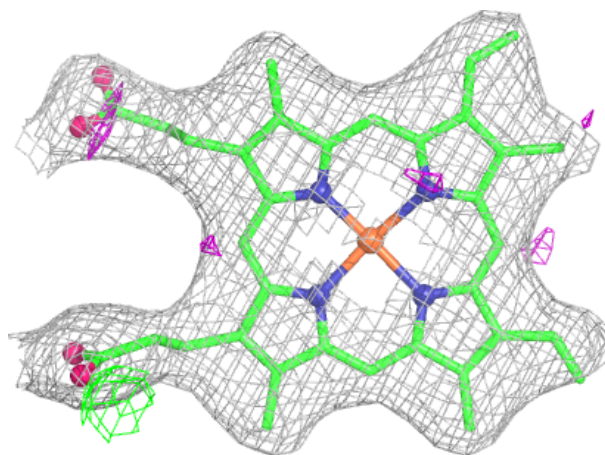
Electron density around HEM F 501:

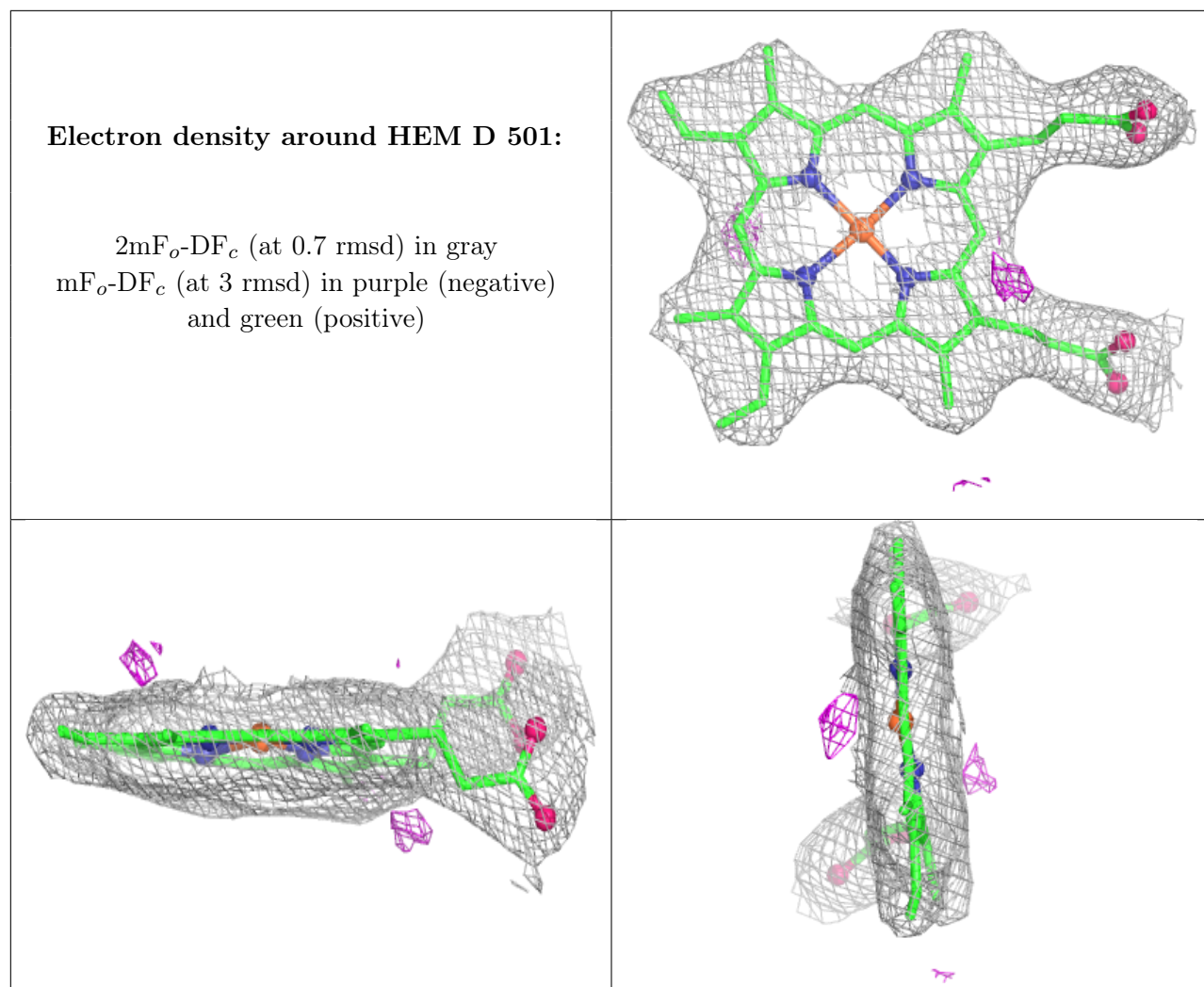
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 501:

$2mF_o-DF_c$ (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.