



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:18 PM UTC

PDB ID : 6CIZ / pdb_00006ciz
Title : Human Cytochrome P450 17A1 in complex with inhibitor: abiraterone C6 nitrile
Authors : Scott, E.E.; Fehl, C.
Deposited on : 2018-02-25
Resolution : 2.60 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

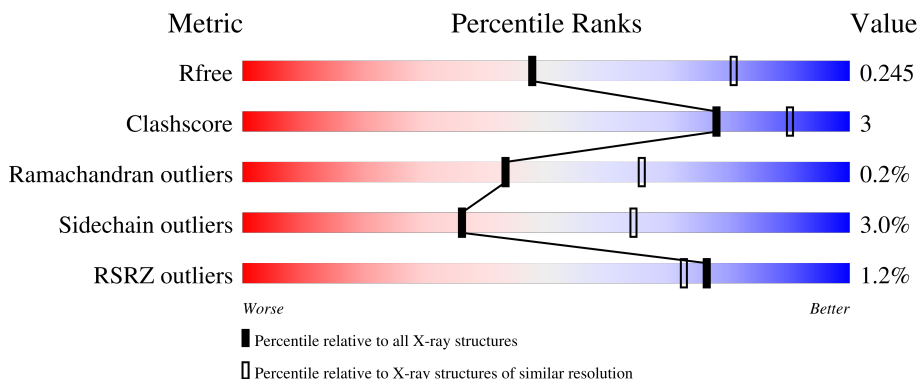
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	87% 7% 5%
1	B	494	86% 9% 5%
1	C	494	89% 7% .
1	D	494	2% 85% 9% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30175 atoms, of which 14760 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	468	Total	C	H	N	O	S	0	0	0
			7408	2391	3680	645	677	15			
1	B	469	Total	C	H	N	O	S	0	0	0
			7377	2397	3639	646	680	15			
1	C	477	Total	C	H	N	O	S	0	0	0
			7479	2432	3684	657	691	15			
1	D	468	Total	C	H	N	O	S	0	0	0
			7368	2393	3637	646	677	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

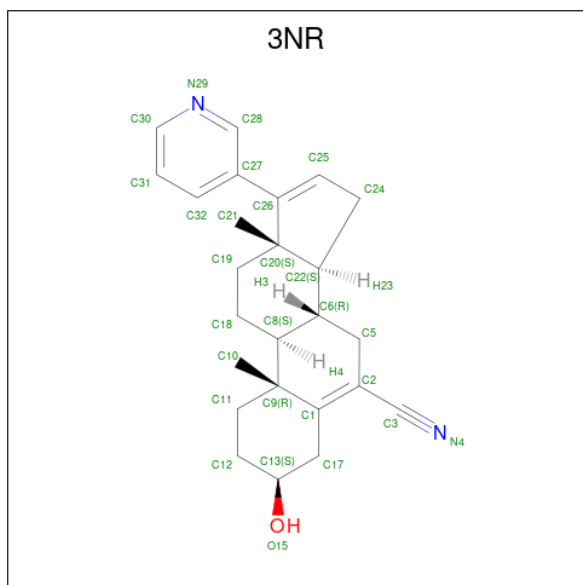
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
2	B	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
2	C	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0



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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 6-cyano-17-(3-pyridyl)-androst-5,16-dien-3-ol (CCD ID: 3NR) (formula: $C_{25}H_{30}N_2O$).



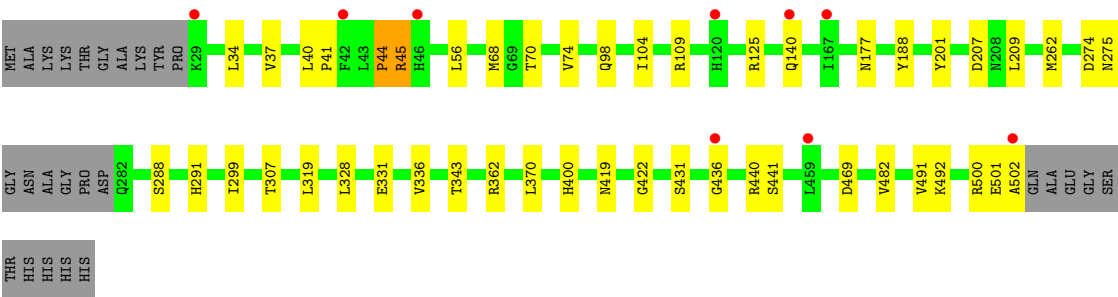
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	25	2	1		
3	B	1	Total	C	N	O	0	0
			28	25	2	1		
3	C	1	Total	C	N	O	0	0
			28	25	2	1		
3	D	1	Total	C	N	O	0	0
			28	25	2	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	38	Total	O	0	0
			38	38		
4	B	41	Total	O	0	0
			41	41		
4	C	40	Total	O	0	0
			40	40		
4	D	20	Total	O	0	0
			20	20		

- 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	89.62Å 153.35Å 169.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.34 – 2.60 38.34 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.34-2.60) 91.3 (38.34-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, R_{free}	0.185 , 0.243 0.189 , 0.245	Depositor DCC
R_{free} test set	3616 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.3	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	30175	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: 3NR, 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	0.11	0/3808	0.30	0/5155
1	B	0.11	0/3819	0.30	0/5170
1	C	0.12	0/3879	0.30	0/5254
1	D	0.12	0/3811	0.32	0/5158
All	All	0.11	0/15317	0.30	0/20737

There are no bond length outliers.

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	3728	3680	3797	22	0
1	B	3738	3639	3804	23	0
1	C	3795	3684	3856	18	0
1	D	3731	3637	3803	25	0
2	A	43	30	30	3	0
2	B	43	30	30	5	0
2	C	43	30	30	2	0
2	D	43	30	30	7	0
3	A	28	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	0	0	0
3	C	28	0	0	0	0
3	D	28	0	0	0	0
4	A	38	0	0	0	0
4	B	41	0	0	0	0
4	C	40	0	0	0	0
4	D	20	0	0	1	0
All	All	15415	14760	15380	86	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 3.

All (86) 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:D:44:PRO:O	1:D:45:ARG:HB2	1.84	0.76
1:A:40:LEU:HD21	1:A:68:MET:HE1	1.68	0.76
1:B:281:ASP:OD1	1:B:282:GLN:N	2.26	0.68
2:C:600:HEM:HHC	2:C:600:HEM:HBB2	1.75	0.67
1:D:288:SER:OG	1:D:291:HIS:ND1	2.24	0.67
1:A:40:LEU:HD12	1:D:68:MET:HE2	1.78	0.65
1:B:274:ASP:C	1:B:280:PRO:HB3	2.22	0.64
1:D:125:ARG:NH1	2:D:600:HEM:O1D	2.32	0.63
1:C:239:ARG:NH1	1:C:240:ASN:OD1	2.31	0.62
1:C:98:GLN:NE2	1:C:103:ASP:OD2	2.33	0.61
1:A:40:LEU:HD21	1:A:68:MET:CE	2.30	0.61
2:B:600:HEM:HBC2	2:B:600:HEM:HMC1	1.81	0.61
2:C:600:HEM:HBC2	2:C:600:HEM:HHD	1.82	0.61
1:D:274:ASP:O	1:D:275:ASN:HB3	2.01	0.60
1:D:209:LEU:HD23	1:D:482:VAL:HG11	1.83	0.59
2:A:600:HEM:HBC2	2:A:600:HEM:HHD	1.86	0.58
2:D:600:HEM:HBC2	2:D:600:HEM:HHD	1.87	0.57
1:B:142:LEU:HD11	1:B:182:ILE:HD11	1.87	0.57
1:B:60:TYR:CD2	1:C:37:VAL:HG21	2.39	0.57
1:B:63:ILE:HG12	1:C:34:LEU:HD22	1.86	0.56
1:C:105:ALA:O	1:C:239:ARG:NH2	2.39	0.55
1:B:60:TYR:CG	1:C:37:VAL:HG21	2.42	0.55
1:A:34:LEU:HD13	1:D:74:VAL:HG22	1.89	0.55
1:A:343:THR:N	1:A:346:ASP:OD2	2.39	0.54
1:A:60:TYR:CG	1:D:37:VAL:HG11	2.42	0.54
2:B:600:HEM:HHA	2:B:600:HEM:HBA2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:600:HEM:HMA2	2:D:600:HEM:HBA1	1.92	0.52
1:A:202:ASN:ND2	3:A:601:3NR:O15	2.41	0.52
1:A:41:PRO:HG3	1:D:37:VAL:O	2.10	0.51
1:B:143:GLU:OE2	1:B:344:ILE:N	2.41	0.51
1:B:330:GLU:O	1:B:334:GLN:HG3	2.11	0.51
2:D:600:HEM:HMB2	2:D:600:HEM:HBB2	1.92	0.50
1:A:370:LEU:HD12	1:A:394:ILE:HB	1.93	0.50
1:B:39:SER:HA	1:C:67:ARG:O	2.12	0.50
1:B:370:LEU:HD22	2:B:600:HEM:HMA1	1.94	0.49
1:B:273:SER:OG	1:B:281:ASP:HB3	2.12	0.49
1:C:105:ALA:HB2	1:C:209:LEU:HD11	1.94	0.49
1:D:98:GLN:HG3	1:D:109:ARG:HD3	1.94	0.49
1:B:40:LEU:HD12	1:C:68:MET:HE2	1.93	0.48
1:B:384:PHE:CG	1:C:34:LEU:HD23	2.48	0.48
1:C:37:VAL:HG13	1:C:37:VAL:O	2.14	0.47
2:A:600:HEM:HBA2	2:A:600:HEM:HHA	1.96	0.47
2:D:600:HEM:HMA2	2:D:600:HEM:CBA	2.44	0.47
1:B:40:LEU:HD21	1:B:68:MET:HE1	1.97	0.47
1:A:351:LEU:HD13	1:A:424:GLN:HA	1.97	0.47
1:D:501:GLU:O	1:D:502:ALA:HB3	2.14	0.46
1:B:156:MET:HE2	1:B:170:PRO:HG3	1.98	0.46
1:C:96:ARG:NH1	1:C:371:ILE:O	2.49	0.46
1:B:105:ALA:O	1:B:239:ARG:NH2	2.47	0.46
1:A:34:LEU:HD13	1:D:74:VAL:CG2	2.46	0.46
1:A:167:ILE:O	1:A:171:VAL:HG12	2.16	0.45
1:A:250:TYR:OH	1:A:264:ASP:OD1	2.34	0.45
1:A:38:GLY:HA3	1:D:40:LEU:HD23	1.99	0.45
1:D:299:ILE:HG23	2:D:600:HEM:HBC1	1.97	0.45
1:A:251:LYS:HA	1:A:267:MET:HE1	1.99	0.45
1:D:262:MET:SD	1:D:299:ILE:HG13	2.58	0.44
1:A:105:ALA:O	1:A:239:ARG:NH2	2.45	0.44
1:D:362:ARG:NH1	1:D:400:HIS:O	2.50	0.44
1:D:419:ASN:OD1	1:D:422:GLY:N	2.46	0.44
1:D:319:LEU:HD21	1:D:491:VAL:HG12	1.99	0.44
1:C:230:GLU:OE1	1:C:230:GLU:N	2.43	0.43
1:D:469:ASP:OD2	1:D:492:LYS:NZ	2.51	0.43
1:B:44:PRO:O	1:B:45:ARG:HB2	2.18	0.43
1:C:209:LEU:HD23	1:C:482:VAL:HG21	2.00	0.43
1:D:370:LEU:HD22	2:D:600:HEM:HMA2	2.00	0.43
1:B:303:GLY:HA2	2:B:600:HEM:HMC3	1.99	0.43
1:A:343:THR:HG22	1:A:345:SER:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:MET:SD	1:A:299:ILE:HG13	2.59	0.42
1:C:198:ILE:HA	1:C:201:TYR:CE2	2.55	0.42
1:D:41:PRO:HD2	4:D:701:HOH:O	2.19	0.42
1:A:136:LYS:O	1:A:137:ASP:C	2.61	0.42
1:B:98:GLN:NE2	1:B:103:ASP:OD2	2.52	0.42
1:B:205:ILE:O	1:B:209:LEU:HB2	2.20	0.42
1:D:177:ASN:OD1	1:D:188:TYR:N	2.50	0.42
1:B:167:ILE:C	1:B:167:ILE:HD12	2.45	0.42
1:A:366:VAL:CG2	2:A:600:HEM:HMB2	2.51	0.41
2:B:600:HEM:HBB2	2:B:600:HEM:HMB2	2.02	0.41
1:C:262:MET:SD	1:C:299:ILE:HG13	2.61	0.41
1:C:273:SER:HA	1:C:281:ASP:OD1	2.20	0.41
1:A:67:ARG:HH21	1:D:41:PRO:HB3	1.85	0.41
1:A:215:VAL:HG21	1:A:393:ILE:HG12	2.02	0.41
1:B:73:THR:CG2	1:B:393:ILE:HD13	2.50	0.41
1:B:136:LYS:HG2	1:B:137:ASP:N	2.35	0.41
1:D:436:GLY:HA3	1:D:441:SER:HA	2.03	0.41
1:D:201:TYR:C	1:D:201:TYR:CD1	2.99	0.40
1:C:371:ILE:O	1:C:372:PRO:C	2.64	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	464/494 (94%)	443 (96%)	21 (4%)	0	100	100
1	B	465/494 (94%)	444 (96%)	21 (4%)	0	100	100
1	C	475/494 (96%)	452 (95%)	22 (5%)	1 (0%)	43	66
1	D	464/494 (94%)	435 (94%)	27 (6%)	2 (0%)	30	51
All	All	1868/1976 (94%)	1774 (95%)	91 (5%)	3 (0%)	43	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	44	PRO
1	D	45	ARG
1	D	44	PRO

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	417/436 (96%)	407 (98%)	10 (2%)	43	70
1	B	419/436 (96%)	407 (97%)	12 (3%)	37	65
1	C	424/436 (97%)	410 (97%)	14 (3%)	33	61
1	D	418/436 (96%)	404 (97%)	14 (3%)	33	61
All	All	1678/1744 (96%)	1628 (97%)	50 (3%)	36	64

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ASP
1	A	207	ASP
1	A	221	LEU
1	A	239	ARG
1	A	244	ASN
1	A	248	GLU
1	A	249	ASN
1	A	284	SER
1	A	319	LEU
1	A	426	ILE
1	B	156	MET
1	B	185	ASN
1	B	216	ASP
1	B	221	LEU
1	B	285	GLU
1	B	339	SER
1	B	344	ILE

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Mol	Chain	Res	Type
1	B	348	ASN
1	B	399	LEU
1	B	430	VAL
1	B	487	ASP
1	B	500	ARG
1	C	37	VAL
1	C	42	PHE
1	C	46	HIS
1	C	75	ILE
1	C	102	LEU
1	C	108	ASN
1	C	194	GLU
1	C	256	SER
1	C	282	GLN
1	C	293	LEU
1	C	344	ILE
1	C	393	ILE
1	C	446	ILE
1	C	497	GLN
1	D	34	LEU
1	D	56	LEU
1	D	70	THR
1	D	104	ILE
1	D	140	GLN
1	D	207	ASP
1	D	307	THR
1	D	328	LEU
1	D	331	GLU
1	D	336	VAL
1	D	343	THR
1	D	431	SER
1	D	440	ARG
1	D	500	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	235	HIS
1	B	78	HIS
1	B	140	GLN
1	B	185	ASN

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Mol	Chain	Res	Type
1	B	200	ASN
1	B	261	ASN
1	C	51	ASN
1	C	52	ASN
1	C	120	HIS
1	C	140	GLN
1	C	401	HIS
1	D	50	HIS
1	D	79	HIS
1	D	185	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 ⓘ

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	1,3	50,50,50	1.40	9 (18%)	67,82,82	1.30	6 (8%)
3	3NR	A	601	2	32,32,32	1.43	5 (15%)	47,50,50	2.38	17 (36%)
3	3NR	B	601	2	32,32,32	1.41	4 (12%)	47,50,50	2.36	15 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	3NR	C	601	2	32,32,32	1.31	4 (12%)	47,50,50	2.45	18 (38%)
3	3NR	D	601	2	32,32,32	1.29	3 (9%)	47,50,50	2.39	16 (34%)
2	HEM	C	600	1,3	50,50,50	1.46	7 (14%)	67,82,82	1.30	10 (14%)
2	HEM	A	600	1,3	50,50,50	1.45	8 (16%)	67,82,82	1.37	12 (17%)
2	HEM	D	600	1,3	50,50,50	1.46	8 (16%)	67,82,82	1.31	10 (14%)

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	1,3	-	6/14/54/54	-
3	3NR	A	601	2	-	0/4/67/67	0/5/5/5
3	3NR	B	601	2	-	1/4/67/67	0/5/5/5
3	3NR	C	601	2	-	0/4/67/67	0/5/5/5
3	3NR	D	601	2	-	0/4/67/67	0/5/5/5
2	HEM	C	600	1,3	-	4/14/54/54	-
2	HEM	A	600	1,3	-	5/14/54/54	-
2	HEM	D	600	1,3	-	3/14/54/54	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	3NR	C20-C26	-5.15	1.49	1.53
3	A	601	3NR	C20-C26	-5.14	1.49	1.53
3	D	601	3NR	C20-C26	-5.04	1.49	1.53
2	D	600	HEM	FE-NC	4.65	2.10	1.95
3	B	601	3NR	C20-C26	-4.60	1.49	1.53
2	A	600	HEM	FE-NC	4.25	2.09	1.95
2	C	600	HEM	FE-NC	3.88	2.08	1.95
3	B	601	3NR	C1-C2	-3.75	1.30	1.35
2	D	600	HEM	FE-ND	3.53	2.05	1.94
2	B	600	HEM	FE-NA	3.45	2.06	1.95
2	C	600	HEM	FE-NA	3.35	2.06	1.95
3	A	601	3NR	C1-C2	-3.27	1.31	1.35
2	A	600	HEM	FE-NA	3.22	2.05	1.95
2	D	600	HEM	CAB-C3B	3.21	1.55	1.47
2	B	600	HEM	CAB-C3B	3.18	1.55	1.47
2	A	600	HEM	CAC-C3C	3.16	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	HEM	CAC-C3C	3.16	1.55	1.47
2	C	600	HEM	CAB-C3B	3.12	1.55	1.47
2	D	600	HEM	CAC-C3C	3.11	1.55	1.47
2	C	600	HEM	FE-NB	3.02	2.04	1.94
2	B	600	HEM	CAC-C3C	3.01	1.55	1.47
2	B	600	HEM	FE-NB	3.01	2.04	1.94
2	B	600	HEM	FE-NC	2.95	2.04	1.95
2	A	600	HEM	CAB-C3B	2.93	1.55	1.47
2	C	600	HEM	FE-ND	2.70	2.03	1.94
3	A	601	3NR	C9-C8	-2.70	1.51	1.56
3	B	601	3NR	C9-C8	-2.65	1.51	1.56
3	D	601	3NR	C1-C2	-2.62	1.32	1.35
2	A	600	HEM	FE-ND	2.59	2.02	1.94
3	C	601	3NR	C9-C1	-2.51	1.50	1.53
2	D	600	HEM	FE-NB	2.47	2.02	1.94
3	C	601	3NR	C9-C8	-2.36	1.52	1.56
2	A	600	HEM	FE-NB	2.35	2.02	1.94
3	B	601	3NR	C9-C1	-2.21	1.50	1.53
3	C	601	3NR	C24-C25	2.19	1.53	1.50
2	B	600	HEM	FE-ND	2.18	2.01	1.94
3	A	601	3NR	C24-C25	2.17	1.53	1.50
3	D	601	3NR	C24-C25	2.16	1.53	1.50
3	A	601	3NR	C9-C1	-2.13	1.50	1.53
2	A	600	HEM	CMD-C2D	2.11	1.55	1.50
2	A	600	HEM	CMA-C3A	2.10	1.55	1.50
2	D	600	HEM	CMD-C2D	2.06	1.55	1.50
2	D	600	HEM	CMC-C2C	2.06	1.55	1.50
2	B	600	HEM	CMC-C2C	2.05	1.55	1.50
2	B	600	HEM	C2A-C3A	-2.05	1.33	1.38
2	D	600	HEM	CMB-C2B	2.02	1.54	1.50
2	B	600	HEM	CMB-C2B	2.01	1.54	1.50
2	C	600	HEM	CMD-C2D	2.01	1.54	1.50

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	3NR	C24-C22-C20	-9.95	97.08	104.05
3	D	601	3NR	C24-C22-C20	-9.89	97.12	104.05
3	B	601	3NR	C24-C22-C20	-9.62	97.31	104.05
3	C	601	3NR	C24-C22-C20	-8.94	97.79	104.05
3	C	601	3NR	C20-C22-C6	-6.00	106.81	113.13
3	B	601	3NR	C24-C22-C6	-4.68	116.67	121.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	3NR	C20-C22-C6	-4.43	108.46	113.13
3	D	601	3NR	C20-C22-C6	-4.41	108.48	113.13
3	B	601	3NR	C20-C22-C6	-4.38	108.52	113.13
3	B	601	3NR	C5-C6-C22	-4.25	105.97	111.22
3	D	601	3NR	C22-C6-C8	-4.06	103.78	109.09
3	A	601	3NR	C24-C22-C6	-4.02	117.37	121.63
3	C	601	3NR	C24-C22-C6	-3.96	117.43	121.63
3	D	601	3NR	C24-C25-C26	-3.95	109.14	112.56
3	A	601	3NR	C24-C25-C26	-3.92	109.16	112.56
3	D	601	3NR	C5-C6-C22	-3.84	106.48	111.22
3	C	601	3NR	C13-C17-C1	-3.80	105.96	112.07
3	C	601	3NR	C22-C6-C8	-3.79	104.13	109.09
3	D	601	3NR	C24-C22-C6	-3.74	117.66	121.63
3	C	601	3NR	C17-C1-C9	3.64	118.61	114.95
3	B	601	3NR	C24-C25-C26	-3.60	109.44	112.56
3	C	601	3NR	C5-C6-C22	-3.56	106.82	111.22
3	A	601	3NR	C5-C6-C22	-3.55	106.83	111.22
3	C	601	3NR	C24-C25-C26	-3.54	109.49	112.56
3	A	601	3NR	C17-C1-C9	3.51	118.48	114.95
3	B	601	3NR	C17-C1-C9	3.43	118.40	114.95
2	B	600	HEM	CAA-C2A-C1A	3.29	131.37	124.94
2	C	600	HEM	C3B-C2B-C1B	3.21	108.82	106.41
3	B	601	3NR	C22-C6-C8	-3.16	104.95	109.09
3	C	601	3NR	C21-C20-C22	-3.15	108.47	112.99
3	B	601	3NR	C17-C1-C2	-3.08	117.63	122.47
3	C	601	3NR	C22-C20-C26	2.98	102.02	99.50
3	D	601	3NR	C13-C17-C1	-2.94	107.35	112.07
3	A	601	3NR	C22-C6-C8	-2.87	105.34	109.09
2	D	600	HEM	CHC-C1C-NC	2.86	127.57	124.45
3	D	601	3NR	C17-C1-C2	-2.85	117.99	122.47
3	A	601	3NR	C13-C17-C1	-2.83	107.52	112.07
2	A	600	HEM	CAA-CBA-CGA	-2.82	106.19	113.67
3	C	601	3NR	C17-C1-C2	-2.80	118.07	122.47
2	B	600	HEM	C4D-ND-C1D	2.78	108.50	105.21
3	D	601	3NR	C17-C1-C9	2.76	117.72	114.95
2	A	600	HEM	C4D-ND-C1D	2.76	108.47	105.21
3	C	601	3NR	C30-N29-C28	2.72	121.62	116.85
2	B	600	HEM	CAA-C2A-C3A	-2.72	120.97	127.07
2	A	600	HEM	CAA-C2A-C1A	2.72	130.25	124.94
3	B	601	3NR	C30-N29-C28	2.72	121.61	116.85
3	A	601	3NR	C30-N29-C28	2.71	121.60	116.85
3	C	601	3NR	C10-C9-C8	-2.71	108.62	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	HEM	CAA-CBA-CGA	-2.71	106.49	113.67
2	B	600	HEM	C3D-C4D-ND	-2.69	107.22	110.17
2	B	600	HEM	C2A-C1A-NA	-2.63	107.23	110.15
3	A	601	3NR	C10-C9-C8	-2.63	108.71	111.66
3	D	601	3NR	C31-C32-C27	-2.61	117.80	120.36
3	A	601	3NR	C18-C19-C20	-2.59	107.27	112.78
2	A	600	HEM	C3D-C4D-ND	-2.58	107.34	110.17
3	B	601	3NR	C21-C20-C22	-2.55	109.33	112.99
2	D	600	HEM	CAC-C3C-C4C	2.55	130.90	124.82
3	C	601	3NR	C8-C9-C1	2.53	112.86	109.29
2	A	600	HEM	C2A-C1A-NA	-2.53	107.35	110.15
2	A	600	HEM	CAC-C3C-C4C	2.52	130.84	124.82
2	D	600	HEM	CHD-C4C-C3C	2.52	129.46	125.21
3	B	601	3NR	C10-C9-C8	-2.52	108.83	111.66
2	C	600	HEM	C1B-NB-C4B	2.52	108.19	105.21
3	A	601	3NR	C17-C1-C2	-2.48	118.58	122.47
3	D	601	3NR	C30-N29-C28	2.45	121.15	116.85
3	D	601	3NR	C21-C20-C22	-2.43	109.50	112.99
2	A	600	HEM	CHD-C4C-C3C	2.42	129.30	125.21
3	B	601	3NR	C8-C9-C1	2.42	112.70	109.29
3	B	601	3NR	C31-C32-C27	-2.42	117.99	120.36
3	B	601	3NR	C18-C19-C20	-2.41	107.65	112.78
3	B	601	3NR	C13-C17-C1	-2.40	108.20	112.07
3	D	601	3NR	C10-C9-C8	-2.40	108.97	111.66
2	B	600	HEM	CHD-C1D-ND	2.40	127.01	124.42
2	C	600	HEM	CHC-C1C-NC	2.39	127.05	124.45
3	C	601	3NR	C18-C8-C9	-2.38	110.14	113.08
3	D	601	3NR	C18-C19-C20	-2.35	107.78	112.78
2	C	600	HEM	C3C-C2C-C1C	2.34	109.26	107.05
3	A	601	3NR	C5-C6-C8	-2.34	108.31	110.90
2	C	600	HEM	CAC-C3C-C4C	2.33	130.38	124.82
3	C	601	3NR	C31-C32-C27	-2.32	118.08	120.36
2	C	600	HEM	C4D-ND-C1D	2.32	107.95	105.21
2	D	600	HEM	CHA-C4D-ND	2.31	127.23	124.37
2	A	600	HEM	CAA-C2A-C3A	-2.28	121.96	127.07
2	A	600	HEM	CHD-C1D-ND	2.28	126.88	124.42
3	D	601	3NR	C8-C9-C1	2.25	112.46	109.29
3	A	601	3NR	C31-C32-C27	-2.24	118.16	120.36
3	C	601	3NR	C18-C19-C20	-2.22	108.06	112.78
3	A	601	3NR	C12-C13-C17	-2.21	107.18	110.29
2	C	600	HEM	C3B-C4B-NB	-2.21	107.88	109.47
2	D	600	HEM	C2D-C1D-ND	-2.19	107.37	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	HEM	CHD-C4C-C3C	2.19	128.90	125.21
2	A	600	HEM	C2D-C1D-ND	-2.17	107.39	109.90
2	C	600	HEM	CHA-C4D-ND	2.17	127.05	124.37
2	C	600	HEM	C2D-C1D-ND	-2.16	107.40	109.90
2	A	600	HEM	CHC-C1C-NC	2.15	126.79	124.45
2	A	600	HEM	CHA-C4D-ND	2.12	126.99	124.37
2	D	600	HEM	C4D-ND-C1D	2.11	107.71	105.21
2	D	600	HEM	CAA-C2A-C1A	-2.08	120.88	124.94
3	C	601	3NR	C12-C13-C17	-2.06	107.39	110.29
3	A	601	3NR	C22-C20-C26	2.06	101.25	99.50
2	D	600	HEM	C3C-C2C-C1C	2.05	108.99	107.05
2	D	600	HEM	CAC-C3C-C2C	-2.05	121.78	128.43
3	A	601	3NR	C21-C20-C22	-2.03	110.08	112.99
3	D	601	3NR	C18-C8-C9	-2.02	110.60	113.08

There are no chirality outliers.

All (19) torsion outliers are listed below:

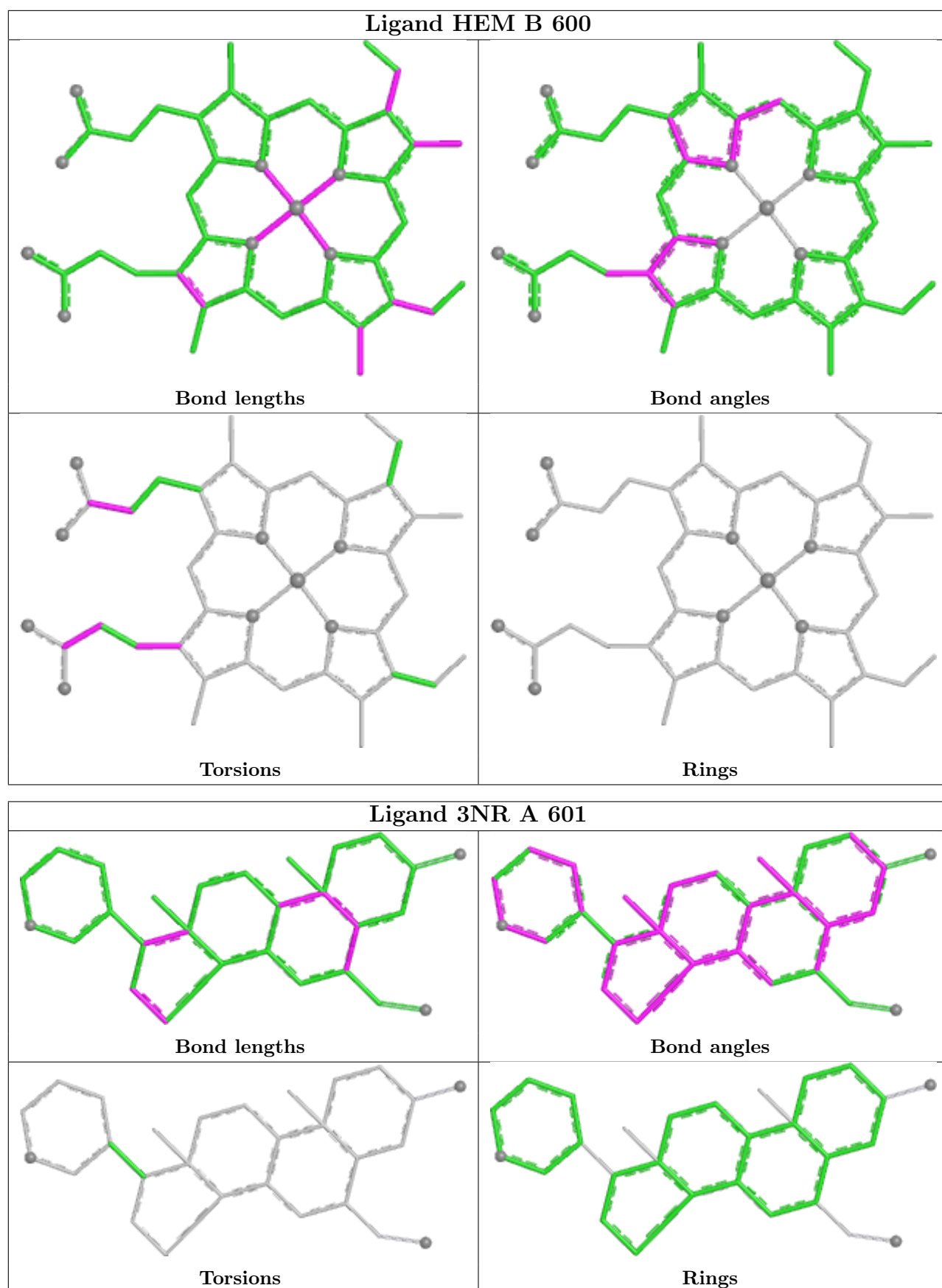
Mol	Chain	Res	Type	Atoms
2	A	600	HEM	C1A-C2A-CAA-CBA
2	D	600	HEM	C3A-C2A-CAA-CBA
2	B	600	HEM	C1A-C2A-CAA-CBA
2	D	600	HEM	C1A-C2A-CAA-CBA
2	A	600	HEM	C3A-C2A-CAA-CBA
2	B	600	HEM	C3A-C2A-CAA-CBA
2	A	600	HEM	C4C-C3C-CAC-CBC
2	C	600	HEM	C4B-C3B-CAB-CBB
2	C	600	HEM	C4C-C3C-CAC-CBC
2	D	600	HEM	C4C-C3C-CAC-CBC
2	B	600	HEM	CAA-CBA-CGA-O1A
2	A	600	HEM	CAA-CBA-CGA-O2A
2	A	600	HEM	CAA-CBA-CGA-O1A
2	B	600	HEM	CAA-CBA-CGA-O2A
3	B	601	3NR	C25-C26-C27-C28
2	C	600	HEM	CAD-CBD-CGD-O2D
2	B	600	HEM	CAD-CBD-CGD-O1D
2	C	600	HEM	CAD-CBD-CGD-O1D
2	B	600	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

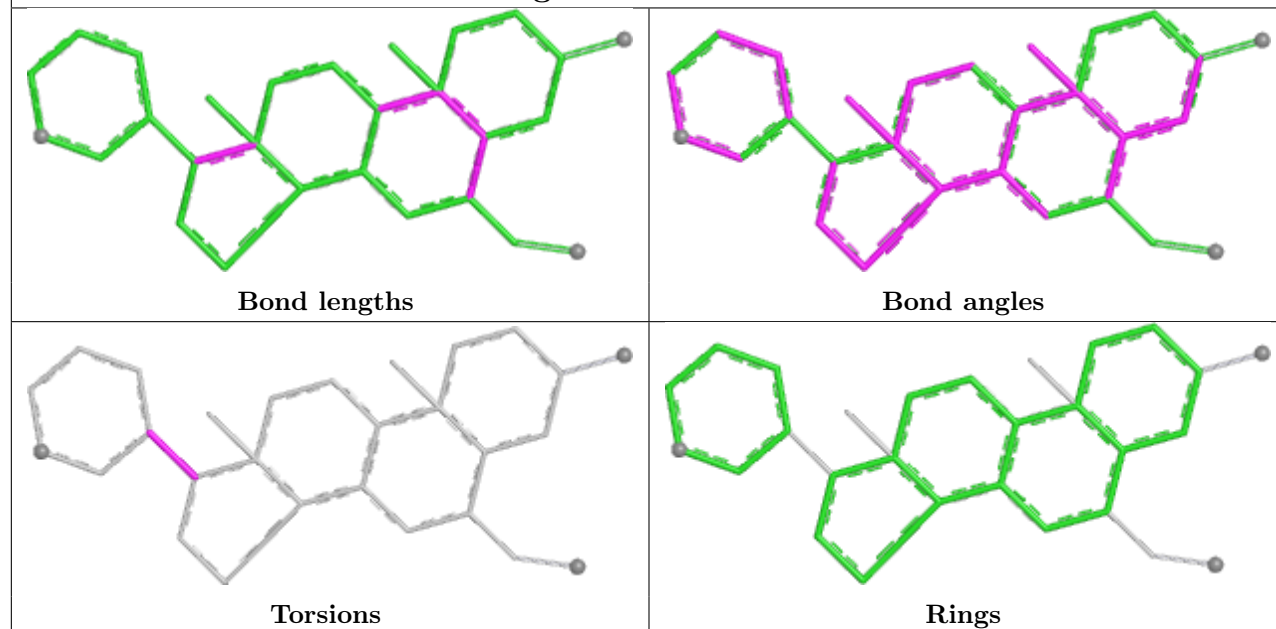
5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	HEM	5	0
3	A	601	3NR	1	0
2	C	600	HEM	2	0
2	A	600	HEM	3	0
2	D	600	HEM	7	0

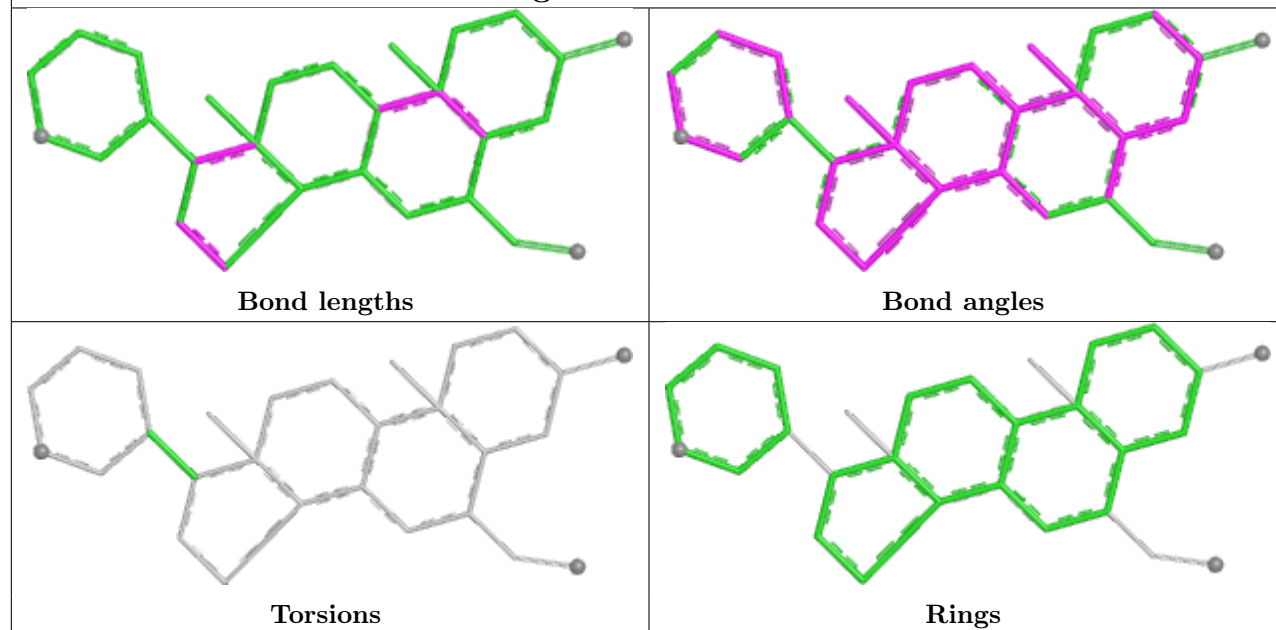
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



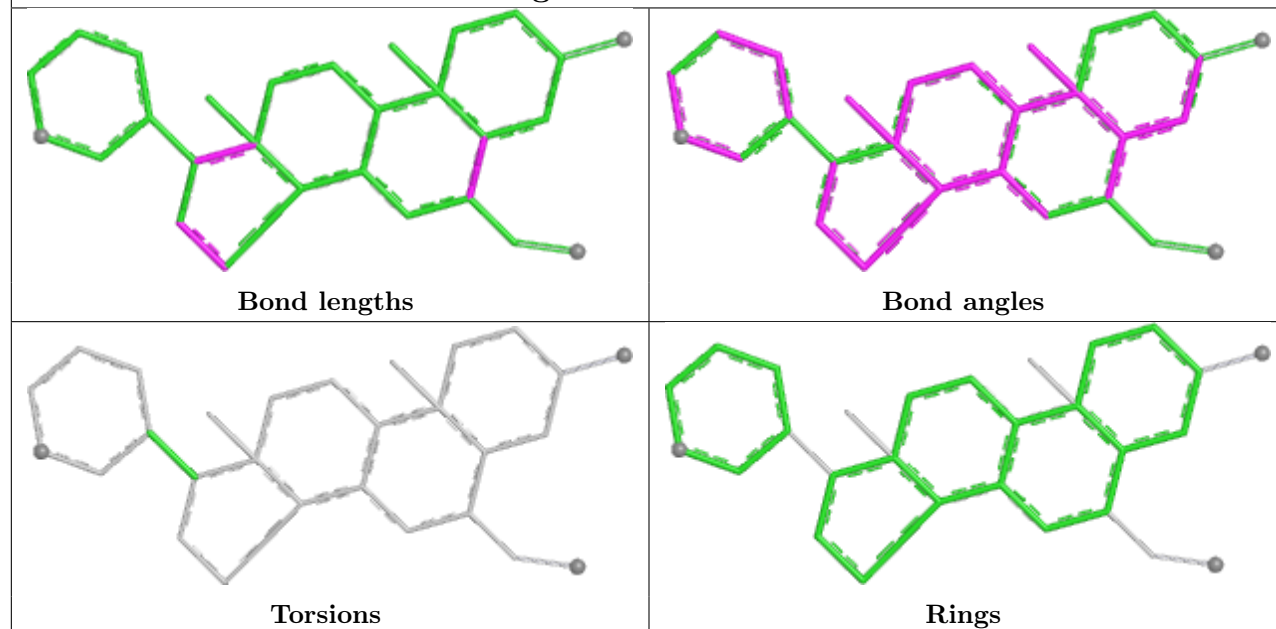
Ligand 3NR B 601



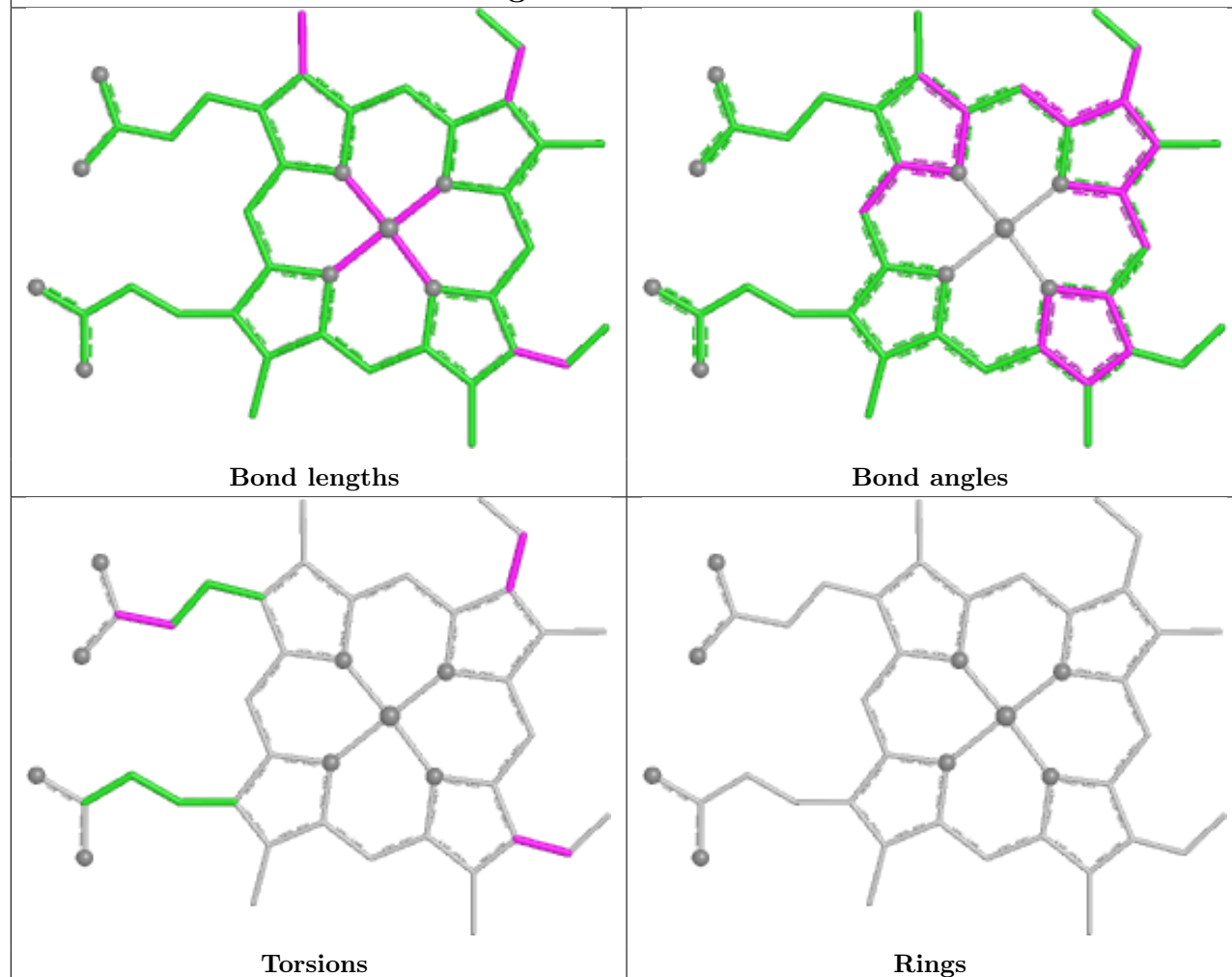
Ligand 3NR C 601

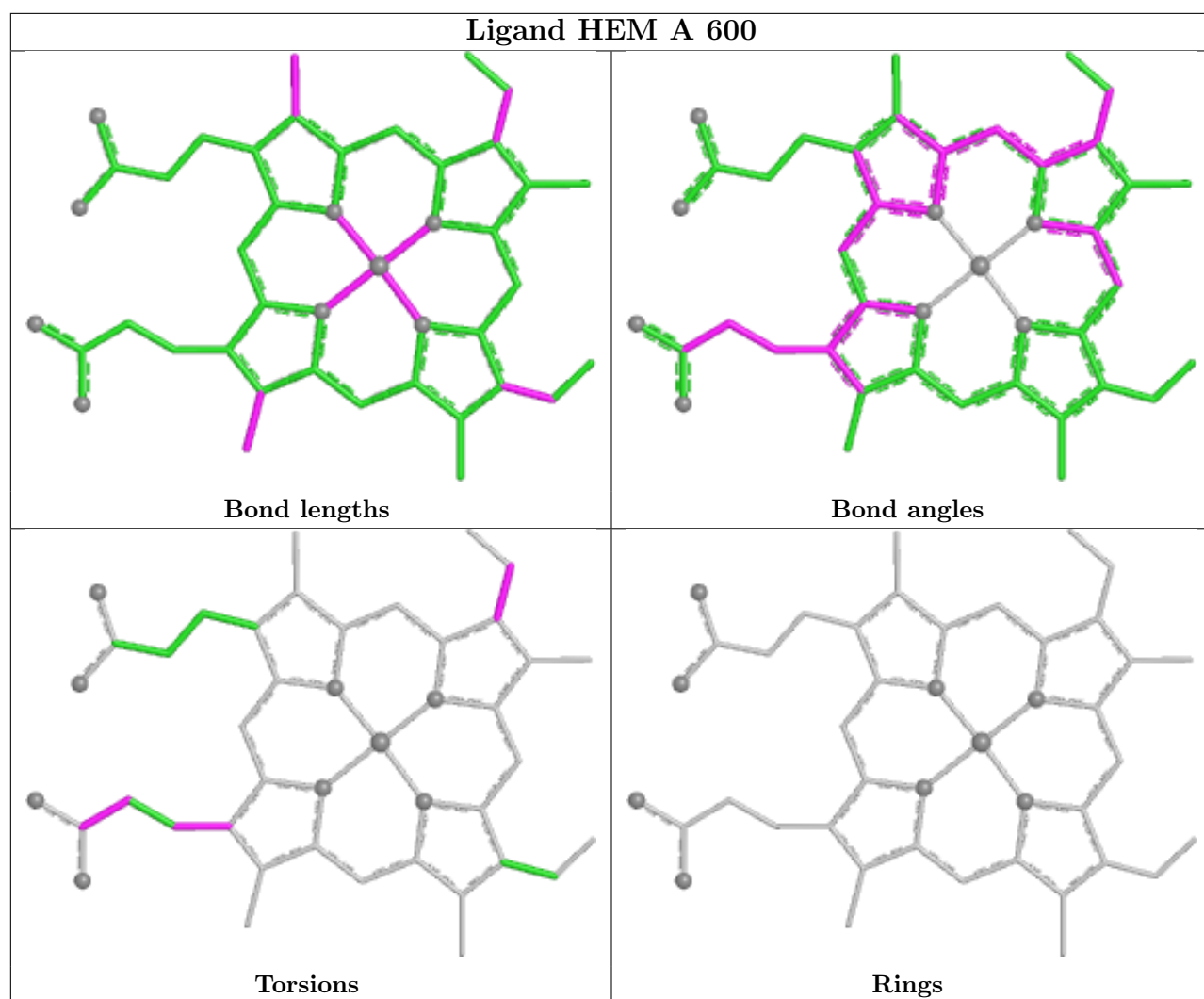


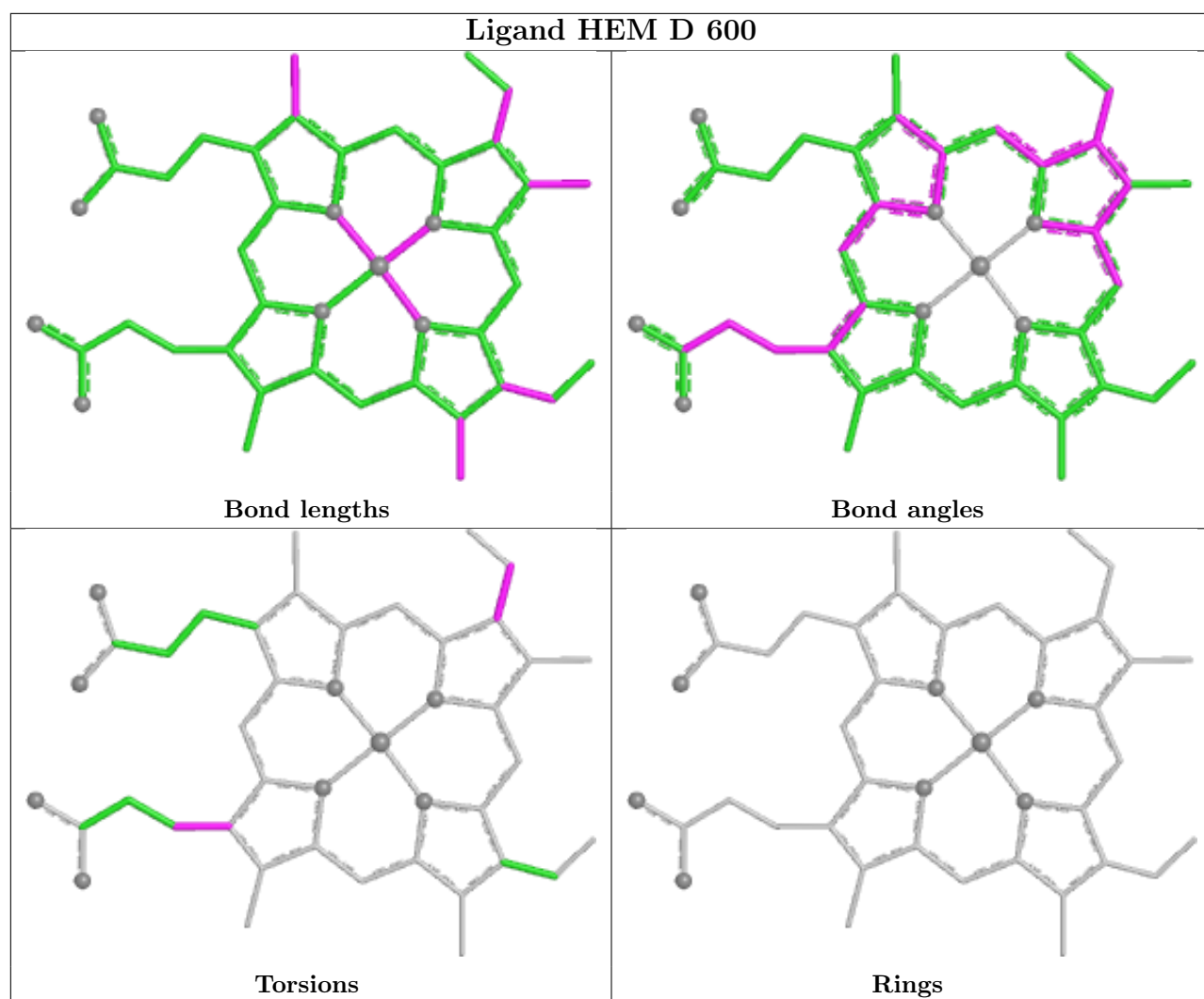
Ligand 3NR D 601



Ligand HEM C 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	468/494 (94%)	-0.11	4 (0%) 81 78	38, 57, 91, 146	0
1	B	469/494 (94%)	-0.15	3 (0%) 85 83	38, 55, 90, 131	0
1	C	477/494 (96%)	-0.05	7 (1%) 72 68	37, 57, 99, 131	0
1	D	468/494 (94%)	0.20	9 (1%) 66 61	41, 66, 108, 137	0
All	All	1882/1976 (95%)	-0.03	23 (1%) 76 73	37, 59, 100, 146	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	504	ALA	3.5
1	D	502	ALA	3.5
1	C	27	TYR	3.3
1	D	29	LYS	2.9
1	D	42	PHE	2.8
1	B	403	GLU	2.6
1	C	316	ALA	2.6
1	C	46	HIS	2.4
1	A	274	ASP	2.4
1	C	277	ASN	2.3
1	D	459	LEU	2.3
1	B	280	PRO	2.3
1	C	42	PHE	2.2
1	D	120	HIS	2.2
1	C	280	PRO	2.2
1	D	436	GLY	2.2
1	A	470	ASP	2.1
1	C	282	GLN	2.1
1	D	46	HIS	2.1
1	D	140	GLN	2.1
1	D	167	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	136	LYS	2.0
1	B	140	GLN	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](#)

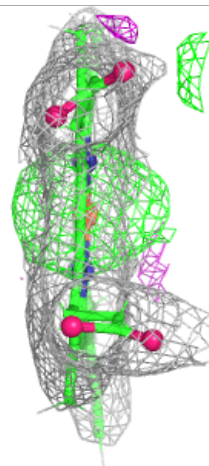
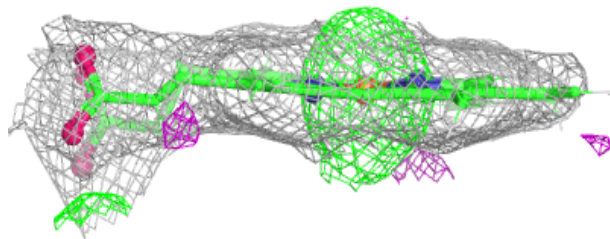
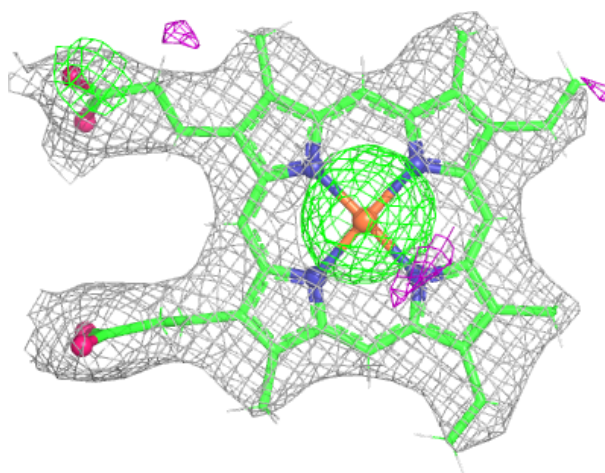
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	D	600	43/43	0.86	0.12	34,49,70,156	0
3	3NR	D	601	28/28	0.94	0.11	33,43,54,55	0
3	3NR	B	601	28/28	0.95	0.09	34,43,51,61	0
3	3NR	C	601	28/28	0.95	0.10	34,42,48,53	0
3	3NR	A	601	28/28	0.95	0.11	29,41,52,63	0
2	HEM	C	600	43/43	0.97	0.09	30,43,54,60	0
2	HEM	A	600	43/43	0.98	0.08	34,44,57,69	0
2	HEM	B	600	43/43	0.98	0.09	27,41,59,63	0

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

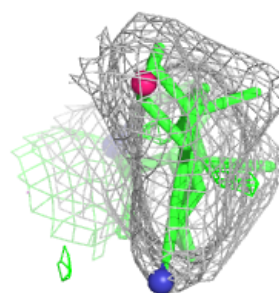
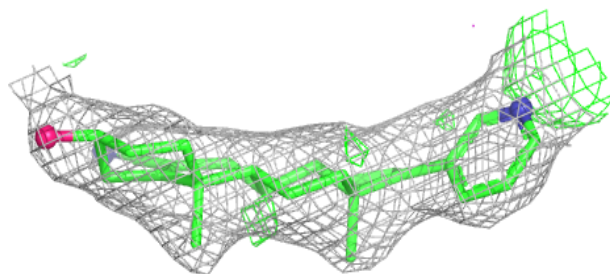
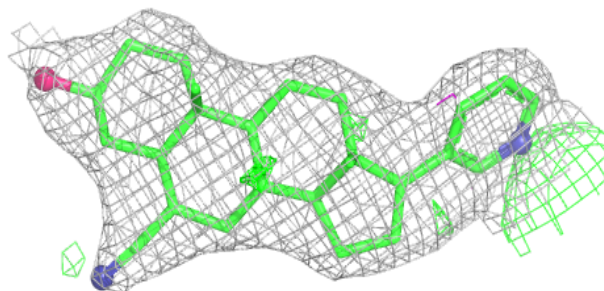
Electron density around HEM D 600:

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

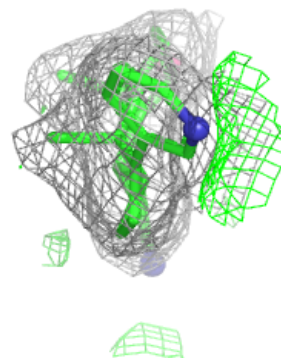
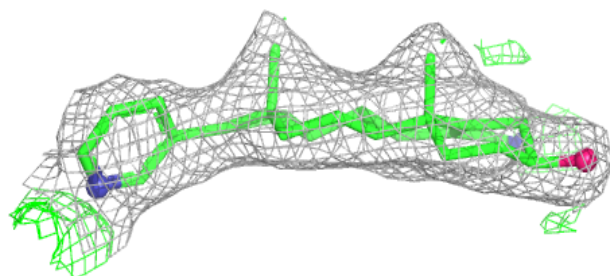
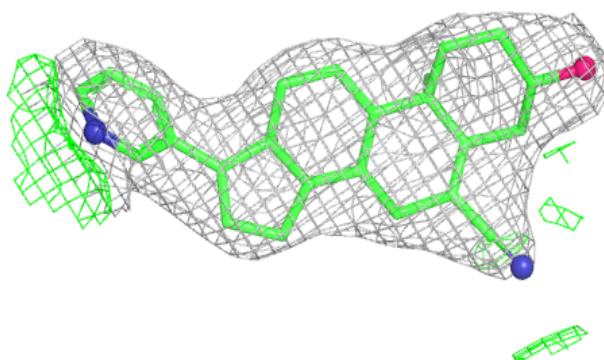


Electron density around 3NR D 601:

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

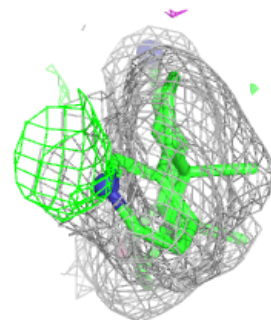
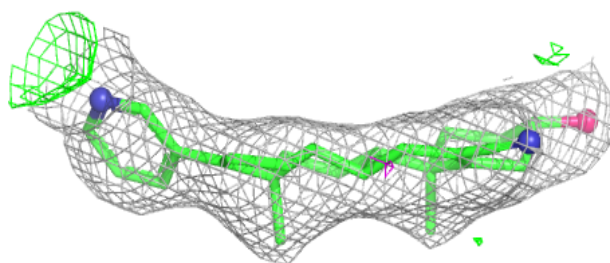
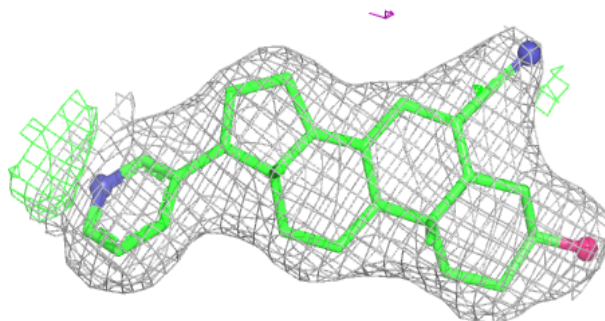
**Electron density around 3NR B 601:**

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

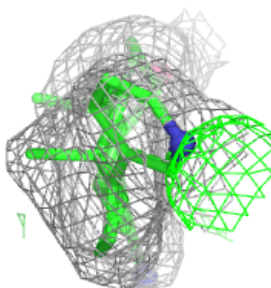
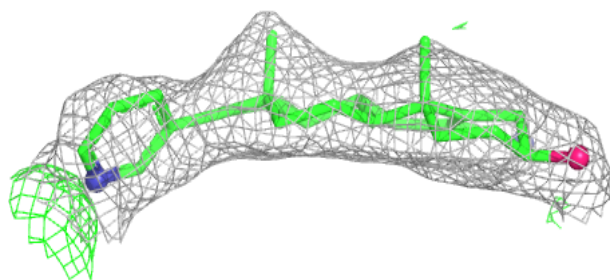
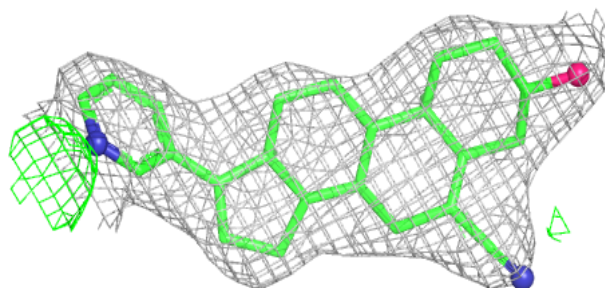


Electron density around 3NR C 601:

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

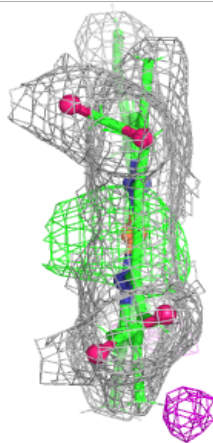
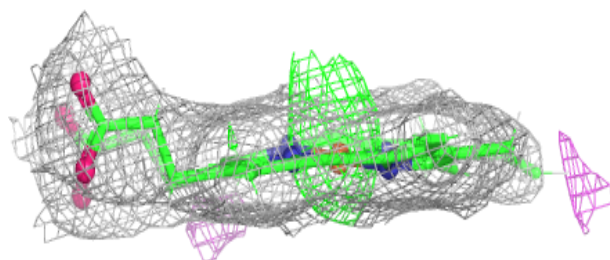
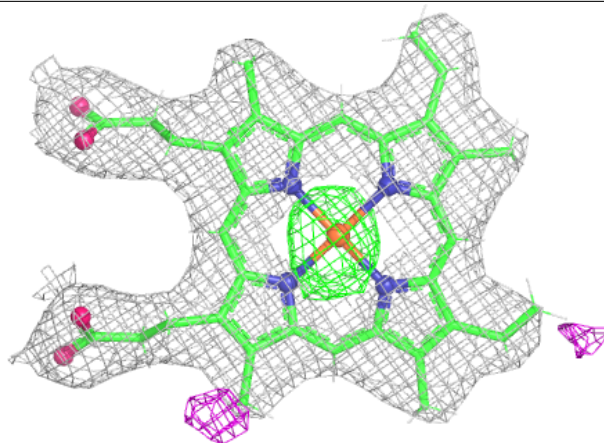
**Electron density around 3NR A 601:**

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



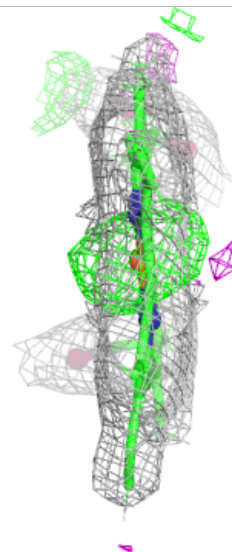
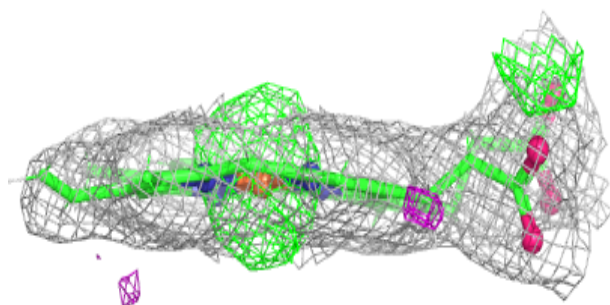
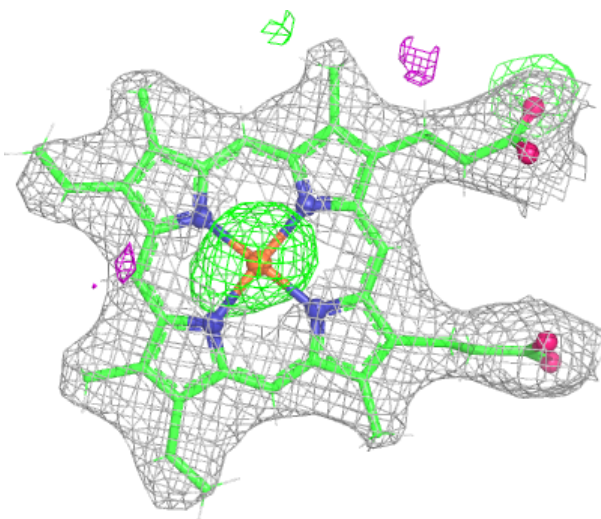
Electron density around HEM C 600:

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



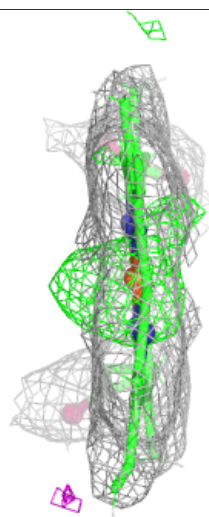
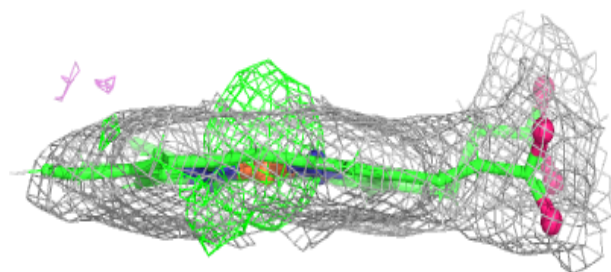
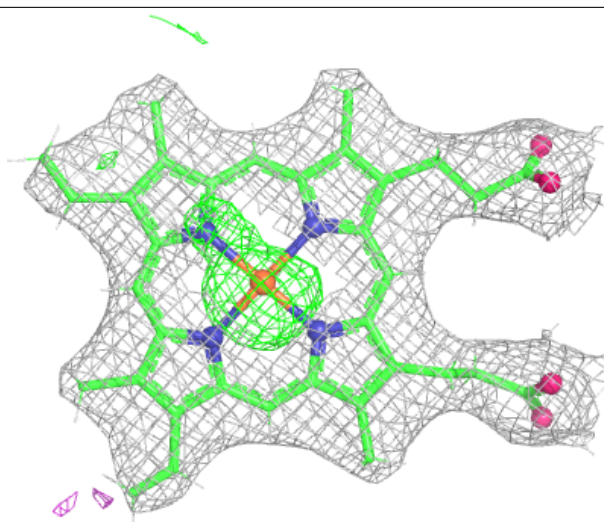
Electron density around HEM A 600:

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



Electron density around HEM 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.