



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 11:26 AM UTC

PDB ID : 5UYS / pdb_00005uys
Title : Human steroidogenic cytochrome P450 17A1 with 3alphaOH-5alpha-abiraterone analog
Authors : Scott, E.E.; Petrunak, E.M.
Deposited on : 2017-02-24
Resolution : 2.39 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

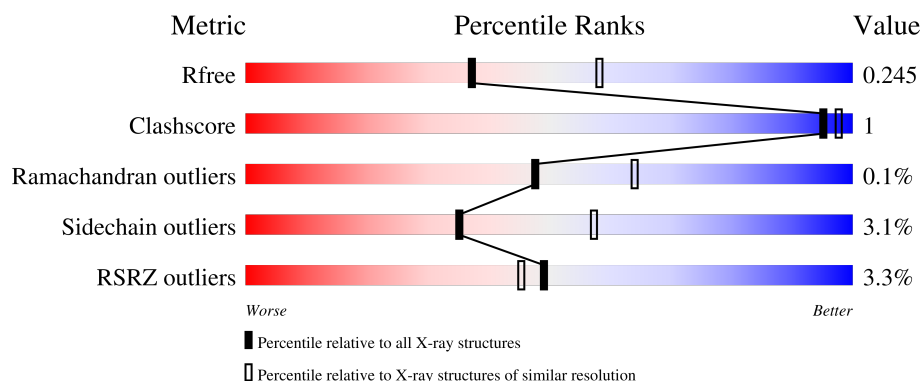
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

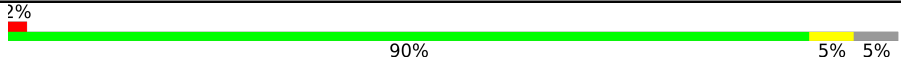
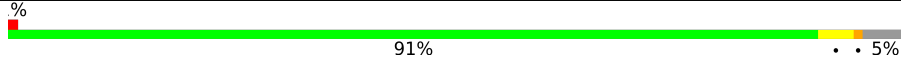
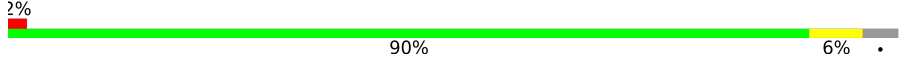
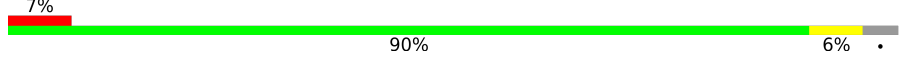
The reported resolution of this entry is 2.39 Å.

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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	 2% 90% 5% 5%
1	B	494	 % 91% . . 5%
1	C	494	 2% 90% 6% .
1	D	494	 7% 90% 6% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31206 atoms, of which 15576 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	471	Total	C	H	N	O	S	0	0	0
			7576	2403	3827	649	682	15			
1	B	470	Total	C	H	N	O	S	0	0	0
			7567	2400	3823	648	681	15			
1	C	473	Total	C	H	N	O	S	0	0	0
			7598	2409	3837	652	685	15			
1	D	473	Total	C	H	N	O	S	0	0	0
			7598	2409	3837	652	685	15			

There are 36 discrepancies between the modelled and reference sequences:

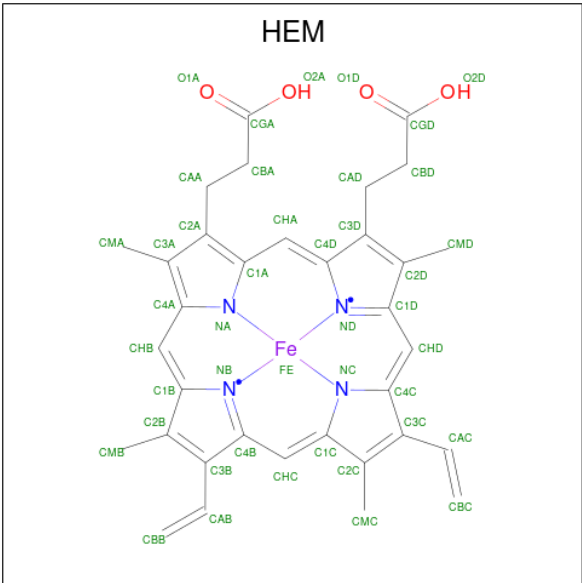
Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	initiating methionine	UNP P05093
A	20	ALA	-	expression tag	UNP P05093
A	21	LYS	-	expression tag	UNP P05093
A	22	LYS	-	expression tag	UNP P05093
A	23	THR	-	expression tag	UNP P05093
A	509	HIS	-	expression tag	UNP P05093
A	510	HIS	-	expression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

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



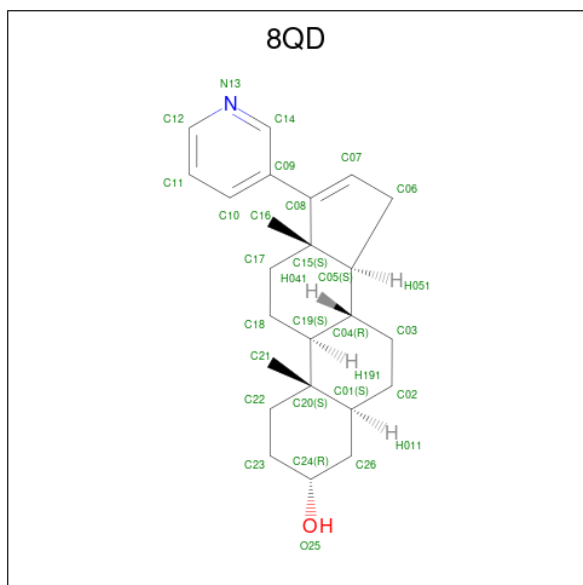
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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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 (3alpha,5alpha,8alpha)-17-(pyridin-3-yl)androst-16-en-3-ol (CCD ID: 8QD) (formula: C₂₄H₃₃NO).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O		0	0
			59	24	33	1	1			
3	B	1	Total	C	H	N	O		0	0
			59	24	33	1	1			
3	C	1	Total	C	H	N	O		0	0
			59	24	33	1	1			
3	D	1	Total	C	H	N	O		0	0
			59	24	33	1	1			

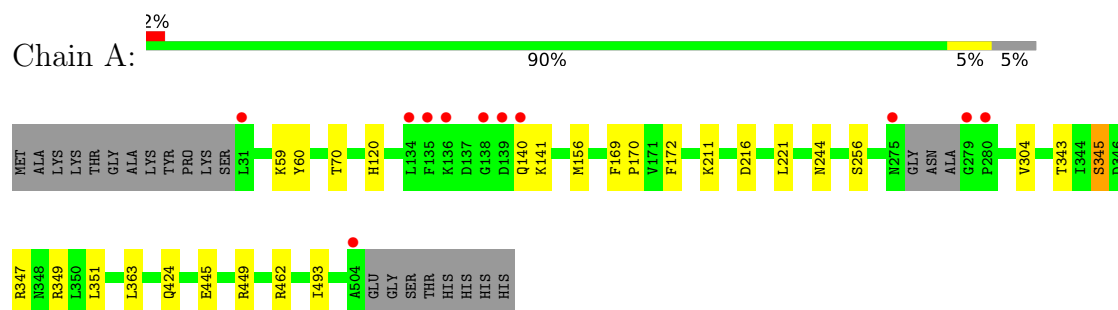
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	103	Total	O	0	0
			103	103		
4	B	93	Total	O	0	0
			93	93		
4	C	84	Total	O	0	0
			84	84		
4	D	59	Total	O	0	0
			59	59		

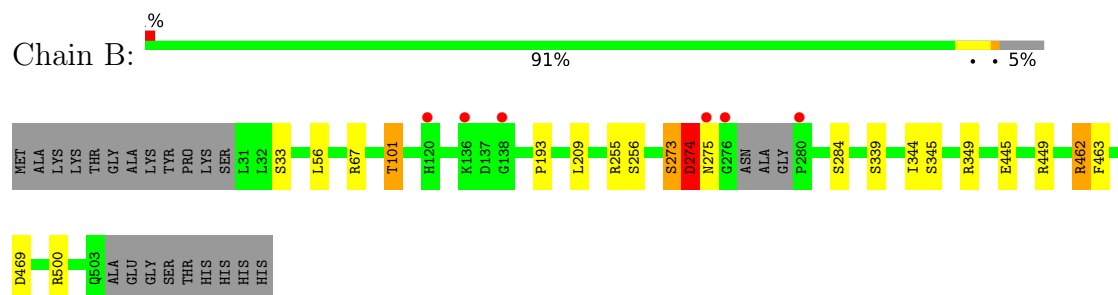
3 Residue-property plots [i](#)

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.

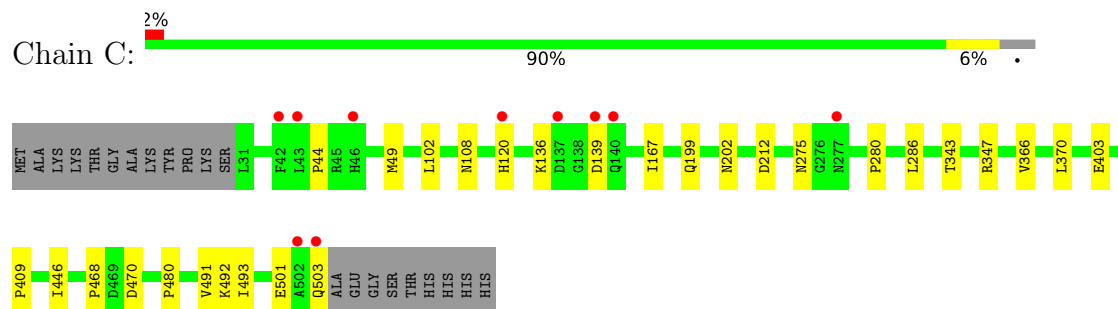
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase



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

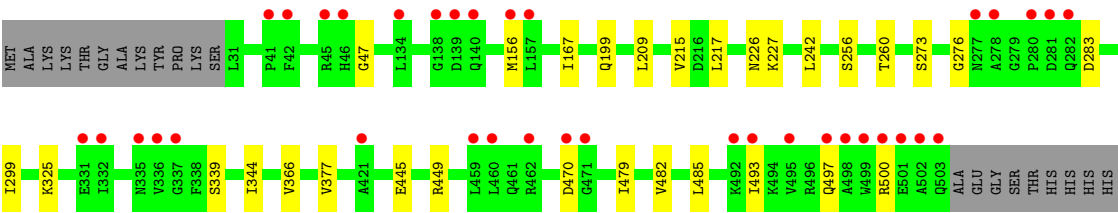


- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase



- 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	89.76Å 153.18Å 168.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.29 – 2.39 39.29 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.29-2.39) 90.2 (39.29-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.190 , 0.245 0.199 , 0.245	Depositor DCC
R_{free} test set	4613 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31206	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: 8QD, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/3830	0.75	0/5186
1	B	0.49	0/3825	0.76	2/5178 (0.0%)
1	C	0.48	0/3843	0.78	1/5205 (0.0%)
1	D	0.46	0/3843	0.78	2/5205 (0.0%)
All	All	0.48	0/15341	0.77	5/20774 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	47	GLY	N-CA-C	-8.43	98.97	111.19
1	B	274	ASP	N-CA-C	-5.99	99.90	109.96
1	D	276	GLY	N-CA-C	-5.45	107.72	115.30
1	B	275	ASN	N-CA-C	5.39	117.49	110.53
1	C	139	ASP	N-CA-C	-5.10	103.75	110.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3749	3827	3812	8	0
1	B	3744	3823	3808	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3761	3837	3822	9	0
1	D	3761	3837	3822	11	0
2	A	43	30	30	1	0
2	B	43	30	30	0	0
2	C	43	30	30	4	0
2	D	43	30	30	3	0
3	A	26	33	0	0	0
3	B	26	33	0	0	0
3	C	26	33	0	0	0
3	D	26	33	0	0	0
4	A	103	0	0	1	0
4	B	93	0	0	1	0
4	C	84	0	0	0	0
4	D	59	0	0	2	0
All	All	15630	15576	15384	37	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 1.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:GLU:OE2	1:B:449:ARG:NH2	2.25	0.69
1:A:120:HIS:ND1	4:A:701:HOH:O	2.28	0.66
1:A:445:GLU:OE2	1:A:449:ARG:NH2	2.29	0.65
2:C:600:HEM:HHC	2:C:600:HEM:HBB2	1.80	0.64
1:B:274:ASP:N	1:B:274:ASP:OD1	2.34	0.60
2:A:600:HEM:HBC2	2:A:600:HEM:HHD	1.84	0.58
2:D:600:HEM:HBC2	2:D:600:HEM:HHD	1.88	0.56
1:A:343:THR:HG22	1:A:345:SER:H	1.74	0.52
1:D:366:VAL:CG2	2:D:600:HEM:HMB2	2.39	0.52
2:C:600:HEM:HBC2	2:C:600:HEM:HHD	1.93	0.50
1:B:101:THR:HG21	1:B:209:LEU:O	2.12	0.49
1:B:273:SER:OG	1:B:284:SER:N	2.47	0.47
1:A:351:LEU:HD13	1:A:424:GLN:HA	1.96	0.47
1:B:469:ASP:N	4:B:705:HOH:O	2.47	0.47
1:C:212:ASP:HA	1:C:480:PRO:HB2	1.96	0.46
1:D:445:GLU:OE2	1:D:449:ARG:NH2	2.49	0.46
1:C:403:GLU:HG2	1:C:409:PRO:HG3	1.96	0.46
1:D:479:ILE:N	1:D:485:LEU:O	2.40	0.46
1:D:299:ILE:HG23	2:D:600:HEM:HBC1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:ARG:HG2	1:B:463:PHE:CZ	2.51	0.45
1:D:226:ASN:HB2	4:D:702:HOH:O	2.15	0.45
1:C:366:VAL:CG2	2:C:600:HEM:HMB2	2.47	0.44
1:A:59:LYS:HE3	1:A:60:TYR:CZ	2.52	0.44
1:A:172:PHE:CE1	1:A:304:VAL:HG11	2.53	0.43
1:C:370:LEU:HD22	2:C:600:HEM:HMA1	2.01	0.43
1:D:273:SER:HB3	1:D:283:ASP:HB2	2.00	0.42
1:A:156:MET:SD	1:B:193:PRO:HB3	2.59	0.42
1:A:169:PHE:HB3	1:A:170:PRO:HD3	2.01	0.42
1:D:215:VAL:HG12	1:D:217:LEU:H	1.85	0.41
1:D:227:LYS:N	4:D:702:HOH:O	2.37	0.41
1:C:468:PRO:HA	1:C:492:LYS:HB2	2.03	0.41
1:D:209:LEU:HD23	1:D:482:VAL:HG11	2.02	0.41
1:C:120:HIS:CD2	1:C:286:LEU:HD22	2.57	0.40
1:C:280:PRO:CD	1:D:377:VAL:HG12	2.51	0.40
1:C:501:GLU:C	1:C:503:GLN:H	2.30	0.40
1:D:470:ASP:OD1	1:D:470:ASP:N	2.54	0.40
1:C:167:ILE:C	1:C:167:ILE:HD12	2.46	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	467/494 (94%)	451 (97%)	16 (3%)	0	100	100
1	B	466/494 (94%)	451 (97%)	15 (3%)	0	100	100
1	C	471/494 (95%)	454 (96%)	15 (3%)	2 (0%)	30	43
1	D	471/494 (95%)	450 (96%)	21 (4%)	0	100	100
All	All	1875/1976 (95%)	1806 (96%)	67 (4%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	44	PRO
1	C	275	ASN

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	419/436 (96%)	405 (97%)	14 (3%)	33	55
1	B	419/436 (96%)	405 (97%)	14 (3%)	33	55
1	C	420/436 (96%)	408 (97%)	12 (3%)	37	60
1	D	420/436 (96%)	408 (97%)	12 (3%)	37	60
All	All	1678/1744 (96%)	1626 (97%)	52 (3%)	35	57

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	THR
1	A	140	GLN
1	A	141	LYS
1	A	211	LYS
1	A	216	ASP
1	A	221	LEU
1	A	244	ASN
1	A	256	SER
1	A	345	SER
1	A	347	ARG
1	A	349	ARG
1	A	363	LEU
1	A	462	ARG
1	A	493	ILE
1	B	33	SER
1	B	56	LEU
1	B	67	ARG
1	B	101	THR
1	B	255	ARG
1	B	256	SER

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Mol	Chain	Res	Type
1	B	273	SER
1	B	274	ASP
1	B	339	SER
1	B	344	ILE
1	B	345	SER
1	B	349	ARG
1	B	462	ARG
1	B	500	ARG
1	C	49	MET
1	C	102	LEU
1	C	108	ASN
1	C	136	LYS
1	C	199	GLN
1	C	202	ASN
1	C	343	THR
1	C	347	ARG
1	C	446	ILE
1	C	470	ASP
1	C	491	VAL
1	C	493	ILE
1	D	156	MET
1	D	167	ILE
1	D	199	GLN
1	D	242	LEU
1	D	256	SER
1	D	260	THR
1	D	325	LYS
1	D	339	SER
1	D	344	ILE
1	D	493	ILE
1	D	497	GLN
1	D	500	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	79	HIS
1	A	199	GLN
1	A	401	HIS
1	A	411	GLN
1	B	108	ASN

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Mol	Chain	Res	Type
1	B	120	HIS
1	B	334	GLN
1	B	376	ASN
1	C	50	HIS
1	C	57	GLN
1	C	108	ASN
1	C	140	GLN
1	C	160	HIS
1	C	268	GLN
1	D	50	HIS
1	D	57	GLN
1	D	407	HIS

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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	B	600	3,1	50,50,50	1.77	7 (14%)	67,82,82	1.23	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	600	3,1	50,50,50	1.81	10 (20%)	67,82,82	1.27	8 (11%)
2	HEM	C	600	3,1	50,50,50	1.80	9 (18%)	67,82,82	1.52	13 (19%)
3	8QD	D	601	2	30,30,30	6.54	20 (66%)	47,47,47	2.92	19 (40%)
3	8QD	A	601	2	30,30,30	6.58	21 (70%)	47,47,47	2.94	16 (34%)
2	HEM	D	600	3,1	50,50,50	1.92	9 (18%)	67,82,82	1.40	10 (14%)
3	8QD	C	601	2	30,30,30	6.37	20 (66%)	47,47,47	2.91	14 (29%)
3	8QD	B	601	2	30,30,30	6.43	21 (70%)	47,47,47	2.92	16 (34%)

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	600	3,1	-	2/14/54/54	-
2	HEM	A	600	3,1	-	1/14/54/54	-
2	HEM	C	600	3,1	-	4/14/54/54	-
3	8QD	D	601	2	-	0/4/62/62	0/5/5/5
3	8QD	A	601	2	-	0/4/62/62	0/5/5/5
2	HEM	D	600	3,1	-	2/14/54/54	-
3	8QD	C	601	2	-	0/4/62/62	0/5/5/5
3	8QD	B	601	2	-	0/4/62/62	0/5/5/5

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	8QD	C07-C08	19.09	1.66	1.33
3	D	601	8QD	C07-C08	19.00	1.65	1.33
3	B	601	8QD	C07-C08	18.57	1.65	1.33
3	C	601	8QD	C07-C08	18.49	1.65	1.33
3	A	601	8QD	C15-C08	-16.24	1.39	1.53
3	D	601	8QD	C06-C07	16.07	1.74	1.50
3	D	601	8QD	C15-C08	-16.05	1.39	1.53
3	A	601	8QD	C06-C07	15.74	1.73	1.50
3	B	601	8QD	C06-C07	15.72	1.73	1.50
3	B	601	8QD	C15-C08	-15.64	1.39	1.53
3	C	601	8QD	C15-C08	-15.30	1.40	1.53
3	C	601	8QD	C06-C07	14.93	1.72	1.50
3	A	601	8QD	C06-C05	-8.87	1.41	1.54
3	B	601	8QD	C06-C05	-8.79	1.41	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	8QD	C06-C05	-8.67	1.42	1.54
3	D	601	8QD	C06-C05	-8.40	1.42	1.54
2	B	600	HEM	C3D-C2D	7.68	1.53	1.36
2	D	600	HEM	C3D-C2D	7.63	1.53	1.36
2	A	600	HEM	C3D-C2D	7.60	1.53	1.36
3	D	601	8QD	C14-C09	7.58	1.51	1.39
3	C	601	8QD	C14-C09	7.42	1.50	1.39
3	A	601	8QD	C14-C09	7.38	1.50	1.39
3	B	601	8QD	C14-C09	7.21	1.50	1.39
2	C	600	HEM	C3D-C2D	7.19	1.52	1.36
3	C	601	8QD	C17-C18	6.60	1.66	1.53
3	A	601	8QD	C17-C18	6.24	1.65	1.53
3	B	601	8QD	C17-C18	6.10	1.65	1.53
3	D	601	8QD	C14-N13	6.05	1.47	1.34
3	C	601	8QD	C14-N13	5.93	1.46	1.34
3	A	601	8QD	C14-N13	5.90	1.46	1.34
3	D	601	8QD	C17-C18	5.88	1.65	1.53
3	D	601	8QD	C10-C09	5.57	1.47	1.39
2	D	600	HEM	FE-NC	5.52	2.13	1.95
3	A	601	8QD	C10-C09	5.43	1.47	1.39
3	B	601	8QD	C14-N13	5.31	1.45	1.34
3	C	601	8QD	C10-C09	5.29	1.47	1.39
3	B	601	8QD	C10-C09	5.26	1.47	1.39
3	C	601	8QD	C04-C19	5.13	1.63	1.53
3	D	601	8QD	C04-C19	5.13	1.63	1.53
3	B	601	8QD	C04-C19	5.11	1.63	1.53
3	A	601	8QD	C04-C19	4.99	1.63	1.53
3	A	601	8QD	C11-C10	4.80	1.47	1.38
3	A	601	8QD	C11-C12	4.80	1.51	1.37
3	D	601	8QD	C11-C12	4.78	1.51	1.37
3	C	601	8QD	C11-C12	4.75	1.51	1.37
3	C	601	8QD	C11-C10	4.73	1.47	1.38
3	B	601	8QD	C12-N13	4.72	1.47	1.33
3	D	601	8QD	C11-C10	4.72	1.47	1.38
3	B	601	8QD	C11-C10	4.67	1.46	1.38
3	A	601	8QD	C15-C05	4.60	1.63	1.54
3	D	601	8QD	C12-N13	4.56	1.46	1.33
3	B	601	8QD	C11-C12	4.45	1.50	1.37
2	D	600	HEM	FE-ND	4.42	2.08	1.94
3	A	601	8QD	C12-N13	4.42	1.46	1.33
3	B	601	8QD	C15-C05	4.41	1.62	1.54
3	C	601	8QD	C12-N13	4.39	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	8QD	C26-C24	4.21	1.59	1.52
3	D	601	8QD	C15-C05	4.12	1.62	1.54
2	B	600	HEM	FE-ND	4.02	2.07	1.94
3	C	601	8QD	C15-C05	3.95	1.62	1.54
3	B	601	8QD	C26-C24	3.82	1.58	1.52
2	A	600	HEM	FE-NC	3.75	2.07	1.95
3	A	601	8QD	C26-C24	3.73	1.58	1.52
2	C	600	HEM	FE-ND	3.71	2.06	1.94
2	C	600	HEM	FE-NB	3.68	2.06	1.94
3	D	601	8QD	C26-C24	3.48	1.58	1.52
3	A	601	8QD	C09-C08	3.47	1.53	1.48
2	C	600	HEM	FE-NC	3.42	2.06	1.95
3	C	601	8QD	C09-C08	3.41	1.53	1.48
2	B	600	HEM	FE-NA	3.38	2.06	1.95
3	B	601	8QD	C03-C02	3.32	1.60	1.52
3	A	601	8QD	C03-C02	3.31	1.60	1.52
2	D	600	HEM	CAB-C3B	3.29	1.56	1.47
3	C	601	8QD	C03-C02	3.27	1.60	1.52
3	C	601	8QD	C20-C01	3.26	1.60	1.55
3	D	601	8QD	C09-C08	3.25	1.53	1.48
2	A	600	HEM	FE-NB	3.21	2.04	1.94
2	B	600	HEM	CAB-C3B	3.20	1.55	1.47
2	A	600	HEM	FE-ND	3.20	2.04	1.94
2	C	600	HEM	CAB-C3B	3.15	1.55	1.47
2	C	600	HEM	CAC-C3C	3.11	1.55	1.47
2	B	600	HEM	FE-NC	3.09	2.05	1.95
3	D	601	8QD	C03-C02	3.08	1.60	1.52
3	B	601	8QD	C20-C01	3.08	1.60	1.55
2	A	600	HEM	CAC-C3C	3.06	1.55	1.47
2	A	600	HEM	CAB-C3B	2.99	1.55	1.47
3	A	601	8QD	C20-C01	2.98	1.60	1.55
3	D	601	8QD	C20-C01	2.96	1.60	1.55
2	D	600	HEM	CAC-C3C	2.89	1.55	1.47
2	B	600	HEM	CAC-C3C	2.87	1.55	1.47
3	B	601	8QD	C22-C23	2.85	1.59	1.53
3	B	601	8QD	C09-C08	2.84	1.52	1.48
2	C	600	HEM	FE-NA	2.82	2.04	1.95
3	A	601	8QD	O25-C24	-2.64	1.35	1.43
2	D	600	HEM	FE-NA	2.46	2.03	1.95
3	D	601	8QD	C22-C23	2.43	1.58	1.53
2	B	600	HEM	CMC-C2C	2.36	1.55	1.50
2	D	600	HEM	CMC-C2C	2.31	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	HEM	CMB-C2B	2.31	1.55	1.50
3	A	601	8QD	C18-C19	2.30	1.57	1.53
3	A	601	8QD	C20-C19	-2.29	1.52	1.56
3	D	601	8QD	O25-C24	-2.27	1.36	1.43
3	C	601	8QD	O25-C24	-2.24	1.36	1.43
3	B	601	8QD	O25-C24	-2.21	1.36	1.43
2	D	600	HEM	CMA-C3A	2.19	1.55	1.50
3	A	601	8QD	C22-C23	2.18	1.57	1.53
3	D	601	8QD	C18-C19	2.15	1.57	1.53
3	C	601	8QD	C22-C23	2.14	1.57	1.53
2	A	600	HEM	FE-NA	2.14	2.02	1.95
3	C	601	8QD	C20-C19	-2.13	1.52	1.56
3	B	601	8QD	C23-C24	2.13	1.56	1.51
2	D	600	HEM	CMB-C2B	2.09	1.55	1.50
2	A	600	HEM	CMB-C2B	2.08	1.55	1.50
2	A	600	HEM	CMC-C2C	2.08	1.55	1.50
3	B	601	8QD	C18-C19	2.07	1.57	1.53
2	A	600	HEM	C2A-C3A	-2.07	1.33	1.38
2	C	600	HEM	O2D-CGD	-2.03	1.24	1.30

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	8QD	C06-C07-C08	-10.81	103.17	112.56
3	D	601	8QD	C06-C07-C08	-10.49	103.46	112.56
3	A	601	8QD	C06-C07-C08	-10.42	103.52	112.56
3	C	601	8QD	C06-C07-C08	-9.74	104.11	112.56
3	D	601	8QD	C05-C15-C08	9.26	107.34	99.50
3	C	601	8QD	C05-C15-C08	8.31	106.54	99.50
3	A	601	8QD	C05-C15-C08	8.17	106.42	99.50
3	B	601	8QD	C05-C15-C08	7.83	106.13	99.50
3	C	601	8QD	C06-C05-C15	6.50	108.60	104.05
3	C	601	8QD	C06-C05-C04	-5.93	115.35	121.63
3	D	601	8QD	C06-C05-C15	5.72	108.05	104.05
3	A	601	8QD	C06-C05-C15	5.48	107.88	104.05
3	A	601	8QD	C06-C05-C04	-5.33	115.98	121.63
3	B	601	8QD	C06-C05-C15	5.11	107.62	104.05
3	B	601	8QD	C06-C05-C04	-5.08	116.24	121.63
2	A	600	HEM	C4D-ND-C1D	5.03	111.17	105.21
3	B	601	8QD	C22-C23-C24	4.98	117.08	110.48
2	D	600	HEM	C4D-ND-C1D	4.86	110.96	105.21
2	C	600	HEM	C4D-ND-C1D	4.71	110.78	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	8QD	C03-C04-C19	4.55	115.97	110.52
3	B	601	8QD	C09-C14-N13	-4.55	116.74	123.50
2	B	600	HEM	C4D-ND-C1D	4.44	110.46	105.21
3	A	601	8QD	C22-C20-C01	4.39	114.04	107.75
3	A	601	8QD	C15-C08-C07	-4.38	105.77	109.66
3	C	601	8QD	C15-C08-C07	-4.38	105.77	109.66
3	D	601	8QD	C15-C08-C07	-4.31	105.83	109.66
3	A	601	8QD	C09-C14-N13	-4.05	117.47	123.50
2	C	600	HEM	CHC-C1C-NC	3.87	128.66	124.45
3	B	601	8QD	C15-C08-C07	-3.84	106.25	109.66
3	A	601	8QD	C22-C23-C24	3.82	115.54	110.48
3	D	601	8QD	C06-C05-C04	-3.79	117.61	121.63
3	D	601	8QD	C09-C14-N13	-3.78	117.88	123.50
3	C	601	8QD	C09-C14-N13	-3.75	117.92	123.50
3	C	601	8QD	C22-C20-C01	3.72	113.08	107.75
3	B	601	8QD	C12-N13-C14	3.61	123.18	116.85
3	C	601	8QD	C16-C15-C17	-3.60	106.99	111.10
3	B	601	8QD	C10-C09-C14	3.57	121.59	117.61
3	A	601	8QD	C12-N13-C14	3.51	123.00	116.85
3	A	601	8QD	C17-C15-C08	-3.50	115.24	119.30
3	D	601	8QD	C17-C15-C08	-3.43	115.33	119.30
3	A	601	8QD	C03-C04-C19	3.36	114.55	110.52
3	D	601	8QD	C22-C20-C01	3.23	112.39	107.75
3	B	601	8QD	C21-C20-C19	-3.16	106.93	111.18
3	B	601	8QD	C01-C26-C24	-3.13	107.99	112.71
3	A	601	8QD	C01-C26-C24	-3.08	108.07	112.71
3	D	601	8QD	C09-C08-C07	3.07	129.04	125.08
3	C	601	8QD	C12-N13-C14	3.07	122.23	116.85
3	D	601	8QD	C12-N13-C14	3.01	122.13	116.85
2	D	600	HEM	CHD-C1D-ND	2.97	127.61	124.42
2	C	600	HEM	CAC-C3C-C4C	2.92	131.79	124.82
3	D	601	8QD	C01-C26-C24	-2.92	108.30	112.71
3	D	601	8QD	C10-C09-C14	2.88	120.82	117.61
2	D	600	HEM	CHD-C4C-C3C	2.79	129.91	125.21
3	A	601	8QD	C10-C09-C14	2.75	120.68	117.61
3	C	601	8QD	C10-C09-C14	2.71	120.63	117.61
2	C	600	HEM	C3C-C2C-C1C	2.70	109.60	107.05
3	A	601	8QD	C16-C15-C17	-2.69	108.02	111.10
3	B	601	8QD	C23-C22-C20	2.65	117.21	112.74
3	D	601	8QD	C03-C04-C19	2.65	113.69	110.52
3	B	601	8QD	C17-C15-C08	-2.62	116.27	119.30
3	C	601	8QD	C15-C05-C04	-2.56	110.43	113.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	HEM	CHA-C4D-ND	2.56	127.53	124.37
2	B	600	HEM	O2A-CGA-CBA	2.55	122.06	114.00
2	D	600	HEM	CAC-C3C-C4C	2.52	130.83	124.82
2	A	600	HEM	CAC-C3C-C4C	2.49	130.76	124.82
2	D	600	HEM	CHC-C4B-NB	2.48	127.09	124.42
2	C	600	HEM	CMD-C2D-C1D	2.47	128.90	125.03
2	C	600	HEM	CHD-C4C-C3C	2.45	129.35	125.21
3	B	601	8QD	C22-C20-C01	2.44	111.25	107.75
3	B	601	8QD	C16-C15-C17	-2.42	108.33	111.10
2	C	600	HEM	CAA-CBA-CGA	-2.42	107.25	113.67
3	C	601	8QD	C01-C26-C24	-2.42	109.06	112.71
3	D	601	8QD	C16-C15-C17	-2.39	108.37	111.10
2	B	600	HEM	CHC-C4B-NB	2.37	126.97	124.42
2	B	600	HEM	O1A-CGA-CBA	-2.36	115.62	123.09
3	C	601	8QD	C16-C15-C08	-2.33	104.14	107.81
3	A	601	8QD	C21-C20-C19	-2.33	108.05	111.18
3	B	601	8QD	C16-C15-C08	-2.32	104.17	107.81
2	B	600	HEM	CAA-CBA-CGA	-2.31	107.53	113.67
2	C	600	HEM	O2A-CGA-CBA	2.25	121.10	114.00
2	D	600	HEM	CHC-C1C-NC	2.23	126.88	124.45
2	C	600	HEM	C3B-C2B-C1B	2.21	108.07	106.41
2	A	600	HEM	CHD-C4C-C3C	2.18	128.88	125.21
2	A	600	HEM	CMD-C2D-C1D	2.15	128.40	125.03
2	D	600	HEM	CHD-C4C-NC	-2.14	122.12	124.45
2	C	600	HEM	CAC-C3C-C2C	-2.14	121.46	128.43
2	D	600	HEM	C2A-C1A-NA	-2.14	107.78	110.15
2	A	600	HEM	CHC-C4B-NB	2.13	126.72	124.42
3	D	601	8QD	C15-C05-C04	-2.13	110.89	113.13
3	D	601	8QD	C16-C15-C05	-2.13	109.93	112.99
3	D	601	8QD	C21-C20-C19	-2.13	108.32	111.18
2	B	600	HEM	CMD-C2D-C1D	2.11	128.34	125.03
2	C	600	HEM	O1A-CGA-CBA	-2.11	116.39	123.09
2	A	600	HEM	CAA-CBA-CGA	-2.10	108.09	113.67
3	D	601	8QD	C03-C02-C01	-2.10	107.77	111.84
2	A	600	HEM	CAC-C3C-C2C	-2.08	121.67	128.43
2	D	600	HEM	CAC-C3C-C2C	-2.06	121.73	128.43
3	A	601	8QD	C05-C06-C07	-2.05	98.10	101.25
3	D	601	8QD	C10-C09-C08	-2.05	117.67	121.04
2	A	600	HEM	CAD-C3D-C4D	2.04	128.25	124.70
2	D	600	HEM	O2A-CGA-CBA	2.03	120.42	114.00
2	C	600	HEM	CAD-CBD-CGD	-2.01	108.35	113.67

There are no chirality outliers.

All (9) torsion outliers are listed below:

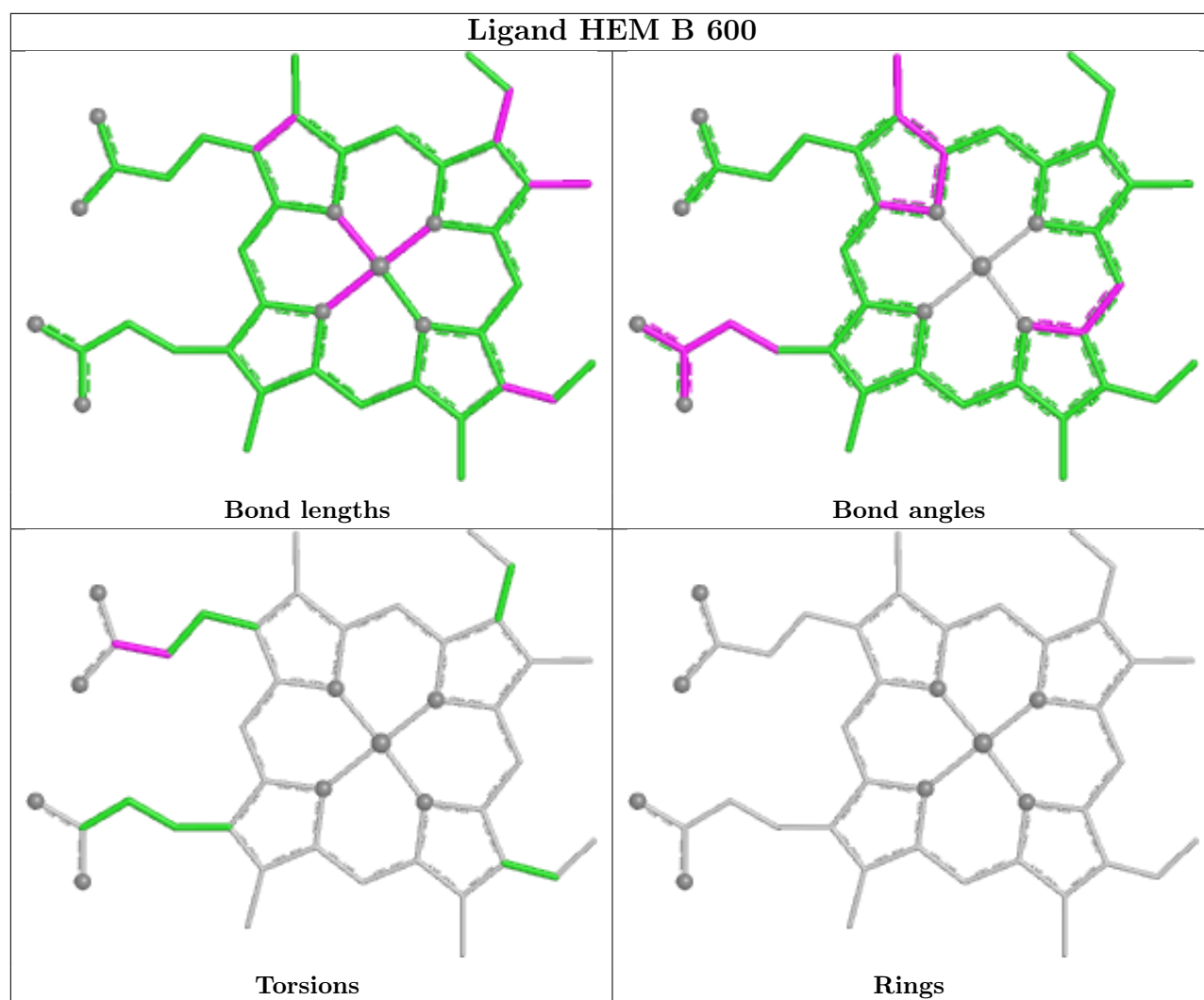
Mol	Chain	Res	Type	Atoms
2	A	600	HEM	C4C-C3C-CAC-CBC
2	C	600	HEM	C4B-C3B-CAB-CBB
2	C	600	HEM	C4C-C3C-CAC-CBC
2	D	600	HEM	C4C-C3C-CAC-CBC
2	C	600	HEM	CAA-CBA-CGA-O2A
2	B	600	HEM	CAD-CBD-CGD-O1D
2	C	600	HEM	CAA-CBA-CGA-O1A
2	B	600	HEM	CAD-CBD-CGD-O2D
2	D	600	HEM	CAA-CBA-CGA-O2A

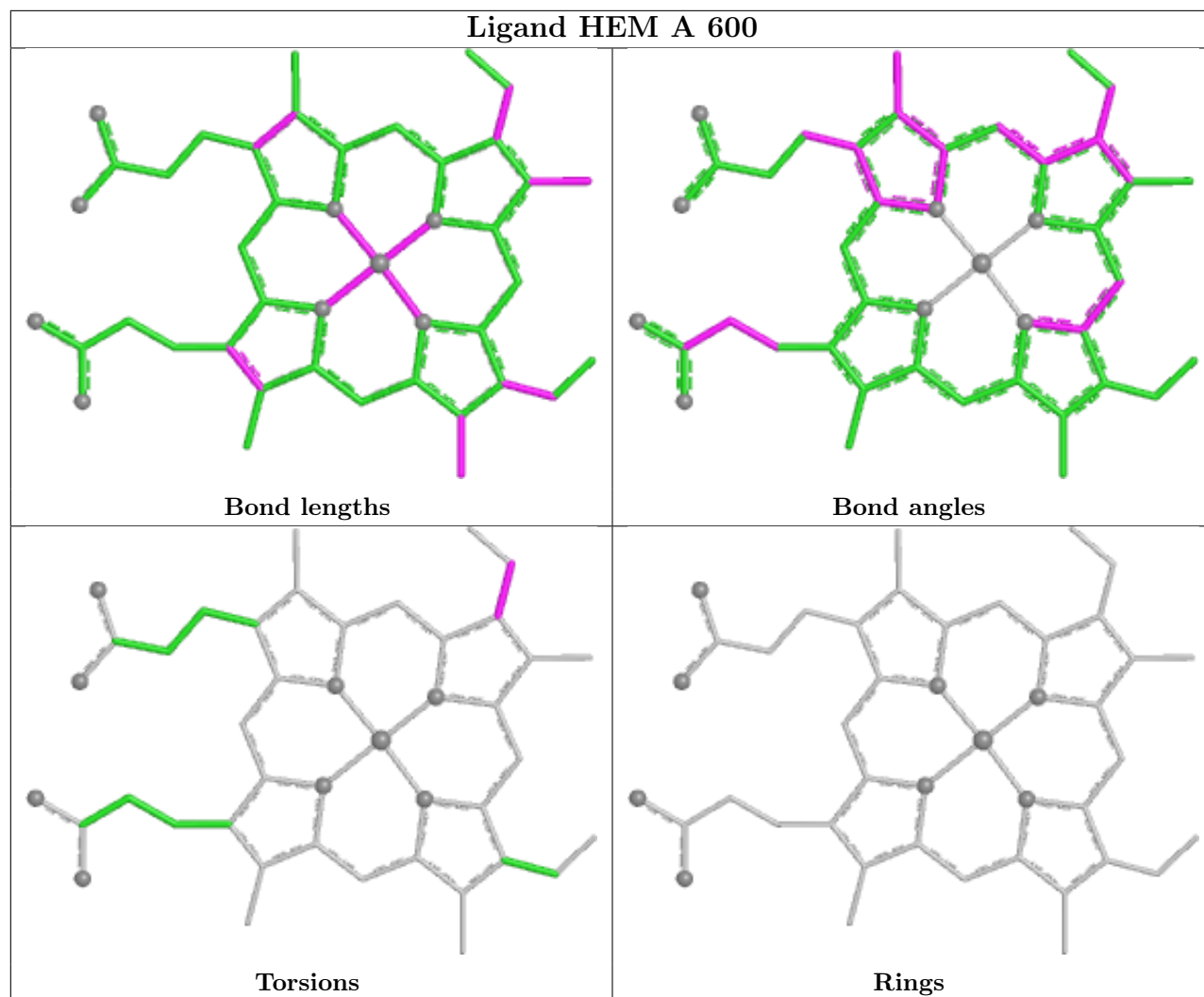
There are no ring outliers.

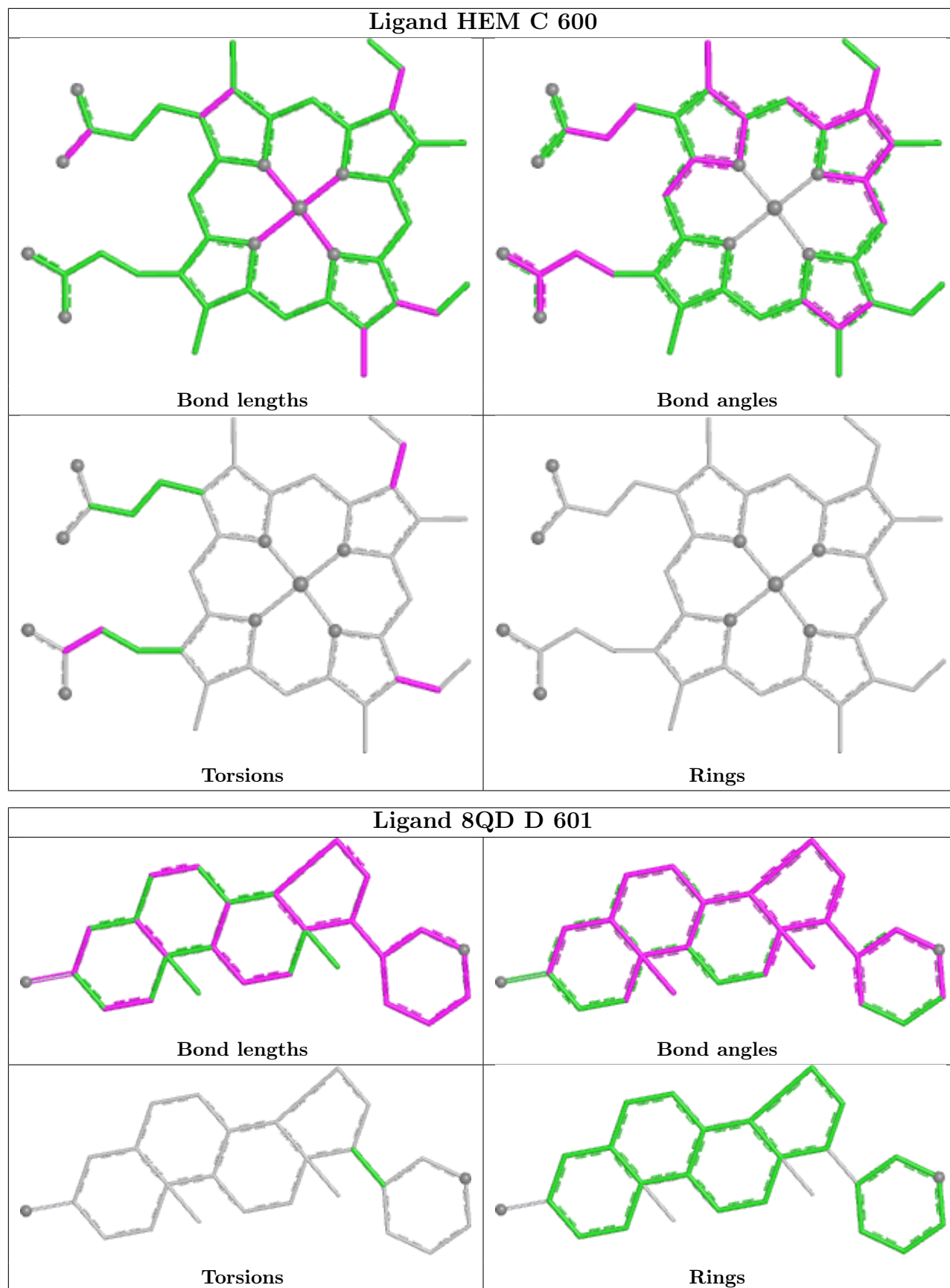
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	HEM	1	0
2	C	600	HEM	4	0
2	D	600	HEM	3	0

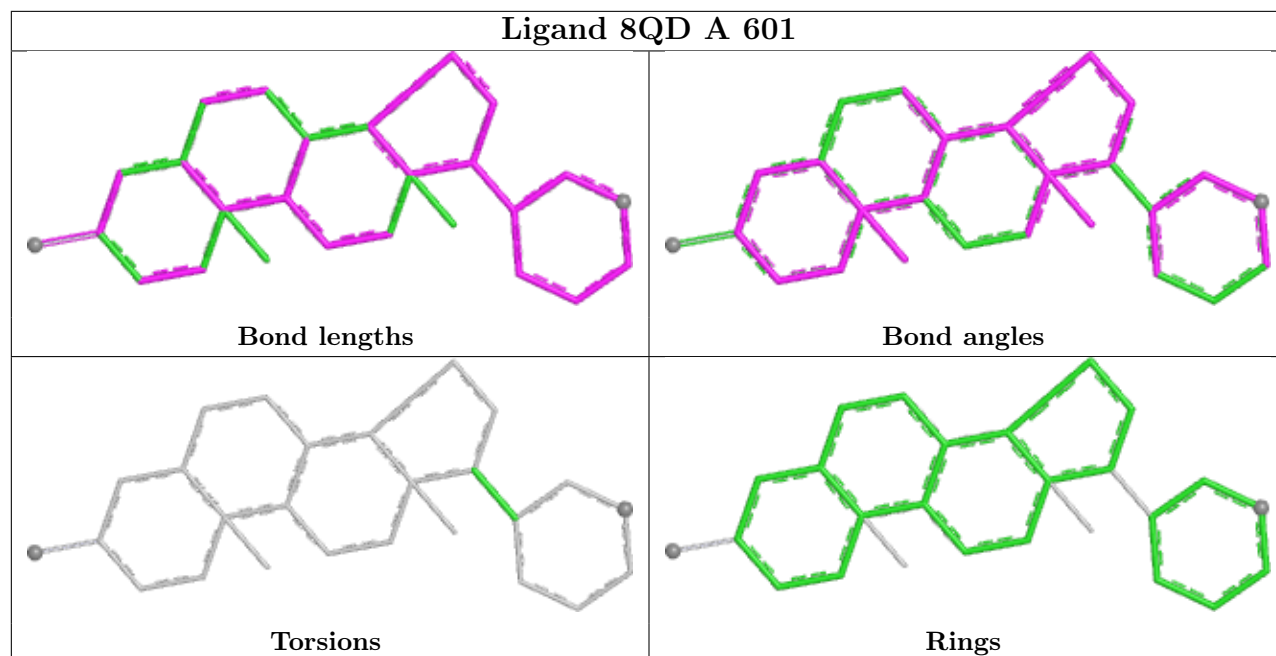
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



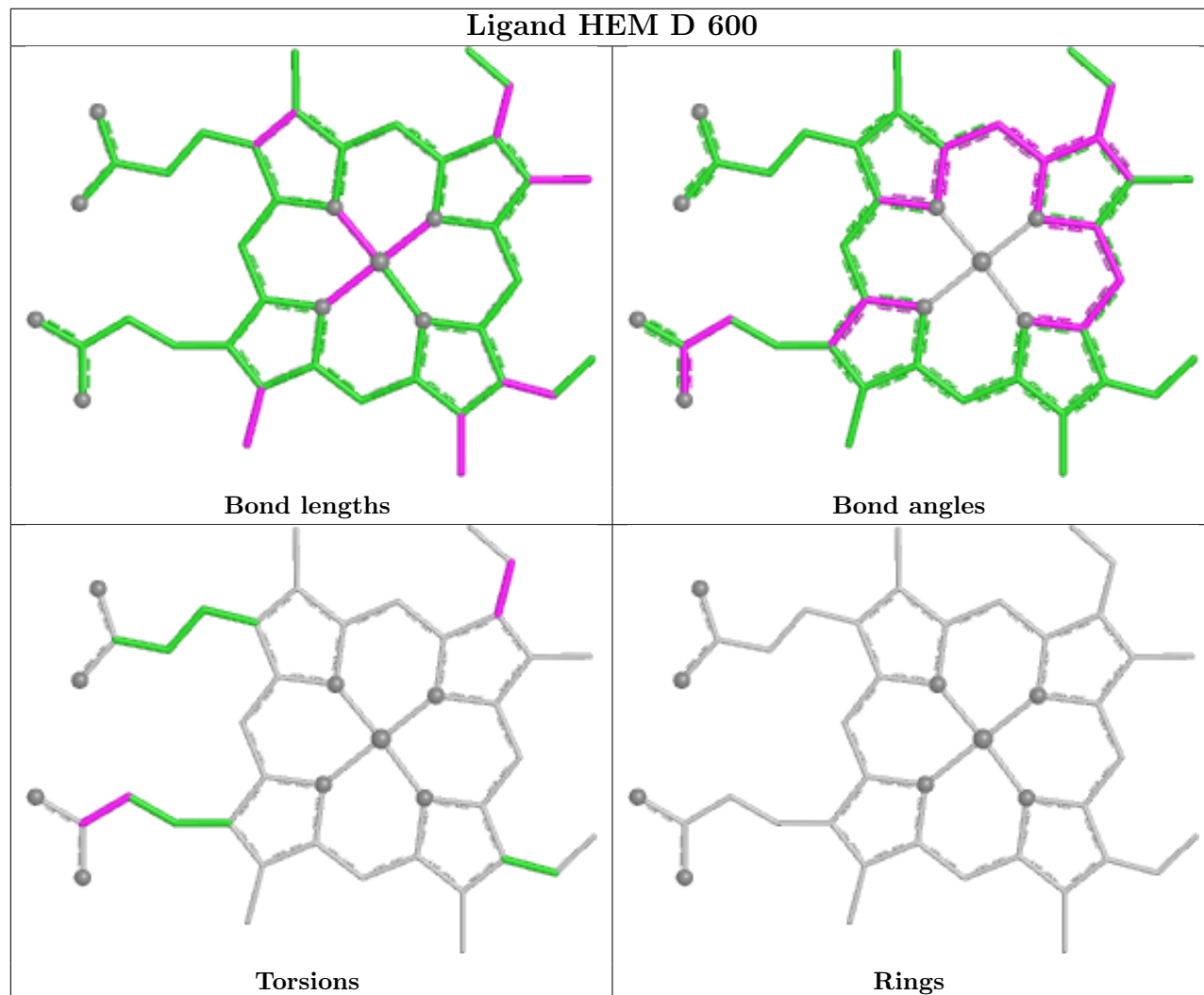


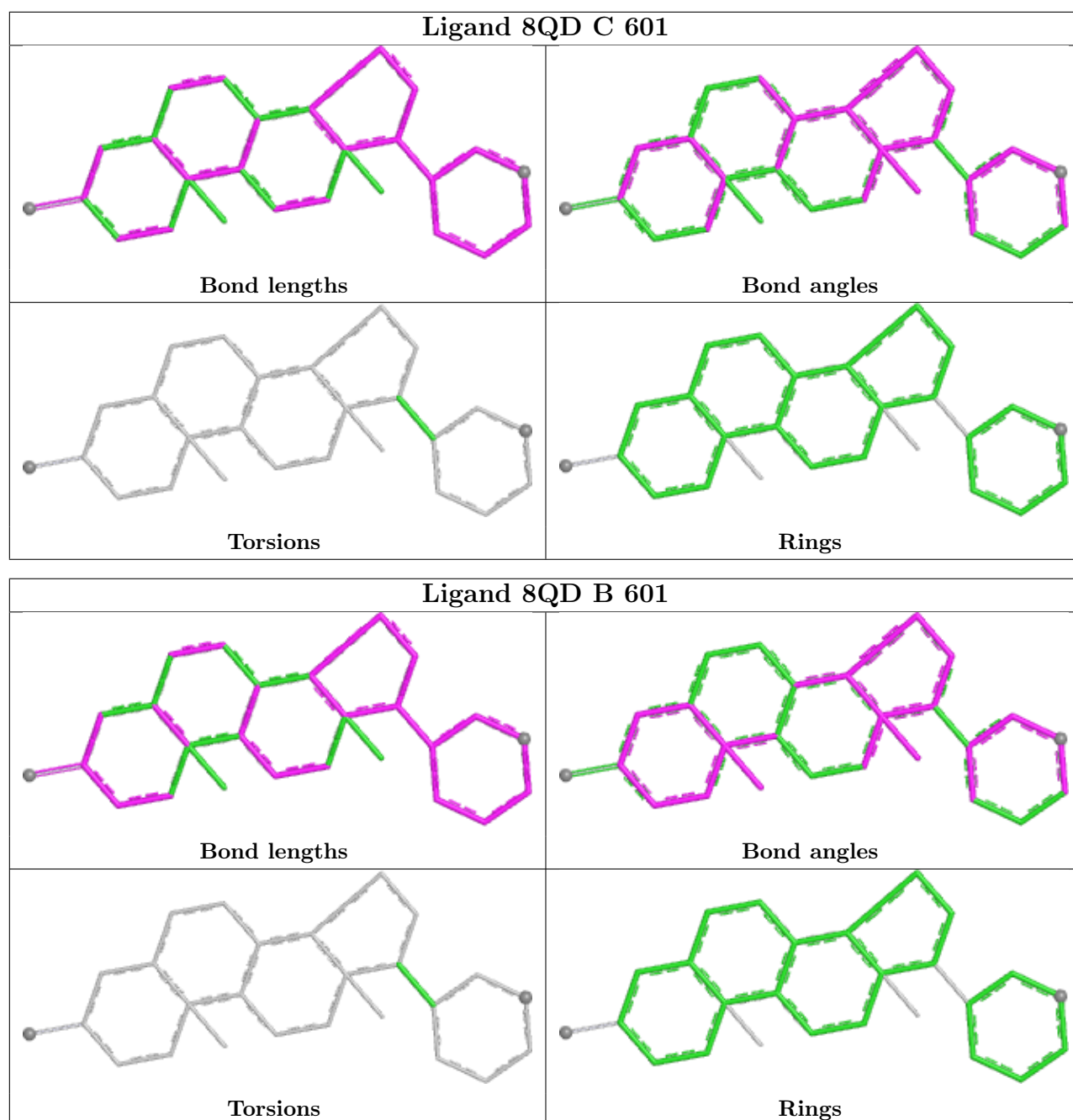


Ligand 8QD A 601



Ligand HEM D 600





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	471/494 (95%)	-0.10	11 (2%) 61 57	26, 41, 70, 107	0
1	B	470/494 (95%)	-0.16	6 (1%) 75 71	24, 39, 72, 99	0
1	C	473/494 (95%)	-0.08	10 (2%) 63 59	25, 40, 71, 106	0
1	D	473/494 (95%)	0.38	36 (7%) 20 16	26, 48, 104, 135	0
All	All	1887/1976 (95%)	0.01	63 (3%) 49 45	24, 41, 84, 135	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	504	ALA	7.3
1	D	499	TRP	4.6
1	D	332	ILE	4.1
1	D	278	ALA	3.8
1	D	459	LEU	3.4
1	D	42	PHE	3.4
1	D	337	GLY	3.3
1	A	138	GLY	3.2
1	A	140	GLN	3.2
1	A	279	GLY	3.2
1	C	140	GLN	3.1
1	D	503	GLN	3.1
1	D	498	ALA	3.1
1	A	280	PRO	3.1
1	D	281	ASP	3.0
1	C	42	PHE	3.0
1	A	275	ASN	3.0
1	B	280	PRO	3.0
1	D	460	LEU	2.9
1	D	462	ARG	2.9
1	C	277	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	46	HIS	2.8
1	D	336	VAL	2.8
1	D	470	ASP	2.8
1	C	139	ASP	2.7
1	D	280	PRO	2.7
1	D	277	ASN	2.6
1	D	331	GLU	2.6
1	D	45	ARG	2.6
1	D	502	ALA	2.5
1	D	501	GLU	2.5
1	A	136	LYS	2.5
1	C	137	ASP	2.5
1	A	135	PHE	2.5
1	D	156	MET	2.5
1	D	139	ASP	2.4
1	D	282	GLN	2.4
1	D	500	ARG	2.4
1	B	276	GLY	2.4
1	B	136	LYS	2.4
1	D	495	VAL	2.4
1	D	41	PRO	2.3
1	C	43	LEU	2.3
1	D	140	GLN	2.3
1	D	493	ILE	2.3
1	D	335	ASN	2.2
1	B	138	GLY	2.2
1	C	46	HIS	2.2
1	C	503	GLN	2.2
1	C	502	ALA	2.2
1	D	138	GLY	2.2
1	D	134	LEU	2.1
1	A	139	ASP	2.1
1	D	492	LYS	2.1
1	A	31	LEU	2.1
1	B	120	HIS	2.1
1	D	497	GLN	2.1
1	D	471	GLY	2.1
1	A	134	LEU	2.1
1	B	275	ASN	2.1
1	C	120	HIS	2.1
1	D	421	ALA	2.0
1	D	157	LEU	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](#)

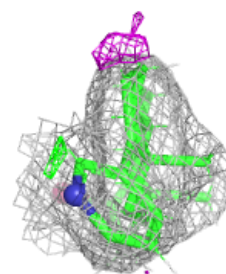
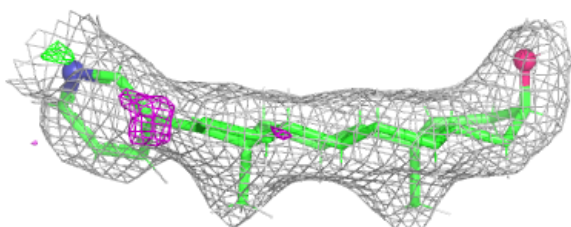
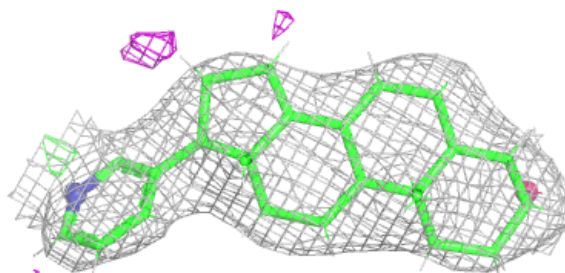
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	8QD	B	601	26/26	0.94	0.09	23,32,42,47	0
3	8QD	C	601	26/26	0.94	0.08	18,29,38,40	0
3	8QD	D	601	26/26	0.94	0.09	22,36,45,47	0
3	8QD	A	601	26/26	0.95	0.09	25,34,42,43	0
2	HEM	C	600	43/43	0.97	0.08	18,29,41,47	0
2	HEM	A	600	43/43	0.98	0.07	21,30,43,52	0
2	HEM	D	600	43/43	0.98	0.07	23,34,48,57	0
2	HEM	B	600	43/43	0.98	0.07	17,28,41,49	0

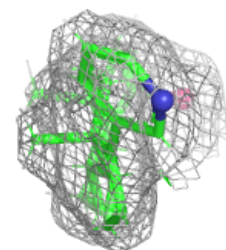
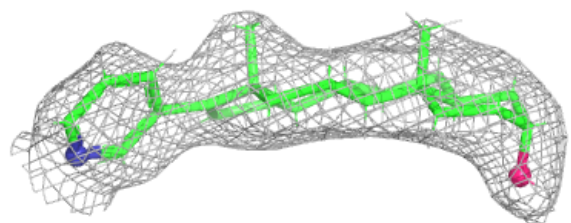
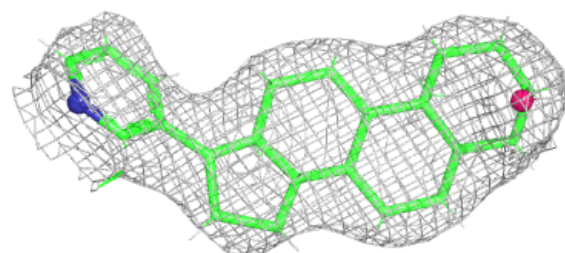
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8QD 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)

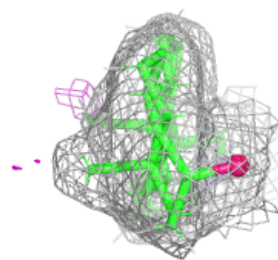
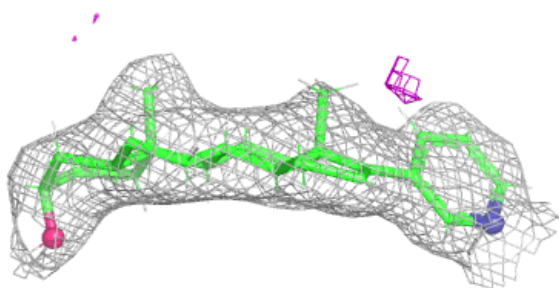
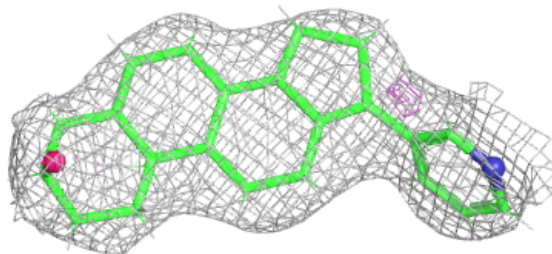
**Electron density around 8QD C 601:**

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

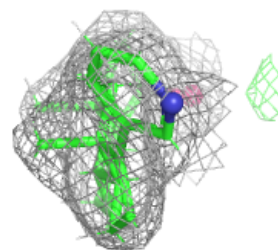
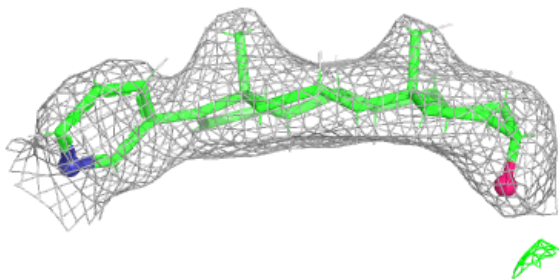
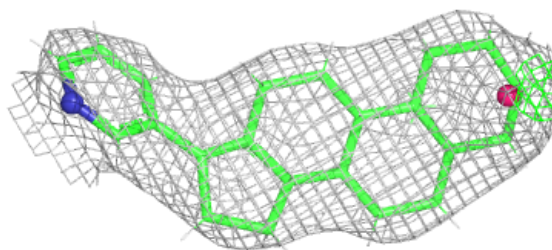


Electron density around 8QD D 601:

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

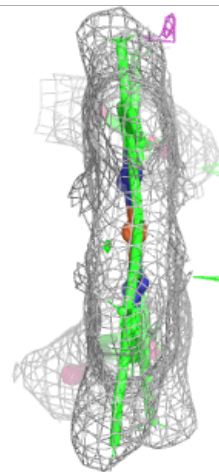
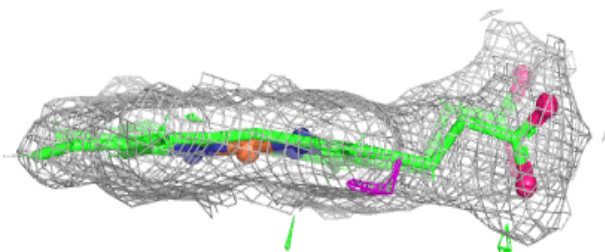
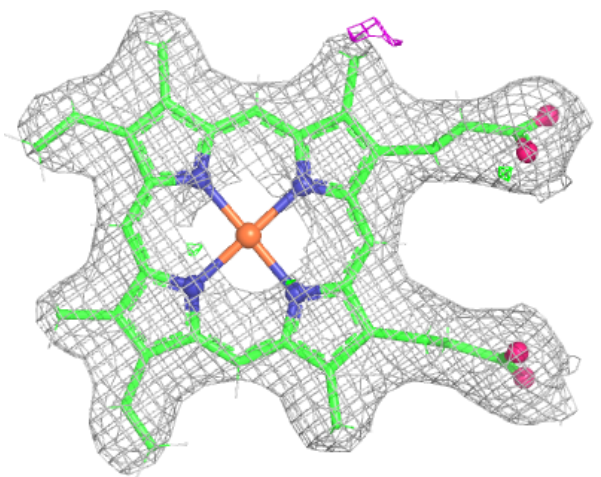
**Electron density around 8QD A 601:**

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



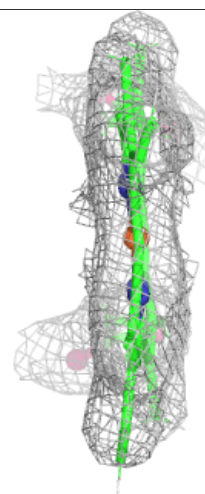
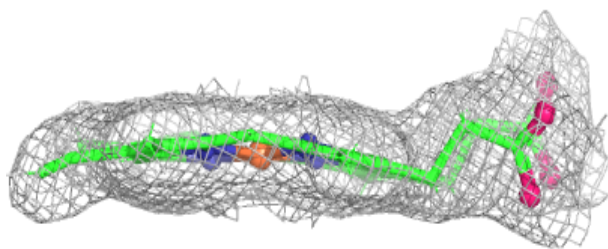
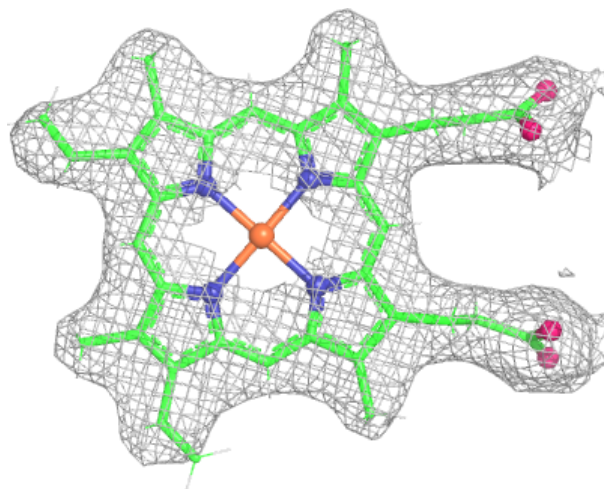
Electron density around HEM C 600:

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



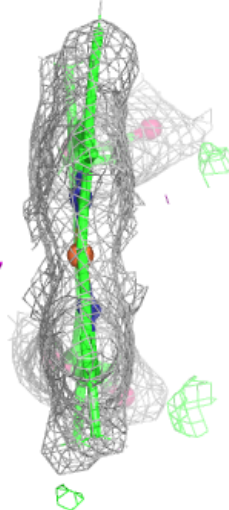
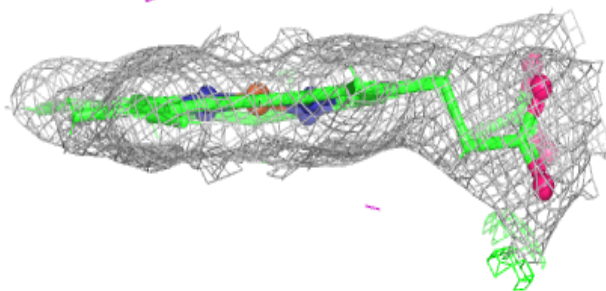
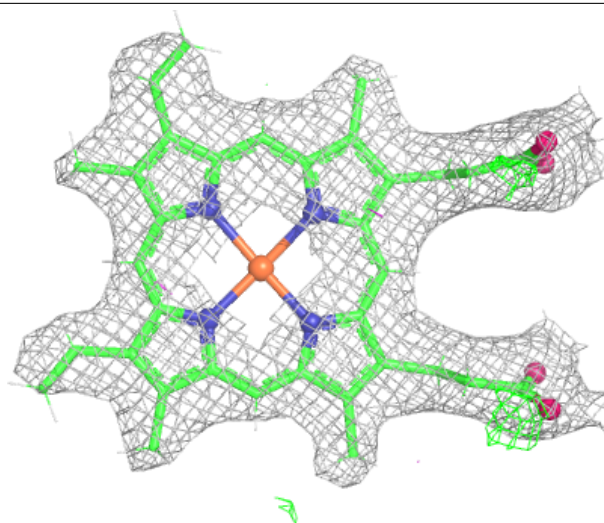
Electron density around HEM A 600:

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



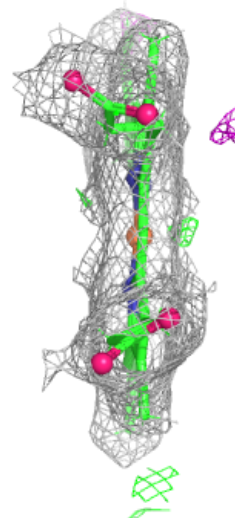
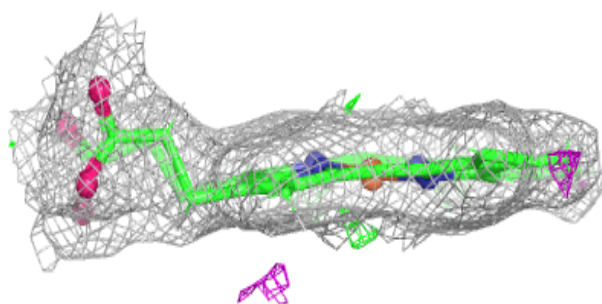
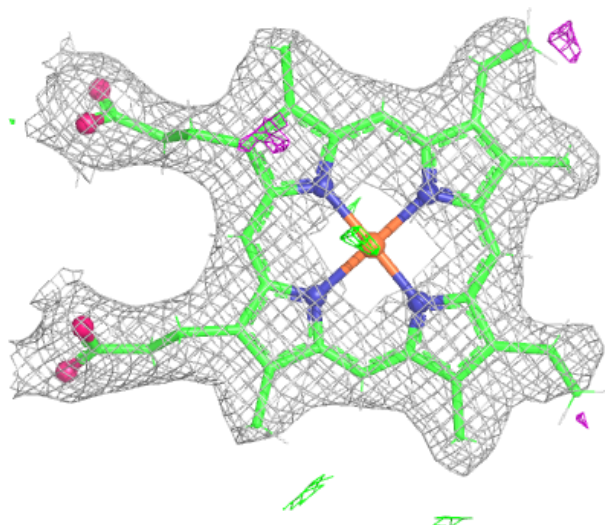
Electron density around HEM D 600:

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



Electron density around HEM B 600:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.