



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 08:10 PM BST

PDB ID : 6CHI
Title : Human Cytochrome P450 17A1 in complex with inhibitor: abiraterone C6 amide
Authors : Scott, E.E.
Deposited on : 2018-02-22
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

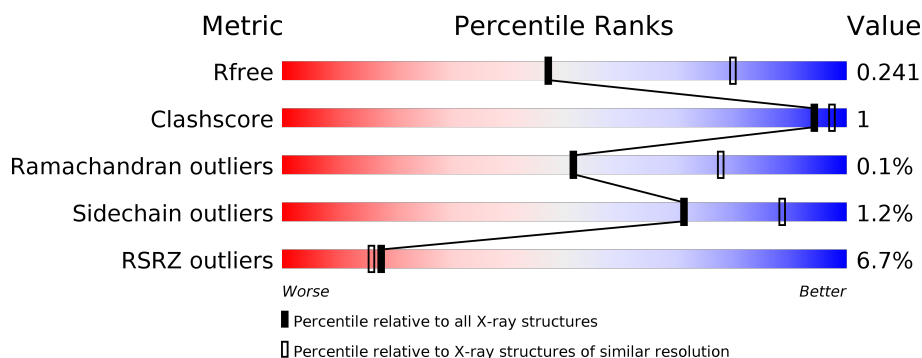
1 Overall quality at a glance

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 on 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	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>6%</div> </div> </div>
1	B	494	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>
1	C	494	<div> <div>7%</div> <div> <div></div> <div>93%</div> <div>•</div> </div> </div>
1	D	494	<div> <div>9%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30100 atoms, of which 14776 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
			7355	2382	3644	642	672	15			
1	B	468	Total	C	H	N	O	S	0	0	0
			7393	2391	3665	645	677	15			
1	C	476	Total	C	H	N	O	S	0	1	0
			7488	2426	3700	656	691	15			
1	D	467	Total	C	H	N	O	S	0	0	0
			7370	2389	3647	644	675	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

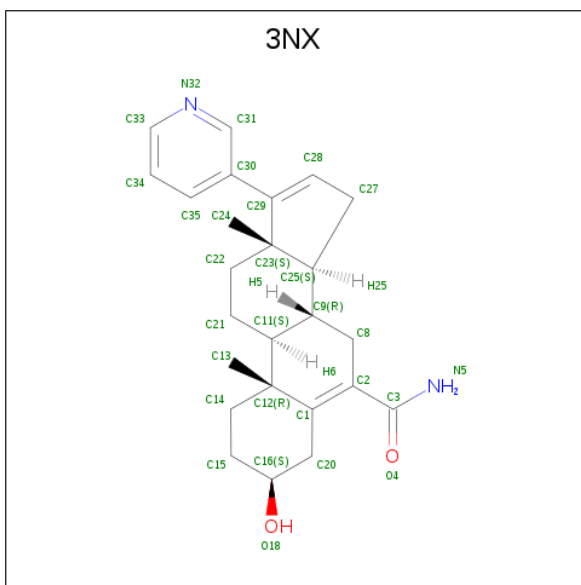
- # HEM

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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 3-hydroxy-17-(3-pyridyl)-androst-5,16-dien-6-amide (three-letter code: 3NX) (formula: $C_{25}H_{32}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			29	25	2	2		
3	B	1	Total	C	N	O	0	0
			29	25	2	2		
3	C	1	Total	C	N	O	0	0
			29	25	2	2		
3	D	1	Total	C	N	O	0	0
			29	25	2	2		

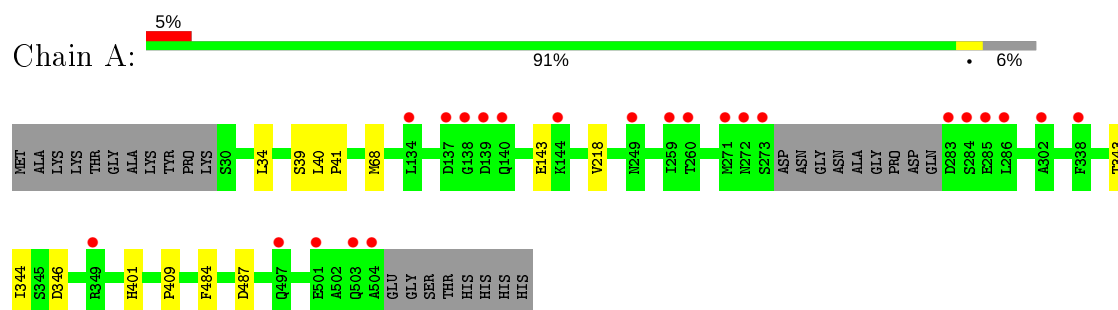
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	25	Total	O	0	0
			25	25		
4	B	16	Total	O	0	0
			16	16		
4	C	29	Total	O	0	0
			29	29		
4	D	16	Total	O	0	0
			16	16		

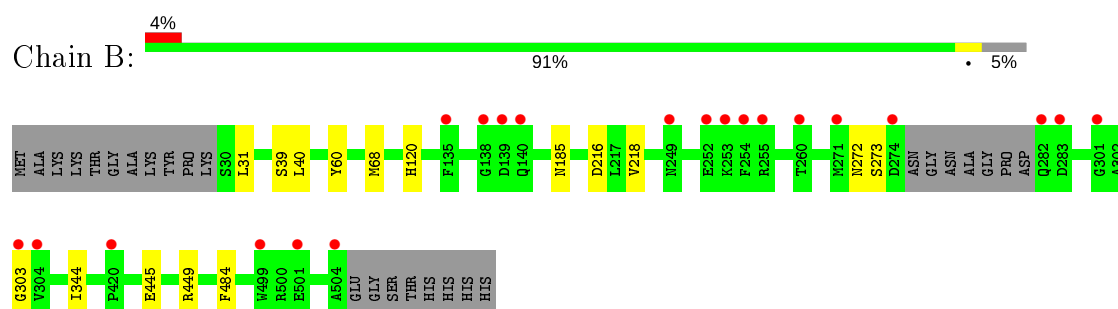
3 Residue-property plots [i](#)

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.

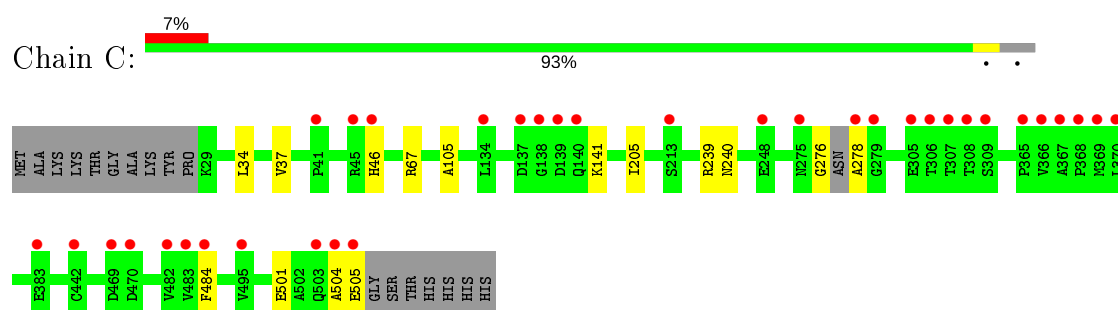
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase



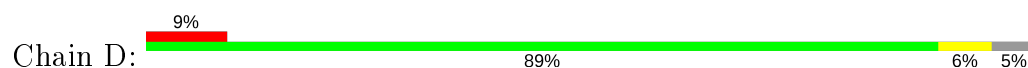
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

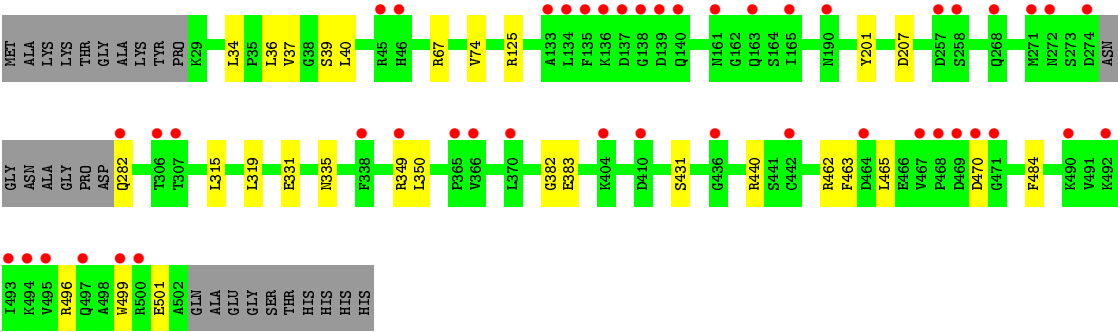


- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase



- 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	89.42Å 154.11Å 167.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.67 – 2.70 39.35 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.67-2.70) 99.5 (39.35-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155:0000)	Depositor
R, R_{free}	0.187 , 0.242 0.188 , 0.241	Depositor DCC
R_{free} test set	3245 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.4	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	0.95	EDS
Total number of atoms	30100	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: HEM, 3NX

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	0.26	1/3791 (0.0%)	0.41	0/5132
1	B	0.27	1/3808 (0.0%)	0.41	0/5155
1	C	0.25	0/3872	0.42	0/5241
1	D	0.26	0/3803	0.42	0/5147
All	All	0.26	2/15274 (0.0%)	0.41	0/20675

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	218	VAL	C-N	7.94	1.49	1.34
1	A	218	VAL	C-N	6.85	1.47	1.34

There are no bond angle outliers.

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	3711	3644	3785	12	0
1	B	3728	3665	3797	7	0
1	C	3788	3700	3853	9	0
1	D	3723	3647	3798	13	0
2	A	43	30	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	30	30	1	0
2	C	43	30	30	2	0
2	D	43	30	30	2	0
3	A	29	0	0	0	0
3	B	29	0	0	0	0
3	C	29	0	0	1	0
3	D	29	0	0	0	0
4	A	25	0	0	0	0
4	B	16	0	0	0	0
4	C	29	0	0	0	0
4	D	16	0	0	1	0
All	All	15324	14776	15353	40	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 (40) 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:A:143:GLU:OE1	1:A:344:ILE:HG22	1.76	0.84
1:C:239:ARG:NH1	1:C:240:ASN:OD1	2.12	0.81
1:A:143:GLU:OE2	1:A:343:THR:HG23	1.84	0.77
1:B:39:SER:HA	1:C:67:ARG:O	1.92	0.70
1:C:34:LEU:HD12	1:C:34:LEU:H	1.64	0.63
2:C:600:HEM:HBB2	2:C:600:HEM:HHC	1.81	0.62
1:D:125:ARG:NH1	2:D:600:HEM:O1D	2.32	0.62
1:A:40:LEU:HD21	1:A:68:MET:CE	2.30	0.62
1:A:143:GLU:OE1	1:A:344:ILE:CG2	2.48	0.61
1:D:315:LEU:HD22	1:D:465:LEU:HD13	1.82	0.61
2:A:600:HEM:HHD	2:A:600:HEM:HBC2	1.83	0.60
2:D:600:HEM:HBC2	2:D:600:HEM:HHD	1.84	0.60
2:C:600:HEM:HHD	2:C:600:HEM:HBC2	1.83	0.59
1:C:501:GLU:O	1:C:505:GLU:HB3	2.04	0.57
1:D:36:LEU:HD11	1:D:39:SER:HB2	1.89	0.54
1:D:462:ARG:HD2	1:D:499:TRP:CE2	2.44	0.53
1:B:40:LEU:HD21	1:B:68:MET:HE1	1.91	0.52
1:D:282:GLN:HB2	4:D:709:HOH:O	2.11	0.51
1:A:39:SER:O	1:A:40:LEU:HD23	2.11	0.50
1:A:343:THR:N	1:A:346:ASP:OD2	2.41	0.49
1:A:39:SER:HA	1:D:67:ARG:O	2.13	0.48
1:B:303:GLY:HA2	2:B:600:HEM:HMC3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:TYR:CG	1:C:37:VAL:HG11	2.50	0.47
1:A:34:LEU:HD13	1:D:74:VAL:HG22	1.97	0.47
1:A:40:LEU:HD21	1:A:68:MET:HE1	1.99	0.45
1:C:276:GLY:O	1:C:278:ALA:N	2.49	0.45
1:A:40:LEU:HD21	1:A:68:MET:HE2	1.99	0.44
1:D:463:PHE:C	1:D:496:ARG:HG3	2.37	0.44
1:C:205:ILE:HD12	3:C:601:3NX:O18	2.18	0.44
1:B:40:LEU:HD21	1:B:68:MET:CE	2.49	0.42
1:D:335:ASN:HB3	1:D:349:ARG:HB3	2.01	0.41
1:D:382:GLY:O	1:D:383:GLU:HB2	2.19	0.41
1:A:41:PRO:HG3	1:D:37:VAL:HG23	2.03	0.41
1:D:331:GLU:HG2	1:D:350:LEU:HD23	2.03	0.41
1:D:462:ARG:HD2	1:D:499:TRP:NE1	2.36	0.41
1:B:272:ASN:O	1:B:273:SER:HB3	2.21	0.40
1:A:401:HIS:HA	1:A:409:PRO:HB2	2.03	0.40
1:C:34:LEU:HD12	1:C:34:LEU:N	2.32	0.40
1:B:445:GLU:OE2	1:B:449:ARG:NH2	2.55	0.40
1:C:105:ALA:O	1:C:239:ARG:NH2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	462/494 (94%)	447 (97%)	15 (3%)	0	100	100
1	B	464/494 (94%)	447 (96%)	17 (4%)	0	100	100
1	C	473/494 (96%)	450 (95%)	22 (5%)	1 (0%)	47	73
1	D	463/494 (94%)	442 (96%)	20 (4%)	1 (0%)	47	73
All	All	1862/1976 (94%)	1786 (96%)	74 (4%)	2 (0%)	51	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	501	GLU
1	C	504	ALA

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%)	413 (100%)	2 (0%)	88	96
1	B	417/436 (96%)	411 (99%)	6 (1%)	67	86
1	C	423/436 (97%)	420 (99%)	3 (1%)	84	94
1	D	417/436 (96%)	408 (98%)	9 (2%)	52	79
All	All	1672/1744 (96%)	1652 (99%)	20 (1%)	71	88

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	484	PHE
1	A	487	ASP
1	B	31	LEU
1	B	120	HIS
1	B	185	ASN
1	B	216	ASP
1	B	344	ILE
1	B	484	PHE
1	C	46	HIS
1	C	141	LYS
1	C	484	PHE
1	D	34	LEU
1	D	40	LEU
1	D	201	TYR
1	D	207	ASP
1	D	319	LEU
1	D	431	SER
1	D	440	ARG
1	D	470	ASP
1	D	484	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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
3	3NX	C	601	2	32,33,33	1.25	4 (12%)	43,52,52	2.53	15 (34%)
3	3NX	D	601	2	32,33,33	1.25	4 (12%)	43,52,52	2.46	15 (34%)
3	3NX	A	601	2	32,33,33	1.24	4 (12%)	43,52,52	2.41	15 (34%)
3	3NX	B	601	2	32,33,33	1.18	4 (12%)	43,52,52	2.39	15 (34%)
2	HEM	A	600	1,3	27,50,50	1.86	4 (14%)	17,82,82	1.46	3 (17%)
2	HEM	C	600	1,3	27,50,50	1.90	5 (18%)	17,82,82	1.51	2 (11%)
2	HEM	B	600	1,3	27,50,50	1.80	5 (18%)	17,82,82	1.72	5 (29%)
2	HEM	D	600	1,3	27,50,50	1.84	5 (18%)	17,82,82	1.66	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	3NX	C	601	2	-	4/7/69/69	0/5/5/5
3	3NX	D	601	2	-	3/7/69/69	0/5/5/5
3	3NX	A	601	2	-	5/7/69/69	0/5/5/5
3	3NX	B	601	2	-	6/7/69/69	0/5/5/5
2	HEM	A	600	1,3	-	0/6/54/54	-
2	HEM	C	600	1,3	-	1/6/54/54	-
2	HEM	B	600	1,3	-	0/6/54/54	-
2	HEM	D	600	1,3	-	0/6/54/54	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	3NX	C23-C29	-4.87	1.48	1.53
3	C	601	3NX	C23-C29	-4.84	1.48	1.53
3	A	601	3NX	C23-C29	-4.73	1.49	1.53
2	D	600	HEM	C3C-C2C	-4.48	1.34	1.40
2	C	600	HEM	C3C-C2C	-4.45	1.34	1.40
3	B	601	3NX	C23-C29	-4.43	1.49	1.53
2	A	600	HEM	C3C-C2C	-4.41	1.34	1.40
2	C	600	HEM	C3B-C2B	-4.25	1.34	1.40
2	A	600	HEM	C3B-CAB	3.83	1.55	1.47
2	D	600	HEM	C3B-CAB	3.80	1.55	1.47
2	B	600	HEM	C3B-CAB	3.80	1.55	1.47
2	C	600	HEM	C3B-CAB	3.78	1.55	1.47
2	A	600	HEM	C3C-CAC	3.76	1.55	1.47
2	C	600	HEM	C3C-CAC	3.75	1.55	1.47
2	B	600	HEM	C3C-CAC	3.74	1.55	1.47
2	D	600	HEM	C3C-CAC	3.71	1.55	1.47
2	B	600	HEM	C3C-C2C	-3.68	1.35	1.40
2	A	600	HEM	C3B-C2B	-3.57	1.35	1.40
2	B	600	HEM	C3B-C2B	-3.52	1.35	1.40
2	D	600	HEM	C3B-C2B	-3.51	1.35	1.40
3	D	601	3NX	C12-C1	-2.34	1.50	1.53
3	A	601	3NX	C12-C1	-2.33	1.50	1.53
3	C	601	3NX	C12-C1	-2.29	1.50	1.53
3	A	601	3NX	C12-C11	-2.27	1.52	1.56
3	D	601	3NX	C12-C11	-2.26	1.52	1.56
3	C	601	3NX	C12-C11	-2.24	1.52	1.56
3	B	601	3NX	C12-C11	-2.23	1.52	1.56
2	B	600	HEM	CAA-C2A	2.20	1.55	1.52
2	C	600	HEM	CAA-C2A	2.16	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	3NX	C27-C28	2.16	1.53	1.50
3	D	601	3NX	C27-C28	2.13	1.53	1.50
3	A	601	3NX	C27-C28	2.13	1.53	1.50
3	B	601	3NX	C12-C1	-2.13	1.50	1.53
2	D	600	HEM	CAA-C2A	2.10	1.55	1.52
3	B	601	3NX	C27-C28	2.00	1.53	1.50

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	3NX	C27-C25-C23	-9.61	96.85	104.05
3	D	601	3NX	C27-C25-C23	-8.78	97.47	104.05
3	A	601	3NX	C27-C25-C23	-8.40	97.75	104.05
3	B	601	3NX	C27-C25-C23	-8.24	97.88	104.05
3	D	601	3NX	C23-C25-C9	-5.79	106.92	113.12
3	B	601	3NX	C23-C25-C9	-5.78	106.94	113.12
3	A	601	3NX	C23-C25-C9	-5.67	107.05	113.12
3	C	601	3NX	C23-C25-C9	-5.63	107.10	113.12
3	D	601	3NX	C27-C28-C29	-4.56	109.12	112.87
3	C	601	3NX	C27-C25-C9	-4.35	116.35	121.57
3	D	601	3NX	C25-C9-C11	-4.25	103.40	109.09
3	C	601	3NX	C27-C28-C29	-4.24	109.38	112.87
3	A	601	3NX	C27-C25-C9	-4.24	116.48	121.57
3	B	601	3NX	C27-C25-C9	-4.22	116.50	121.57
3	B	601	3NX	C27-C28-C29	-4.19	109.42	112.87
3	A	601	3NX	C27-C28-C29	-4.08	109.52	112.87
3	D	601	3NX	C27-C25-C9	-3.54	117.32	121.57
3	C	601	3NX	C24-C23-C25	-3.48	107.84	112.98
3	D	601	3NX	C8-C9-C25	-3.43	107.00	111.18
2	B	600	HEM	CMC-C2C-C3C	3.42	131.08	124.68
3	B	601	3NX	C8-C9-C25	-3.41	107.02	111.18
3	C	601	3NX	C16-C20-C1	-3.31	106.37	112.05
3	A	601	3NX	C33-N32-C31	3.23	122.44	116.85
3	C	601	3NX	C8-C9-C25	-3.22	107.25	111.18
3	B	601	3NX	C33-N32-C31	3.21	122.40	116.85
2	D	600	HEM	CMB-C2B-C3B	3.20	130.66	124.68
3	C	601	3NX	C33-N32-C31	3.10	122.21	116.85
3	A	601	3NX	C25-C9-C11	-3.07	104.98	109.09
3	A	601	3NX	C8-C9-C25	-3.03	107.48	111.18
3	A	601	3NX	C16-C20-C1	-3.00	106.90	112.05
3	B	601	3NX	C16-C20-C1	-2.98	106.95	112.05
2	B	600	HEM	CMB-C2B-C3B	2.97	130.23	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	HEM	CAA-CBA-CGA	-2.96	107.71	112.67
3	B	601	3NX	C25-C23-C29	2.94	102.21	99.70
3	D	601	3NX	C24-C23-C25	-2.92	108.66	112.98
3	B	601	3NX	C21-C22-C23	-2.90	106.46	112.74
3	C	601	3NX	C25-C9-C11	-2.89	105.22	109.09
2	A	600	HEM	CMB-C2B-C3B	2.81	129.93	124.68
3	D	601	3NX	C11-C12-C1	2.80	113.29	109.27
3	D	601	3NX	C33-N32-C31	2.79	121.68	116.85
3	A	601	3NX	C13-C12-C11	-2.79	108.36	111.68
3	C	601	3NX	C25-C23-C29	2.78	102.07	99.70
3	A	601	3NX	C11-C12-C1	2.77	113.26	109.27
3	A	601	3NX	C24-C23-C25	-2.77	108.89	112.98
3	A	601	3NX	C21-C22-C23	-2.77	106.75	112.74
3	C	601	3NX	C13-C12-C11	-2.77	108.38	111.68
3	D	601	3NX	C13-C12-C11	-2.74	108.41	111.68
3	B	601	3NX	C24-C23-C25	-2.73	108.95	112.98
3	B	601	3NX	C25-C9-C11	-2.73	105.44	109.09
3	A	601	3NX	C25-C23-C29	2.70	102.00	99.70
2	B	600	HEM	CAA-CBA-CGA	-2.69	108.17	112.67
3	B	601	3NX	C13-C12-C11	-2.66	108.50	111.68
3	D	601	3NX	C16-C20-C1	-2.64	107.53	112.05
3	A	601	3NX	C21-C11-C12	-2.62	109.63	113.08
2	C	600	HEM	CMA-C3A-C4A	-2.59	124.48	128.46
3	C	601	3NX	C21-C22-C23	-2.58	107.16	112.74
3	D	601	3NX	C25-C23-C29	2.55	101.87	99.70
3	B	601	3NX	C11-C12-C1	2.53	112.91	109.27
3	C	601	3NX	C21-C11-C12	-2.52	109.75	113.08
3	D	601	3NX	C21-C11-C12	-2.52	109.76	113.08
3	D	601	3NX	C21-C22-C23	-2.48	107.37	112.74
3	A	601	3NX	C30-C31-N32	-2.38	119.97	123.49
3	C	601	3NX	C11-C12-C1	2.38	112.69	109.27
3	D	601	3NX	C34-C35-C30	-2.37	117.54	120.34
3	B	601	3NX	C30-C31-N32	-2.33	120.05	123.49
3	C	601	3NX	C30-C31-N32	-2.23	120.19	123.49
2	A	600	HEM	CBD-CAD-C3D	-2.22	108.39	112.48
2	D	600	HEM	CMA-C3A-C4A	-2.21	125.07	128.46
3	B	601	3NX	C21-C11-C12	-2.20	110.18	113.08
2	D	600	HEM	CMD-C2D-C1D	-2.16	125.14	128.46
2	D	600	HEM	C4A-C3A-C2A	2.12	108.47	107.00
2	B	600	HEM	CMD-C2D-C1D	-2.10	125.23	128.46
2	A	600	HEM	CAA-CBA-CGA	-2.01	109.29	112.67
2	B	600	HEM	CMA-C3A-C4A	-2.01	125.38	128.46

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	601	3NX	C1-C2-C3-N5
3	A	601	3NX	C1-C2-C3-N5
3	B	601	3NX	C23-C29-C30-C31
3	A	601	3NX	C28-C29-C30-C31
3	B	601	3NX	C23-C29-C30-C35
3	B	601	3NX	C28-C29-C30-C31
3	A	601	3NX	C28-C29-C30-C35
3	C	601	3NX	C1-C2-C3-N5
3	B	601	3NX	C1-C2-C3-N5
2	C	600	HEM	C1A-C2A-CAA-CBA
3	C	601	3NX	C8-C2-C3-O4
3	B	601	3NX	C8-C2-C3-O4
3	B	601	3NX	C28-C29-C30-C35
3	A	601	3NX	C23-C29-C30-C35
3	C	601	3NX	C28-C29-C30-C31
3	C	601	3NX	C28-C29-C30-C35
3	A	601	3NX	C23-C29-C30-C31
3	D	601	3NX	C28-C29-C30-C31
3	D	601	3NX	C28-C29-C30-C35

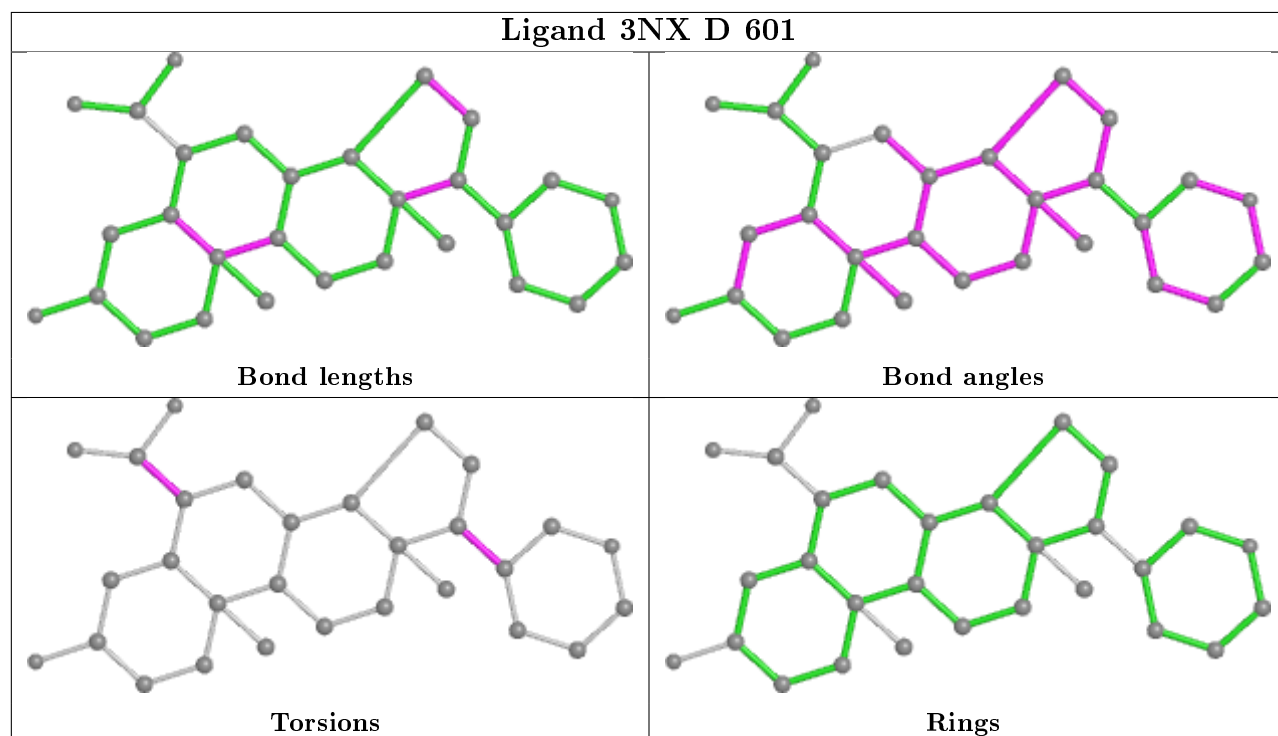
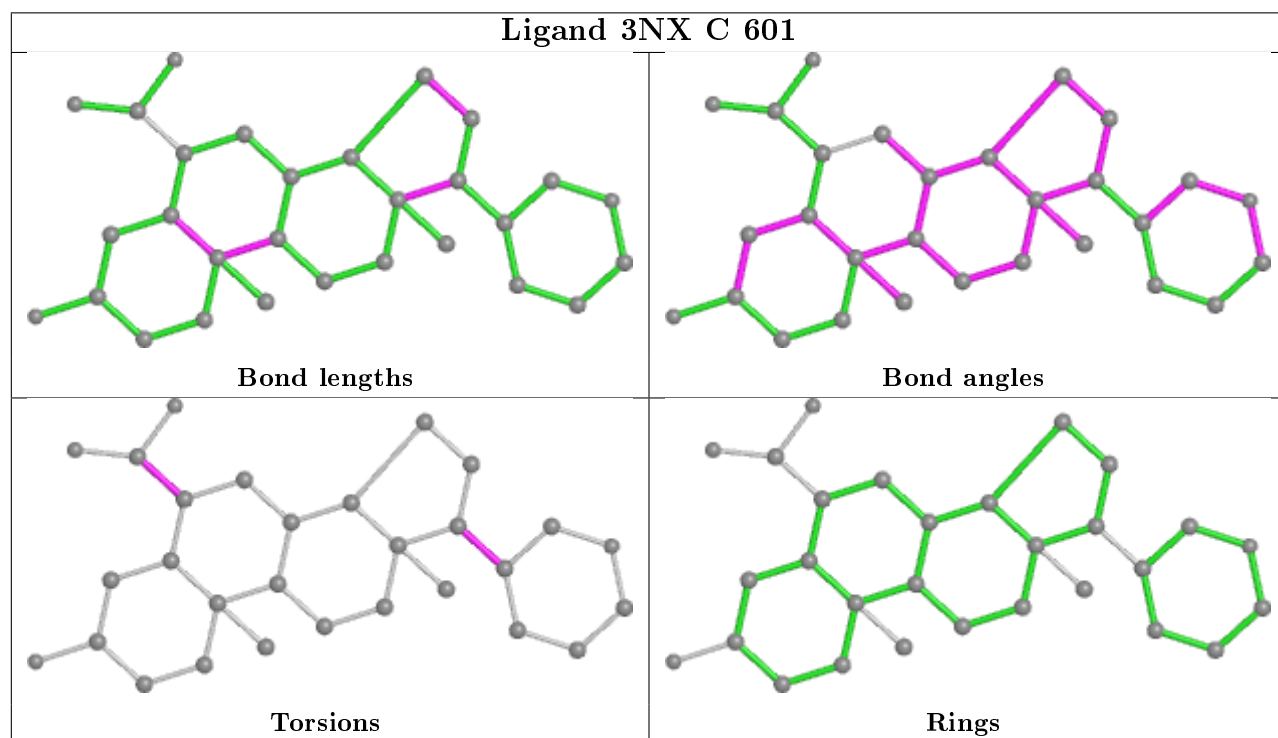
There are no ring outliers.

5 monomers are involved in 7 short contacts:

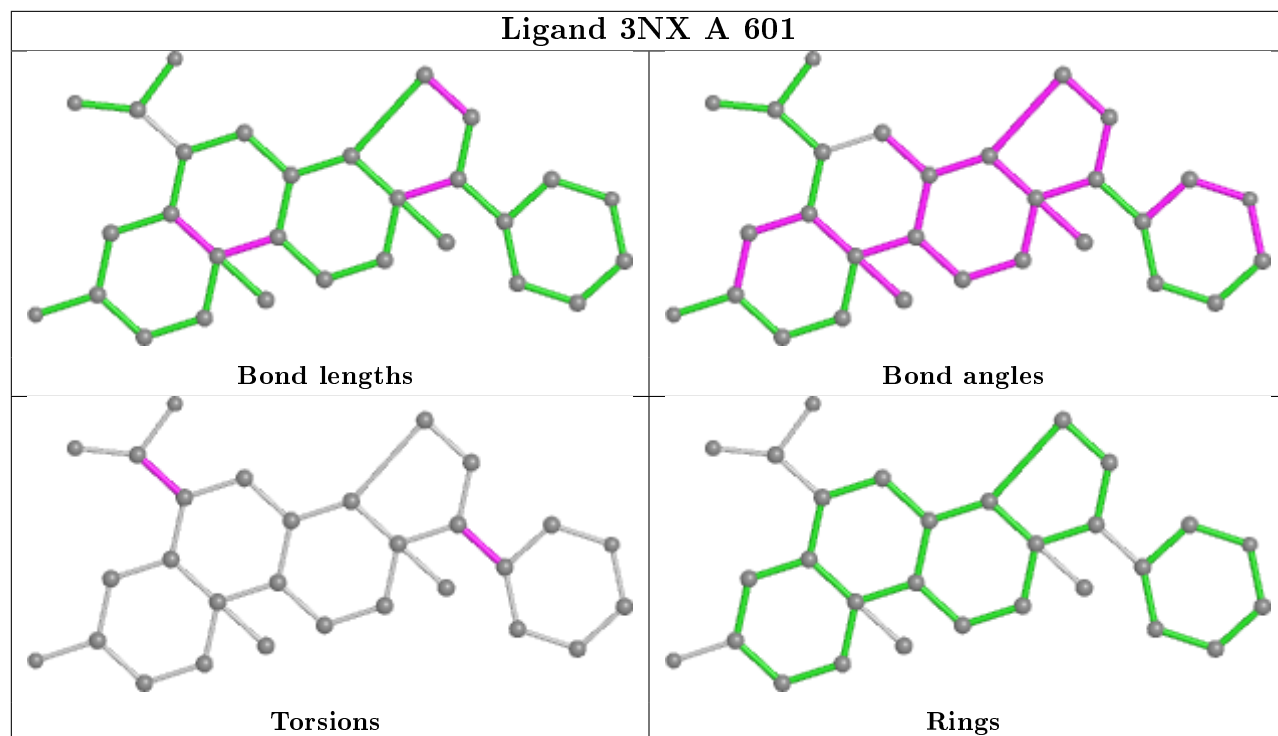
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	3NX	1	0
2	A	600	HEM	1	0
2	C	600	HEM	2	0
2	B	600	HEM	1	0
2	D	600	HEM	2	0

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.

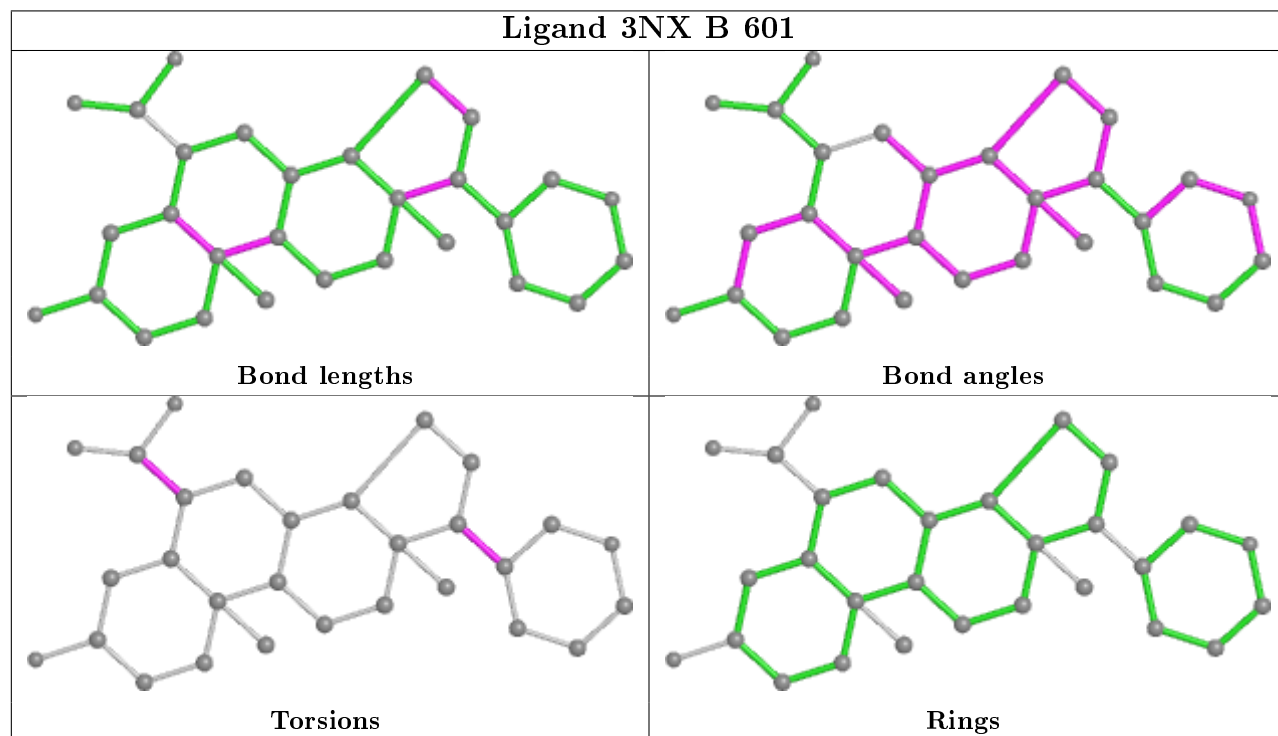
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

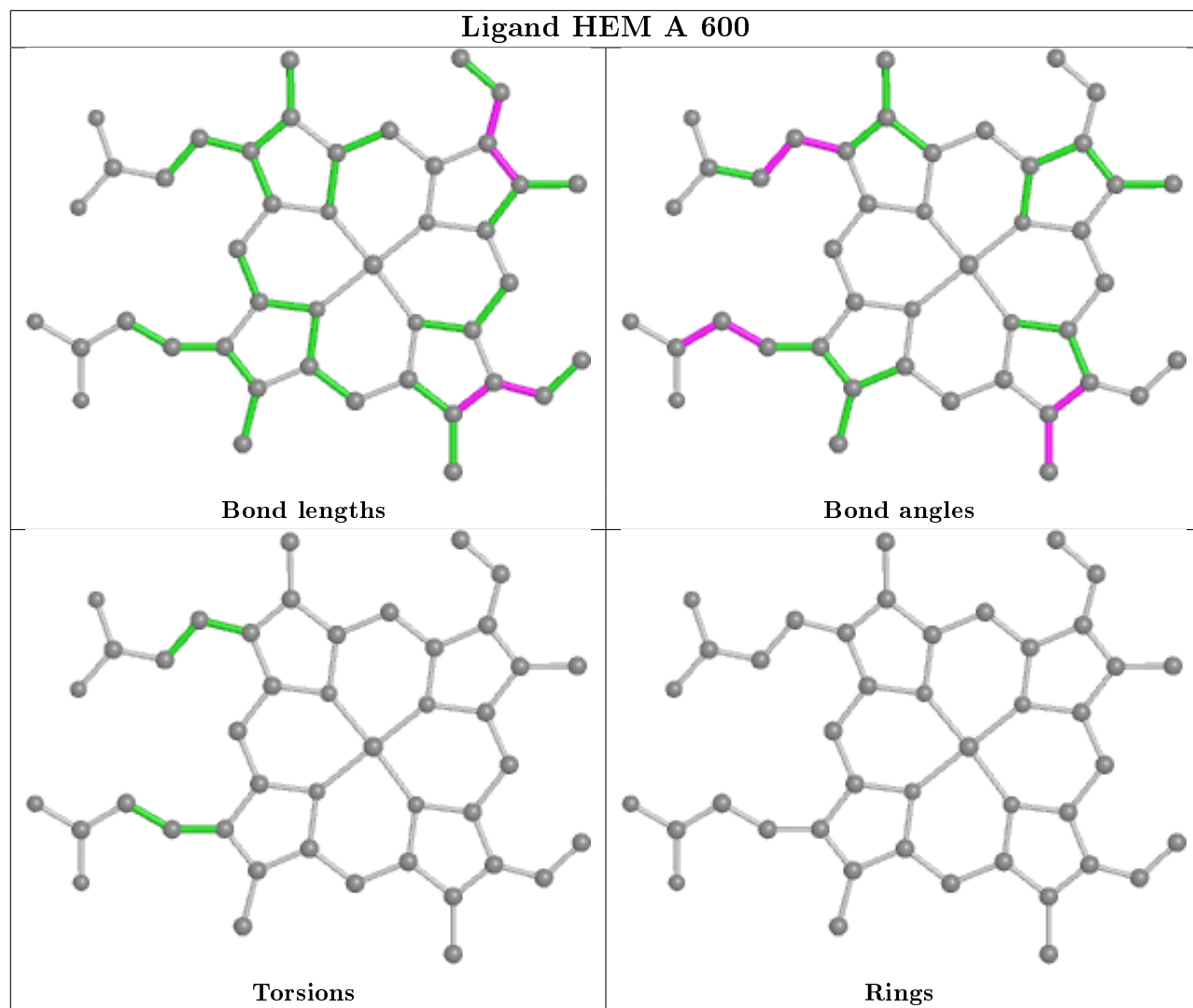


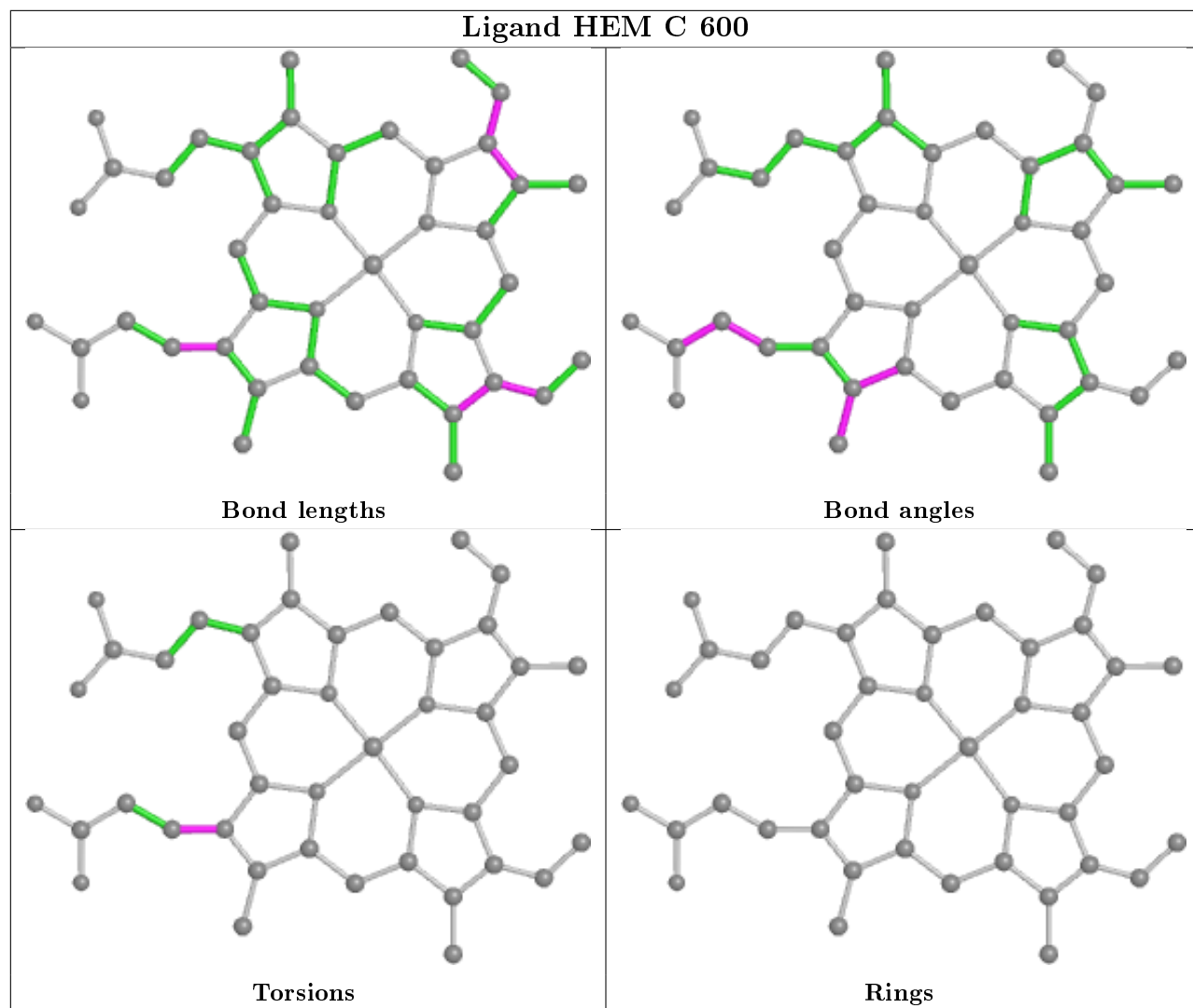
Ligand 3NX A 601

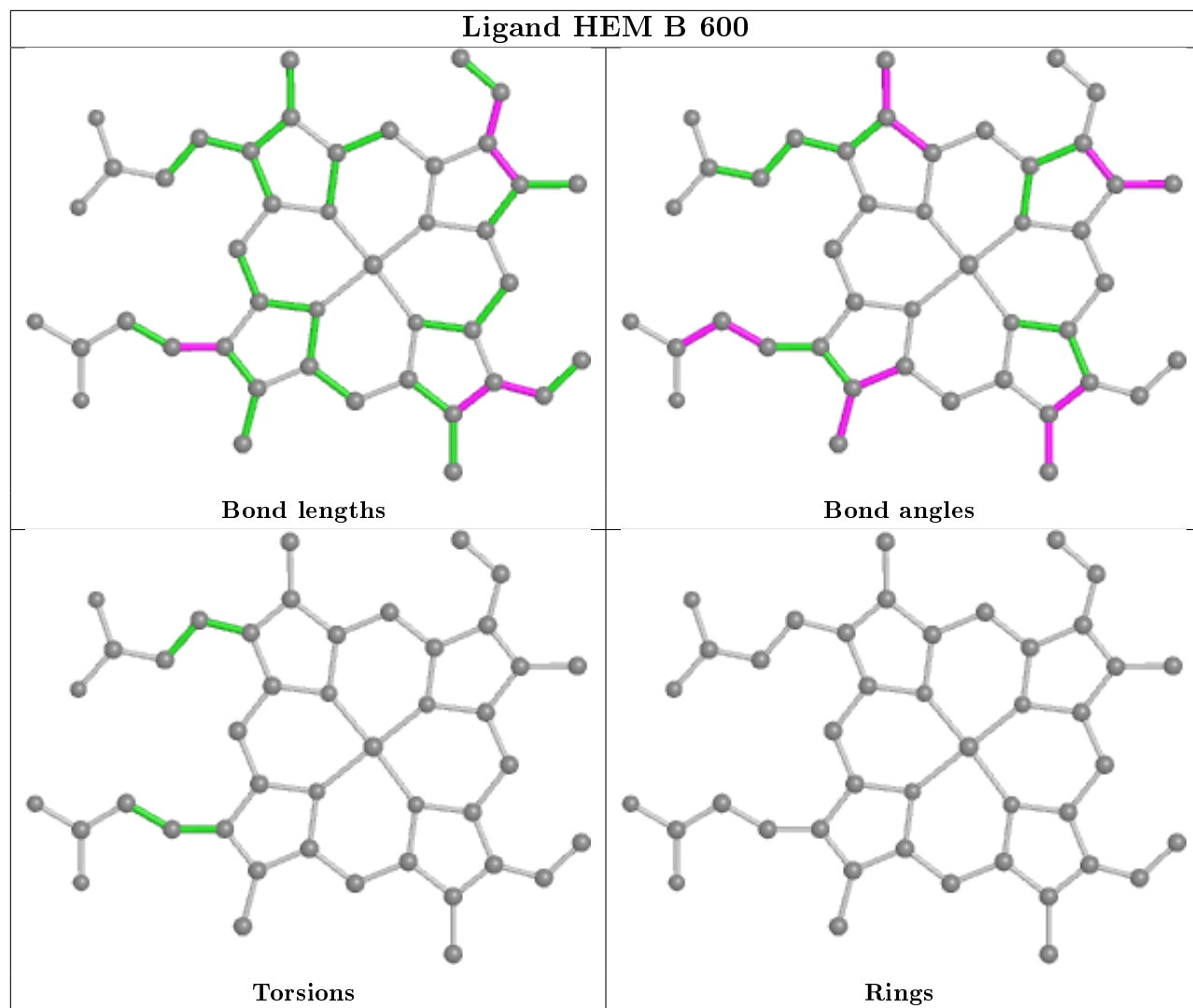


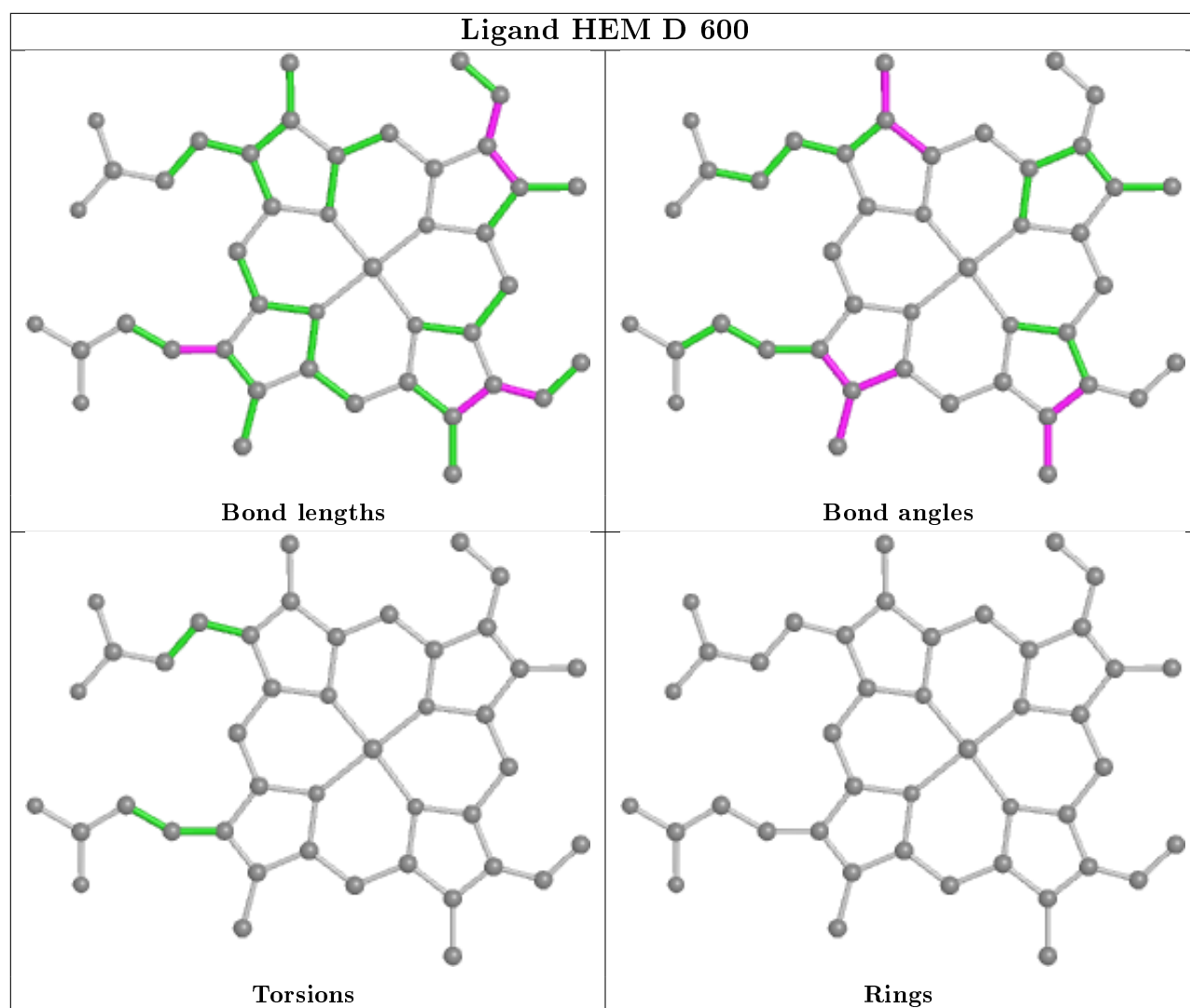
Ligand 3NX B 601











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

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	466/494 (94%)	0.37	23 (4%) 29 28	38, 54, 83, 125	0
1	B	468/494 (94%)	0.32	21 (4%) 33 31	35, 53, 89, 126	0
1	C	476/494 (96%)	0.43	35 (7%) 14 12	34, 52, 89, 144	0
1	D	467/494 (94%)	0.57	46 (9%) 7 5	39, 60, 96, 128	0
All	All	1877/1976 (94%)	0.42	125 (6%) 17 16	34, 55, 90, 144	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	139	ASP	6.9
1	A	139	ASP	6.7
1	B	139	ASP	5.8
1	B	140	GLN	5.7
1	C	45	ARG	5.4
1	A	140	GLN	5.3
1	D	46	HIS	5.3
1	D	140	GLN	4.9
1	D	470	ASP	4.9
1	D	271	MET	4.6
1	B	138	GLY	4.6
1	A	271	MET	4.6
1	D	137	ASP	4.5
1	D	139	ASP	4.5
1	A	284	SER	4.3
1	D	471	GLY	4.3
1	D	138	GLY	4.2
1	D	45	ARG	4.1
1	C	138	GLY	4.0
1	A	137	ASP	4.0
1	B	255	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	279	GLY	3.8
1	A	138	GLY	3.8
1	D	282	GLN	3.7
1	D	274	ASP	3.7
1	C	46	HIS	3.7
1	C	366	VAL	3.6
1	B	254	PHE	3.6
1	A	497	GLN	3.6
1	D	469	ASP	3.5
1	C	504	ALA	3.4
1	A	504	ALA	3.4
1	D	500	ARG	3.3
1	D	497	GLN	3.3
1	C	278	ALA	3.3
1	B	249	ASN	3.2
1	D	134	LEU	3.1
1	B	252	GLU	3.1
1	C	275	ASN	3.1
1	C	470	ASP	3.1
1	C	306	THR	3.1
1	D	467	VAL	3.1
1	C	442	CYS	3.1
1	C	134	LEU	3.0
1	B	274	ASP	3.0
1	A	259	ILE	2.9
1	C	367	ALA	2.9
1	D	272	ASN	2.9
1	A	273	SER	2.9
1	C	137	ASP	2.9
1	C	248	GLU	2.8
1	D	442	CYS	2.8
1	B	504	ALA	2.8
1	A	285	GLU	2.8
1	A	134	LEU	2.8
1	D	436	GLY	2.7
1	D	136	LYS	2.7
1	A	501	GLU	2.7
1	C	482	VAL	2.7
1	A	283	ASP	2.7
1	C	140	GLN	2.7
1	B	135	PHE	2.6
1	B	271	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	163	GLN	2.6
1	D	468	PRO	2.6
1	D	349	ARG	2.6
1	C	307	THR	2.5
1	A	286	LEU	2.5
1	A	302	ALA	2.5
1	D	493	ILE	2.5
1	D	133	ALA	2.5
1	C	469	ASP	2.5
1	C	368	PRO	2.4
1	D	366	VAL	2.4
1	B	499	TRP	2.4
1	D	492	LYS	2.4
1	C	484	PHE	2.4
1	C	503	GLN	2.4
1	D	338	PHE	2.4
1	C	213	SER	2.4
1	D	257	ASP	2.4
1	B	253	LYS	2.4
1	A	249	ASN	2.4
1	C	305	GLU	2.4
1	D	135	PHE	2.4
1	D	495	VAL	2.4
1	D	494	LYS	2.3
1	D	161	ASN	2.3
1	B	301	GLY	2.3
1	C	505	GLU	2.3
1	B	303	GLY	2.3
1	C	369	MET	2.2
1	C	383	GLU	2.2
1	B	501	GLU	2.2
1	D	258	SER	2.2
1	C	41	PRO	2.2
1	D	307	THR	2.2
1	C	483	VAL	2.2
1	A	272	ASN	2.2
1	A	349	ARG	2.2
1	B	420	PRO	2.2
1	C	308	THR	2.2
1	D	306	THR	2.2
1	A	503	GLN	2.2
1	D	490	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	309	SER	2.2
1	A	260	THR	2.2
1	D	165	ILE	2.1
1	C	495	VAL	2.1
1	D	365	PRO	2.1
1	D	410	ASP	2.1
1	B	304	VAL	2.1
1	C	370	LEU	2.1
1	D	404	LYS	2.1
1	B	283	ASP	2.1
1	A	144	LYS	2.1
1	D	190	ASN	2.1
1	A	338	PHE	2.1
1	D	464	ASP	2.1
1	B	282	GLN	2.0
1	D	268	GLN	2.0
1	C	365	PRO	2.0
1	D	370	LEU	2.0
1	D	499	TRP	2.0
1	B	260	THR	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 monosaccharides 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.

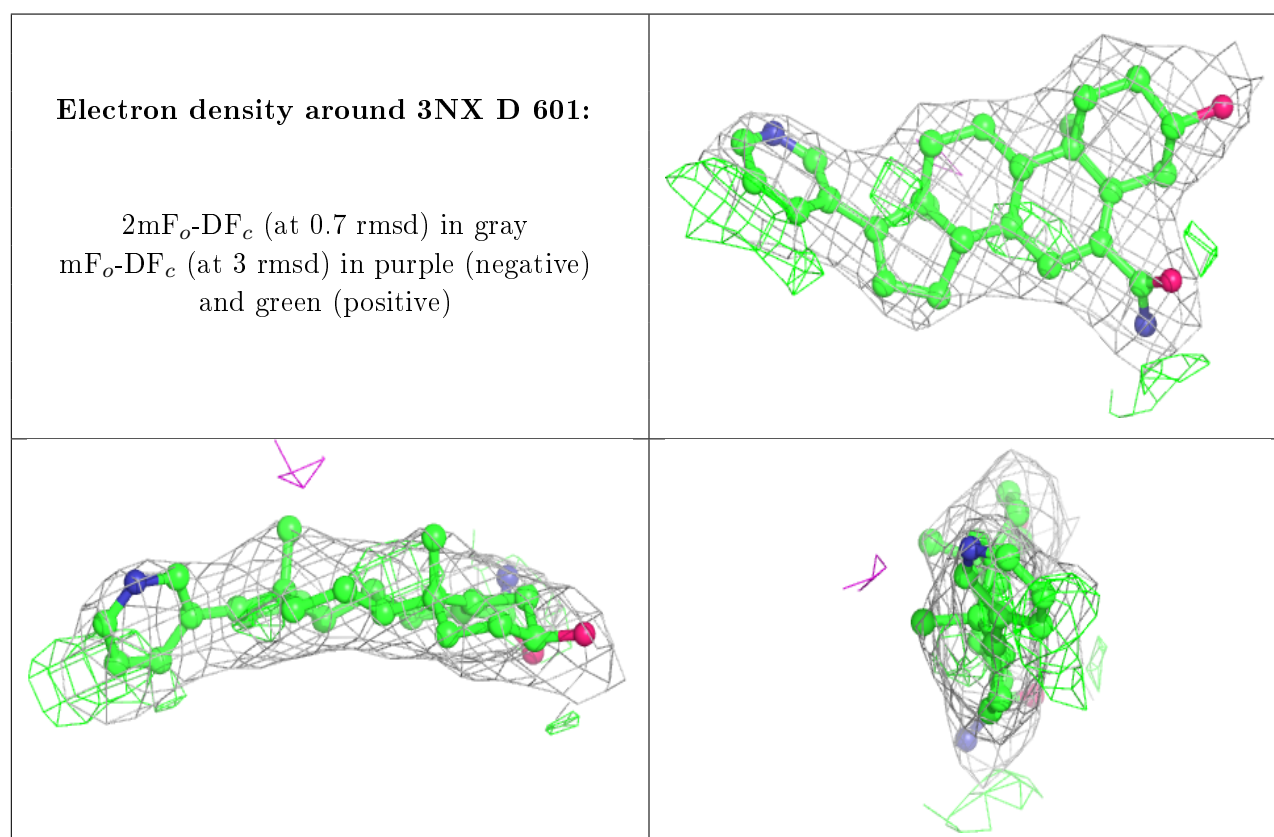
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	3NX	D	601	29/29	0.91	0.33	32,47,57,71	0
3	3NX	C	601	29/29	0.94	0.34	33,40,50,62	0
3	3NX	A	601	29/29	0.95	0.35	38,48,56,66	0

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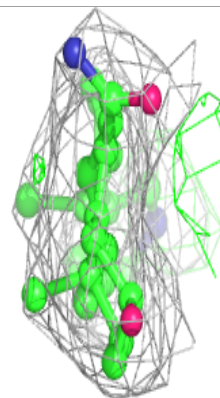
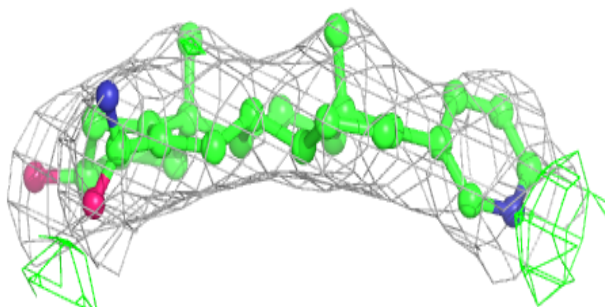
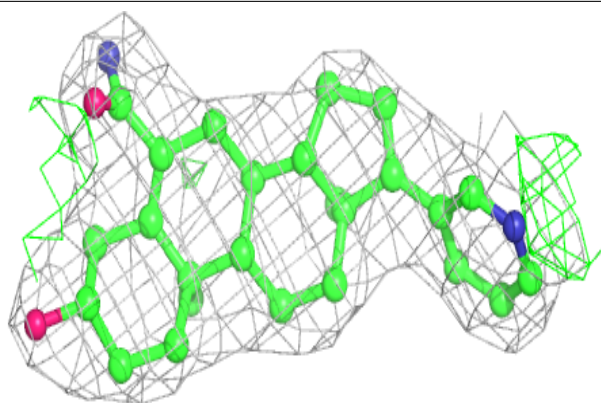
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	3NX	B	601	29/29	0.96	0.32	31,44,51,67	0
2	HEM	D	600	43/43	0.96	0.33	37,56,68,74	0
2	HEM	B	600	43/43	0.97	0.30	33,47,61,68	0
2	HEM	C	600	43/43	0.97	0.31	29,44,56,65	0
2	HEM	A	600	43/43	0.98	0.32	36,47,62,68	0

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.

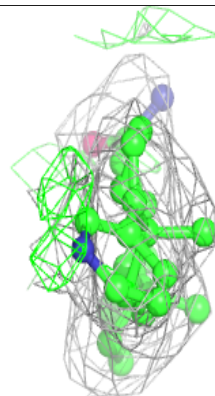
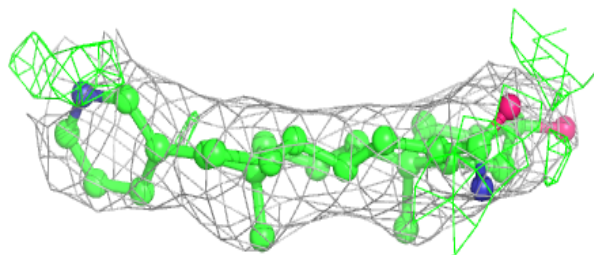
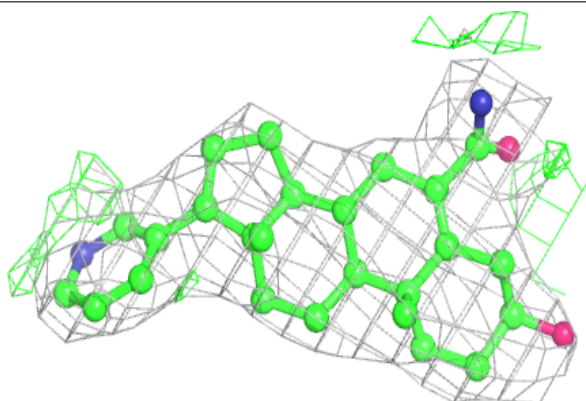


Electron density around 3NX C 601:

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

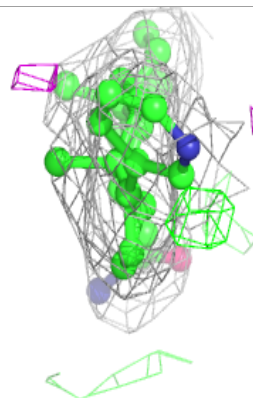
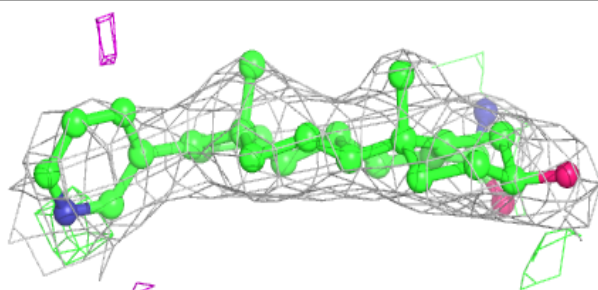
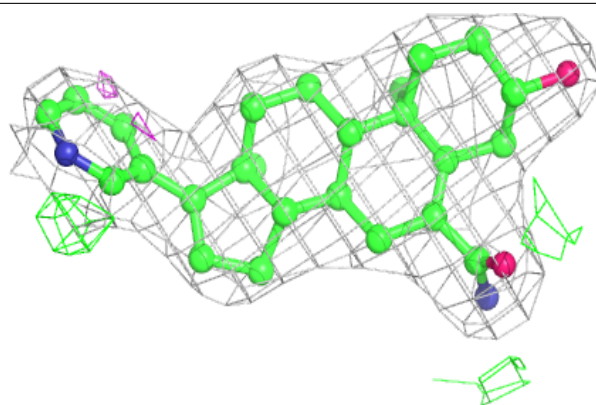
**Electron density around 3NX A 601:**

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



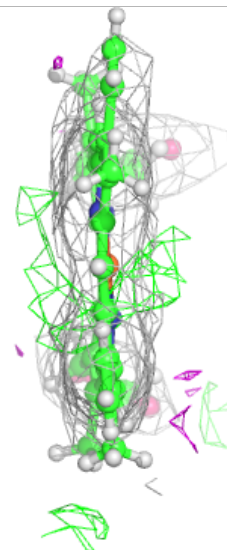
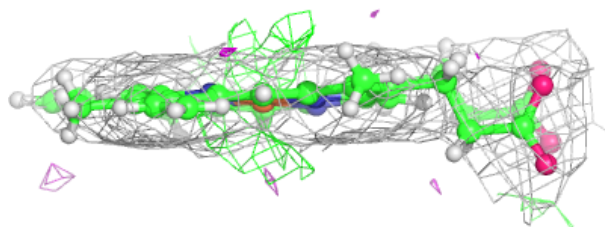
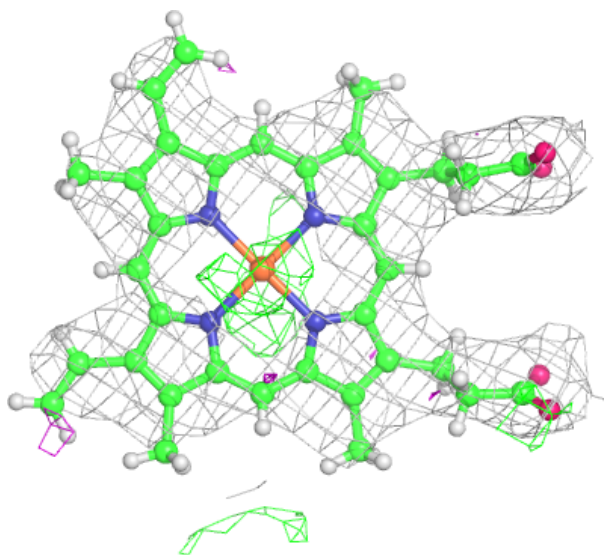
Electron density around 3NX B 601:

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



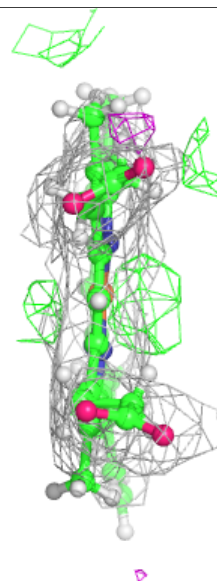
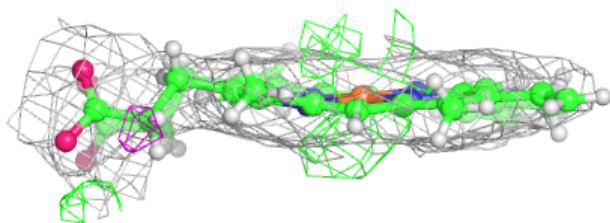
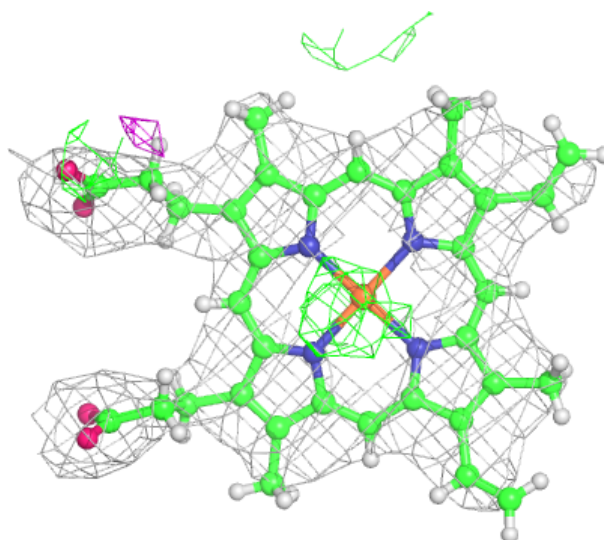
Electron density around HEM D 600:

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



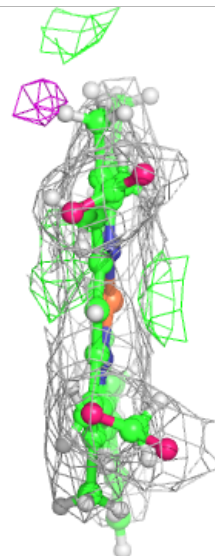
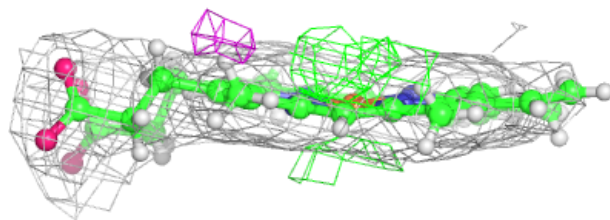
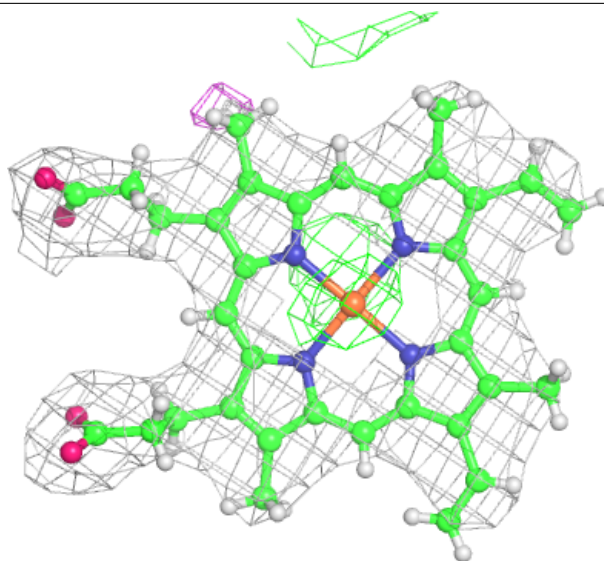
Electron density around HEM B 600:

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



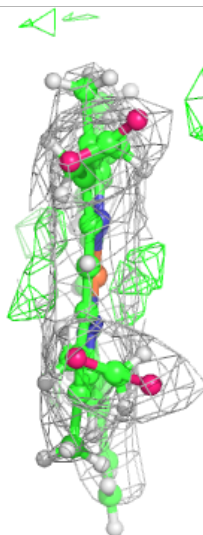
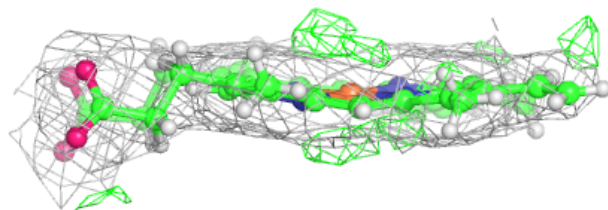
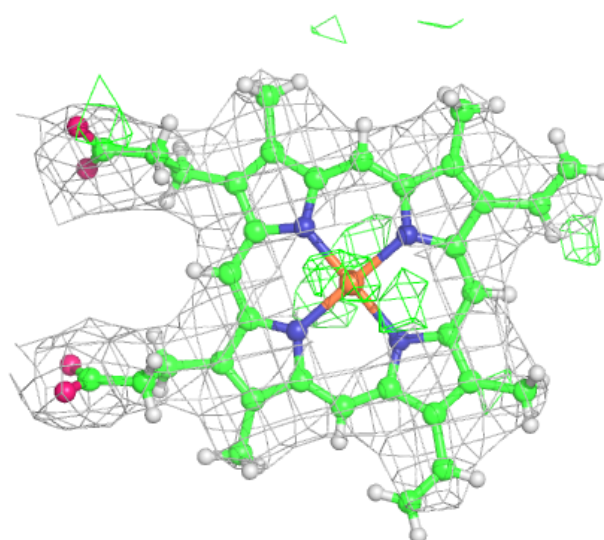
Electron density around HEM C 600:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.