



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:44 PM UTC

PDB ID : 8FDA / pdb_00008fda
Title : Human Cytochrome P450 17A1 in complex with steroidal isonitrile inhibitor
Authors : Richard, A.M.; Scott, E.E.
Deposited on : 2022-12-02
Resolution : 2.20 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

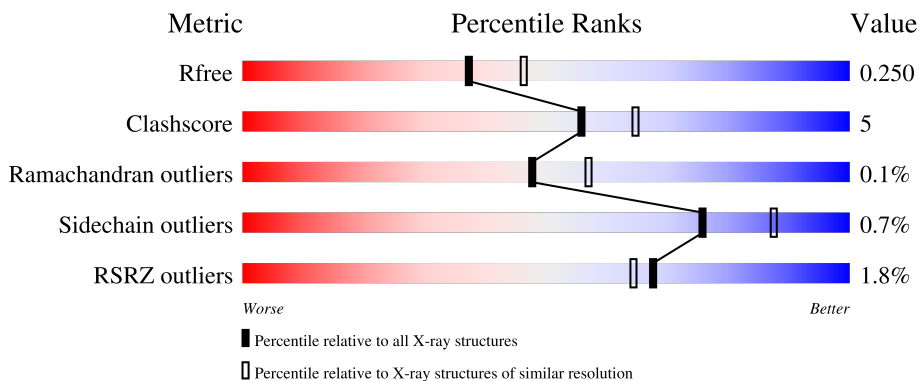
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


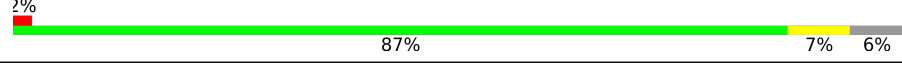
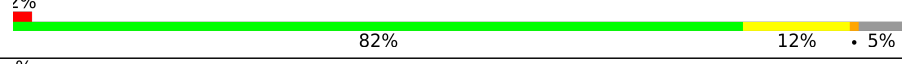

The reported resolution of this entry is 2.20 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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% 85% 10% 5%
1	B	494	 2% 87% 7% 6%
1	C	494	 2% 82% 12% 5%
1	D	494	 2% 87% 7% 6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 30965 atoms, of which 15498 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	
			Total	C	H	N	O				S
1	A	467	7524	2390	3802	644	673	15	0	0	0
1	B	465	7487	2379	3781	641	671	15	0	0	0
1	C	467	7523	2391	3797	645	675	15	0	1	0
1	D	466	7505	2385	3788	643	674	15	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

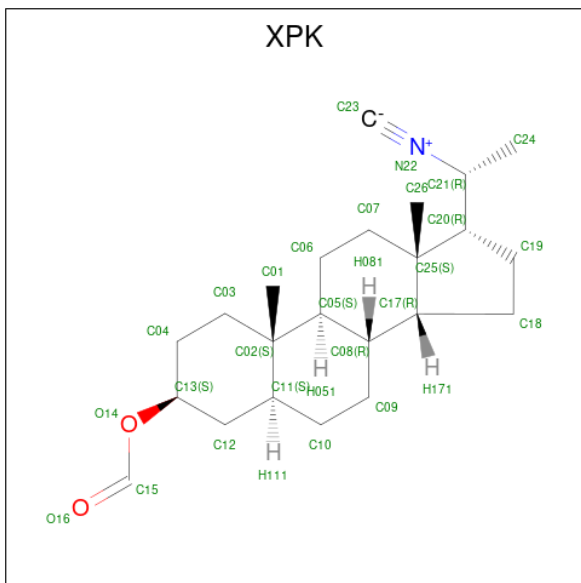
Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	initiating methionine	UNP P05093
A	20	ALA	-	expression tag	UNP P05093
A	21	LYS	-	expression tag	UNP P05093
A	22	LYS	-	expression tag	UNP P05093
A	23	THR	-	expression tag	UNP P05093
A	509	HIS	-	expression tag	UNP P05093
A	510	HIS	-	expression 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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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 [(1 {R})-1-[(3 {S},5 {S},8 {R},9 {S},10 {S},13 {S},17 {R})-3-methanoyloxy-10,13-dimethyl-1,2,3,4,5,6,7,8,9,11,12,13,14,15,16,17-hexadecahydrocyclopenta[a]phenanthren-17-yl]ethyl]-methylidyne-azanium (CCD ID: XPK) (formula: C₂₃H₃₅NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			61	23	35	1	2		
3	B	1	Total	C	H	N	O	0	0
			61	23	35	1	2		
3	C	1	Total	C	H	N	O	0	0
			61	23	35	1	2		
3	C	1	Total	C	H	N	O	0	0
			61	23	35	1	2		
3	D	1	Total	C	H	N	O	0	0
			61	23	35	1	2		
3	D	1	Total	C	H	N	O	0	0
			61	23	35	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	70	Total	O	0	0
			70	70		

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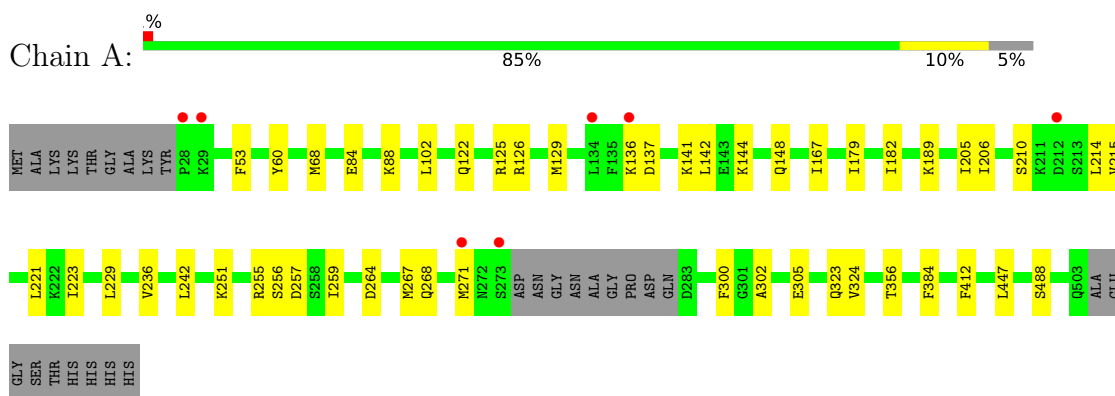
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	76	Total 76	O 76	0	0
4	C	48	Total 48	O 48	0	0
4	D	74	Total 74	O 74	0	0

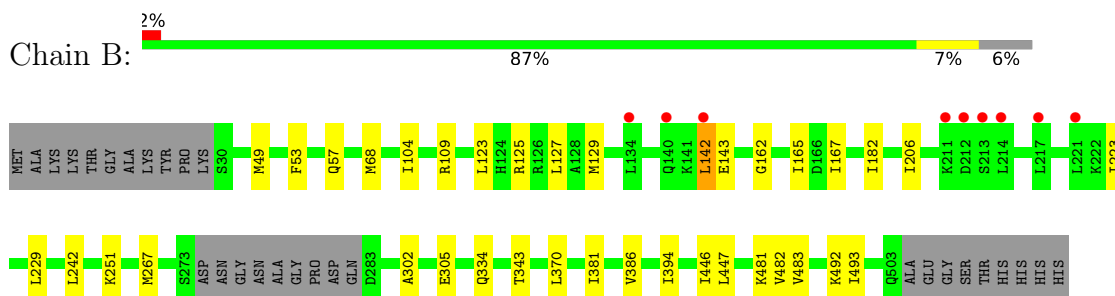
3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

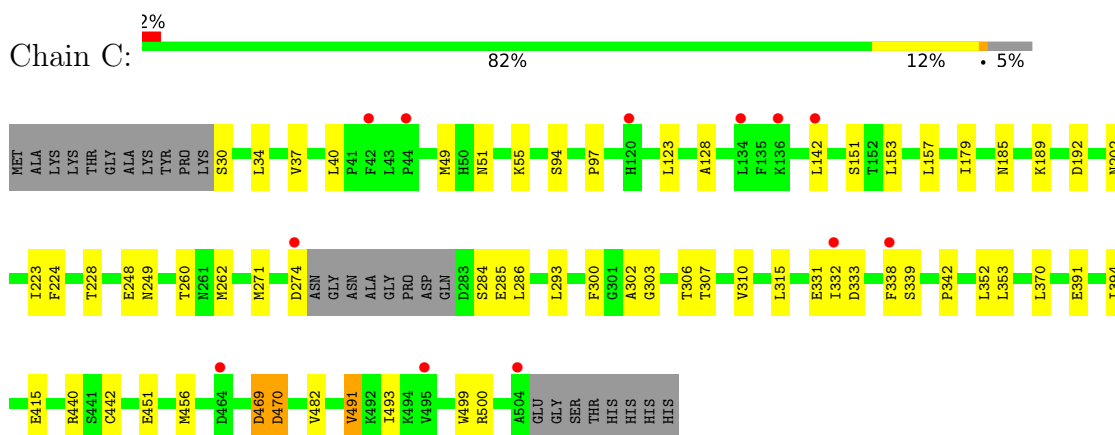
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase




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

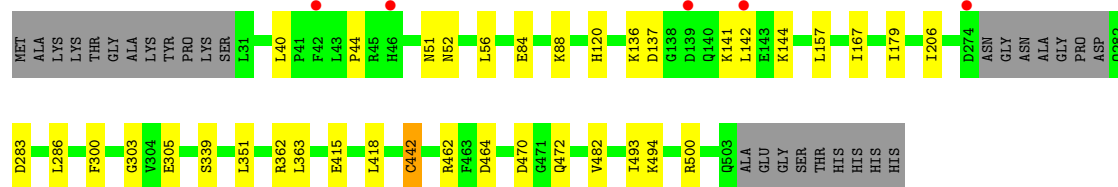


- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase



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

Chain D:  %



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.13Å 152.28Å 171.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.96 – 2.20 38.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.96-2.20) 84.8 (38.96-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.78 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.216 , 0.259 (Not available) , 0.250	Depositor DCC
R_{free} test set	2000 reflections (1.77%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtrriage
Anisotropy	0.585	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	30965	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0514e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.17	0/3803	0.33	0/5147
1	B	0.22	0/3786	0.36	0/5125
1	C	0.25	0/3810	0.36	0/5158
1	D	0.26	1/3797 (0.0%)	0.33	0/5140
All	All	0.23	1/15196 (0.0%)	0.34	0/20570

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	442	CYS	C-O	-6.17	1.16	1.23

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	3722	3802	3801	40	0
1	B	3706	3781	3780	27	0
1	C	3726	3797	3796	46	0
1	D	3717	3788	3787	27	0
2	A	43	30	30	1	0
2	B	43	30	30	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	43	30	30	5	0
2	D	43	30	30	5	0
3	A	26	35	0	1	0
3	B	26	35	0	2	0
3	C	52	70	0	3	0
3	D	52	70	0	5	0
4	A	70	0	0	0	0
4	B	76	0	0	2	0
4	C	48	0	0	5	0
4	D	74	0	0	0	0
All	All	15467	15498	15284	144	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (144) 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:C:315:LEU:CD1	1:C:456:MET:HE1	2.18	0.73
1:A:68:MET:HE1	1:C:40:LEU:HD12	1.71	0.71
1:B:165:ILE:HD11	1:B:493:ILE:HD12	1.72	0.70
1:C:500:ARG:HG2	1:C:500:ARG:HH11	1.57	0.69
1:A:447:LEU:HD23	2:A:600:HEM:HBC2	1.74	0.69
2:D:600:HEM:HBB2	2:D:600:HEM:HHC	1.75	0.68
1:A:189:LYS:HD2	1:A:189:LYS:H	1.57	0.68
1:C:353:LEU:HD11	1:C:456:MET:HB3	1.76	0.68
2:C:600:HEM:HHC	2:C:600:HEM:HBB2	1.78	0.64
1:B:68:MET:SD	1:D:40:LEU:HD12	2.39	0.63
1:A:142:LEU:HD11	1:A:182:ILE:HD11	1.81	0.62
1:C:315:LEU:HD11	1:C:456:MET:HE1	1.80	0.61
1:A:142:LEU:HD21	1:A:447:LEU:HD13	1.82	0.61
1:D:442:CYS:HB2	2:D:600:HEM:NA	2.16	0.60
1:D:362:ARG:NH2	1:D:363:LEU:HD13	2.17	0.59
1:C:415:GLU:OE1	1:C:415:GLU:N	2.36	0.58
1:A:255:ARG:HB3	1:A:257:ASP:OD1	2.02	0.58
2:C:600:HEM:HBC2	2:C:600:HEM:HMC2	1.85	0.58
1:C:128:ALA:HA	1:C:262:MET:HE2	1.86	0.58
1:B:109:ARG:HH11	1:B:109:ARG:HG3	1.69	0.57
1:A:102:LEU:HD21	1:A:214:LEU:HD21	1.87	0.57
2:B:600:HEM:HBB2	2:B:600:HEM:HMB2	1.86	0.56
1:B:447:LEU:HD23	2:B:600:HEM:HBC2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ARG:HG2	1:A:129:MET:HE2	1.87	0.55
1:C:274:ASP:OD1	1:C:284:SER:OG	2.24	0.55
1:C:97:PRO:HG3	1:C:391:GLU:HG3	1.87	0.55
1:C:307:THR:HG21	1:C:451:GLU:OE1	2.07	0.55
1:C:500:ARG:HG2	1:C:500:ARG:NH1	2.21	0.55
1:D:464:ASP:HB2	1:D:494:LYS:HE3	1.90	0.53
1:C:333:ASP:OD1	1:C:338:PHE:CE1	2.62	0.52
1:C:370:LEU:HD12	1:C:394:ILE:HB	1.92	0.52
1:B:381:ILE:HD12	1:B:386:VAL:HG21	1.91	0.51
1:C:482:VAL:HG22	3:C:601:XPX:C26	2.41	0.51
1:B:206:ILE:HD11	1:B:305:GLU:HG3	1.90	0.51
1:B:125:ARG:HG2	1:B:129:MET:HE2	1.92	0.51
2:B:600:HEM:NA	3:B:601:XPX:C23	2.74	0.51
1:A:356:THR:HG23	1:A:412:PHE:HZ	1.75	0.51
1:A:256:SER:OG	1:A:271:MET:HE1	2.10	0.51
1:C:185:ASN:OD1	1:C:260:THR:OG1	2.28	0.51
1:A:221:LEU:HD21	1:A:229:LEU:HG	1.93	0.50
1:A:206:ILE:HD11	1:A:305:GLU:HG3	1.94	0.50
1:C:293:LEU:C	1:C:293:LEU:HD23	2.36	0.50
1:C:303:GLY:HA2	2:C:600:HEM:HMC2	1.93	0.50
1:C:179:ILE:HG21	1:C:300:PHE:HA	1.92	0.50
1:A:256:SER:OG	1:A:271:MET:SD	2.70	0.50
1:D:52:ASN:HB3	3:D:602:XPX:C04	2.42	0.50
1:D:56:LEU:HD22	3:D:602:XPX:C01	2.40	0.50
1:C:442:CYS:HB2	2:C:600:HEM:NA	2.27	0.49
1:B:109:ARG:HG3	1:B:109:ARG:NH1	2.25	0.49
1:C:223:ILE:HD12	1:C:224:PHE:CE2	2.47	0.49
1:D:470:ASP:OD1	1:D:472:GLN:N	2.46	0.49
1:D:157:LEU:HD22	1:D:493:ILE:HD13	1.95	0.49
2:D:600:HEM:HBC2	2:D:600:HEM:HMC2	1.93	0.49
1:B:482:VAL:HG13	1:B:483:VAL:HG23	1.94	0.48
1:A:122:GLN:O	1:A:122:GLN:OE1	2.31	0.48
1:B:370:LEU:HD22	1:B:394:ILE:HB	1.95	0.48
1:C:285:GLU:OE2	4:C:701:HOH:O	2.20	0.48
1:C:491:VAL:HG13	1:C:493:ILE:HD11	1.95	0.48
1:C:331:GLU:OE1	1:C:352:LEU:HB3	2.14	0.48
1:B:142:LEU:HD21	1:B:182:ILE:HD11	1.95	0.48
2:B:600:HEM:HBC2	2:B:600:HEM:HMC2	1.96	0.48
1:A:126:ARG:HA	1:A:129:MET:HE3	1.96	0.48
1:A:141:LYS:HB3	1:A:144:LYS:HD2	1.96	0.48
1:A:259:ILE:O	1:A:259:ILE:HD12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ALA:HB2	3:A:601:XPX:C18	2.43	0.47
2:B:600:HEM:HBB2	2:B:600:HEM:CMB	2.43	0.47
1:C:353:LEU:HD11	1:C:456:MET:CB	2.43	0.47
1:D:179:ILE:HG21	1:D:300:PHE:HA	1.95	0.47
2:D:600:HEM:C4A	3:D:601:XPX:C23	2.92	0.47
1:B:125:ARG:CG	1:B:129:MET:HE2	2.45	0.47
1:D:136:LYS:O	1:D:137:ASP:OD1	2.32	0.47
1:B:165:ILE:HD11	1:B:493:ILE:CD1	2.43	0.47
1:D:303:GLY:HA2	2:D:600:HEM:HMC2	1.95	0.47
1:C:189:LYS:HA	1:C:189:LYS:HD2	1.75	0.47
1:D:482:VAL:HG22	3:D:601:XPX:C26	2.44	0.47
1:A:167:ILE:C	1:A:167:ILE:HD12	2.40	0.47
1:C:332:ILE:HD11	1:C:342:PRO:HG3	1.97	0.46
1:A:251:LYS:HA	1:A:267:MET:HE1	1.97	0.46
1:C:469:ASP:O	1:C:470:ASP:OD1	2.34	0.46
1:D:500:ARG:HH11	1:D:500:ARG:HG2	1.80	0.46
1:C:202:ASN:ND2	3:C:601:XPX:C15	2.79	0.46
1:B:446:ILE:HG22	4:B:729:HOH:O	2.16	0.46
1:C:248:GLU:HG3	1:C:249:ASN:N	2.31	0.45
1:D:470:ASP:OD1	1:D:472:GLN:HB2	2.16	0.45
1:A:215:VAL:O	1:A:215:VAL:HG12	2.15	0.45
1:B:104:ILE:HD12	1:B:229:LEU:HD22	1.98	0.45
1:A:142:LEU:HD21	1:A:447:LEU:CD1	2.45	0.45
1:A:148:GLN:NE2	1:A:148:GLN:HA	2.31	0.45
1:A:242:LEU:C	1:A:242:LEU:HD23	2.42	0.45
1:C:192:ASP:O	4:C:702:HOH:O	2.21	0.45
1:A:205:ILE:HD11	1:A:236:VAL:HG23	1.99	0.45
1:C:415:GLU:H	1:C:415:GLU:CD	2.21	0.44
1:C:228:THR:OG1	4:C:704:HOH:O	2.21	0.44
1:B:57:GLN:NE2	4:B:708:HOH:O	2.49	0.44
1:B:162:GLY:O	1:B:492:LYS:NZ	2.50	0.44
1:C:338:PHE:CD2	1:C:499:TRP:HA	2.51	0.44
2:C:600:HEM:O1A	4:C:703:HOH:O	2.21	0.44
1:A:53:PHE:HE2	1:A:215:VAL:HG11	1.83	0.44
1:A:84:GLU:HA	1:A:88:LYS:HB2	1.98	0.44
1:A:179:ILE:HG21	1:A:300:PHE:HA	2.00	0.44
1:B:123:LEU:HD11	1:B:127:LEU:HD11	2.00	0.44
1:A:268:GLN:O	1:A:271:MET:HG2	2.17	0.44
1:D:84:GLU:HA	1:D:88:LYS:HB2	2.00	0.44
1:A:323:GLN:HG2	1:A:324:VAL:N	2.32	0.44
1:D:206:ILE:HD11	1:D:305:GLU:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:TYR:CG	1:C:37:VAL:HG11	2.52	0.44
1:D:283:ASP:HA	1:D:286:LEU:CD1	2.48	0.43
1:A:256:SER:OG	1:A:271:MET:CE	2.66	0.43
1:A:60:TYR:CD2	1:C:37:VAL:HG11	2.53	0.43
1:A:256:SER:HG	1:A:271:MET:HE1	1.83	0.43
1:D:52:ASN:HB3	3:D:602:XPX:C03	2.47	0.43
1:A:136:LYS:O	1:A:137:ASP:OD1	2.36	0.43
1:B:223:ILE:HG23	1:D:44:PRO:HG2	2.00	0.43
1:C:30:SER:O	4:C:705:HOH:O	2.21	0.43
1:D:120:HIS:CG	1:D:286:LEU:HD23	2.53	0.43
1:A:141:LYS:CB	1:A:144:LYS:HD2	2.49	0.43
1:C:51:ASN:O	1:C:55:LYS:HG3	2.19	0.42
1:C:128:ALA:HA	1:C:262:MET:CE	2.48	0.42
1:B:251:LYS:HA	1:B:267:MET:HE1	2.01	0.42
2:B:600:HEM:HBC2	2:B:600:HEM:CMC	2.49	0.42
1:C:271:MET:HE3	1:C:271:MET:HB3	1.85	0.42
1:A:259:ILE:HA	1:A:264:ASP:HB3	2.02	0.42
1:C:123:LEU:HD22	1:C:286:LEU:HD12	2.01	0.42
1:C:94:SER:O	1:C:440:ARG:HD3	2.20	0.42
1:D:167:ILE:C	1:D:167:ILE:HD12	2.45	0.42
1:B:242:LEU:HD23	1:B:242:LEU:C	2.44	0.42
1:B:143:GLU:OE2	1:B:343:THR:HB	2.20	0.41
1:B:167:ILE:C	1:B:167:ILE:HD12	2.45	0.41
1:A:384:PHE:HB3	1:C:34:LEU:HG	2.03	0.41
1:D:415:GLU:H	1:D:415:GLU:CD	2.27	0.41
1:B:49:MET:CE	1:B:53:PHE:CZ	3.03	0.41
1:D:120:HIS:CD2	1:D:286:LEU:HD23	2.55	0.41
1:C:153:LEU:HD11	1:C:157:LEU:HD11	2.02	0.41
1:C:306:THR:O	1:C:310:VAL:HG23	2.21	0.41
1:D:283:ASP:HA	1:D:286:LEU:HD12	2.02	0.41
1:A:189:LYS:HD2	1:A:189:LYS:N	2.32	0.41
1:B:334:GLN:O	1:B:334:GLN:HG3	2.21	0.41
1:D:470:ASP:OD1	1:D:470:ASP:C	2.64	0.41
1:D:462:ARG:HE	1:D:462:ARG:HB2	1.71	0.41
1:B:481:LYS:C	1:B:483:VAL:N	2.77	0.40
1:A:223:ILE:CG2	1:C:49:MET:HE1	2.51	0.40
1:B:302:ALA:HB2	3:B:601:XPX:C18	2.52	0.40
1:C:302:ALA:HB2	3:C:601:XPX:C18	2.51	0.40
1:D:351:LEU:HB3	1:D:418:LEU:HD21	2.03	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	463/494 (94%)	446 (96%)	17 (4%)	0	100	100
1	B	461/494 (93%)	444 (96%)	17 (4%)	0	100	100
1	C	464/494 (94%)	448 (97%)	14 (3%)	2 (0%)	30	34
1	D	462/494 (94%)	451 (98%)	11 (2%)	0	100	100
All	All	1850/1976 (94%)	1789 (97%)	59 (3%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	470	ASP
1	C	469	ASP

5.3.2 Protein sidechains [i](#)

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%)	415 (100%)	2 (0%)	81	90
1	B	415/436 (95%)	414 (100%)	1 (0%)	87	94
1	C	417/436 (96%)	413 (99%)	4 (1%)	68	81
1	D	416/436 (95%)	411 (99%)	5 (1%)	63	78
All	All	1665/1744 (96%)	1653 (99%)	12 (1%)	76	87

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	SER
1	A	488	SER
1	B	142	LEU
1	C	142	LEU
1	C	151	SER
1	C	339	SER
1	C	491	VAL
1	D	51	ASN
1	D	141	LYS
1	D	142	LEU
1	D	144	LYS
1	D	339	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	148	GLN
1	A	199	GLN
1	A	202	ASN
1	A	208	ASN
1	A	268	GLN
1	A	376	ASN
1	A	407	HIS
1	A	408	GLN
1	B	57	GLN
1	B	202	ASN
1	B	235	HIS
1	B	376	ASN
1	B	450	GLN
1	C	50	HIS
1	C	202	ASN
1	C	244	ASN
1	C	402	ASN
1	D	50	HIS
1	D	140	GLN
1	D	148	GLN
1	D	190	ASN
1	D	202	ASN
1	D	244	ASN
1	D	282	GLN
1	D	411	GLN
1	D	497	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	XPK	D	602	-	27,29,29	5.22	15 (55%)	39,45,45	2.10	16 (41%)
2	HEM	C	600	1	50,50,50	1.44	6 (12%)	67,82,82	1.21	5 (7%)
2	HEM	B	600	1	50,50,50	1.39	5 (10%)	67,82,82	1.00	2 (2%)
2	HEM	D	600	1	50,50,50	1.39	6 (12%)	67,82,82	1.17	5 (7%)
3	XPK	C	601	-	27,29,29	5.23	16 (59%)	39,45,45	1.87	10 (25%)
3	XPK	A	601	-	27,29,29	5.23	16 (59%)	39,45,45	1.55	4 (10%)
2	HEM	A	600	1	50,50,50	1.85	11 (22%)	67,82,82	2.08	22 (32%)
3	XPK	D	601	-	27,29,29	5.32	15 (55%)	39,45,45	1.85	11 (28%)
3	XPK	B	601	-	27,29,29	5.29	16 (59%)	39,45,45	1.75	9 (23%)
3	XPK	C	602	-	27,29,29	5.30	17 (62%)	39,45,45	2.07	13 (33%)

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	XPK	D	602	-	-	6/7/67/67	0/4/4/4
2	HEM	C	600	1	-	1/14/54/54	-
2	HEM	B	600	1	-	0/14/54/54	-
2	HEM	D	600	1	-	1/14/54/54	-
3	XPK	C	601	-	-	3/7/67/67	0/4/4/4
3	XPK	A	601	-	-	4/7/67/67	0/4/4/4
2	HEM	A	600	1	-	1/14/54/54	-
3	XPK	D	601	-	-	0/7/67/67	0/4/4/4
3	XPK	B	601	-	-	0/7/67/67	0/4/4/4
3	XPK	C	602	-	-	2/7/67/67	0/4/4/4

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	XPK	C25-C20	-15.57	1.26	1.55
3	D	602	XPK	C25-C20	-15.33	1.26	1.55
3	A	601	XPK	C25-C20	-15.32	1.26	1.55
3	B	601	XPK	C25-C20	-15.31	1.26	1.55
3	D	601	XPK	C25-C20	-15.20	1.27	1.55
3	C	601	XPK	C25-C20	-14.48	1.28	1.55
3	B	601	XPK	C18-C17	-12.86	1.28	1.54
3	C	602	XPK	C18-C17	-12.34	1.29	1.54
3	A	601	XPK	C18-C17	-12.09	1.29	1.54
3	D	602	XPK	C18-C17	-11.98	1.29	1.54
3	D	601	XPK	C18-C17	-11.97	1.30	1.54
3	C	601	XPK	C18-C17	-11.94	1.30	1.54
3	D	602	XPK	C06-C05	10.13	1.70	1.53
3	C	602	XPK	C06-C05	10.06	1.70	1.53
3	D	601	XPK	C06-C05	9.46	1.69	1.53
3	C	601	XPK	C25-C17	9.44	1.72	1.55
3	A	601	XPK	C06-C05	9.44	1.69	1.53
3	D	601	XPK	C25-C17	9.32	1.72	1.55
3	C	602	XPK	C25-C17	9.28	1.72	1.55
3	D	602	XPK	C25-C17	9.23	1.72	1.55
3	B	601	XPK	C25-C17	9.14	1.71	1.55
3	C	601	XPK	C06-C05	9.10	1.68	1.53
3	B	601	XPK	C06-C05	9.05	1.68	1.53
3	A	601	XPK	C25-C17	8.85	1.71	1.55
3	C	601	XPK	O14-C13	-8.39	1.35	1.46
3	D	601	XPK	O14-C13	-8.29	1.36	1.46
3	B	601	XPK	O14-C13	-8.17	1.36	1.46
3	A	601	XPK	O14-C13	-8.03	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	XPK	O14-C13	-6.80	1.37	1.46
3	D	602	XPK	O14-C13	-6.44	1.38	1.46
3	D	601	XPK	C19-C20	5.57	1.65	1.54
3	C	601	XPK	C19-C20	5.44	1.65	1.54
2	A	600	HEM	FE-NA	5.43	2.13	1.95
2	A	600	HEM	FE-NC	5.36	2.12	1.95
3	C	602	XPK	C19-C20	5.00	1.64	1.54
3	A	601	XPK	C19-C20	4.97	1.64	1.54
3	D	602	XPK	C19-C20	4.80	1.64	1.54
3	B	601	XPK	C19-C20	4.76	1.64	1.54
3	C	601	XPK	O14-C15	4.53	1.43	1.33
3	D	601	XPK	O14-C15	4.51	1.42	1.33
3	C	602	XPK	O14-C15	4.51	1.42	1.33
3	B	601	XPK	O14-C15	4.50	1.42	1.33
3	A	601	XPK	O14-C15	4.41	1.42	1.33
3	D	602	XPK	C07-C06	4.27	1.61	1.53
3	D	602	XPK	O14-C15	4.27	1.42	1.33
2	C	600	HEM	FE-NB	4.09	2.07	1.94
2	A	600	HEM	CAC-C3C	4.08	1.58	1.47
3	D	602	XPK	C08-C17	4.00	1.61	1.53
3	A	601	XPK	C07-C06	3.99	1.61	1.53
3	C	601	XPK	C07-C06	3.97	1.61	1.53
2	A	600	HEM	FE-NB	3.96	2.07	1.94
3	D	601	XPK	C07-C06	3.91	1.61	1.53
3	C	602	XPK	C08-C17	3.82	1.60	1.53
3	C	602	XPK	C07-C06	3.77	1.60	1.53
2	B	600	HEM	FE-NA	3.72	2.07	1.95
3	D	601	XPK	C08-C17	3.59	1.60	1.53
3	D	601	XPK	C20-C21	3.49	1.62	1.53
3	B	601	XPK	C07-C06	3.48	1.60	1.53
3	C	601	XPK	C08-C17	3.47	1.60	1.53
2	D	600	HEM	FE-NA	3.44	2.06	1.95
2	C	600	HEM	FE-NA	3.36	2.06	1.95
3	A	601	XPK	C08-C17	3.35	1.59	1.53
3	C	601	XPK	C20-C21	3.29	1.61	1.53
3	C	601	XPK	C03-C04	3.23	1.59	1.53
3	D	601	XPK	C03-C04	3.23	1.59	1.53
3	B	601	XPK	C08-C17	3.22	1.59	1.53
2	D	600	HEM	CAC-C3C	3.21	1.56	1.47
2	C	600	HEM	CAC-C3C	3.18	1.55	1.47
2	D	600	HEM	CAB-C3B	3.07	1.55	1.47
2	B	600	HEM	CAB-C3B	3.05	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	HEM	FE-NB	3.04	2.04	1.94
2	C	600	HEM	FE-ND	2.99	2.04	1.94
3	A	601	XPK	C03-C04	2.97	1.59	1.53
2	B	600	HEM	CAC-C3C	2.96	1.55	1.47
2	C	600	HEM	CAB-C3B	2.95	1.55	1.47
3	B	601	XPK	C20-C21	2.93	1.60	1.53
2	A	600	HEM	CAB-C3B	2.93	1.55	1.47
3	B	601	XPK	C09-C10	2.93	1.60	1.52
3	C	602	XPK	C03-C04	2.92	1.59	1.53
3	C	602	XPK	C20-C21	2.85	1.60	1.53
3	D	602	XPK	C20-C21	2.83	1.60	1.53
3	D	602	XPK	C09-C10	2.80	1.59	1.52
3	D	602	XPK	C07-C25	2.79	1.59	1.54
3	D	601	XPK	C09-C10	2.79	1.59	1.52
3	C	602	XPK	C09-C10	2.76	1.59	1.52
3	B	601	XPK	C03-C04	2.75	1.58	1.53
2	A	600	HEM	CMB-C2B	2.73	1.56	1.50
3	C	601	XPK	C09-C10	2.72	1.59	1.52
3	C	601	XPK	C02-C11	2.72	1.59	1.55
2	B	600	HEM	FE-NC	2.68	2.04	1.95
2	A	600	HEM	FE-ND	2.67	2.03	1.94
3	D	602	XPK	C03-C04	2.65	1.58	1.53
3	D	601	XPK	C12-C13	2.65	1.58	1.52
3	A	601	XPK	C20-C21	2.62	1.60	1.53
3	C	601	XPK	C12-C13	2.61	1.58	1.52
3	B	601	XPK	C02-C11	2.60	1.59	1.55
3	A	601	XPK	C09-C10	2.59	1.59	1.52
2	A	600	HEM	CMA-C3A	2.53	1.55	1.50
3	D	601	XPK	C02-C11	2.50	1.59	1.55
3	C	601	XPK	C07-C25	2.42	1.58	1.54
3	A	601	XPK	C02-C11	2.41	1.59	1.55
3	C	602	XPK	C04-C13	2.39	1.57	1.51
3	B	601	XPK	C04-C13	2.39	1.57	1.51
3	B	601	XPK	C12-C13	2.38	1.57	1.52
3	C	601	XPK	C04-C13	2.34	1.57	1.51
3	A	601	XPK	C07-C25	2.33	1.58	1.54
2	A	600	HEM	CMC-C2C	2.32	1.55	1.50
2	D	600	HEM	FE-ND	2.32	2.02	1.94
3	D	601	XPK	C04-C13	2.27	1.57	1.51
2	C	600	HEM	FE-NC	2.21	2.02	1.95
3	B	601	XPK	C07-C25	2.17	1.57	1.54
3	C	602	XPK	C08-C05	2.17	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	XPK	C12-C13	2.17	1.57	1.52
3	C	602	XPK	C07-C25	2.16	1.57	1.54
3	D	602	XPK	C08-C05	2.16	1.57	1.53
2	A	600	HEM	C1C-C2C	2.15	1.49	1.45
3	C	602	XPK	C12-C13	2.15	1.57	1.52
3	A	601	XPK	C04-C13	2.09	1.56	1.51
3	D	602	XPK	C12-C13	2.09	1.57	1.52
2	A	600	HEM	C4C-NC	-2.09	1.35	1.39
3	C	602	XPK	C02-C11	2.04	1.58	1.55
2	D	600	HEM	FE-NC	2.02	2.01	1.95
2	B	600	HEM	FE-ND	2.01	2.01	1.94

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	XPK	C05-C08-C17	4.97	115.58	109.09
3	C	601	XPK	C20-C25-C17	4.78	105.58	100.10
2	A	600	HEM	CHC-C4B-NB	4.58	129.35	124.42
3	D	602	XPK	O14-C15-O16	-4.50	119.93	125.70
2	A	600	HEM	C3B-C4B-NB	-4.46	106.26	109.47
3	B	601	XPK	C20-C25-C17	4.45	105.21	100.10
2	A	600	HEM	C4B-C3B-C2B	4.38	111.30	107.28
3	C	602	XPK	O14-C15-O16	-4.30	120.18	125.70
2	A	600	HEM	CHD-C1D-ND	4.23	128.97	124.42
3	B	601	XPK	C05-C08-C17	4.10	114.44	109.09
3	C	602	XPK	C05-C08-C17	4.06	114.39	109.09
3	C	602	XPK	C07-C25-C20	-3.99	110.72	116.60
3	D	601	XPK	C05-C08-C17	3.99	114.30	109.09
3	A	601	XPK	O14-C15-O16	-3.85	120.76	125.70
3	B	601	XPK	O14-C15-O16	-3.83	120.79	125.70
3	D	602	XPK	C07-C25-C20	-3.81	110.98	116.60
3	C	602	XPK	C05-C02-C11	3.79	113.78	108.51
3	D	602	XPK	C12-C13-C04	3.78	116.25	111.53
3	D	601	XPK	C18-C17-C08	-3.70	113.19	119.10
3	A	601	XPK	C05-C08-C17	3.70	113.92	109.09
2	A	600	HEM	C3D-C4D-ND	-3.69	106.13	110.17
2	A	600	HEM	C2A-C1A-NA	-3.68	106.06	110.15
2	A	600	HEM	CHC-C1C-NC	-3.67	120.45	124.45
2	A	600	HEM	CHB-C4A-NA	3.64	130.46	123.86
3	A	601	XPK	C18-C17-C08	-3.57	113.40	119.10
3	D	601	XPK	C20-C25-C17	3.54	104.16	100.10
3	C	602	XPK	C02-C05-C08	3.50	115.99	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	HEM	C3B-C2B-C1B	-3.48	103.80	106.41
2	A	600	HEM	C4D-ND-C1D	3.45	109.30	105.21
3	C	602	XPK	C06-C05-C08	-3.41	107.02	111.78
3	D	601	XPK	O14-C15-O16	-3.39	121.36	125.70
3	D	602	XPK	C06-C05-C08	-3.38	107.06	111.78
3	C	602	XPK	C18-C17-C08	-3.37	113.72	119.10
3	C	601	XPK	O14-C13-C04	3.27	112.84	107.86
2	D	600	HEM	C3B-C2B-C1B	3.24	108.84	106.41
3	C	602	XPK	C18-C17-C25	3.22	107.63	103.84
3	B	601	XPK	C07-C25-C20	-3.17	111.94	116.60
3	C	602	XPK	C01-C02-C05	-3.15	106.94	111.18
3	D	602	XPK	C02-C05-C08	3.14	115.62	112.43
3	C	601	XPK	O14-C15-O16	-3.14	121.68	125.70
3	D	601	XPK	O14-C13-C04	3.13	112.62	107.86
3	B	601	XPK	C18-C17-C08	-3.11	114.14	119.10
2	C	600	HEM	C3B-C2B-C1B	3.10	108.74	106.41
2	A	600	HEM	CHC-C1C-C2C	3.09	131.91	125.49
3	C	602	XPK	C07-C25-C17	3.07	111.84	107.25
3	D	601	XPK	C07-C25-C17	3.06	111.83	107.25
2	A	600	HEM	O1D-CGD-CBD	-3.03	113.49	123.09
2	A	600	HEM	CBA-CAA-C2A	-3.03	104.16	112.53
3	D	602	XPK	C18-C17-C08	-2.99	114.32	119.10
2	A	600	HEM	O2D-CGD-CBD	2.94	123.30	114.00
3	D	602	XPK	C05-C02-C11	2.94	112.60	108.51
3	D	602	XPK	C05-C08-C17	2.92	112.90	109.09
3	D	602	XPK	C25-C17-C08	-2.91	110.29	114.41
3	D	602	XPK	C18-C17-C25	2.86	107.20	103.84
3	B	601	XPK	C03-C02-C11	2.82	111.79	107.75
3	D	601	XPK	C07-C25-C20	-2.81	112.46	116.60
3	D	601	XPK	C03-C02-C11	2.81	111.78	107.75
3	D	602	XPK	C11-C12-C13	2.77	117.14	111.65
3	C	601	XPK	C18-C17-C08	-2.77	114.69	119.10
3	D	602	XPK	C07-C25-C17	2.75	111.35	107.25
2	A	600	HEM	CHA-C1A-C2A	2.74	131.30	125.30
3	C	601	XPK	C03-C02-C11	2.71	111.64	107.75
3	B	601	XPK	C01-C02-C05	-2.71	107.53	111.18
3	C	602	XPK	C03-C04-C13	2.69	114.72	110.33
2	D	600	HEM	C1B-NB-C4B	2.67	108.37	105.21
2	C	600	HEM	CAA-CBA-CGA	-2.66	106.61	113.67
2	A	600	HEM	CAC-C3C-C4C	-2.65	118.50	124.82
3	C	602	XPK	C20-C25-C17	2.63	103.12	100.10
2	B	600	HEM	C3B-C2B-C1B	2.63	108.38	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	XPK	C01-C02-C05	-2.60	107.68	111.18
2	A	600	HEM	CMA-C3A-C4A	-2.54	121.56	125.42
2	C	600	HEM	C3B-C4B-NB	-2.53	107.65	109.47
2	C	600	HEM	C1B-NB-C4B	2.50	108.17	105.21
3	D	602	XPK	C03-C04-C13	2.48	114.38	110.33
2	A	600	HEM	C2D-C1D-ND	-2.47	107.05	109.90
3	D	602	XPK	C09-C08-C05	2.45	113.46	110.52
3	A	601	XPK	C07-C25-C20	-2.44	113.01	116.60
3	B	601	XPK	C07-C25-C17	2.43	110.88	107.25
2	D	600	HEM	C3B-C4B-NB	-2.41	107.74	109.47
3	D	601	XPK	C26-C25-C17	-2.35	107.41	111.68
2	A	600	HEM	C1B-NB-C4B	2.30	107.93	105.21
3	C	601	XPK	C26-C25-C20	-2.29	107.52	111.68
3	D	602	XPK	C12-C11-C02	2.26	115.06	112.66
3	C	601	XPK	C07-C25-C17	2.22	110.57	107.25
3	D	601	XPK	C18-C17-C25	2.20	106.43	103.84
2	B	600	HEM	CHD-C1D-ND	2.20	126.79	124.42
2	A	600	HEM	CHA-C4D-C3D	2.18	129.24	125.23
3	D	602	XPK	C01-C02-C05	-2.17	108.25	111.18
2	A	600	HEM	CHB-C4A-C3A	-2.15	121.19	127.43
3	C	602	XPK	C12-C13-C04	2.14	114.20	111.53
3	C	601	XPK	C12-C13-C04	-2.11	108.90	111.53
2	D	600	HEM	CHA-C4D-ND	2.06	126.91	124.37
3	C	601	XPK	C02-C05-C08	-2.06	110.34	112.43
2	D	600	HEM	CHC-C1C-NC	2.03	126.67	124.45
2	C	600	HEM	CHB-C1B-NB	2.02	126.86	124.37
3	B	601	XPK	C07-C06-C05	-2.02	109.71	113.14
2	A	600	HEM	CHB-C1B-NB	-2.00	121.89	124.37

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	XPK	C19-C20-C21-C24
3	A	601	XPK	C19-C20-C21-N22
3	A	601	XPK	C25-C20-C21-C24
3	A	601	XPK	C25-C20-C21-N22
3	C	601	XPK	C19-C20-C21-C24
3	C	602	XPK	C12-C13-O14-C15
3	C	602	XPK	O16-C15-O14-C13
3	D	602	XPK	O16-C15-O14-C13
3	D	602	XPK	C19-C20-C21-C24

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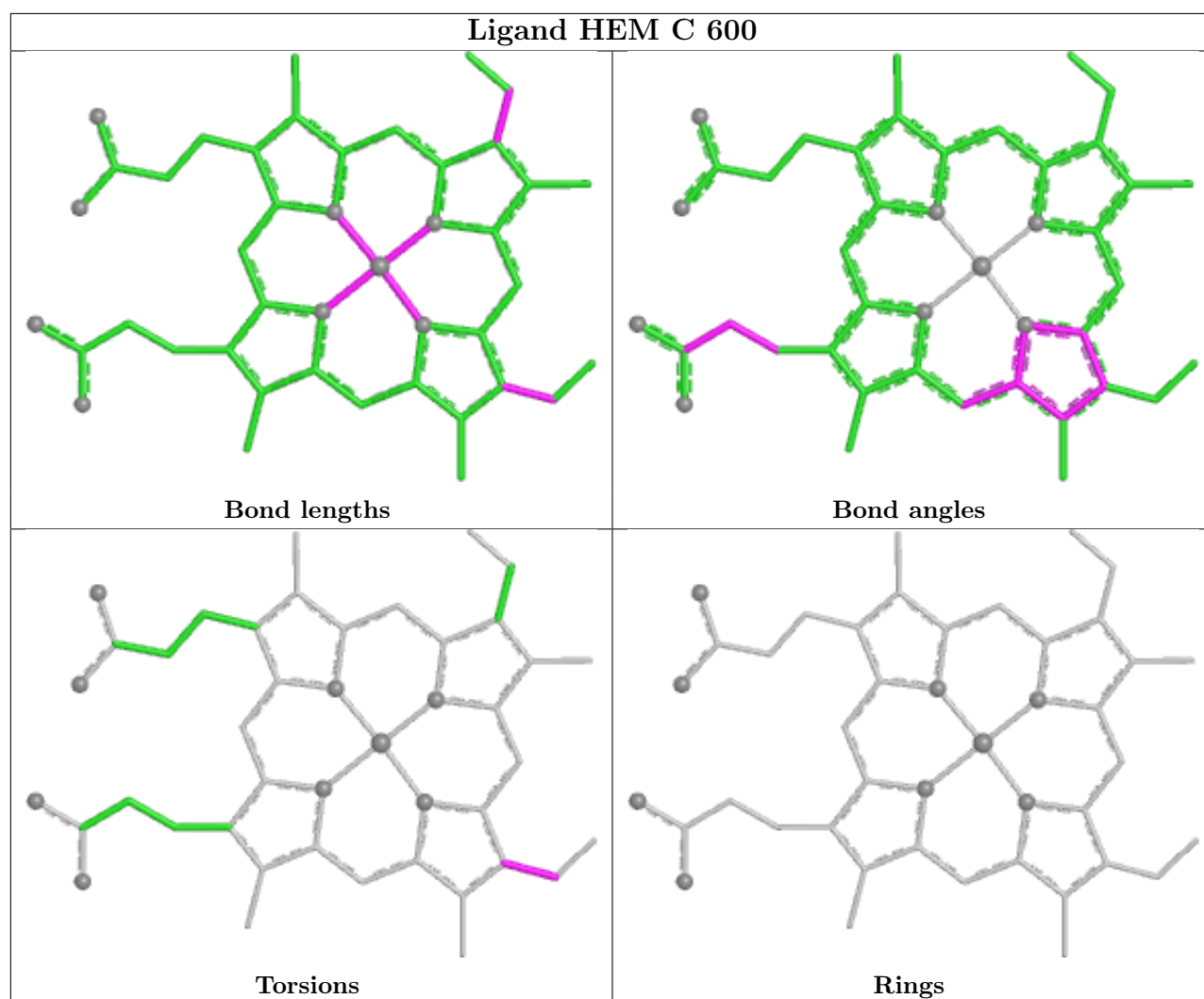
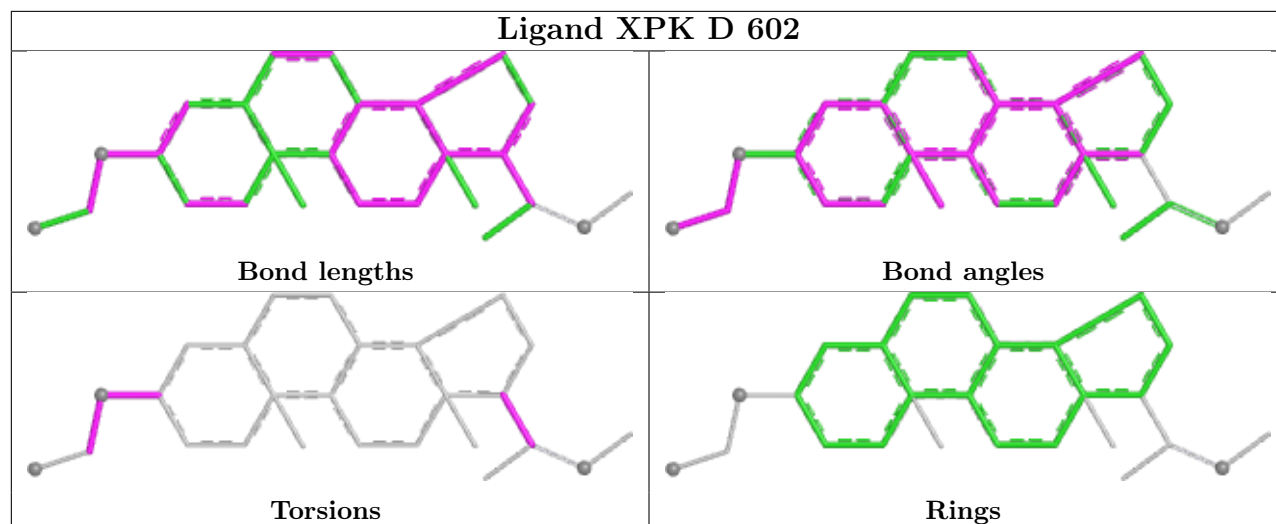
Mol	Chain	Res	Type	Atoms
3	D	602	XPK	C19-C20-C21-N22
3	D	602	XPK	C25-C20-C21-C24
3	D	602	XPK	C25-C20-C21-N22
2	C	600	HEM	C4B-C3B-CAB-CBB
2	D	600	HEM	C4B-C3B-CAB-CBB
3	D	602	XPK	C12-C13-O14-C15
3	C	601	XPK	C25-C20-C21-C24
2	A	600	HEM	CAD-CBD-CGD-O2D
3	C	601	XPK	C25-C20-C21-N22

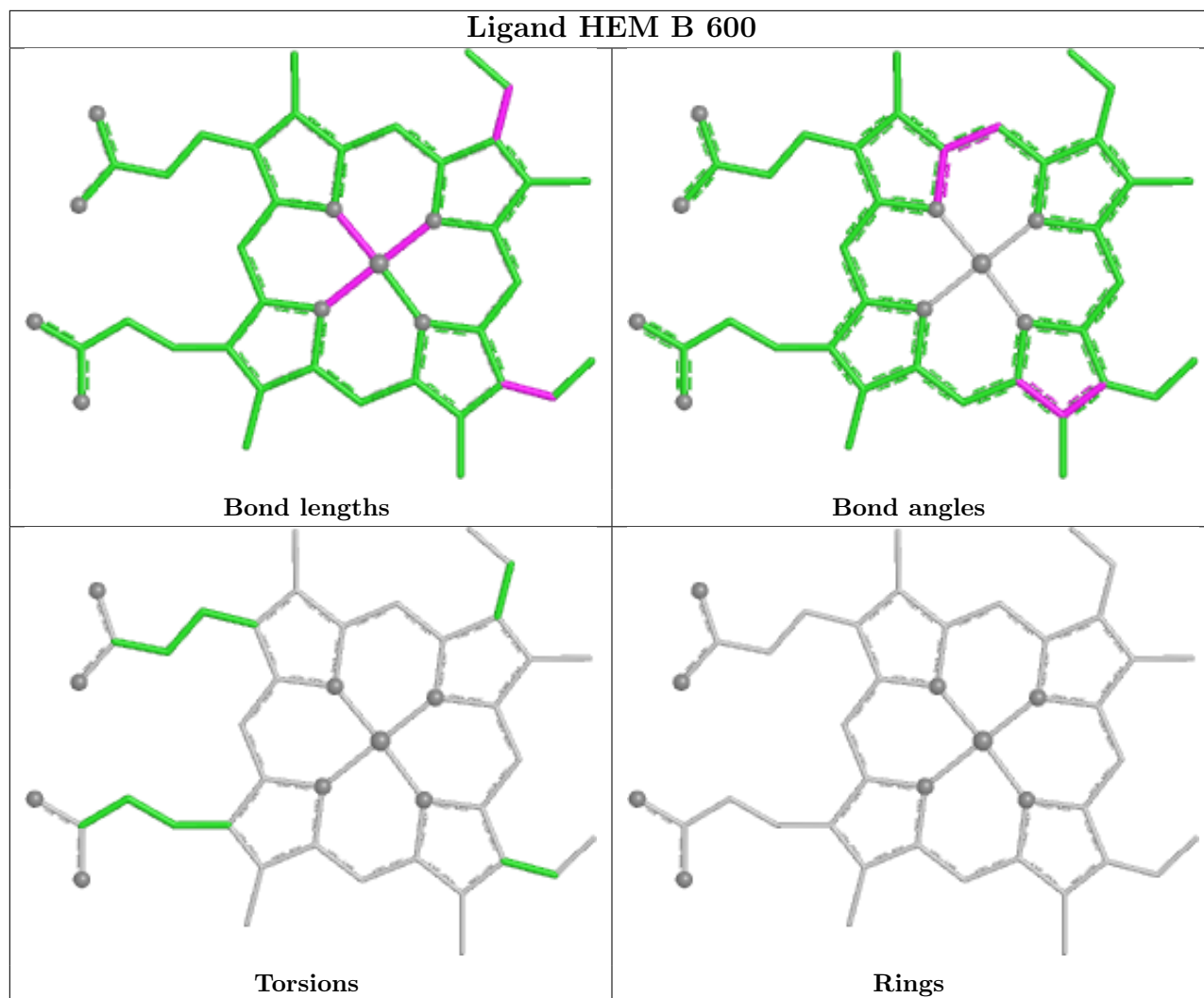
There are no ring outliers.

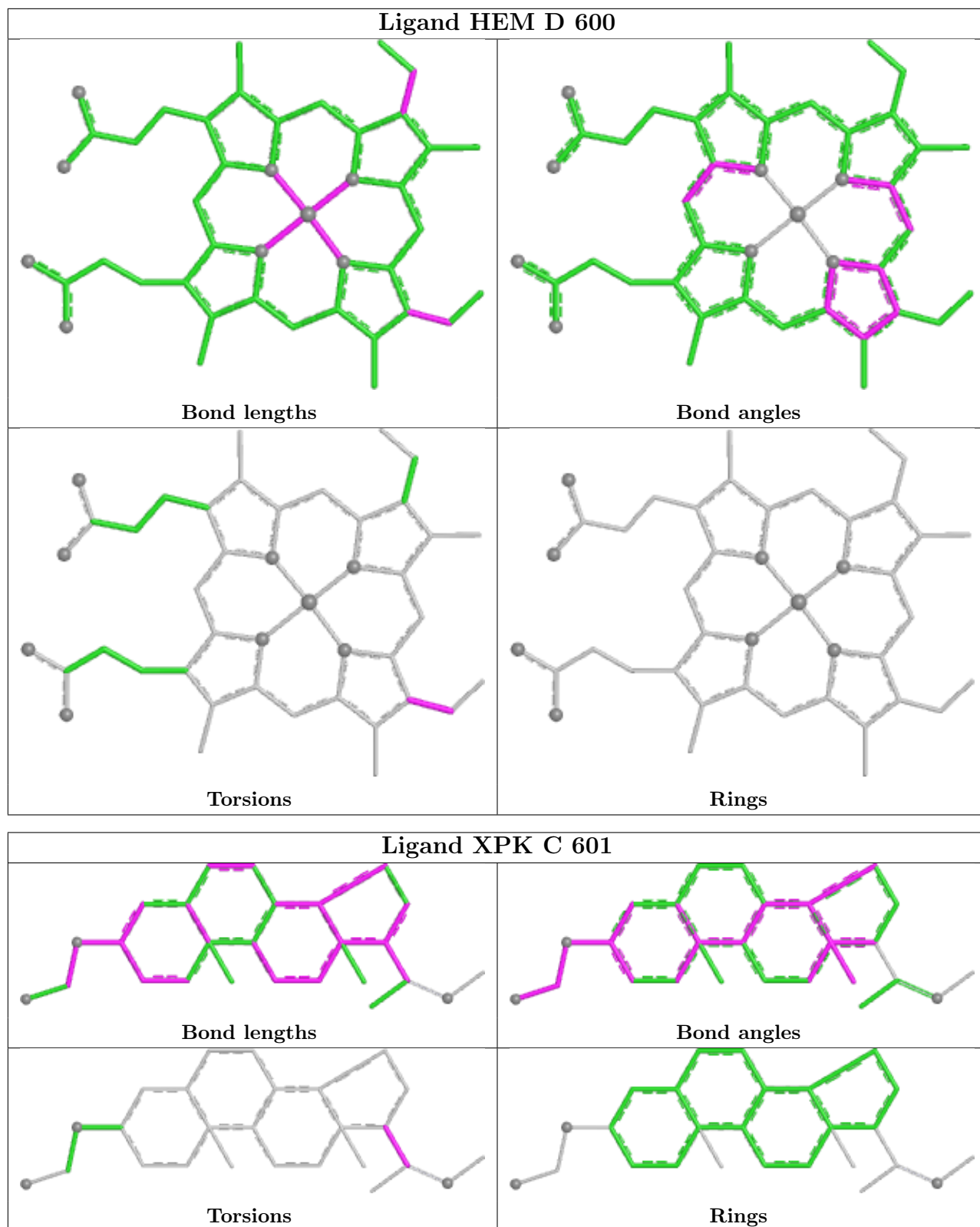
9 monomers are involved in 26 short contacts:

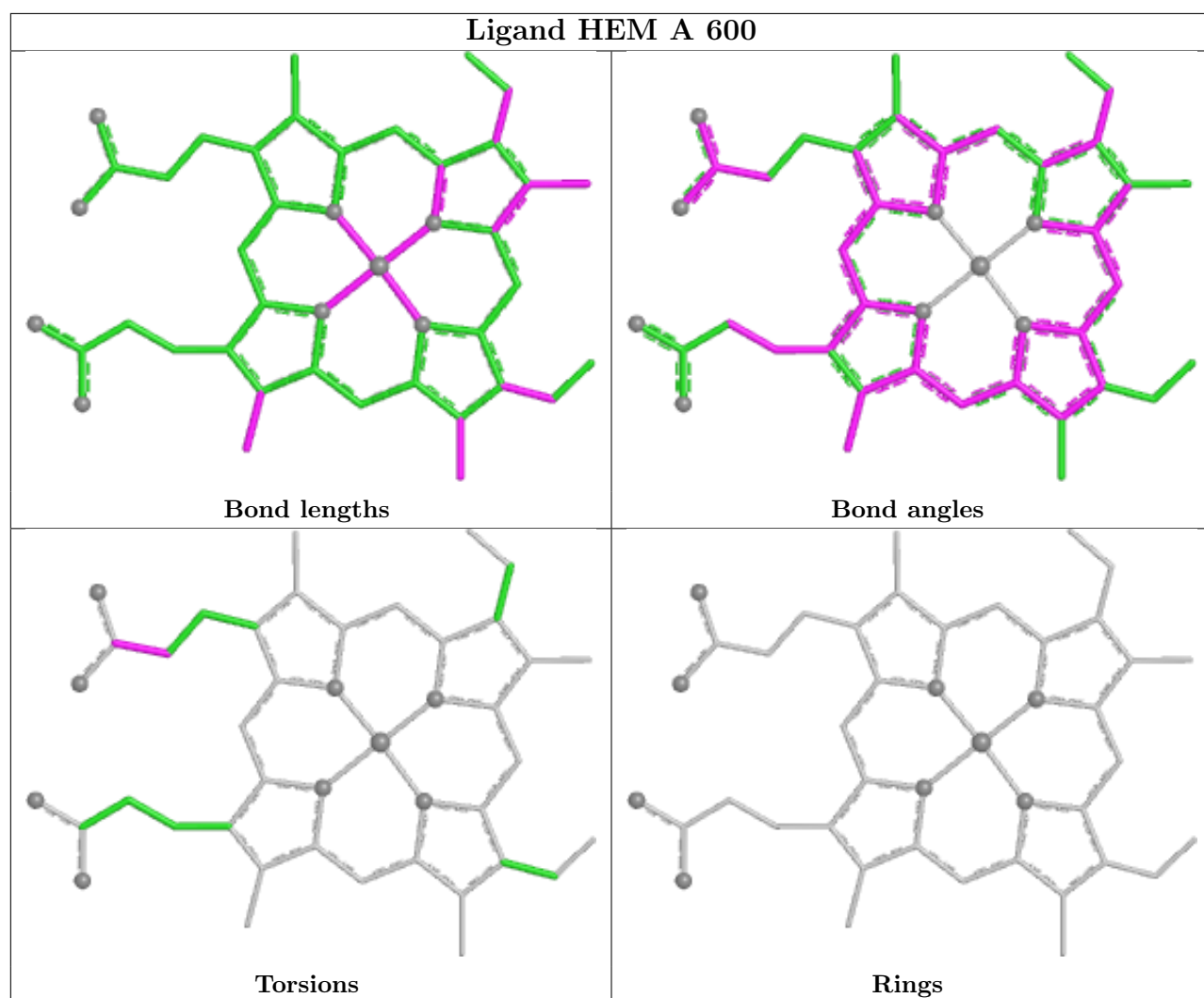
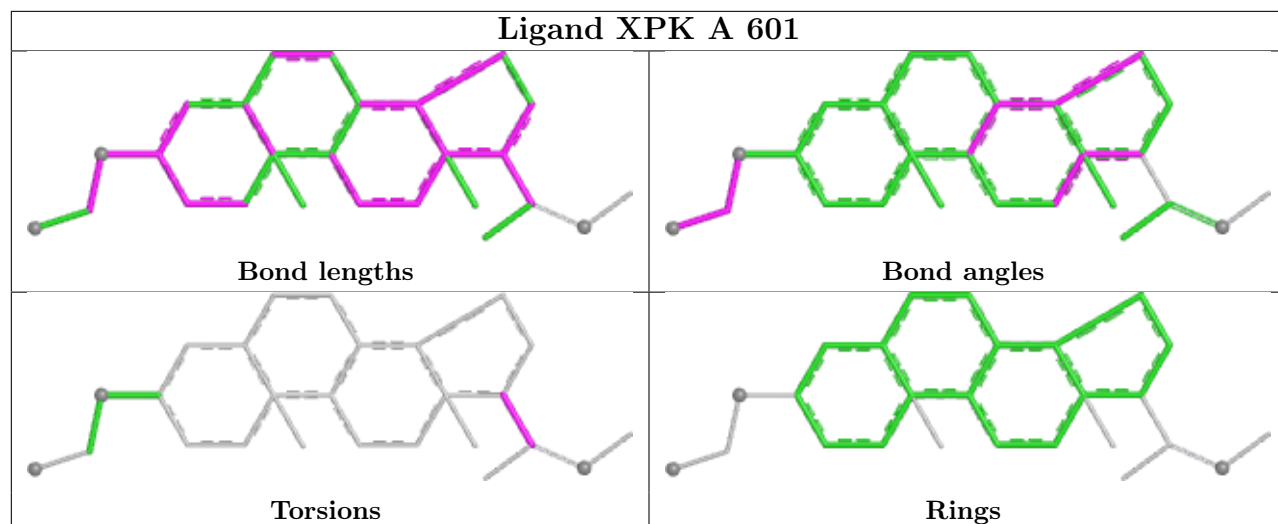
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	602	XPK	3	0
2	C	600	HEM	5	0
2	B	600	HEM	6	0
2	D	600	HEM	5	0
3	C	601	XPK	3	0
3	A	601	XPK	1	0
2	A	600	HEM	1	0
3	D	601	XPK	2	0
3	B	601	XPK	2	0

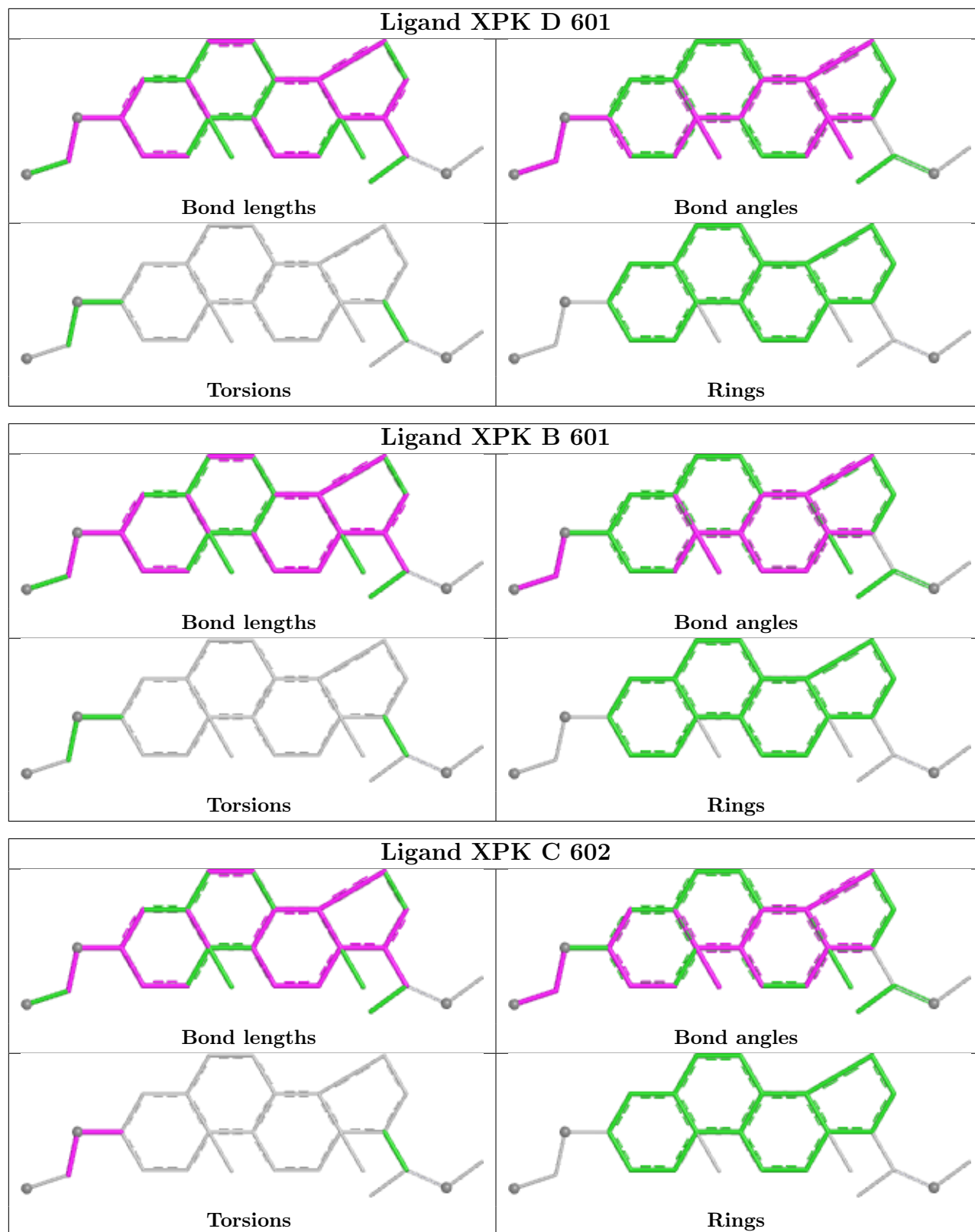
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	467/494 (94%)	0.21	7 (1%) 72 69	38, 56, 81, 110	0
1	B	465/494 (94%)	0.15	9 (1%) 66 63	40, 55, 78, 112	0
1	C	467/494 (94%)	0.47	12 (2%) 57 54	41, 64, 95, 125	1 (0%)
1	D	466/494 (94%)	0.26	5 (1%) 78 76	42, 59, 83, 115	0
All	All	1865/1976 (94%)	0.27	33 (1%) 67 64	38, 58, 88, 125	1 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	504	ALA	3.4
1	D	139	ASP	3.3
1	D	274	ASP	3.3
1	A	28	PRO	3.3
1	C	42	PHE	3.1
1	C	495	VAL	3.0
1	B	213	SER	2.9
1	A	134	LEU	2.8
1	D	42	PHE	2.8
1	C	134	LEU	2.7
1	B	212	ASP	2.7
1	C	274	ASP	2.7
1	D	142	LEU	2.5
1	B	142	LEU	2.4
1	A	29	LYS	2.4
1	C	120[A]	HIS	2.4
1	C	338	PHE	2.3
1	D	46	HIS	2.3
1	A	212	ASP	2.2
1	B	134	LEU	2.2
1	C	44	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	140	GLN	2.2
1	C	464	ASP	2.1
1	C	136	LYS	2.1
1	A	273	SER	2.1
1	B	211	LYS	2.1
1	B	214	LEU	2.1
1	B	221	LEU	2.1
1	C	142	LEU	2.0
1	A	136	LYS	2.0
1	A	271	MET	2.0
1	B	217	LEU	2.0
1	C	332	ILE	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](#)

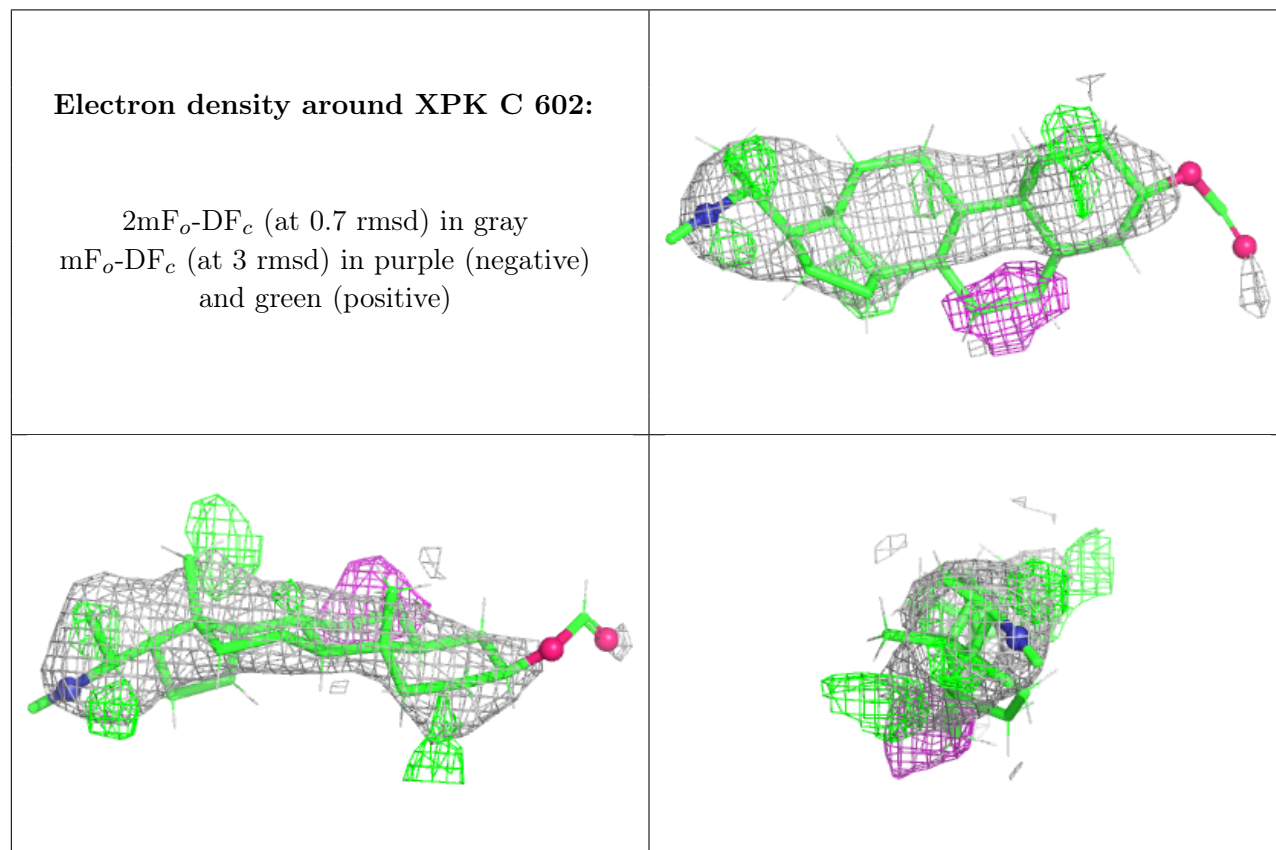
There are no oligosaccharides in this entry.

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.

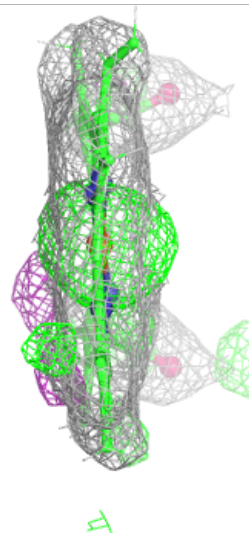
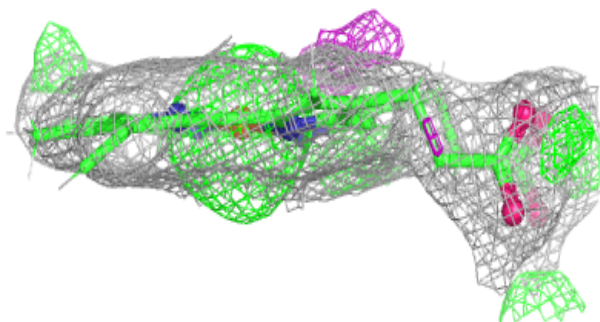
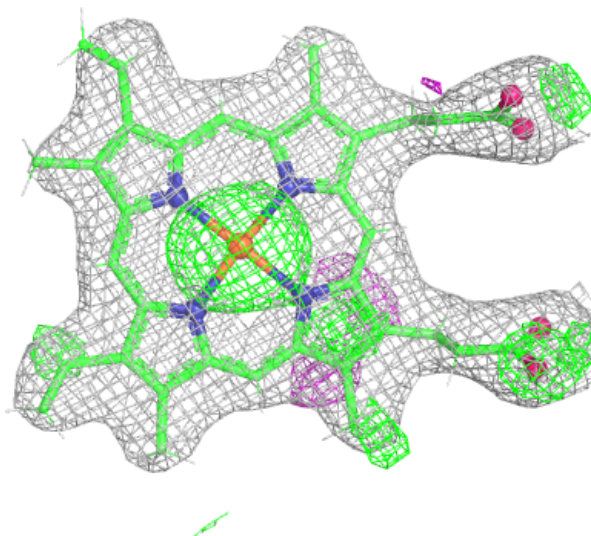
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	XPK	C	602	26/26	0.79	0.25	65,83,98,104	61
2	HEM	A	600	43/43	0.81	0.15	34,51,64,173	0
3	XPK	D	602	26/26	0.82	0.25	66,82,101,102	61
3	XPK	B	601	26/26	0.86	0.14	42,56,71,86	0
3	XPK	D	601	26/26	0.87	0.15	49,61,70,77	0
2	HEM	C	600	43/43	0.88	0.11	34,49,76,123	0
3	XPK	C	601	26/26	0.90	0.14	49,64,73,85	0
3	XPK	A	601	26/26	0.91	0.13	42,61,75,76	0
2	HEM	B	600	43/43	0.94	0.09	29,46,57,87	0
2	HEM	D	600	43/43	0.97	0.08	32,45,59,72	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.



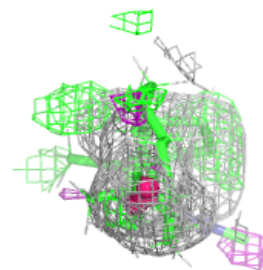
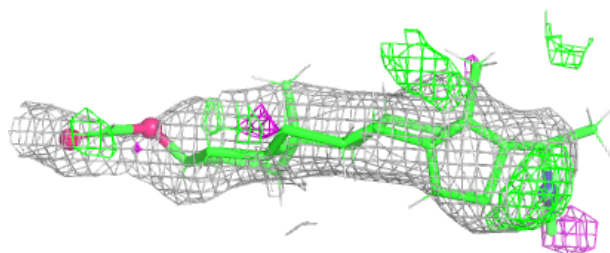
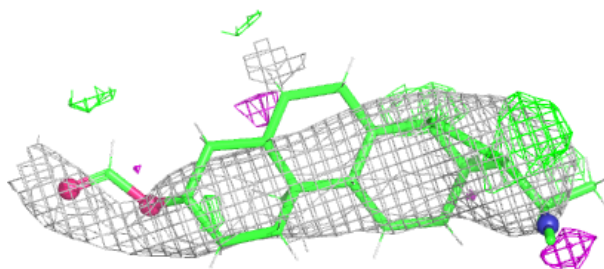
Electron density around HEM A 600:

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

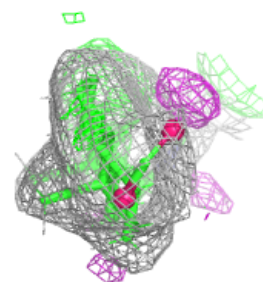
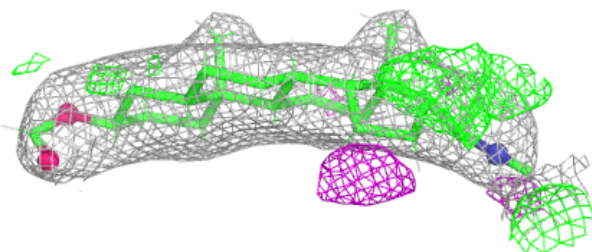
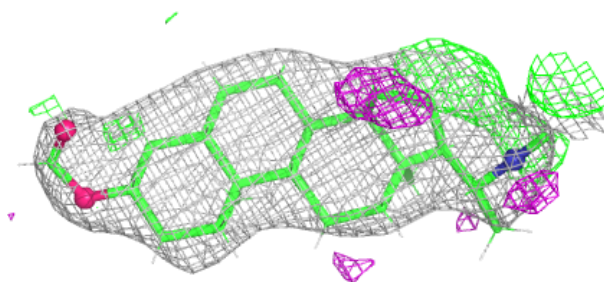


Electron density around XPK D 602:

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

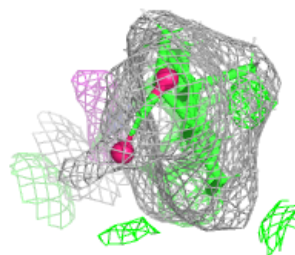
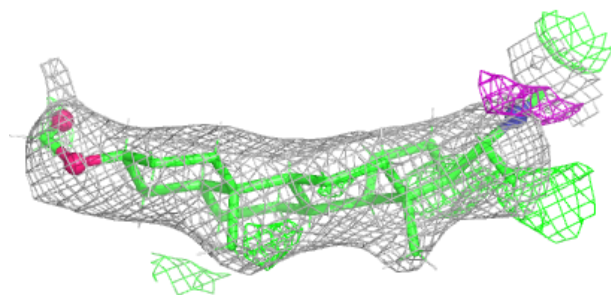
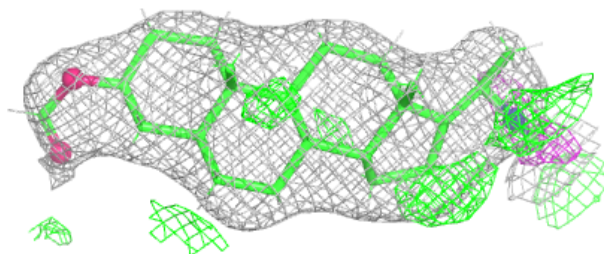
**Electron density around XPK B 601:**

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

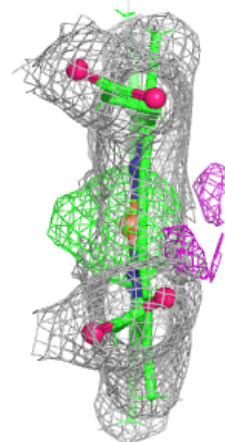
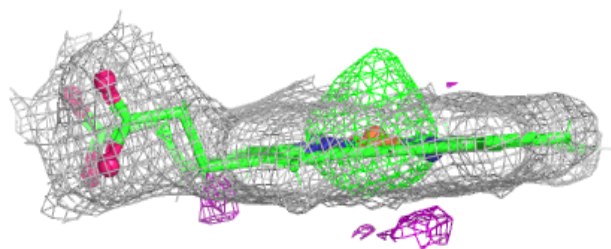
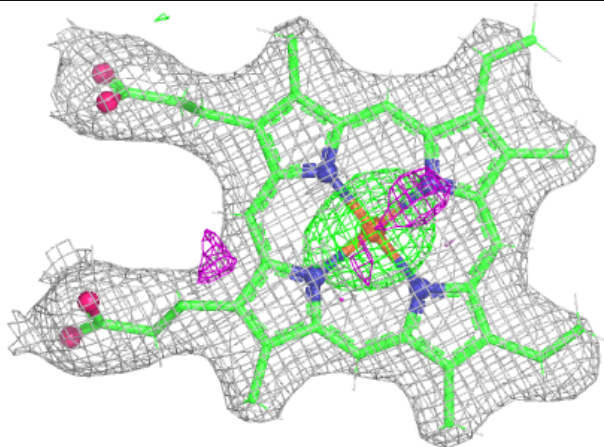


Electron density around XPK D 601:

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

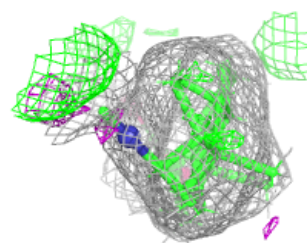
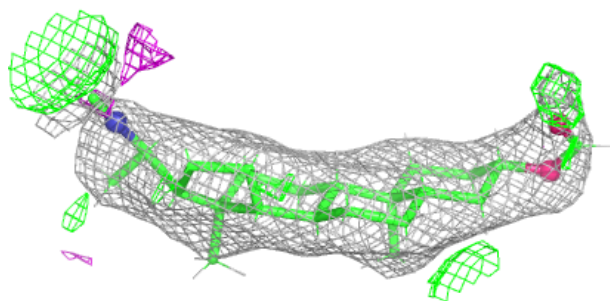
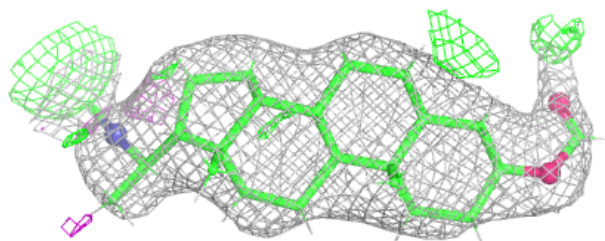
**Electron density around HEM C 600:**

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

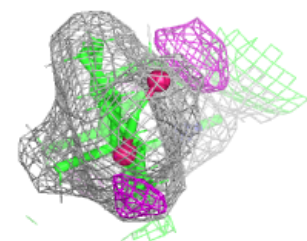
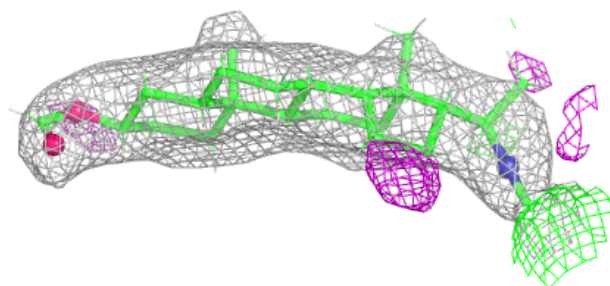
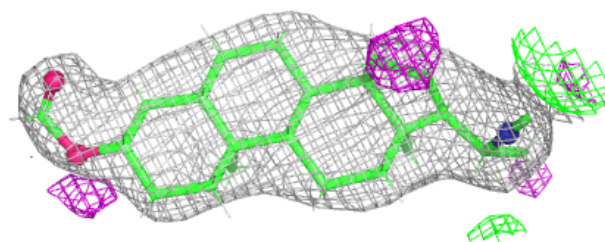


Electron density around XPK C 601:

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and green (positive)

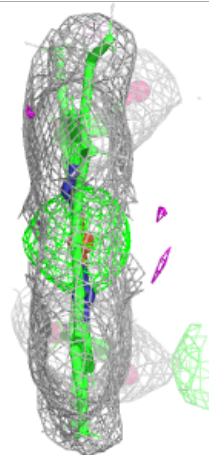
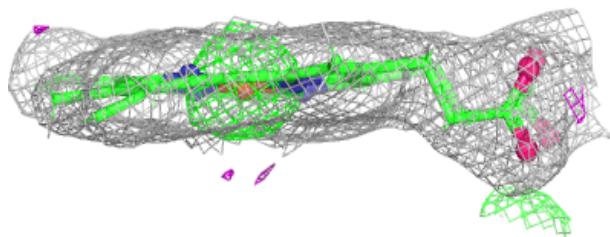
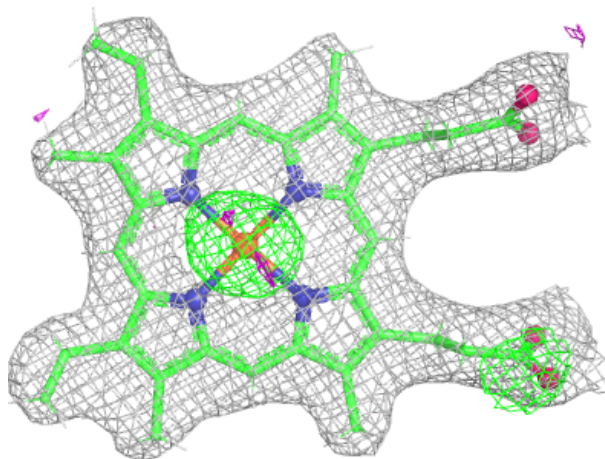
**Electron density around XPK A 601:**

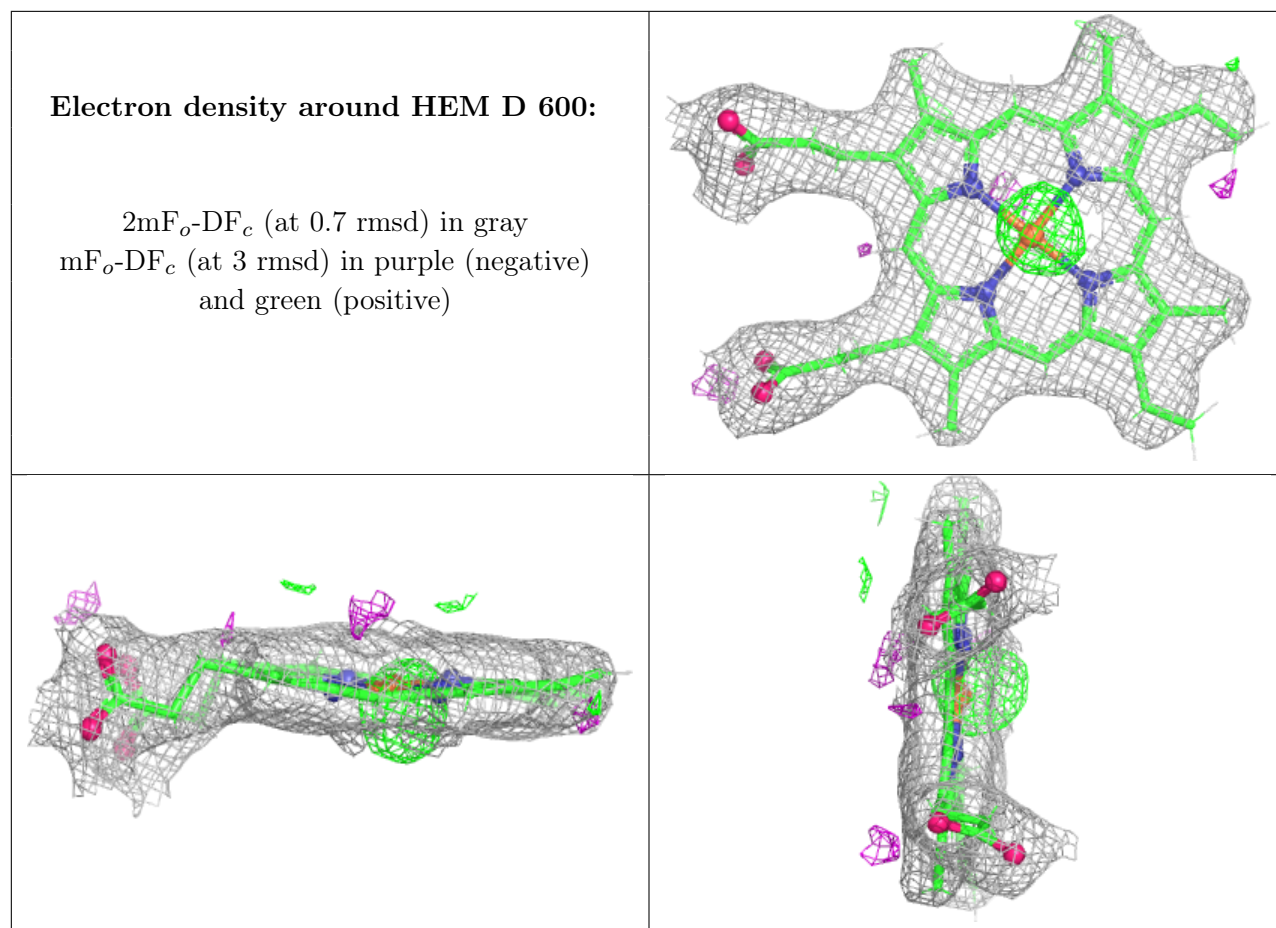
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.