



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:14 AM UTC

PDB ID : 6WR0 / pdb_00006wr0
Title : Human steroidogenic cytochrome P450 17A1 with 3-keto-delta4-abiraterone analog
Authors : Petrunak, E.M.; Bart, A.G.; Scott, E.E.
Deposited on : 2020-04-29
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (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

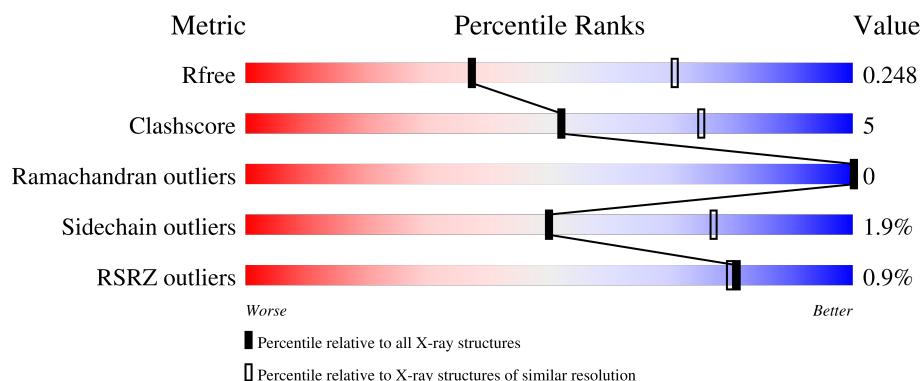
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	494	 83% 11% • 6%
1	B	494	 78% 15% • 6%
1	C	494	 2% 78% 16% • •
1	D	494	 2% 81% 13% • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30722 atoms, of which 15420 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 Steroid 17-alpha-hydroxylase/17,20 lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	466	Total	C	H	N	O	S	0	0	0
			7500	2383	3787	642	673	15			
1	B	465	Total	C	H	N	O	S	0	0	0
			7488	2380	3780	641	672	15			
1	C	474	Total	C	H	N	O	S	0	0	0
			7595	2412	3828	653	687	15			
1	D	466	Total	C	H	N	O	S	0	0	0
			7506	2385	3789	643	674	15			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	initiating methionine	UNP P05093
A	20	ALA	-	expression tag	UNP P05093
A	21	LYS	-	expression tag	UNP P05093
A	22	LYS	-	expression tag	UNP P05093
A	23	THR	-	expression tag	UNP P05093
A	509	HIS	-	expression tag	UNP P05093
A	510	HIS	-	expression tag	UNP P05093
A	511	HIS	-	expression tag	UNP P05093
A	512	HIS	-	expression tag	UNP P05093
B	19	MET	-	initiating methionine	UNP P05093
B	20	ALA	-	expression tag	UNP P05093
B	21	LYS	-	expression tag	UNP P05093
B	22	LYS	-	expression tag	UNP P05093
B	23	THR	-	expression tag	UNP P05093
B	509	HIS	-	expression tag	UNP P05093
B	510	HIS	-	expression tag	UNP P05093
B	511	HIS	-	expression tag	UNP P05093
B	512	HIS	-	expression tag	UNP P05093
C	19	MET	-	initiating methionine	UNP P05093
C	20	ALA	-	expression tag	UNP P05093
C	21	LYS	-	expression tag	UNP P05093

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Chain	Residue	Modelled	Actual	Comment	Reference
C	22	LYS	-	expression tag	UNP P05093
C	23	THR	-	expression tag	UNP P05093
C	509	HIS	-	expression tag	UNP P05093
C	510	HIS	-	expression tag	UNP P05093
C	511	HIS	-	expression tag	UNP P05093
C	512	HIS	-	expression tag	UNP P05093
D	19	MET	-	initiating methionine	UNP P05093
D	20	ALA	-	expression tag	UNP P05093
D	21	LYS	-	expression tag	UNP P05093
D	22	LYS	-	expression tag	UNP P05093
D	23	THR	-	expression tag	UNP P05093
D	509	HIS	-	expression tag	UNP P05093
D	510	HIS	-	expression tag	UNP P05093
D	511	HIS	-	expression tag	UNP P05093
D	512	HIS	-	expression tag	UNP P05093

- # HEM

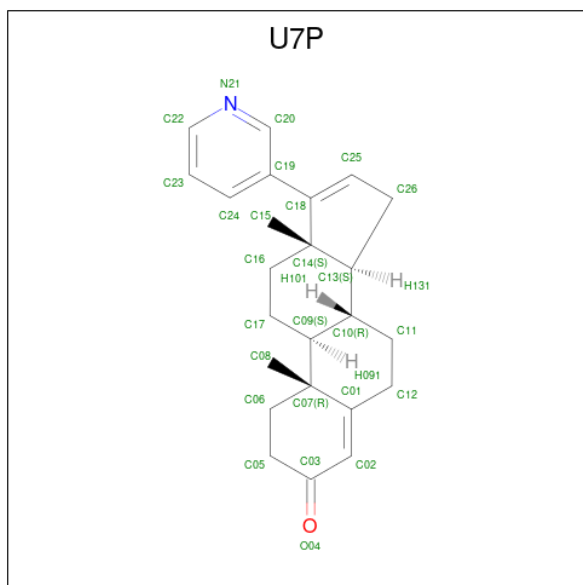
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
2	B	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
2	C	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	D	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 3 is (8alpha)-17-(pyridin-3-yl)androsta-4,16-dien-3-one (CCD ID: U7P) (formula: C₂₄H₂₉NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			55	24	29	1	1		
3	B	1	Total	C	H	N	O	0	0
			55	24	29	1	1		
3	C	1	Total	C	H	N	O	0	0
			55	24	29	1	1		
3	D	1	Total	C	H	N	O	0	0
			55	24	29	1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

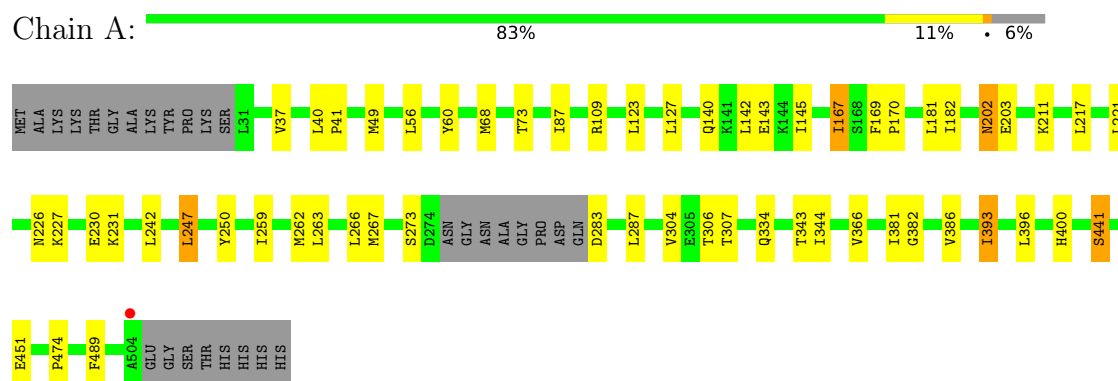
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	28	Total 28	O 28	0	0
5	B	38	Total 38	O 38	0	0
5	C	33	Total 33	O 33	0	0
5	D	19	Total 19	O 19	0	0

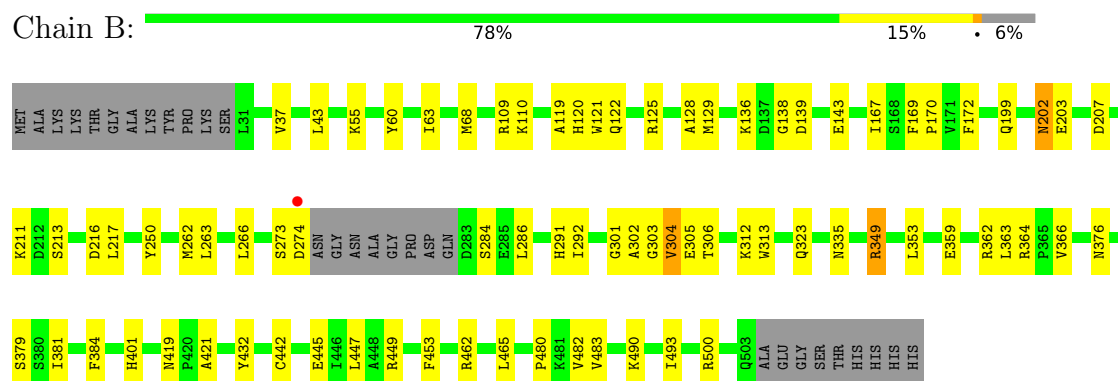
3 Residue-property plots [i](#)

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.

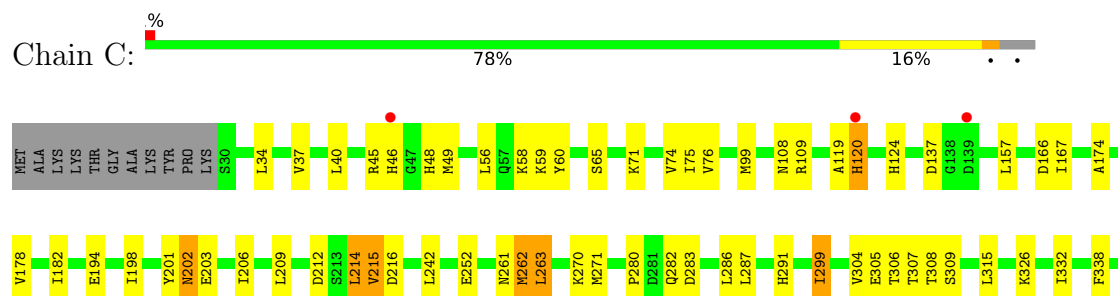
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

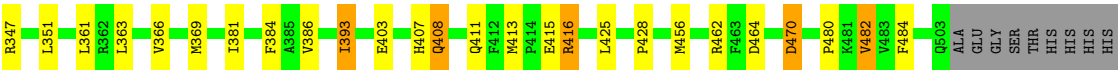


- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

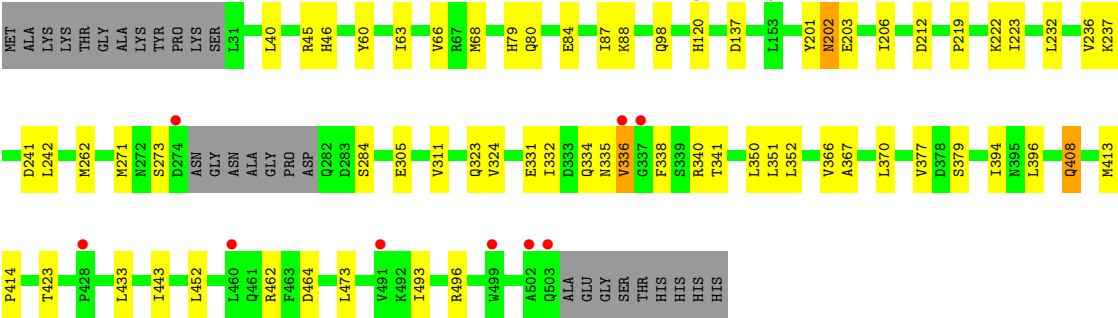
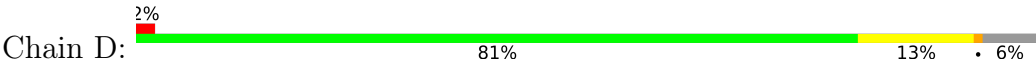


- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase





● Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.35Å 152.98Å 168.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.81 – 2.70 39.81 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.81-2.70) 90.8 (39.81-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.209 , 0.246 0.211 , 0.248	Depositor DCC
R_{free} test set	3264 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	30722	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, HEM, U7P

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	0.87	8/3793 (0.2%)	0.74	7/5135 (0.1%)
1	B	1.12	25/3788 (0.7%)	0.83	10/5128 (0.2%)
1	C	1.17	29/3849 (0.8%)	0.97	25/5213 (0.5%)
1	D	0.97	11/3797 (0.3%)	0.90	12/5140 (0.2%)
All	All	1.04	73/15227 (0.5%)	0.86	54/20616 (0.3%)

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	413	MET	C-O	-10.30	1.15	1.24
1	C	212	ASP	C-O	-7.76	1.17	1.24
1	C	49	MET	N-CA	-7.35	1.36	1.46
1	B	109	ARG	C-O	-7.27	1.14	1.23
1	D	379	SER	C-O	-6.96	1.17	1.24
1	B	143	GLU	C-O	-6.91	1.15	1.24
1	A	202	ASN	C-O	-6.76	1.16	1.24
1	C	215	VAL	C-O	-6.74	1.17	1.23
1	C	306	THR	C-O	-6.74	1.16	1.24
1	C	75	ILE	C-O	-6.73	1.16	1.24
1	D	98	GLN	C-O	-6.60	1.15	1.24
1	A	203	GLU	CA-C	-6.56	1.44	1.52
1	C	263	LEU	C-O	-6.54	1.16	1.24
1	C	408	GLN	C-O	-6.53	1.15	1.24
1	D	341	THR	C-N	6.50	1.42	1.33
1	A	393	ILE	C-O	-6.43	1.17	1.24
1	D	212	ASP	C-O	-6.35	1.18	1.24
1	B	303	GLY	CA-C	-6.29	1.45	1.52
1	B	119	ALA	CA-C	-6.25	1.44	1.52
1	B	384	PHE	C-O	-6.13	1.16	1.23
1	D	367	ALA	C-O	-6.09	1.17	1.24
1	C	203	GLU	N-CA	-5.97	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	202	ASN	C-O	-5.72	1.17	1.24
1	C	326	LYS	C-O	-5.67	1.17	1.24
1	B	203	GLU	N-CA	-5.64	1.39	1.46
1	B	301	GLY	C-O	-5.63	1.17	1.23
1	C	76	VAL	C-O	-5.63	1.18	1.24
1	C	416	ARG	CA-C	-5.62	1.44	1.52
1	C	299	ILE	C-O	-5.61	1.17	1.24
1	A	167	ILE	C-O	-5.59	1.17	1.24
1	D	120	HIS	C-O	-5.59	1.17	1.24
1	C	305	GLU	CA-C	-5.58	1.45	1.52
1	B	55	LYS	C-O	-5.53	1.17	1.24
1	B	121	TRP	C-O	-5.51	1.17	1.24
1	B	376	ASN	CA-C	-5.50	1.45	1.52
1	C	74	VAL	C-O	-5.50	1.18	1.24
1	B	312	LYS	C-O	-5.49	1.17	1.24
1	A	203	GLU	C-O	-5.47	1.17	1.24
1	D	222	LYS	C-O	-5.46	1.16	1.24
1	B	207	ASP	C-O	-5.45	1.17	1.24
1	B	207	ASP	C-N	-5.44	1.25	1.33
1	A	203	GLU	N-CA	-5.41	1.39	1.46
1	A	230	GLU	C-O	-5.36	1.17	1.24
1	D	203	GLU	N-CA	-5.35	1.40	1.46
1	C	484	PHE	C-O	-5.35	1.17	1.23
1	B	379	SER	C-O	-5.34	1.19	1.24
1	C	308	THR	C-O	-5.34	1.17	1.24
1	C	120	HIS	C-O	-5.31	1.18	1.24
1	B	302	ALA	C-O	-5.30	1.17	1.24
1	B	323	GLN	C-O	-5.26	1.18	1.24
1	C	56	LEU	C-O	-5.25	1.17	1.24
1	A	441	SER	C-N	-5.25	1.26	1.33
1	B	465	LEU	C-O	-5.25	1.17	1.24
1	B	203	GLU	C-O	-5.25	1.17	1.24
1	C	304	VAL	CA-CB	-5.24	1.49	1.55
1	C	216	ASP	C-O	-5.22	1.17	1.24
1	B	122	GLN	C-O	-5.22	1.18	1.24
1	C	262	MET	C-O	-5.22	1.18	1.24
1	C	307	THR	C-O	-5.21	1.18	1.24
1	C	291	HIS	C-O	-5.20	1.17	1.24
1	B	306	THR	C-O	-5.18	1.17	1.24
1	B	119	ALA	C-O	-5.16	1.18	1.24
1	D	202	ASN	C-O	-5.15	1.18	1.24
1	D	66	VAL	C-O	-5.14	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	381	ILE	C-O	-5.13	1.18	1.24
1	C	203	GLU	CA-C	-5.13	1.46	1.52
1	B	304	VAL	C-O	-5.12	1.18	1.23
1	C	309	SER	C-O	-5.11	1.18	1.24
1	B	199	GLN	N-CA	-5.05	1.40	1.46
1	C	361	LEU	C-O	-5.05	1.17	1.24
1	B	490	LYS	C-O	-5.04	1.17	1.23
1	D	262	MET	C-O	-5.02	1.18	1.24
1	C	120	HIS	N-CA	-5.02	1.40	1.46

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ILE	N-CA-C	10.58	121.42	111.48
1	C	305	GLU	N-CA-C	9.67	121.90	111.36
1	A	87	ILE	CB-CA-C	-9.57	103.58	111.71
1	D	87	ILE	N-CA-C	8.91	118.66	111.62
1	B	305	GLU	N-CA-C	7.89	119.96	111.36
1	D	87	ILE	CB-CA-C	-7.43	104.44	111.05
1	C	214	LEU	N-CA-C	7.15	120.68	109.96
1	D	335	ASN	N-CA-C	6.87	118.85	111.36
1	D	79	HIS	CA-C-N	6.77	129.36	120.28
1	D	79	HIS	C-N-CA	6.77	129.36	120.28
1	C	384	PHE	N-CA-C	6.77	121.07	110.17
1	C	291	HIS	N-CA-C	-6.75	103.39	111.69
1	D	79	HIS	N-CA-C	6.71	118.60	111.28
1	C	304	VAL	N-CA-C	6.69	118.03	111.67
1	C	166	ASP	N-CA-C	-6.59	98.50	109.24
1	C	45	ARG	N-CA-C	-6.57	100.55	110.28
1	B	462	ARG	N-CA-C	6.52	121.52	113.50
1	C	108	ASN	N-CA-C	6.42	118.42	110.91
1	D	45	ARG	N-CA-C	-6.33	104.30	111.14
1	C	411	GLN	N-CA-C	6.26	120.25	110.17
1	C	65	SER	N-CA-C	6.10	118.98	109.52
1	B	109	ARG	N-CA-C	6.06	119.78	111.54
1	C	413	MET	CA-C-N	6.01	125.69	119.56
1	C	413	MET	C-N-CA	6.01	125.69	119.56
1	C	411	GLN	CA-C-N	5.94	131.14	122.41
1	C	411	GLN	C-N-CA	5.94	131.14	122.41
1	A	259	ILE	CB-CA-C	-5.88	103.01	111.19
1	B	203	GLU	CA-C-N	5.78	126.35	120.00
1	B	203	GLU	C-N-CA	5.78	126.35	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	203	GLU	CA-C-N	5.66	126.26	119.98
1	D	203	GLU	C-N-CA	5.66	126.26	119.98
1	B	304	VAL	N-CA-C	5.55	116.61	111.45
1	D	423	THR	N-CA-C	5.52	120.17	113.38
1	A	287	LEU	N-CA-C	5.42	118.97	111.55
1	B	480	PRO	CB-CA-C	-5.42	107.32	111.87
1	B	349	ARG	CB-CG-CD	-5.40	98.87	111.30
1	C	464	ASP	N-CA-C	-5.40	100.44	109.24
1	C	363	LEU	N-CA-C	5.37	117.22	111.36
1	C	74	VAL	CB-CA-C	-5.37	102.65	110.81
1	D	473	LEU	CA-C-N	-5.36	114.43	119.85
1	D	473	LEU	C-N-CA	-5.36	114.43	119.85
1	C	203	GLU	CA-C-N	5.31	125.84	120.00
1	C	203	GLU	C-N-CA	5.31	125.84	120.00
1	C	462	ARG	N-CA-C	5.30	120.02	113.50
1	C	415	GLU	CA-C-N	5.29	129.54	120.72
1	C	415	GLU	C-N-CA	5.29	129.54	120.72
1	A	382	GLY	O-C-N	5.24	127.54	122.41
1	B	138	GLY	N-CA-C	5.22	117.47	110.43
1	A	203	GLU	CA-C-N	5.12	125.66	119.98
1	A	203	GLU	C-N-CA	5.12	125.66	119.98
1	C	415	GLU	N-CA-C	5.11	119.14	113.01
1	C	76	VAL	CA-C-N	5.07	131.34	121.41
1	C	76	VAL	C-N-CA	5.07	131.34	121.41
1	B	139	ASP	N-CA-C	-5.03	105.88	111.36

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	3713	3787	3785	39	0
1	B	3708	3780	3779	38	0
1	C	3767	3828	3827	39	0
1	D	3717	3789	3787	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	43	30	30	8	0
2	B	43	30	30	6	0
2	C	43	30	30	5	0
2	D	43	30	30	5	0
3	A	26	29	0	1	0
3	B	26	29	0	1	0
3	C	26	29	0	0	0
3	D	26	29	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	28	0	0	2	0
5	B	38	0	0	0	0
5	C	33	0	0	1	0
5	D	19	0	0	0	0
All	All	15302	15420	15298	156	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 5.

All (156) 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:601:HEM:HHC	2:C:601:HEM:HBB2	1.41	1.00
2:A:600:HEM:HBB2	2:A:600:HEM:HMB2	1.44	0.97
2:A:600:HEM:HBC2	2:A:600:HEM:HHD	1.44	0.96
2:A:600:HEM:HBB2	2:A:600:HEM:CMB	2.12	0.80
2:C:601:HEM:HBC2	2:C:601:HEM:HHD	1.64	0.79
1:C:198:ILE:HA	1:C:201:TYR:CE2	2.23	0.74
1:A:68:MET:HE1	1:D:40:LEU:HD12	1.71	0.73
1:B:68:MET:HE1	1:C:40:LEU:HD12	1.76	0.68
2:D:601:HEM:HBA1	2:D:601:HEM:HMA1	1.78	0.65
1:A:140:GLN:HG2	1:A:140:GLN:O	1.98	0.63
1:D:370:LEU:HD12	1:D:394:ILE:HB	1.79	0.63
1:D:331:GLU:OE2	1:D:350:LEU:HA	1.99	0.62
1:C:482:VAL:HG13	5:C:705:HOH:O	2.00	0.61
1:A:56:LEU:HD22	1:A:60:TYR:CD2	2.36	0.61
1:A:167:ILE:C	1:A:167:ILE:HD12	2.26	0.60
2:D:601:HEM:HBC2	2:D:601:HEM:HHD	1.85	0.59
1:A:40:LEU:HD12	1:D:68:MET:HE2	1.82	0.59
1:D:332:ILE:HA	1:D:350:LEU:HD21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:HEM:HBC2	2:B:601:HEM:HMC2	1.85	0.58
2:C:601:HEM:HBB2	2:C:601:HEM:CHC	2.19	0.58
1:D:206:ILE:HD11	1:D:305:GLU:HG3	1.85	0.58
1:A:142:LEU:HD11	1:A:182:ILE:HD11	1.85	0.58
1:D:408:GLN:HB3	1:D:413:MET:CE	2.33	0.58
1:B:60:TYR:CG	1:C:37:VAL:HG11	2.39	0.57
2:D:601:HEM:HBA1	2:D:601:HEM:CMA	2.33	0.57
1:D:273:SER:OG	1:D:284:SER:HB3	2.05	0.57
1:A:211:LYS:O	1:A:211:LYS:HD2	2.05	0.56
1:D:338:PHE:N	1:D:338:PHE:CD1	2.73	0.55
1:A:306:THR:HG21	3:A:601:U7P:N21	2.23	0.54
1:C:262:MET:HE3	1:C:299:ILE:HG21	1.89	0.54
1:D:408:GLN:CB	1:D:413:MET:HE1	2.38	0.54
1:D:493:ILE:HG23	1:D:493:ILE:O	2.07	0.53
1:A:37:VAL:HG12	1:D:60:TYR:CD1	2.43	0.53
1:A:68:MET:CE	1:D:40:LEU:HD12	2.38	0.53
1:C:157:LEU:HD21	1:C:167:ILE:HG22	1.91	0.53
1:C:366:VAL:CG2	2:C:601:HEM:HMB2	2.39	0.53
1:A:227:LYS:O	1:A:231:LYS:HG3	2.09	0.53
1:C:124:HIS:HE1	1:C:286:LEU:O	1.91	0.53
1:B:445:GLU:OE2	1:B:449:ARG:NH2	2.42	0.52
1:C:59:LYS:O	1:C:59:LYS:HG3	2.09	0.52
1:B:266:LEU:HD13	1:B:292:ILE:HG23	1.92	0.51
1:A:123:LEU:HD11	1:A:127:LEU:HD11	1.92	0.51
1:A:381:ILE:HG13	1:A:386:VAL:HG21	1.92	0.51
1:D:323:GLN:H	1:D:323:GLN:CD	2.17	0.51
1:C:407:HIS:CE1	1:C:408:GLN:HG3	2.45	0.51
1:C:280:PRO:HG2	1:D:377:VAL:HG12	1.91	0.51
1:A:334:GLN:HG3	1:A:334:GLN:O	2.09	0.51
1:B:110:LYS:HD3	1:B:291:HIS:CD2	2.46	0.51
1:B:442:CYS:HB2	2:B:601:HEM:NA	2.25	0.51
2:B:601:HEM:HBB2	2:B:601:HEM:HMB2	1.91	0.51
1:A:221:LEU:HD12	1:A:226:ASN:OD1	2.11	0.51
1:C:48:HIS:CE1	1:C:480:PRO:HD3	2.46	0.50
1:B:120:HIS:HB3	1:B:286:LEU:HD22	1.93	0.50
1:A:366:VAL:CG2	2:A:600:HEM:HMB2	2.41	0.50
1:B:335:ASN:O	1:B:349:ARG:NH1	2.44	0.50
1:A:167:ILE:C	1:A:167:ILE:CD1	2.85	0.50
1:B:273:SER:OG	1:B:284:SER:HB2	2.11	0.50
1:C:252:GLU:HA	1:C:252:GLU:OE2	2.13	0.49
1:C:209:LEU:HD23	1:C:482:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:LEU:HD23	1:C:456:MET:HE1	1.95	0.49
1:B:136:LYS:O	1:B:136:LYS:HD3	2.12	0.49
1:B:172:PHE:CE2	1:B:304:VAL:HG11	2.47	0.49
1:B:500:ARG:HG2	1:B:500:ARG:HH11	1.78	0.49
1:D:352:LEU:O	1:D:352:LEU:HG	2.11	0.49
1:C:351:LEU:HD22	1:C:425:LEU:HG	1.95	0.49
2:A:600:HEM:HMB2	2:A:600:HEM:CBB	2.29	0.49
1:B:167:ILE:C	1:B:167:ILE:HD12	2.38	0.48
1:A:56:LEU:HD22	1:A:60:TYR:HD2	1.77	0.48
1:B:273:SER:O	1:B:274:ASP:HB2	2.13	0.48
1:B:128:ALA:HA	1:B:262:MET:HE2	1.96	0.48
1:B:353:LEU:HD23	1:B:453:PHE:CE1	2.48	0.48
1:B:419:ASN:HD21	1:B:421:ALA:HB3	1.77	0.48
2:B:601:HEM:HBB2	2:B:601:HEM:CMB	2.42	0.48
1:C:470:ASP:OD1	1:C:470:ASP:N	2.46	0.48
1:C:109:ARG:HH11	1:C:109:ARG:HG3	1.77	0.48
1:C:194:GLU:CD	1:C:242:LEU:HD11	2.38	0.48
1:A:41:PRO:CB	1:A:56:LEU:HD11	2.43	0.48
1:B:63:ILE:HG12	1:C:34:LEU:HD22	1.96	0.47
1:A:307:THR:HG21	1:A:451:GLU:OE1	2.13	0.47
1:B:363:LEU:HD23	1:B:401:HIS:NE2	2.29	0.47
1:A:41:PRO:HB2	1:A:56:LEU:HD11	1.96	0.47
1:B:37:VAL:HG12	1:C:60:TYR:CD1	2.50	0.47
1:A:366:VAL:HG21	2:A:600:HEM:HMB2	1.95	0.47
2:B:601:HEM:HBC2	2:B:601:HEM:CMC	2.45	0.47
1:C:167:ILE:HD12	1:C:167:ILE:C	2.40	0.47
1:B:313:TRP:CZ3	1:B:364:ARG:HG3	2.49	0.47
2:D:601:HEM:CMA	2:D:601:HEM:CBA	2.92	0.47
1:B:362:ARG:HB2	1:B:432:TYR:HE1	1.80	0.46
1:A:250:TYR:CD2	1:A:263:LEU:HD23	2.50	0.46
1:D:336:VAL:HG23	1:D:340:ARG:NH1	2.30	0.46
1:A:169:PHE:HB3	1:A:170:PRO:HD3	1.97	0.46
1:B:447:LEU:HD23	2:B:601:HEM:HBC2	1.97	0.46
1:A:273:SER:O	1:A:273:SER:OG	2.34	0.46
1:A:109:ARG:HH11	1:A:109:ARG:HG2	1.80	0.45
1:C:270:LYS:HD3	1:C:287:LEU:HB2	1.98	0.45
1:B:211:LYS:C	1:B:211:LYS:HD3	2.41	0.45
1:B:493:ILE:O	1:B:493:ILE:HG23	2.15	0.45
1:C:120:HIS:CE1	1:C:124:HIS:CE1	3.04	0.45
1:C:381:ILE:HD12	1:C:386:VAL:HG21	1.98	0.45
1:D:408:GLN:HB2	1:D:413:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LEU:O	1:A:267:MET:HG2	2.17	0.45
1:C:369:MET:HE2	1:C:393:ILE:HG21	1.99	0.45
1:B:172:PHE:CD2	1:B:304:VAL:HG11	2.52	0.45
2:C:601:HEM:HHH	2:C:601:HEM:CBH	2.41	0.44
1:A:396:LEU:HD11	1:A:400:HIS:NE2	2.32	0.44
1:B:169:PHE:HB3	1:B:170:PRO:HD3	1.98	0.44
1:D:324:VAL:HG11	1:D:414:PRO:HG2	1.99	0.44
1:A:247:LEU:N	1:A:247:LEU:HD23	2.33	0.44
1:C:338:PHE:CD1	1:C:338:PHE:N	2.86	0.44
1:B:136:LYS:HD3	1:B:136:LYS:C	2.43	0.43
1:A:262:MET:O	1:A:266:LEU:HD12	2.18	0.43
1:A:211:LYS:HD2	1:A:211:LYS:C	2.43	0.43
1:B:43:LEU:HD21	1:C:71:LYS:HD2	2.01	0.43
1:D:84:GLU:HG3	1:D:88:LYS:HE3	2.00	0.43
2:A:600:HEM:HBC2	2:A:600:HEM:CHD	2.23	0.43
1:D:242:LEU:C	1:D:242:LEU:HD23	2.43	0.43
1:B:366:VAL:HG13	1:B:483:VAL:HG13	2.00	0.43
1:C:198:ILE:HA	1:C:201:TYR:CD2	2.53	0.43
1:A:474:PRO:HB3	1:A:489:PHE:CG	2.54	0.43
1:B:60:TYR:CD2	1:C:37:VAL:HG11	2.53	0.43
1:B:202:ASN:ND2	3:B:602:U7P:O04	2.52	0.42
1:D:311:VAL:HG23	1:D:452:LEU:HD23	2.01	0.42
1:A:304:VAL:HG21	5:A:725:HOH:O	2.17	0.42
1:A:242:LEU:C	1:A:242:LEU:HD23	2.45	0.42
1:B:359:GLU:HA	1:B:359:GLU:OE1	2.20	0.42
1:B:363:LEU:HD22	1:B:364:ARG:HH12	1.85	0.42
1:D:464:ASP:OD1	1:D:496:ARG:HG2	2.19	0.42
1:A:109:ARG:NH1	5:A:701:HOH:O	2.52	0.42
1:A:145:ILE:HG23	1:A:181:LEU:HD13	2.02	0.42
1:C:271:MET:HE2	1:C:271:MET:HB3	1.85	0.42
1:C:416:ARG:HG2	1:C:428:PRO:HG3	2.00	0.42
1:B:250:TYR:CD1	1:B:263:LEU:HD23	2.55	0.42
1:C:282:GLN:HG2	1:C:283:ASP:N	2.35	0.42
1:D:237:LYS:HE3	1:D:241:ASP:OD2	2.20	0.42
1:D:366:VAL:CG2	2:D:601:HEM:HMB2	2.50	0.42
1:C:58:LYS:HA	1:C:58:LYS:HD3	1.87	0.41
1:C:182:ILE:O	1:C:261:ASN:HB2	2.20	0.41
1:C:119:ALA:HB1	1:C:286:LEU:HD11	2.02	0.41
1:D:206:ILE:CD1	1:D:305:GLU:HG3	2.50	0.41
1:D:396:LEU:HD11	1:D:433:LEU:O	2.20	0.41
1:A:143:GLU:OE2	1:A:343:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:GLU:OE2	1:D:351:LEU:N	2.53	0.41
2:A:600:HEM:HHA	2:A:600:HEM:HAA1	1.89	0.41
1:D:232:LEU:O	1:D:236:VAL:HG23	2.20	0.41
1:D:331:GLU:OE2	1:D:350:LEU:CA	2.68	0.41
1:C:109:ARG:HG3	1:C:109:ARG:NH1	2.35	0.41
1:C:99:MET:HE1	1:C:214:LEU:HD22	2.02	0.41
1:C:174:ALA:O	1:C:178:VAL:HG23	2.21	0.40
1:D:271:MET:HE2	1:D:271:MET:HB3	1.97	0.40
1:A:49:MET:HE1	1:A:217:LEU:HG	2.01	0.40
1:A:344:ILE:HD12	1:A:344:ILE:HG23	1.85	0.40
1:B:217:LEU:HA	1:B:217:LEU:HD23	1.89	0.40
1:D:219:PRO:HG2	1:D:223:ILE:HG23	2.03	0.40
1:B:125:ARG:O	1:B:129:MET:HG3	2.21	0.40
1:B:493:ILE:O	1:B:493:ILE:CG2	2.70	0.40
1:D:63:ILE:O	1:D:63:ILE:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	462/494 (94%)	450 (97%)	12 (3%)	0	100	100
1	B	461/494 (93%)	446 (97%)	15 (3%)	0	100	100
1	C	472/494 (96%)	458 (97%)	14 (3%)	0	100	100
1	D	462/494 (94%)	448 (97%)	14 (3%)	0	100	100
All	All	1857/1976 (94%)	1802 (97%)	55 (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	415/436 (95%)	409 (99%)	6 (1%)	59	82
1	B	415/436 (95%)	411 (99%)	4 (1%)	68	86
1	C	421/436 (97%)	409 (97%)	12 (3%)	37	67
1	D	416/436 (95%)	406 (98%)	10 (2%)	43	72
All	All	1667/1744 (96%)	1635 (98%)	32 (2%)	50	77

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	THR
1	A	202	ASN
1	A	247	LEU
1	A	283	ASP
1	A	393	ILE
1	A	441	SER
1	B	202	ASN
1	B	213	SER
1	B	216	ASP
1	B	482	VAL
1	C	46	HIS
1	C	137	ASP
1	C	202	ASN
1	C	206	ILE
1	C	215	VAL
1	C	263	LEU
1	C	332	ILE
1	C	347	ARG
1	C	393	ILE
1	C	403	GLU
1	C	470	ASP
1	C	482	VAL
1	D	46	HIS
1	D	80	GLN

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Mol	Chain	Res	Type
1	D	137	ASP
1	D	201	TYR
1	D	202	ASN
1	D	334	GLN
1	D	336	VAL
1	D	408	GLN
1	D	443	ILE
1	D	462	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	HIS
1	A	472	GLN
1	B	202	ASN
1	B	208	ASN
1	B	249	ASN
1	B	348	ASN
1	C	52	ASN
1	C	321	ASN
1	C	401	HIS
1	D	50	HIS
1	D	108	ASN
1	D	321	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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
2	HEM	B	601	1,3	50,50,50	1.45	9 (18%)	67,82,82	1.18	6 (8%)
3	U7P	D	602	2	30,30,30	6.28	22 (73%)	47,47,47	2.93	18 (38%)
3	U7P	B	602	2	30,30,30	6.14	22 (73%)	47,47,47	2.64	21 (44%)
3	U7P	A	601	2	30,30,30	6.15	22 (73%)	47,47,47	2.98	16 (34%)
3	U7P	C	602	2	30,30,30	6.10	22 (73%)	47,47,47	2.90	14 (29%)
2	HEM	C	601	1,3	50,50,50	1.77	12 (24%)	67,82,82	1.68	16 (23%)
2	HEM	A	600	3	50,50,50	1.79	14 (28%)	67,82,82	1.83	19 (28%)
2	HEM	D	601	1,3	50,50,50	2.45	19 (38%)	67,82,82	2.21	27 (40%)

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	B	601	1,3	-	2/14/54/54	-
3	U7P	D	602	2	-	0/4/62/62	0/5/5/5
3	U7P	B	602	2	-	2/4/62/62	0/5/5/5
3	U7P	A	601	2	-	2/4/62/62	0/5/5/5
3	U7P	C	602	2	-	2/4/62/62	0/5/5/5
2	HEM	C	601	1,3	-	3/14/54/54	-
2	HEM	A	600	3	-	1/14/54/54	-
2	HEM	D	601	1,3	-	5/14/54/54	-

All (142) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	U7P	C25-C18	19.91	1.67	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	U7P	C25-C18	19.81	1.67	1.33
3	A	601	U7P	C25-C18	19.39	1.66	1.33
3	C	602	U7P	C25-C18	18.99	1.65	1.33
3	C	602	U7P	C14-C18	-17.55	1.37	1.53
3	A	601	U7P	C14-C18	-16.57	1.38	1.53
3	D	602	U7P	C14-C18	-11.37	1.43	1.53
3	B	602	U7P	C14-C18	-11.25	1.43	1.53
3	D	602	U7P	C02-C01	11.12	1.50	1.34
3	B	602	U7P	C02-C01	10.06	1.48	1.34
3	D	602	U7P	C26-C25	9.65	1.64	1.50
3	B	602	U7P	C26-C25	9.14	1.63	1.50
3	A	601	U7P	C02-C01	9.05	1.47	1.34
3	C	602	U7P	C02-C01	8.91	1.47	1.34
3	B	602	U7P	C14-C13	7.85	1.69	1.54
3	A	601	U7P	C26-C25	7.64	1.61	1.50
3	D	602	U7P	C16-C17	7.60	1.68	1.53
3	C	602	U7P	C26-C25	7.48	1.61	1.50
3	D	602	U7P	C20-C19	7.47	1.51	1.39
3	B	602	U7P	C20-C19	7.39	1.50	1.39
3	D	602	U7P	C14-C13	7.07	1.67	1.54
3	B	602	U7P	C16-C17	7.04	1.67	1.53
2	D	601	HEM	C1B-NB	-6.53	1.29	1.40
2	D	601	HEM	C1C-C2C	-6.34	1.32	1.45
3	A	601	U7P	C16-C17	6.30	1.66	1.53
3	C	602	U7P	C16-C14	-6.22	1.42	1.54
3	C	602	U7P	C16-C17	5.95	1.65	1.53
3	D	602	U7P	C20-N21	5.78	1.46	1.34
3	A	601	U7P	C07-C09	-5.78	1.46	1.56
3	D	602	U7P	C23-C24	5.72	1.48	1.38
3	A	601	U7P	C14-C13	5.64	1.65	1.54
3	B	602	U7P	C10-C09	5.60	1.64	1.53
3	B	602	U7P	C20-N21	5.55	1.46	1.34
3	B	602	U7P	C23-C24	5.51	1.48	1.38
2	C	601	HEM	FE-NB	5.49	2.11	1.94
3	A	601	U7P	C20-C19	5.28	1.47	1.39
3	D	602	U7P	C10-C09	5.28	1.63	1.53
3	B	602	U7P	C12-C01	5.28	1.59	1.50
3	A	601	U7P	C16-C14	-5.24	1.44	1.54
3	C	602	U7P	C14-C13	5.21	1.64	1.54
3	A	601	U7P	C10-C13	-5.17	1.43	1.53
3	D	602	U7P	C24-C19	5.05	1.47	1.39
3	D	602	U7P	C12-C01	4.97	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	U7P	C23-C22	4.93	1.51	1.37
3	B	602	U7P	C23-C22	4.84	1.51	1.37
3	B	602	U7P	C24-C19	4.77	1.46	1.39
2	D	601	HEM	C4B-NB	-4.69	1.29	1.38
3	C	602	U7P	C15-C14	-4.58	1.47	1.54
3	C	602	U7P	C07-C09	-4.58	1.48	1.56
3	C	602	U7P	C20-C19	4.49	1.46	1.39
3	C	602	U7P	C10-C13	-4.48	1.45	1.53
3	D	602	U7P	C22-N21	4.46	1.46	1.33
2	A	600	HEM	C1B-NB	-4.41	1.32	1.40
3	B	602	U7P	C22-N21	4.38	1.46	1.33
3	C	602	U7P	O04-C03	-4.20	1.16	1.23
2	A	600	HEM	FE-NB	4.09	2.07	1.94
2	D	601	HEM	C4D-ND	-4.00	1.33	1.40
3	A	601	U7P	C08-C07	-4.00	1.48	1.54
3	A	601	U7P	C10-C09	3.92	1.61	1.53
3	C	602	U7P	C10-C09	3.92	1.61	1.53
2	D	601	HEM	O2A-CGA	-3.91	1.17	1.30
2	D	601	HEM	C1C-NC	-3.91	1.32	1.39
3	A	601	U7P	C22-N21	3.90	1.44	1.33
2	C	601	HEM	C1B-NB	-3.90	1.33	1.40
2	D	601	HEM	FE-ND	-3.83	1.83	1.94
3	D	602	U7P	C16-C14	-3.82	1.47	1.54
3	A	601	U7P	O04-C03	-3.77	1.17	1.23
3	A	601	U7P	C15-C14	-3.75	1.48	1.54
2	C	601	HEM	FE-NC	3.75	2.07	1.95
2	B	601	HEM	FE-NA	3.75	2.07	1.95
3	C	602	U7P	C08-C07	-3.72	1.48	1.54
2	A	600	HEM	FE-NC	3.68	2.07	1.95
2	D	601	HEM	O2D-CGD	-3.67	1.18	1.30
3	D	602	U7P	C02-C03	3.55	1.53	1.45
3	A	601	U7P	C20-N21	3.53	1.41	1.34
2	A	600	HEM	C4D-ND	-3.50	1.34	1.40
3	B	602	U7P	C02-C03	3.49	1.53	1.45
3	C	602	U7P	C20-N21	3.47	1.41	1.34
3	B	602	U7P	C16-C14	-3.47	1.47	1.54
2	B	601	HEM	FE-NC	3.45	2.06	1.95
3	A	601	U7P	C23-C22	3.41	1.47	1.37
2	C	601	HEM	C4D-ND	-3.39	1.34	1.40
3	A	601	U7P	C23-C24	3.37	1.44	1.38
2	D	601	HEM	C3D-C2D	-3.36	1.29	1.36
2	D	601	HEM	C1B-C2B	-3.36	1.37	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	HEM	C1A-C2A	-3.34	1.37	1.44
2	A	600	HEM	C1C-C2C	-3.34	1.38	1.45
3	D	602	U7P	C19-C18	3.31	1.53	1.48
3	C	602	U7P	C22-N21	3.30	1.43	1.33
3	C	602	U7P	C12-C01	3.26	1.55	1.50
2	A	600	HEM	FE-ND	-3.25	1.84	1.94
3	D	602	U7P	C17-C09	3.23	1.59	1.53
2	C	601	HEM	C1C-C2C	-3.21	1.39	1.45
2	B	601	HEM	FE-NB	3.21	2.04	1.94
3	B	602	U7P	C07-C09	-3.17	1.51	1.56
3	A	601	U7P	C12-C01	3.17	1.55	1.50
3	C	602	U7P	C23-C22	3.16	1.46	1.37
3	A	601	U7P	C06-C07	-3.12	1.48	1.54
2	D	601	HEM	C4A-NA	-3.05	1.33	1.39
2	A	600	HEM	C4B-NB	-3.04	1.32	1.38
2	D	601	HEM	C1D-ND	-3.03	1.32	1.38
3	A	601	U7P	C24-C19	3.03	1.44	1.39
3	C	602	U7P	C23-C24	3.02	1.44	1.38
2	B	601	HEM	CAB-C3B	2.95	1.55	1.47
2	C	601	HEM	FE-ND	-2.93	1.85	1.94
3	D	602	U7P	C07-C09	-2.89	1.51	1.56
3	D	602	U7P	C05-C03	2.88	1.56	1.50
3	C	602	U7P	C11-C10	-2.84	1.48	1.53
2	A	600	HEM	C3C-C4C	-2.79	1.41	1.46
2	C	601	HEM	C4B-NB	-2.76	1.33	1.38
3	B	602	U7P	C17-C09	2.76	1.58	1.53
2	B	601	HEM	CAC-C3C	2.72	1.54	1.47
2	D	601	HEM	C2A-C3A	-2.69	1.31	1.38
3	C	602	U7P	C24-C19	2.68	1.43	1.39
2	D	601	HEM	C3C-C4C	-2.63	1.41	1.46
2	B	601	HEM	FE-ND	2.63	2.03	1.94
3	B	602	U7P	C19-C18	2.63	1.52	1.48
2	D	601	HEM	FE-NC	2.59	2.03	1.95
2	A	600	HEM	C1A-C2A	-2.58	1.39	1.44
2	C	601	HEM	C3C-C4C	-2.57	1.41	1.46
3	A	601	U7P	C11-C10	-2.55	1.48	1.53
3	B	602	U7P	C05-C03	2.54	1.55	1.50
2	C	601	HEM	O2D-CGD	-2.54	1.22	1.30
2	C	601	HEM	C1D-ND	-2.47	1.34	1.38
2	C	601	HEM	O2A-CGA	-2.45	1.22	1.30
3	D	602	U7P	C10-C13	-2.44	1.49	1.53
2	D	601	HEM	CHB-C4A	-2.41	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	U7P	C10-C13	-2.41	1.49	1.53
2	B	601	HEM	CMB-C2B	2.37	1.55	1.50
2	A	600	HEM	O2D-CGD	-2.37	1.23	1.30
2	A	600	HEM	C1D-ND	-2.32	1.34	1.38
2	D	601	HEM	CHC-C1C	-2.30	1.33	1.38
3	C	602	U7P	C06-C07	-2.29	1.50	1.54
2	A	600	HEM	C1B-C2B	-2.27	1.39	1.44
3	B	602	U7P	C11-C12	2.16	1.57	1.53
2	A	600	HEM	O2A-CGA	-2.14	1.23	1.30
2	A	600	HEM	C1C-NC	-2.13	1.35	1.39
3	D	602	U7P	C08-C07	-2.13	1.51	1.54
2	D	601	HEM	C4C-NC	-2.07	1.35	1.39
2	B	601	HEM	CMD-C2D	2.07	1.55	1.50
2	B	601	HEM	CMA-C3A	2.05	1.55	1.50
2	C	601	HEM	C1A-C2A	-2.02	1.40	1.44

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	U7P	C13-C14-C18	12.50	110.09	99.50
3	C	602	U7P	C13-C14-C18	11.23	109.01	99.50
3	A	601	U7P	C13-C14-C18	10.24	108.17	99.50
3	C	602	U7P	C26-C25-C18	-8.81	104.91	112.56
3	A	601	U7P	C26-C25-C18	-8.27	105.38	112.56
3	D	602	U7P	C26-C25-C18	-7.74	105.84	112.56
3	C	602	U7P	C01-C02-C03	-6.73	113.25	123.67
3	A	601	U7P	C14-C18-C19	-6.62	118.38	125.39
3	B	602	U7P	C13-C14-C18	6.51	105.01	99.50
3	B	602	U7P	C15-C14-C16	-6.31	103.89	111.10
3	B	602	U7P	C26-C25-C18	-5.99	107.36	112.56
3	A	601	U7P	C01-C02-C03	-5.90	114.55	123.67
2	D	601	HEM	CHC-C4B-NB	5.54	130.38	124.42
3	B	602	U7P	C26-C13-C14	5.43	107.85	104.05
2	A	600	HEM	CHC-C4B-NB	5.41	130.25	124.42
3	D	602	U7P	C15-C14-C13	-4.95	105.88	112.99
3	A	601	U7P	C06-C07-C09	-4.77	102.42	108.74
3	A	601	U7P	C15-C14-C18	-4.71	100.41	107.81
3	A	601	U7P	C26-C13-C14	4.55	107.23	104.05
3	B	602	U7P	C14-C13-C10	-4.51	108.38	113.13
2	D	601	HEM	C4B-C3B-C2B	-4.49	103.16	107.28
3	D	602	U7P	C07-C09-C10	4.48	119.27	112.71
2	A	600	HEM	CHD-C1D-ND	4.48	129.24	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	HEM	CHC-C4B-NB	4.46	129.22	124.42
2	D	601	HEM	CHD-C1D-ND	4.30	129.05	124.42
2	D	601	HEM	CMB-C2B-C1B	-4.17	118.52	125.03
3	D	602	U7P	C26-C13-C10	4.15	126.03	121.63
3	C	602	U7P	C06-C07-C01	4.12	115.84	108.74
3	A	601	U7P	C19-C20-N21	-4.08	117.43	123.50
3	C	602	U7P	C15-C14-C13	-4.01	107.23	112.99
2	D	601	HEM	CAC-C3C-C4C	3.98	134.33	124.82
2	C	601	HEM	CHD-C1D-ND	3.92	128.64	124.42
2	D	601	HEM	CHA-C4D-ND	3.91	129.20	124.37
2	D	601	HEM	CHA-C4D-C3D	-3.83	118.16	125.23
3	C	602	U7P	C06-C07-C09	-3.76	103.77	108.74
2	A	600	HEM	CHB-C1B-NB	3.74	128.99	124.37
2	C	601	HEM	C1B-NB-C4B	3.69	109.58	105.21
2	D	601	HEM	O2A-CGA-O1A	-3.67	113.89	123.33
2	D	601	HEM	CHB-C1B-NB	3.66	128.89	124.37
2	D	601	HEM	O2D-CGD-O1D	-3.57	114.16	123.33
3	D	602	U7P	C13-C26-C25	3.53	106.68	101.25
3	B	602	U7P	C11-C10-C09	3.47	114.68	110.52
3	D	602	U7P	C22-N21-C20	3.45	122.89	116.85
2	C	601	HEM	CHA-C4D-ND	3.44	128.62	124.37
2	A	600	HEM	CHA-C4D-ND	3.40	128.57	124.37
2	D	601	HEM	C1B-NB-C4B	3.40	109.23	105.21
3	A	601	U7P	C24-C19-C20	3.36	121.35	117.61
3	B	602	U7P	C06-C07-C01	3.34	114.50	108.74
3	C	602	U7P	C26-C13-C14	3.32	106.37	104.05
3	A	601	U7P	C22-N21-C20	3.29	122.62	116.85
2	A	600	HEM	C1B-NB-C4B	3.23	109.03	105.21
3	B	602	U7P	C15-C14-C13	-3.19	108.41	112.99
3	D	602	U7P	C15-C14-C16	-3.18	107.47	111.10
2	D	601	HEM	O2D-CGD-CBD	3.16	123.99	114.00
2	C	601	HEM	C3B-C4B-NB	-3.16	107.20	109.47
3	C	602	U7P	C15-C14-C16	-3.13	107.53	111.10
2	B	601	HEM	CHC-C4B-NB	3.11	127.77	124.42
3	B	602	U7P	C22-N21-C20	3.10	122.27	116.85
2	D	601	HEM	C1A-CHA-C4D	-3.09	118.98	126.25
3	D	602	U7P	C15-C14-C18	-3.07	102.99	107.81
2	C	601	HEM	CHB-C1B-NB	3.06	128.15	124.37
2	D	601	HEM	CAC-C3C-C2C	-3.04	118.54	128.43
3	B	602	U7P	C01-C02-C03	-3.04	118.97	123.67
2	D	601	HEM	CAB-C3B-C2B	3.03	138.28	128.43
3	B	602	U7P	C09-C10-C13	3.02	113.03	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	HEM	CAA-CBA-CGA	-2.98	105.76	113.67
3	C	602	U7P	C15-C14-C18	-2.98	103.13	107.81
3	B	602	U7P	C08-C07-C01	-2.96	103.86	108.38
3	A	601	U7P	C14-C13-C10	-2.93	110.05	113.13
2	A	600	HEM	CHD-C1D-C2D	-2.92	120.42	125.03
3	D	602	U7P	C14-C18-C25	-2.89	107.09	109.66
2	A	600	HEM	O2A-CGA-CBA	2.86	123.04	114.00
3	D	602	U7P	C01-C02-C03	-2.85	119.26	123.67
2	A	600	HEM	CBA-CAA-C2A	2.84	120.38	112.53
2	A	600	HEM	O2A-CGA-O1A	-2.84	116.04	123.33
3	C	602	U7P	C05-C03-C02	2.81	121.00	116.73
2	A	600	HEM	C3B-C4B-NB	-2.77	107.48	109.47
3	C	602	U7P	C14-C18-C25	-2.76	107.20	109.66
3	B	602	U7P	C19-C20-N21	-2.72	119.46	123.50
3	B	602	U7P	C05-C03-C02	2.69	120.81	116.73
3	B	602	U7P	C26-C13-C10	2.68	124.48	121.63
3	A	601	U7P	C06-C07-C01	2.68	113.37	108.74
3	D	602	U7P	C11-C10-C13	-2.68	107.63	112.08
2	D	601	HEM	C3B-C2B-C1B	2.68	108.42	106.41
3	C	602	U7P	C14-C13-C10	-2.63	110.36	113.13
2	D	601	HEM	CMD-C2D-C1D	2.62	129.12	125.03
3	A	601	U7P	C15-C14-C16	-2.57	108.17	111.10
2	B	601	HEM	C2A-C1A-NA	-2.57	107.30	110.15
3	B	602	U7P	C14-C18-C25	-2.56	107.38	109.66
2	B	601	HEM	C1B-NB-C4B	2.56	108.24	105.21
2	D	601	HEM	CHC-C4B-C3B	-2.54	120.00	125.07
2	B	601	HEM	C4D-ND-C1D	2.53	108.21	105.21
2	A	600	HEM	C1A-CHA-C4D	-2.53	120.30	126.25
3	A	601	U7P	C09-C07-C01	2.51	113.33	109.65
3	B	602	U7P	C17-C09-C07	-2.49	110.01	113.08
2	B	601	HEM	C3D-C4D-ND	-2.49	107.44	110.17
3	B	602	U7P	C07-C09-C10	2.46	116.31	112.71
3	C	602	U7P	C11-C12-C01	-2.46	107.42	111.93
3	D	602	U7P	C19-C20-N21	-2.46	119.85	123.50
2	D	601	HEM	CHD-C1D-C2D	-2.44	121.18	125.03
3	B	602	U7P	C16-C14-C13	2.42	112.63	108.88
2	C	601	HEM	CHA-C4D-C3D	-2.41	120.79	125.23
2	D	601	HEM	CAD-C3D-C4D	2.41	128.89	124.70
2	A	600	HEM	C4C-CHD-C1D	-2.35	121.02	126.02
2	D	601	HEM	CHA-C1A-NA	2.32	128.08	123.86
3	A	601	U7P	C07-C09-C10	-2.32	109.32	112.71
2	D	601	HEM	CHD-C4C-C3C	2.31	129.11	125.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	U7P	C05-C06-C07	2.31	117.44	113.42
2	A	600	HEM	CHA-C1A-NA	2.31	128.04	123.86
2	C	601	HEM	CHD-C1D-C2D	-2.28	121.43	125.03
2	A	600	HEM	CHA-C4D-C3D	-2.26	121.06	125.23
2	A	600	HEM	CHB-C1B-C2B	-2.26	120.54	126.95
3	D	602	U7P	C06-C07-C09	-2.25	105.76	108.74
2	A	600	HEM	CHD-C4C-NC	2.25	126.90	124.45
2	D	601	HEM	C3D-C4D-ND	2.24	112.63	110.17
3	B	602	U7P	C15-C14-C18	-2.24	104.28	107.81
2	C	601	HEM	C1A-CHA-C4D	-2.22	121.03	126.25
2	D	601	HEM	C4C-CHD-C1D	-2.21	121.31	126.02
2	C	601	HEM	O2D-CGD-O1D	-2.21	117.64	123.33
3	C	602	U7P	O04-C03-C02	-2.21	117.67	121.65
2	C	601	HEM	O2A-CGA-O1A	-2.21	117.66	123.33
2	D	601	HEM	CHC-C1C-NC	2.19	126.84	124.45
2	A	600	HEM	O2D-CGD-O1D	-2.19	117.70	123.33
3	D	602	U7P	C06-C07-C01	2.16	112.46	108.74
3	B	602	U7P	C16-C14-C18	2.13	121.76	119.30
2	C	601	HEM	CAD-C3D-C4D	2.12	128.40	124.70
2	D	601	HEM	O2A-CGA-CBA	2.12	120.70	114.00
2	B	601	HEM	C3B-C4B-NB	-2.11	107.96	109.47
3	D	602	U7P	C05-C03-C02	2.09	119.91	116.73
2	D	601	HEM	CMA-C3A-C4A	2.09	128.60	125.42
2	C	601	HEM	O2D-CGD-CBD	2.07	120.55	114.00
2	C	601	HEM	CHD-C4C-NC	2.07	126.71	124.45
2	C	601	HEM	O2A-CGA-CBA	2.06	120.52	114.00
2	C	601	HEM	CBA-CAA-C2A	2.06	118.22	112.53
2	A	600	HEM	C4A-CHB-C1B	-2.05	121.42	126.25
3	D	602	U7P	C11-C10-C09	-2.04	108.07	110.52
3	A	601	U7P	C08-C07-C09	-2.03	109.38	111.66

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	HEM	C1A-C2A-CAA-CBA
2	D	601	HEM	C3A-C2A-CAA-CBA
2	C	601	HEM	C4B-C3B-CAB-CBB
2	C	601	HEM	C4C-C3C-CAC-CBC
3	A	601	U7P	C14-C18-C19-C20
2	A	600	HEM	C4C-C3C-CAC-CBC
2	D	601	HEM	C4C-C3C-CAC-CBC

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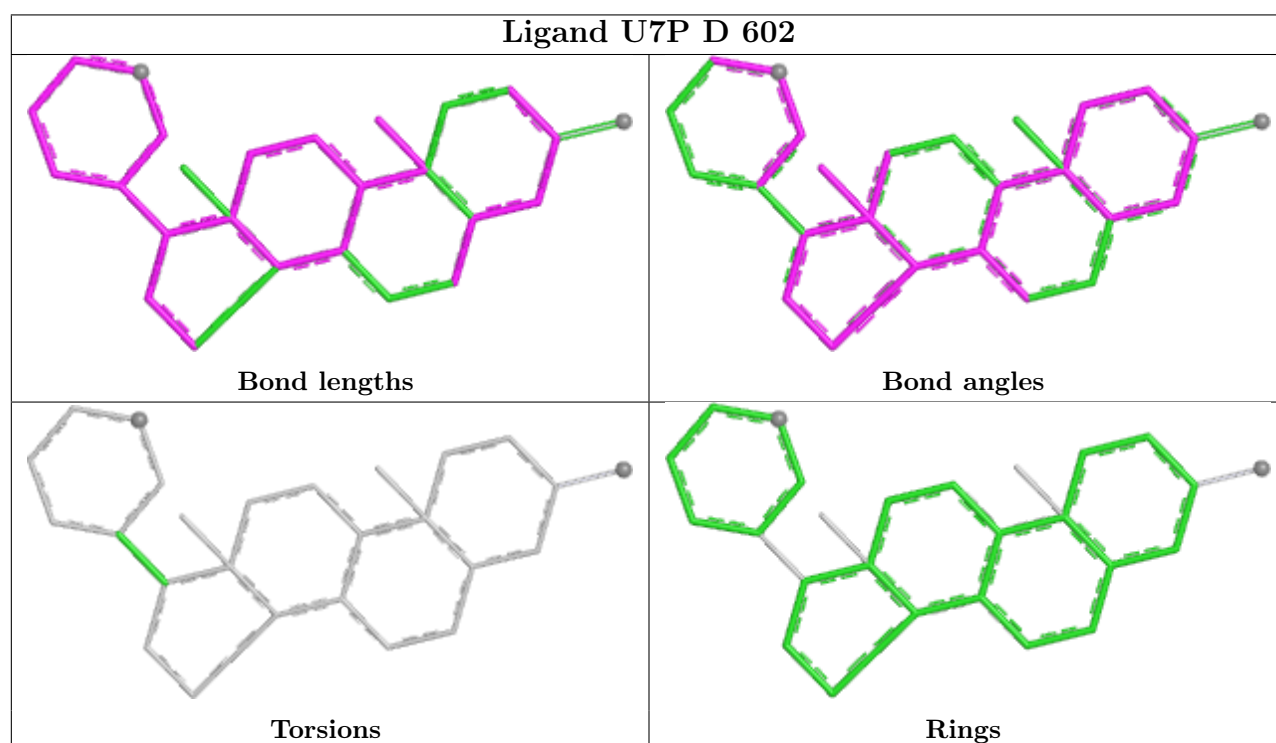
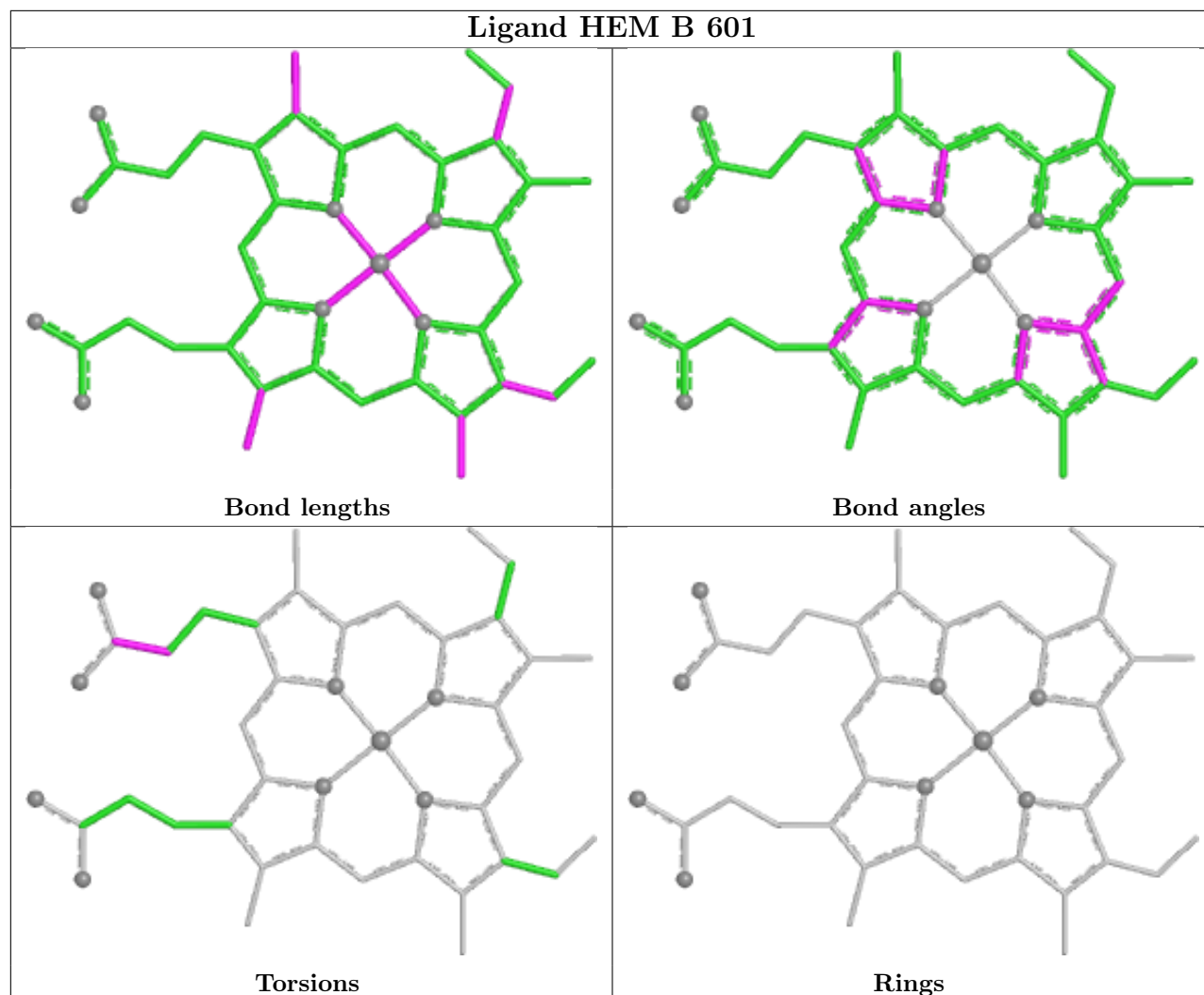
Mol	Chain	Res	Type	Atoms
3	C	602	U7P	C14-C18-C19-C20
3	A	601	U7P	C14-C18-C19-C24
3	C	602	U7P	C14-C18-C19-C24
3	B	602	U7P	C25-C18-C19-C24
2	B	601	HEM	CAD-CBD-CGD-O1D
3	B	602	U7P	C25-C18-C19-C20
2	B	601	HEM	CAD-CBD-CGD-O2D
2	C	601	HEM	CAD-CBD-CGD-O1D
2	D	601	HEM	CAD-CBD-CGD-O2D
2	D	601	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

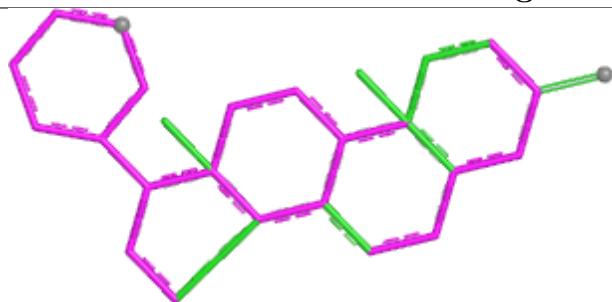
6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	HEM	6	0
3	B	602	U7P	1	0
3	A	601	U7P	1	0
2	C	601	HEM	5	0
2	A	600	HEM	8	0
2	D	601	HEM	5	0

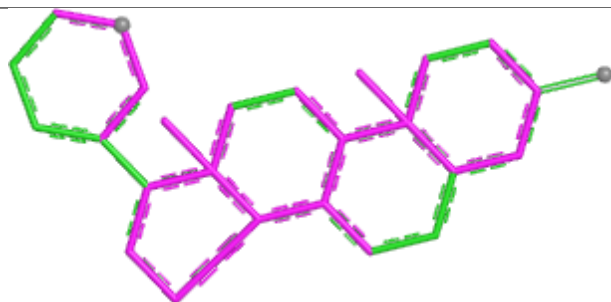
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



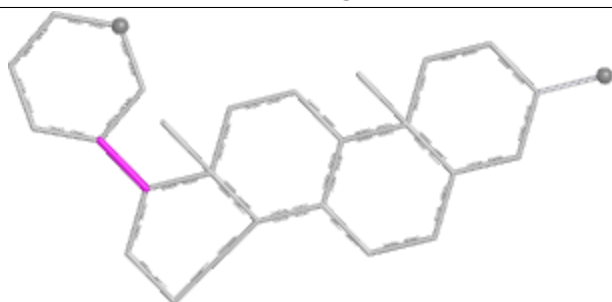
Ligand U7P B 602



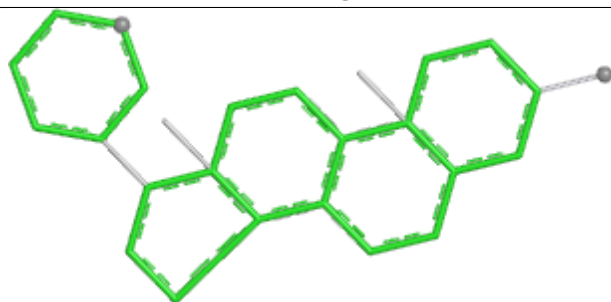
Bond lengths



Bond angles

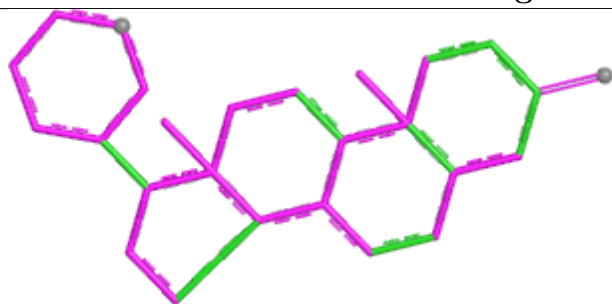


Torsions

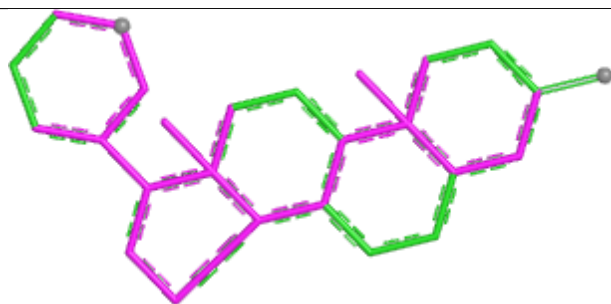


Rings

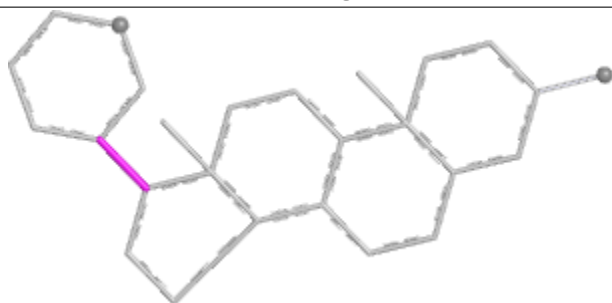
Ligand U7P A 601



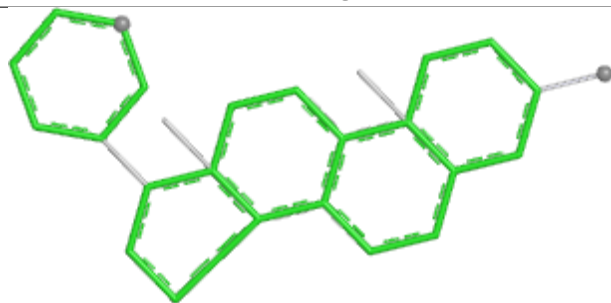
Bond lengths



Bond angles

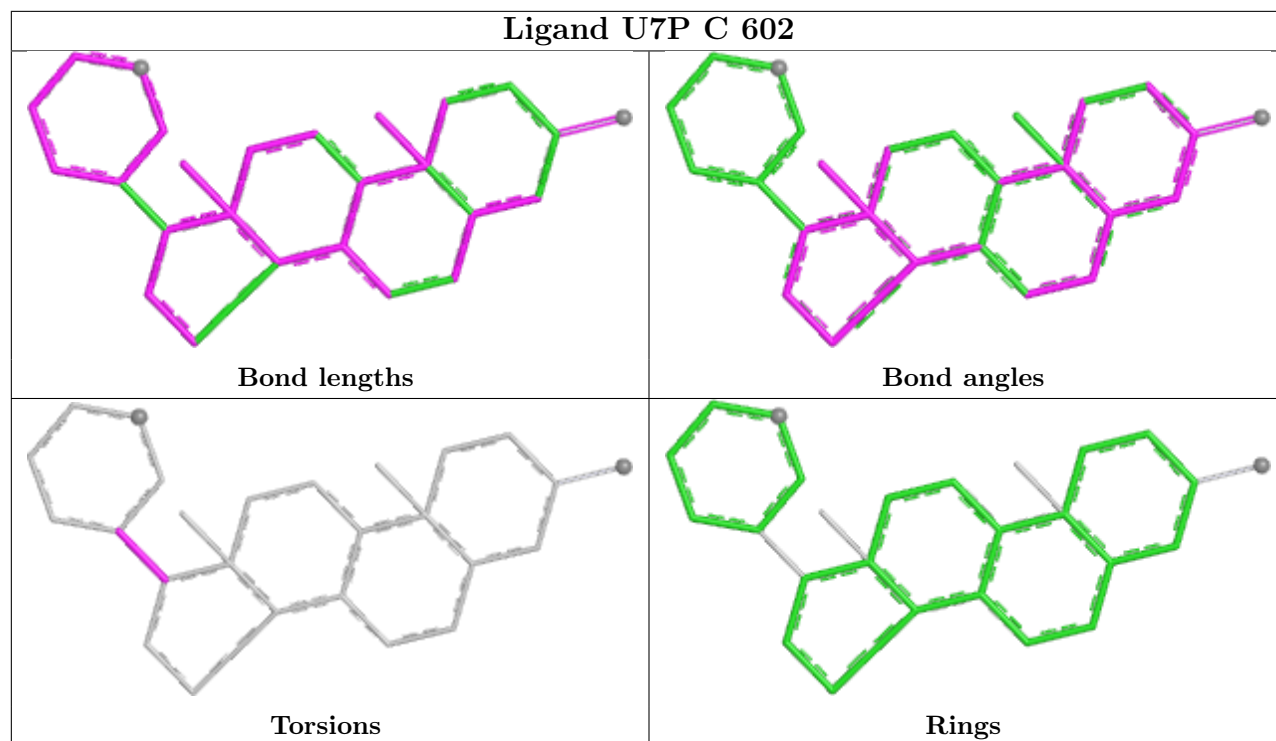


Torsions

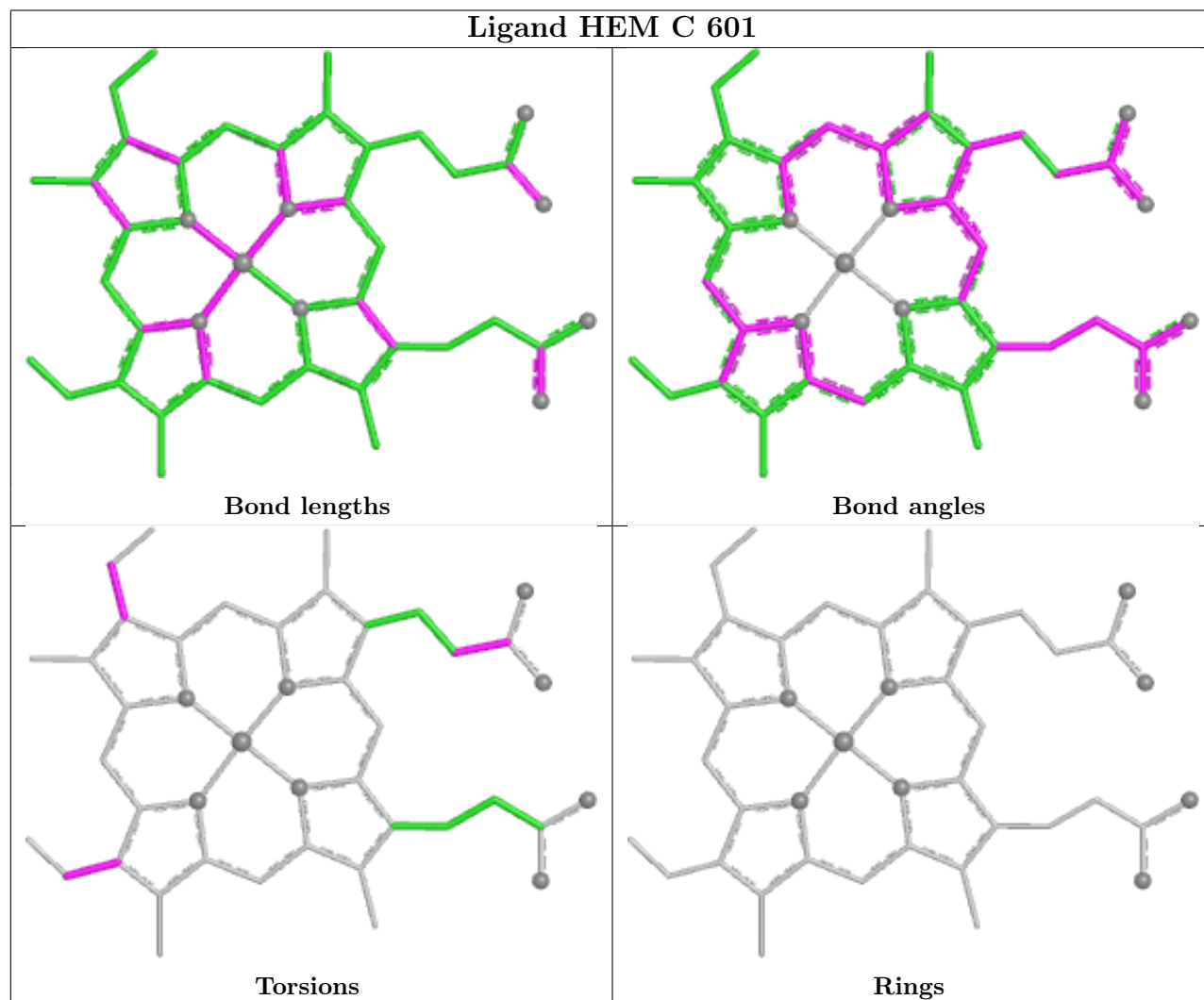


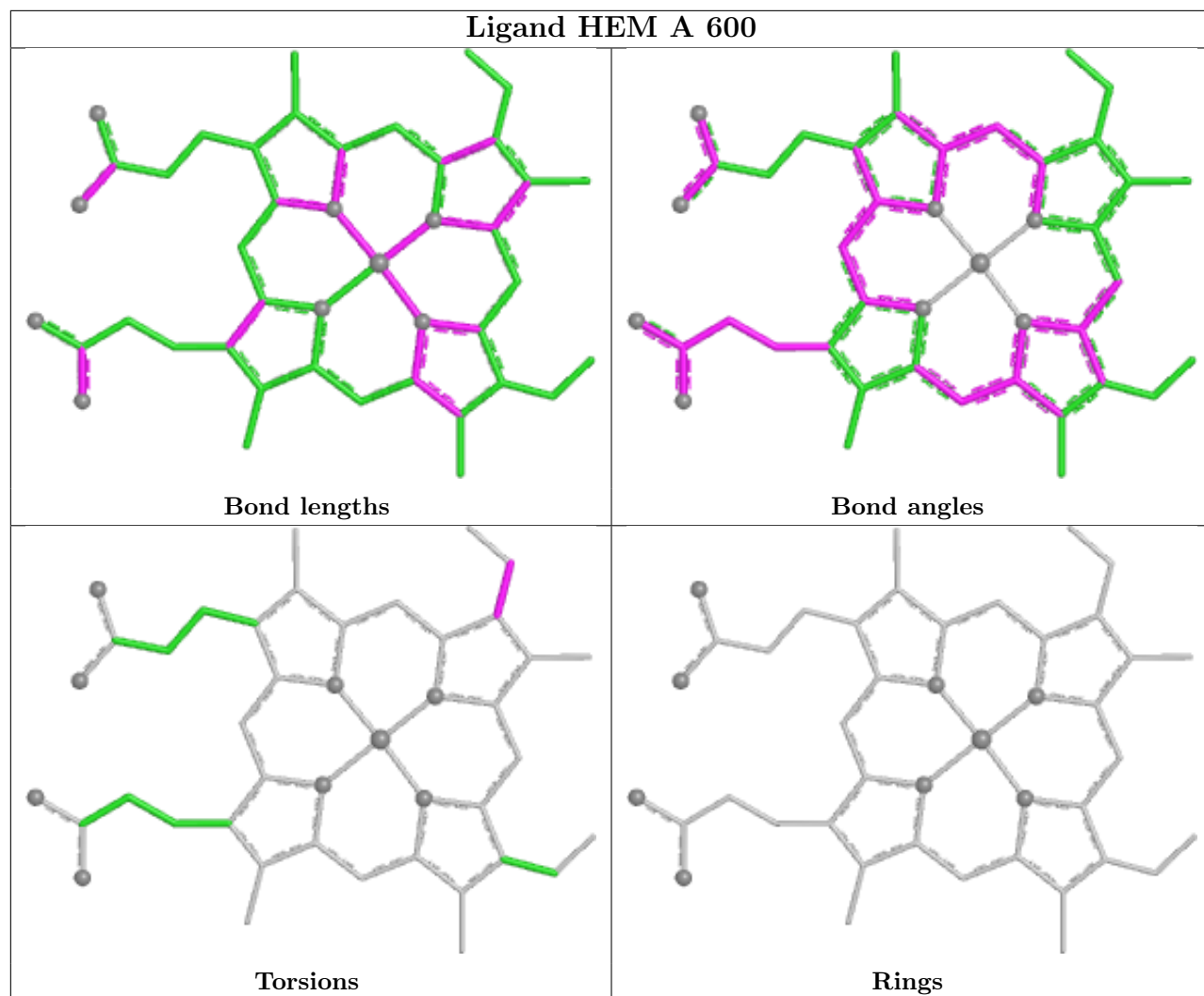
Rings

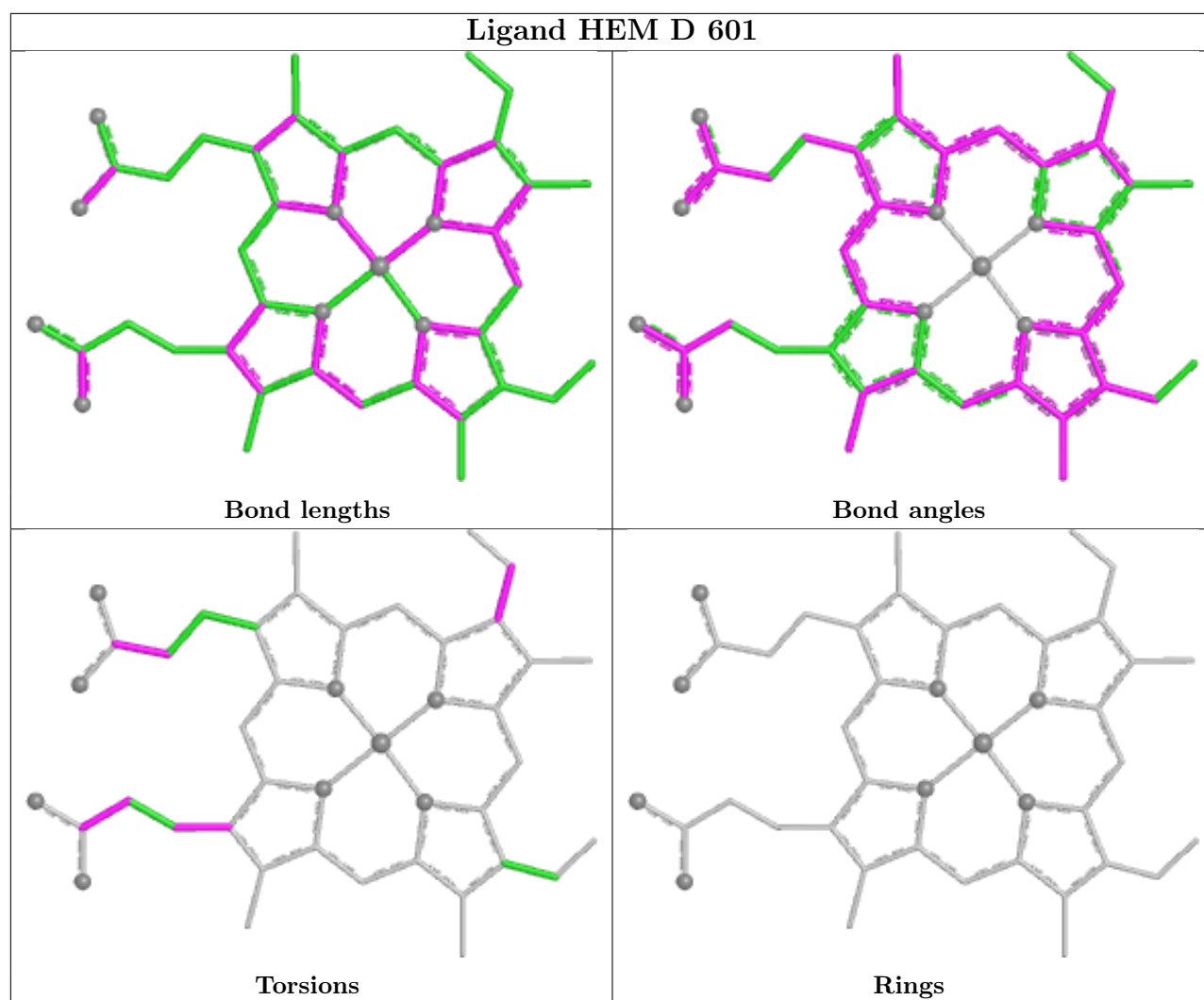
Ligand U7P C 602



Ligand HEM C 601







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	466/494 (94%)	-0.01	1 (0%) 91 90	42, 57, 85, 116	0
1	B	465/494 (94%)	-0.02	1 (0%) 91 90	41, 56, 85, 110	0
1	C	474/494 (95%)	0.05	3 (0%) 85 85	41, 58, 89, 105	0
1	D	466/494 (94%)	0.32	11 (2%) 59 56	42, 64, 103, 116	0
All	All	1871/1976 (94%)	0.09	16 (0%) 81 80	41, 58, 94, 116	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	504	ALA	4.1
1	C	46	HIS	3.0
1	C	120	HIS	2.7
1	D	337	GLY	2.6
1	B	274	ASP	2.5
1	D	460	LEU	2.5
1	D	499	TRP	2.4
1	D	274	ASP	2.4
1	D	153	LEU	2.3
1	D	503	GLN	2.2
1	D	336	VAL	2.2
1	D	491	VAL	2.2
1	D	502	ALA	2.1
1	D	120	HIS	2.1
1	C	139	ASP	2.1
1	D	428	PRO	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](#)

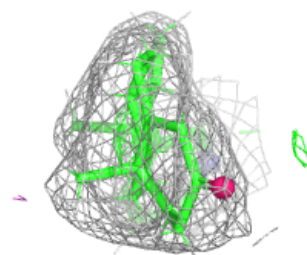
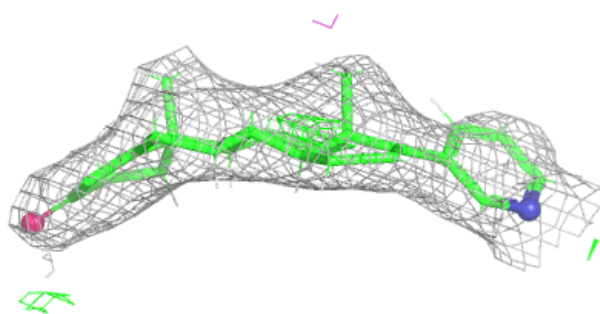
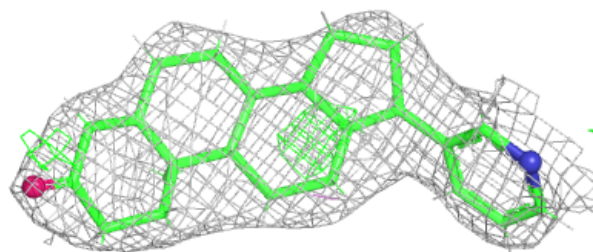
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	CL	D	603	1/1	0.90	0.09	49,49,49,49	0
4	CL	C	603	1/1	0.91	0.15	57,57,57,57	0
3	U7P	D	602	26/26	0.92	0.13	43,53,60,61	0
3	U7P	B	602	26/26	0.92	0.13	41,51,60,62	0
3	U7P	C	602	26/26	0.92	0.11	37,48,59,59	0
3	U7P	A	601	26/26	0.93	0.11	45,54,62,66	0
4	CL	B	603	1/1	0.95	0.16	60,60,60,60	0
2	HEM	D	601	43/43	0.96	0.09	43,53,64,67	0
2	HEM	A	600	43/43	0.96	0.10	42,51,62,63	0
2	HEM	B	601	43/43	0.97	0.09	39,44,54,56	0
2	HEM	C	601	43/43	0.97	0.08	35,43,52,54	0

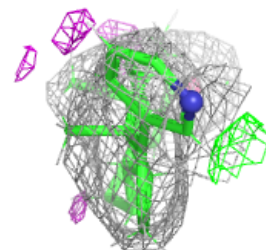
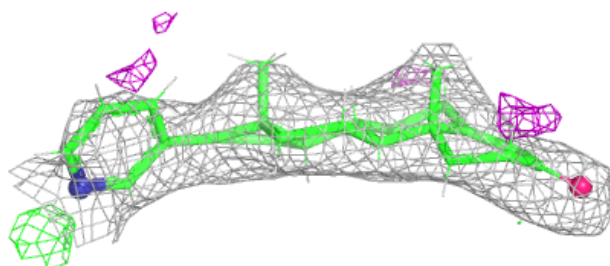
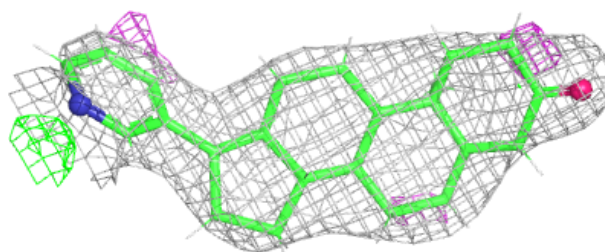
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around U7P D 602:

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

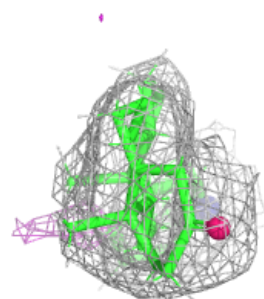
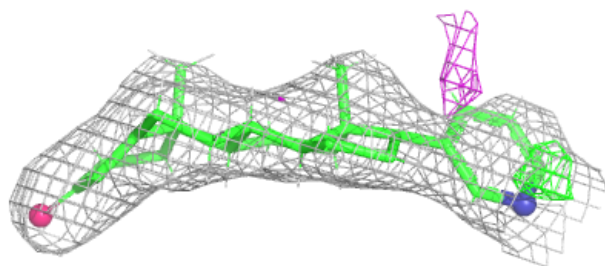
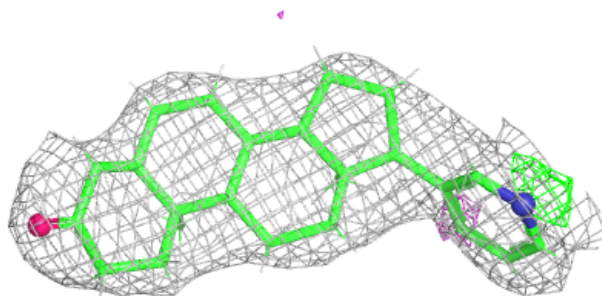
**Electron density around U7P B 602:**

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

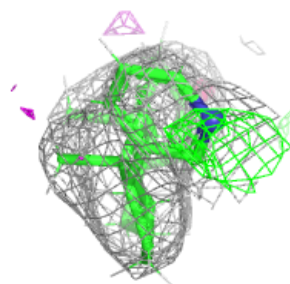
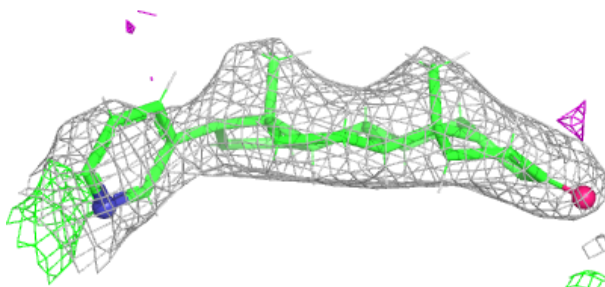
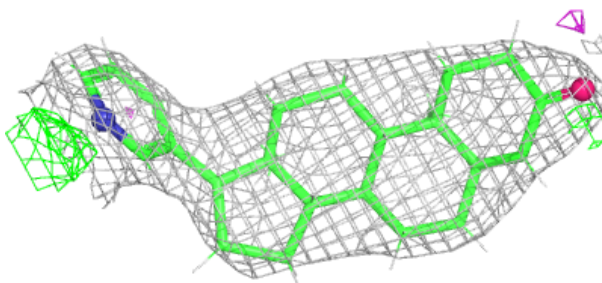


Electron density around U7P C 602:

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

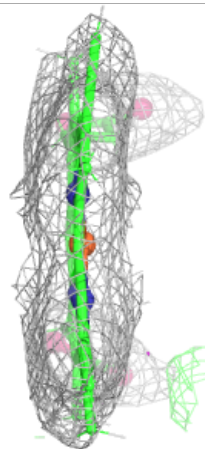
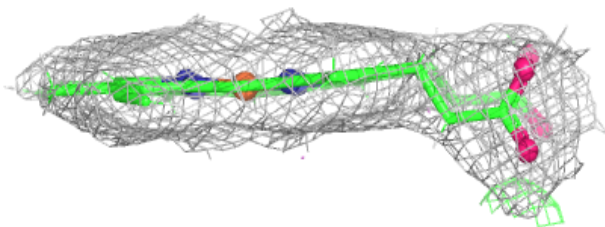
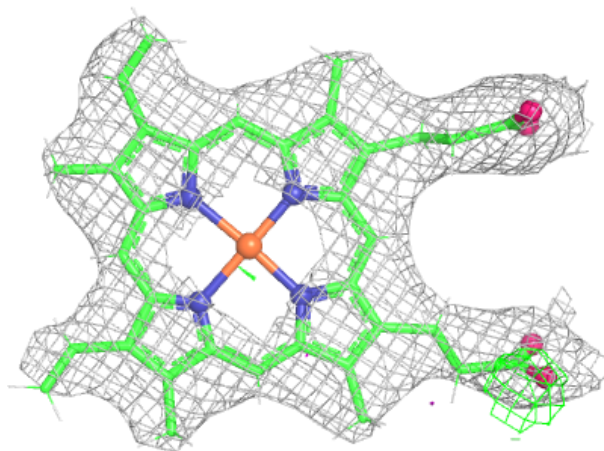
**Electron density around U7P A 601:**

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



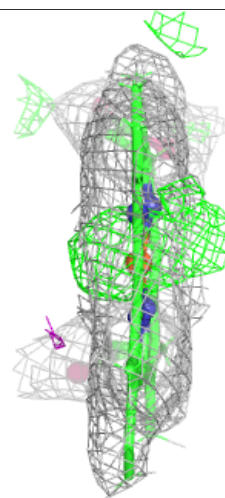
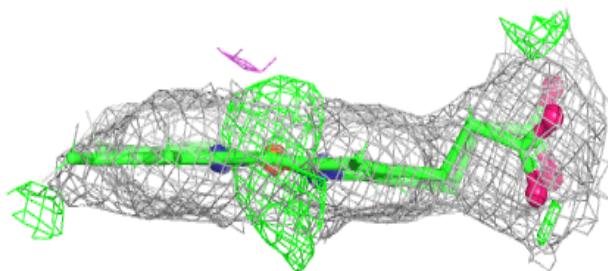
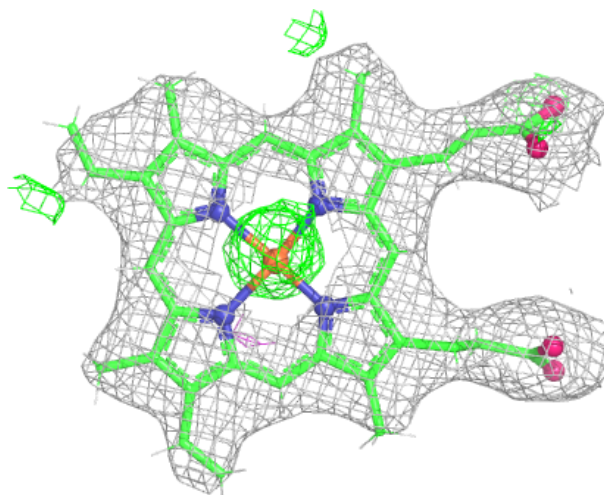
Electron density around HEM D 601:

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



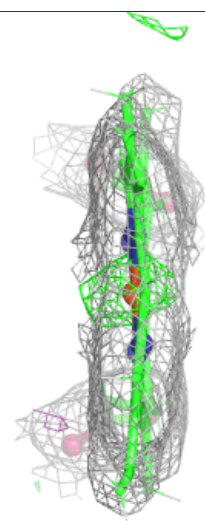
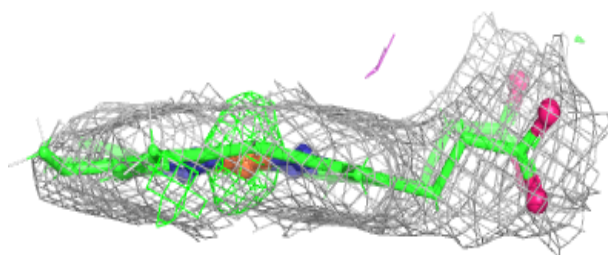
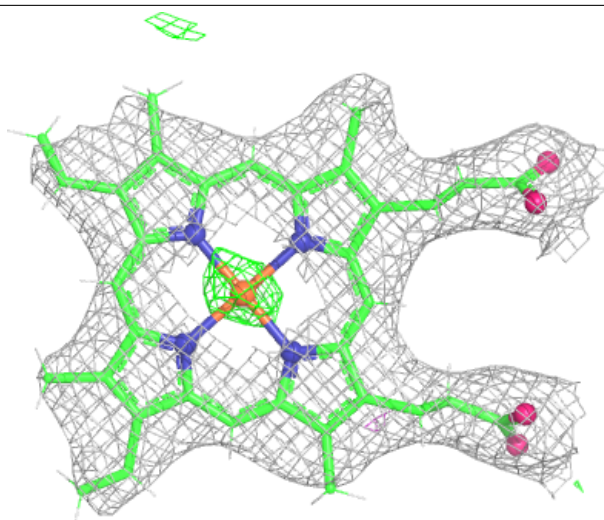
Electron density around HEM A 600:

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and green (positive)



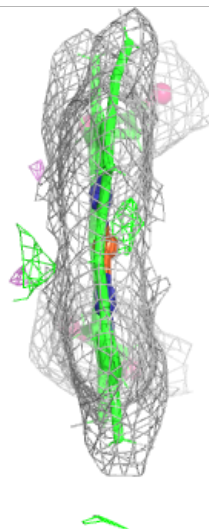
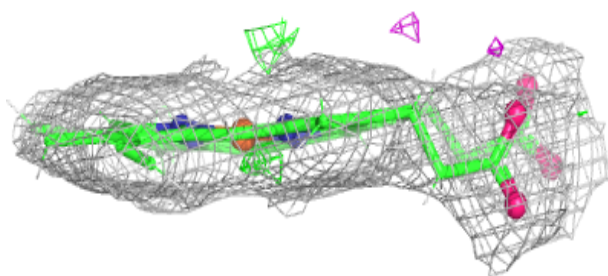
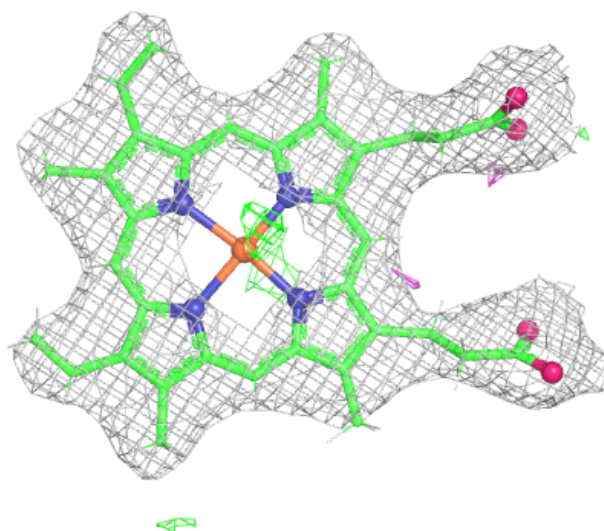
Electron density around HEM B 601:

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



Electron density around HEM C 601:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.