



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 03:37 PM EDT

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

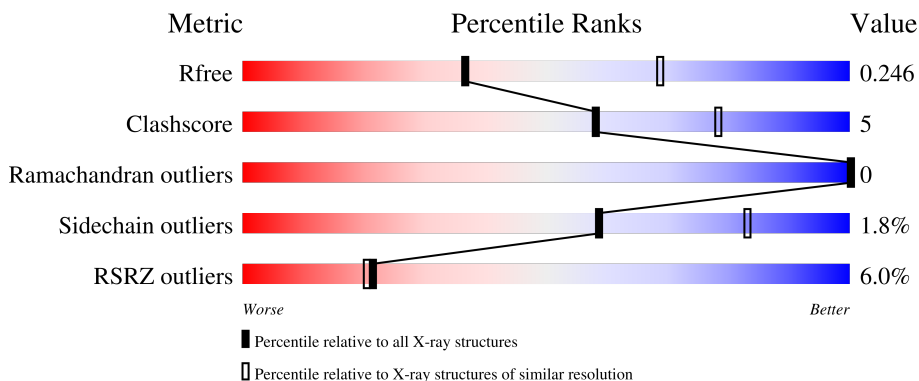
1 Overall quality at a glance

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 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	
1	B	494	
1	C	494	
1	D	494	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 30722 atoms, of which 15420 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Steroid 17-alpha-hydroxylase/17,20 lyase.

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

There are 36 discrepancies between the modelled and reference sequences:

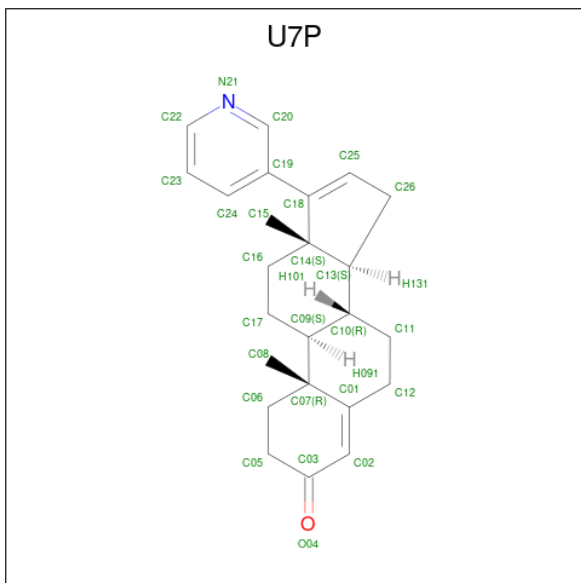
Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	initiating methionine	UNP P05093
A	20	ALA	-	expression tag	UNP P05093
A	21	LYS	-	expression tag	UNP P05093
A	22	LYS	-	expression tag	UNP P05093
A	23	THR	-	expression tag	UNP P05093
A	509	HIS	-	expression tag	UNP P05093
A	510	HIS	-	expression 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	
			Total	C	Fe	H	N			O
2	D	1	73	34	1	30	4	4	0	0

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



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

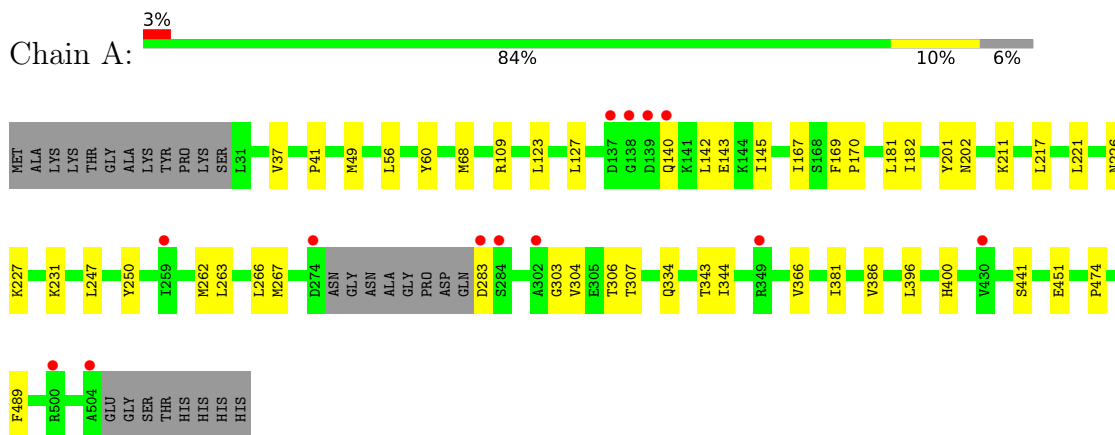
- Molecule 5 is water.

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

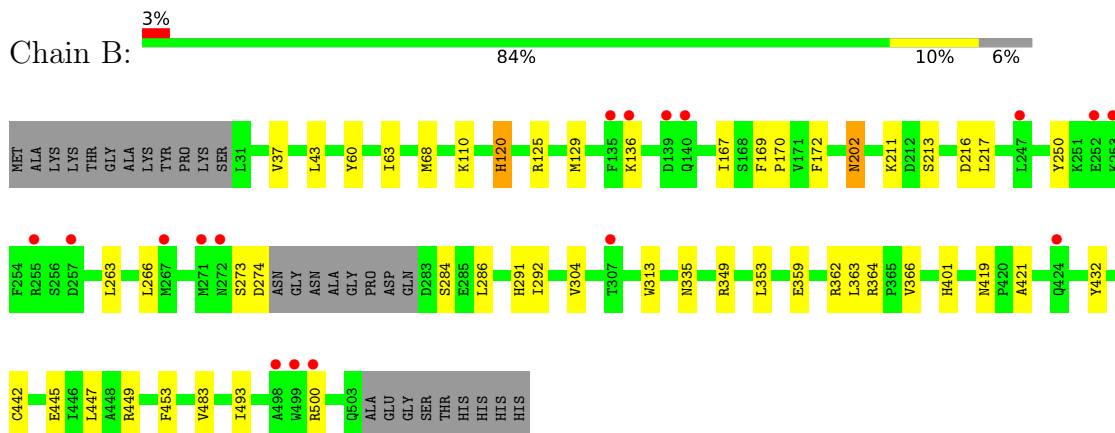
3 Residue-property plots [i](#)

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

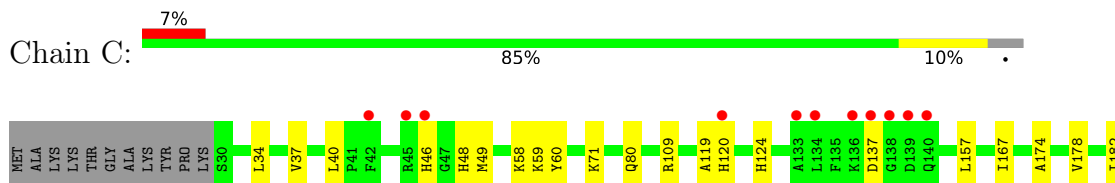
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

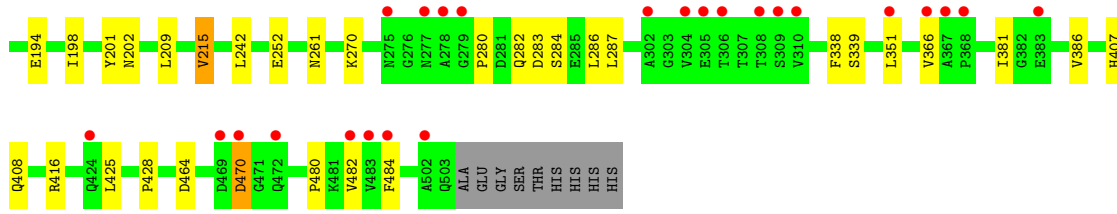


- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

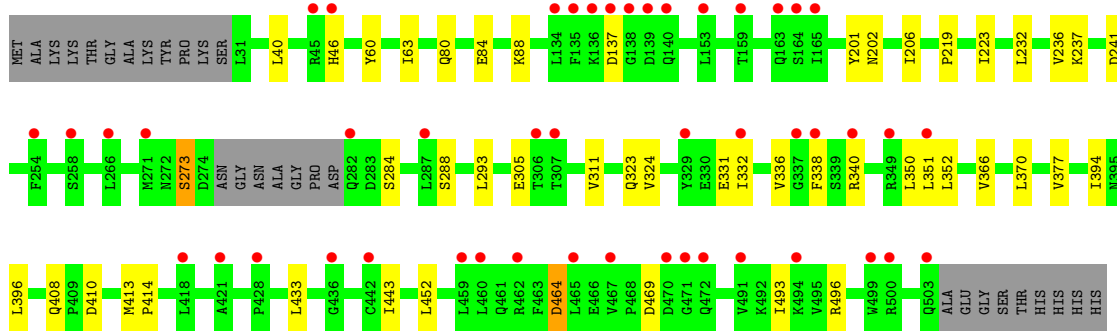
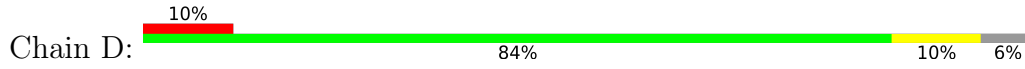


- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.35Å 152.98Å 168.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.81 – 2.70 39.81 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.81-2.70) 90.8 (39.81-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.209 , 0.246 0.209 , 0.246	Depositor DCC
R_{free} test set	3264 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtrriage
Anisotropy	0.588	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	30722	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.65	0/3793	0.66	0/5135
1	B	0.85	0/3788	0.70	0/5128
1	C	0.85	0/3849	0.75	0/5213
1	D	0.70	0/3797	0.74	0/5140
All	All	0.77	0/15227	0.71	0/20616

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	3713	3787	3785	36	0
1	B	3708	3780	3779	37	0
1	C	3767	3828	3827	36	0
1	D	3717	3789	3787	31	0
2	A	43	30	30	9	0
2	B	43	30	30	6	0
2	C	43	30	30	5	0
2	D	43	30	30	5	0
3	A	26	29	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	26	29	0	1	0
3	C	26	29	0	0	0
3	D	26	29	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	28	0	0	2	0
5	B	38	0	0	0	0
5	C	33	0	0	1	0
5	D	19	0	0	0	0
All	All	15302	15420	15298	147	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 (147) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:601:HEM:HHC	2:C:601:HEM:HBB2	1.41	1.00
2:A:600:HEM:HBB2	2:A:600:HEM:HMB2	1.44	0.97
2:A:600:HEM:HBC2	2:A:600:HEM:HHB	1.44	0.96
2:A:600:HEM:HBB2	2:A:600:HEM:CMB	2.12	0.80
2:C:601:HEM:HBC2	2:C:601:HEM:HHB	1.64	0.79
1:C:198:ILE:HA	1:C:201:TYR:CE2	2.23	0.74
2:D:601:HEM:HBA1	2:D:601:HEM:HMA1	1.78	0.65
1:A:140:GLN:HG2	1:A:140:GLN:O	1.98	0.64
1:D:370:LEU:HD12	1:D:394:ILE:HB	1.79	0.63
1:D:331:GLU:OE2	1:D:350:LEU:HA	1.99	0.62
1:C:482:VAL:HG13	5:C:705:HOH:O	2.00	0.61
1:A:56:LEU:HD22	1:A:60:TYR:CD2	2.36	0.61
2:D:601:HEM:HBC2	2:D:601:HEM:HHB	1.85	0.59
1:D:332:ILE:HA	1:D:350:LEU:HD21	1.84	0.59
2:B:601:HEM:HBC2	2:B:601:HEM:HMC2	1.85	0.58
2:C:601:HEM:HBB2	2:C:601:HEM:CHC	2.19	0.58
1:D:206:ILE:HD11	1:D:305:GLU:HG3	1.85	0.58
1:A:142:LEU:HD11	1:A:182:ILE:HD11	1.85	0.58
1:D:408:GLN:HB3	1:D:413:MET:CE	2.33	0.58
1:B:60:TYR:CG	1:C:37:VAL:HG11	2.39	0.57
2:D:601:HEM:HBA1	2:D:601:HEM:CMA	2.33	0.57
1:D:273:SER:OG	1:D:284:SER:HB3	2.05	0.57
1:A:211:LYS:O	1:A:211:LYS:HD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ILE:C	1:A:167:ILE:HD12	2.26	0.55
1:D:338:PHE:N	1:D:338:PHE:CD1	2.73	0.55
1:A:306:THR:HG21	3:A:601:U7P:N21	2.23	0.54
1:D:493:ILE:HG23	1:D:493:ILE:O	2.07	0.53
1:A:37:VAL:HG12	1:D:60:TYR:CD1	2.43	0.53
1:A:68:MET:CE	1:D:40:LEU:HD12	2.38	0.53
1:C:157:LEU:HD21	1:C:167:ILE:HG22	1.91	0.53
1:C:366:VAL:CG2	2:C:601:HEM:HMB2	2.39	0.53
1:A:227:LYS:O	1:A:231:LYS:HG3	2.09	0.53
1:C:124:HIS:HE1	1:C:286:LEU:O	1.91	0.53
1:B:445:GLU:OE2	1:B:449:ARG:NH2	2.42	0.52
1:C:59:LYS:O	1:C:59:LYS:HG3	2.09	0.52
1:B:266:LEU:HD13	1:B:292:ILE:HG23	1.92	0.51
1:A:123:LEU:HD11	1:A:127:LEU:HD11	1.92	0.51
1:A:381:ILE:HG13	1:A:386:VAL:HG21	1.92	0.51
1:C:407:HIS:CE1	1:C:408:GLN:HG3	2.45	0.51
1:C:280:PRO:HG2	1:D:377:VAL:HG12	1.91	0.51
1:A:334:GLN:HG3	1:A:334:GLN:O	2.09	0.51
1:B:110:LYS:HD3	1:B:291:HIS:CD2	2.46	0.51
1:B:442:CYS:HB2	2:B:601:HEM:NA	2.25	0.51
2:B:601:HEM:HBB2	2:B:601:HEM:HMB2	1.91	0.51
1:A:221:LEU:HD12	1:A:226:ASN:OD1	2.11	0.51
1:C:48:HIS:CE1	1:C:480:PRO:HD3	2.46	0.50
1:B:120:HIS:HB3	1:B:286:LEU:HD22	1.93	0.50
1:A:366:VAL:CG2	2:A:600:HEM:HMB2	2.41	0.50
1:B:335:ASN:O	1:B:349:ARG:NH1	2.44	0.50
1:B:273:SER:OG	1:B:284:SER:HB2	2.11	0.50
1:D:352:LEU:O	1:D:352:LEU:HG	2.11	0.49
1:C:252:GLU:HA	1:C:252:GLU:OE2	2.13	0.49
1:C:209:LEU:HD23	1:C:482:VAL:HG11	1.93	0.49
1:B:136:LYS:O	1:B:136:LYS:HD3	2.12	0.49
1:B:172:PHE:CE2	1:B:304:VAL:HG11	2.47	0.49
1:B:500:ARG:HG2	1:B:500:ARG:HH11	1.78	0.49
1:C:351:LEU:HD22	1:C:425:LEU:HG	1.95	0.49
2:A:600:HEM:HMB2	2:A:600:HEM:CBB	2.29	0.49
1:A:56:LEU:HD22	1:A:60:TYR:HD2	1.77	0.48
1:B:273:SER:O	1:B:274:ASP:HB2	2.13	0.48
1:B:353:LEU:HD23	1:B:453:PHE:CE1	2.48	0.48
1:B:419:ASN:HD21	1:B:421:ALA:HB3	1.77	0.48
2:B:601:HEM:HBB2	2:B:601:HEM:CMB	2.42	0.48
1:C:470:ASP:OD1	1:C:470:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:MET:HE1	1:D:40:LEU:HD12	1.94	0.48
1:C:109:ARG:HH11	1:C:109:ARG:HG3	1.77	0.48
1:A:41:PRO:CB	1:A:56:LEU:HD11	2.43	0.48
1:B:63:ILE:HG12	1:C:34:LEU:HD22	1.96	0.47
1:A:307:THR:HG21	1:A:451:GLU:OE1	2.13	0.47
1:B:363:LEU:HD23	1:B:401:HIS:NE2	2.29	0.47
1:A:41:PRO:HB2	1:A:56:LEU:HD11	1.96	0.47
1:B:37:VAL:HG12	1:C:60:TYR:CD1	2.50	0.47
1:A:366:VAL:HG21	2:A:600:HEM:HMB2	1.95	0.47
2:B:601:HEM:HBC2	2:B:601:HEM:CMC	2.45	0.47
1:B:313:TRP:CZ3	1:B:364:ARG:HG3	2.49	0.47
1:D:323:GLN:H	1:D:323:GLN:CD	2.17	0.47
2:D:601:HEM:CMA	2:D:601:HEM:CBA	2.92	0.47
1:B:362:ARG:HB2	1:B:432:TYR:HE1	1.80	0.46
1:A:250:TYR:CD2	1:A:263:LEU:HD23	2.50	0.46
1:D:336:VAL:HG23	1:D:340:ARG:NH1	2.30	0.46
1:A:169:PHE:HB3	1:A:170:PRO:HD3	1.97	0.46
1:B:447:LEU:HD23	2:B:601:HEM:HBC2	1.97	0.46
1:A:109:ARG:HH11	1:A:109:ARG:HG2	1.80	0.45
1:C:270:LYS:HD3	1:C:287:LEU:HB2	1.98	0.45
1:B:493:ILE:O	1:B:493:ILE:HG23	2.15	0.45
1:C:120:HIS:CE1	1:C:124:HIS:CE1	3.04	0.45
1:A:167:ILE:C	1:A:167:ILE:CD1	2.85	0.45
1:C:381:ILE:HD12	1:C:386:VAL:HG21	1.98	0.45
1:A:263:LEU:O	1:A:267:MET:HG2	2.17	0.45
1:B:172:PHE:CD2	1:B:304:VAL:HG11	2.52	0.45
2:C:601:HEM:HHD	2:C:601:HEM:CBC	2.41	0.44
1:A:396:LEU:HD11	1:A:400:HIS:NE2	2.32	0.44
1:B:169:PHE:HB3	1:B:170:PRO:HD3	1.98	0.44
1:D:324:VAL:HG11	1:D:414:PRO:HG2	1.99	0.44
1:A:247:LEU:N	1:A:247:LEU:HD23	2.33	0.44
1:A:303:GLY:HA2	2:A:600:HEM:HMC2	1.98	0.44
1:B:167:ILE:C	1:B:167:ILE:HD12	2.38	0.44
1:C:338:PHE:CD1	1:C:338:PHE:N	2.86	0.44
1:A:262:MET:O	1:A:266:LEU:HD12	2.18	0.43
1:B:43:LEU:HD21	1:C:71:LYS:HD2	2.01	0.43
1:D:84:GLU:HG3	1:D:88:LYS:HE3	2.00	0.43
2:A:600:HEM:HBC2	2:A:600:HEM:CHD	2.23	0.43
1:B:366:VAL:HG13	1:B:483:VAL:HG13	2.00	0.43
1:C:194:GLU:CD	1:C:242:LEU:HD11	2.38	0.43
1:C:198:ILE:HA	1:C:201:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:PRO:HB3	1:A:489:PHE:CG	2.54	0.43
1:B:60:TYR:CD2	1:C:37:VAL:HG11	2.53	0.43
1:C:49:MET:HE1	1:C:215:VAL:CG2	2.49	0.43
1:B:68:MET:CE	1:C:40:LEU:HD12	2.49	0.43
1:A:49:MET:HE1	1:A:217:LEU:HG	1.99	0.42
1:B:202:ASN:ND2	3:B:602:U7P:O04	2.52	0.42
1:D:311:VAL:HG23	1:D:452:LEU:HD23	2.01	0.42
1:A:304:VAL:HG21	5:A:725:HOH:O	2.17	0.42
1:D:408:GLN:CB	1:D:413:MET:HE1	2.49	0.42
1:B:359:GLU:HA	1:B:359:GLU:OE1	2.20	0.42
1:B:363:LEU:HD22	1:B:364:ARG:HH12	1.85	0.42
1:C:167:ILE:HD12	1:C:167:ILE:C	2.40	0.42
1:D:464:ASP:OD1	1:D:496:ARG:HG2	2.19	0.42
1:A:109:ARG:NH1	5:A:701:HOH:O	2.52	0.42
1:A:145:ILE:HG23	1:A:181:LEU:HD13	2.02	0.42
1:C:416:ARG:HG2	1:C:428:PRO:HG3	2.00	0.42
1:D:408:GLN:CB	1:D:413:MET:CE	2.98	0.42
1:B:250:TYR:CD1	1:B:263:LEU:HD23	2.55	0.42
1:C:282:GLN:HG2	1:C:283:ASP:N	2.35	0.42
1:D:237:LYS:HE3	1:D:241:ASP:OD2	2.20	0.42
1:D:366:VAL:CG2	2:D:601:HEM:HMB2	2.50	0.42
1:C:58:LYS:HA	1:C:58:LYS:HD3	1.87	0.41
1:B:68:MET:HE1	1:C:40:LEU:HD12	2.01	0.41
1:C:182:ILE:O	1:C:261:ASN:HB2	2.20	0.41
1:C:119:ALA:HB1	1:C:286:LEU:HD11	2.02	0.41
1:D:206:ILE:CD1	1:D:305:GLU:HG3	2.50	0.41
1:D:396:LEU:HD11	1:D:433:LEU:O	2.20	0.41
1:A:143:GLU:OE2	1:A:343:THR:HG22	2.21	0.41
1:D:331:GLU:OE2	1:D:351:LEU:N	2.53	0.41
2:A:600:HEM:HHA	2:A:600:HEM:HAA1	1.89	0.41
1:D:232:LEU:O	1:D:236:VAL:HG23	2.20	0.41
1:D:331:GLU:OE2	1:D:350:LEU:CA	2.68	0.41
1:C:109:ARG:HG3	1:C:109:ARG:NH1	2.35	0.41
1:D:408:GLN:HB3	1:D:413:MET:HE3	2.03	0.41
1:B:211:LYS:HD3	1:B:211:LYS:C	2.41	0.41
1:C:174:ALA:O	1:C:178:VAL:HG23	2.21	0.40
1:A:344:ILE:HD12	1:A:344:ILE:HG23	1.85	0.40
1:B:217:LEU:HA	1:B:217:LEU:HD23	1.89	0.40
1:D:219:PRO:HG2	1:D:223:ILE:HG23	2.03	0.40
1:B:125:ARG:O	1:B:129:MET:HG3	2.21	0.40
1:B:493:ILE:O	1:B:493:ILE:CG2	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ILE:O	1:D:63:ILE:HG23	2.22	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%)	450 (97%)	12 (3%)	0	100	100
1	B	461/494 (93%)	446 (97%)	15 (3%)	0	100	100
1	C	472/494 (96%)	458 (97%)	14 (3%)	0	100	100
1	D	462/494 (94%)	448 (97%)	14 (3%)	0	100	100
All	All	1857/1976 (94%)	1802 (97%)	55 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [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	415/436 (95%)	411 (99%)	4 (1%)	76	91
1	B	415/436 (95%)	411 (99%)	4 (1%)	76	91
1	C	421/436 (97%)	411 (98%)	10 (2%)	49	77
1	D	416/436 (95%)	404 (97%)	12 (3%)	42	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1667/1744 (96%)	1637 (98%)	30 (2%)	59 83

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	TYR
1	A	202	ASN
1	A	283	ASP
1	A	441	SER
1	B	120	HIS
1	B	202	ASN
1	B	213	SER
1	B	216	ASP
1	C	46	HIS
1	C	80	GLN
1	C	137	ASP
1	C	202	ASN
1	C	215	VAL
1	C	284	SER
1	C	339	SER
1	C	464	ASP
1	C	470	ASP
1	C	484	PHE
1	D	46	HIS
1	D	80	GLN
1	D	137	ASP
1	D	201	TYR
1	D	202	ASN
1	D	273	SER
1	D	288	SER
1	D	293	LEU
1	D	410	ASP
1	D	443	ILE
1	D	464	ASP
1	D	469	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	B	202	ASN

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Mol	Chain	Res	Type
1	C	124	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	B	601	3,1	41,50,50	1.49	5 (12%)	45,82,82	1.49	8 (17%)
3	U7P	A	601	2	30,30,30	5.84	22 (73%)	44,47,47	2.86	14 (31%)
3	U7P	D	602	2	30,30,30	6.00	22 (73%)	44,47,47	2.96	17 (38%)
2	HEM	A	600	3	41,50,50	1.60	10 (24%)	45,82,82	2.07	13 (28%)
2	HEM	D	601	3,1	41,50,50	2.35	14 (34%)	45,82,82	2.47	20 (44%)
3	U7P	B	602	2	30,30,30	5.87	22 (73%)	44,47,47	2.62	18 (40%)
3	U7P	C	602	2	30,30,30	5.78	22 (73%)	44,47,47	2.94	14 (31%)
2	HEM	C	601	3,1	41,50,50	1.53	9 (21%)	45,82,82	1.86	13 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	601	3,1	-	2/12/54/54	-
3	U7P	A	601	2	-	2/4/62/62	0/5/5/5
3	U7P	D	602	2	-	0/4/62/62	0/5/5/5
2	HEM	A	600	3	-	1/12/54/54	-
2	HEM	D	601	3,1	-	6/12/54/54	-
3	U7P	B	602	2	-	2/4/62/62	0/5/5/5
3	U7P	C	602	2	-	2/4/62/62	0/5/5/5
2	HEM	C	601	3,1	-	3/12/54/54	-

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	U7P	C25-C18	19.12	1.67	1.33
3	B	602	U7P	C25-C18	19.02	1.67	1.33
3	A	601	U7P	C25-C18	18.61	1.66	1.33
3	C	602	U7P	C25-C18	18.23	1.65	1.33
3	C	602	U7P	C14-C18	-15.95	1.37	1.53
3	A	601	U7P	C14-C18	-15.05	1.38	1.53
3	D	602	U7P	C02-C01	10.60	1.50	1.34
3	D	602	U7P	C14-C18	-10.28	1.43	1.53
3	B	602	U7P	C14-C18	-10.17	1.43	1.53
3	D	602	U7P	C26-C25	9.73	1.64	1.50
3	B	602	U7P	C02-C01	9.59	1.48	1.34
3	B	602	U7P	C26-C25	9.22	1.63	1.50
3	A	601	U7P	C02-C01	8.62	1.47	1.34
3	C	602	U7P	C02-C01	8.49	1.47	1.34
3	A	601	U7P	C26-C25	7.73	1.61	1.50
3	B	602	U7P	C14-C13	7.59	1.69	1.54
3	C	602	U7P	C26-C25	7.57	1.61	1.50
3	D	602	U7P	C20-C19	7.50	1.51	1.39
3	B	602	U7P	C20-C19	7.42	1.50	1.39
3	D	602	U7P	C16-C17	7.11	1.68	1.53
3	D	602	U7P	C14-C13	6.84	1.67	1.54
3	B	602	U7P	C16-C17	6.59	1.67	1.53
2	D	601	HEM	C1B-NB	-6.59	1.29	1.40
3	C	602	U7P	C16-C14	-5.98	1.42	1.54
3	A	601	U7P	C16-C17	5.90	1.66	1.53
3	D	602	U7P	C20-N21	5.66	1.46	1.34
3	C	602	U7P	C16-C17	5.57	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	U7P	C10-C09	5.51	1.64	1.53
3	A	601	U7P	C07-C09	-5.47	1.46	1.56
3	A	601	U7P	C14-C13	5.46	1.65	1.54
3	B	602	U7P	C20-N21	5.44	1.46	1.34
3	A	601	U7P	C20-C19	5.31	1.47	1.39
3	D	602	U7P	C10-C09	5.20	1.63	1.53
3	A	601	U7P	C10-C13	-5.09	1.43	1.53
3	B	602	U7P	C12-C01	5.04	1.59	1.50
3	C	602	U7P	C14-C13	5.03	1.64	1.54
3	A	601	U7P	C16-C14	-5.03	1.44	1.54
3	D	602	U7P	C23-C22	4.77	1.51	1.37
3	D	602	U7P	C12-C01	4.74	1.58	1.50
3	B	602	U7P	C23-C22	4.69	1.51	1.37
3	D	602	U7P	C23-C24	4.64	1.48	1.38
2	B	601	HEM	C3C-C2C	-4.58	1.34	1.40
3	D	602	U7P	C24-C19	4.54	1.47	1.39
3	C	602	U7P	C20-C19	4.51	1.46	1.39
3	B	602	U7P	C23-C24	4.47	1.48	1.38
2	A	600	HEM	C1B-NB	-4.47	1.32	1.40
2	D	601	HEM	C3C-C2C	-4.44	1.34	1.40
2	D	601	HEM	C4B-NB	-4.44	1.29	1.38
3	C	602	U7P	C10-C13	-4.41	1.45	1.53
3	C	602	U7P	C15-C14	-4.37	1.47	1.54
3	C	602	U7P	C07-C09	-4.34	1.48	1.56
2	D	601	HEM	C2C-C1C	-4.32	1.32	1.42
3	B	602	U7P	C24-C19	4.28	1.46	1.39
3	D	602	U7P	C22-N21	4.27	1.46	1.33
3	B	602	U7P	C22-N21	4.19	1.46	1.33
3	C	602	U7P	O04-C03	-4.07	1.16	1.23
2	D	601	HEM	C4D-ND	-4.05	1.33	1.40
2	C	601	HEM	C1B-NB	-3.95	1.33	1.40
3	A	601	U7P	C10-C09	3.86	1.61	1.53
3	C	602	U7P	C10-C09	3.86	1.61	1.53
2	D	601	HEM	O2A-CGA	-3.82	1.17	1.30
3	A	601	U7P	C08-C07	-3.81	1.48	1.54
3	A	601	U7P	C22-N21	3.74	1.44	1.33
3	D	602	U7P	C16-C14	-3.67	1.47	1.54
3	A	601	U7P	O04-C03	-3.66	1.17	1.23
2	D	601	HEM	O2D-CGD	-3.59	1.18	1.30
3	A	601	U7P	C15-C14	-3.57	1.48	1.54
2	D	601	HEM	C1B-C2B	-3.55	1.37	1.44
2	A	600	HEM	C4D-ND	-3.55	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	U7P	C08-C07	-3.55	1.48	1.54
3	D	602	U7P	C02-C03	3.46	1.53	1.45
3	A	601	U7P	C20-N21	3.46	1.41	1.34
2	C	601	HEM	C4D-ND	-3.44	1.34	1.40
3	B	602	U7P	C02-C03	3.41	1.53	1.45
3	C	602	U7P	C20-N21	3.40	1.41	1.34
2	D	601	HEM	C3D-C2D	-3.36	1.29	1.36
2	B	601	HEM	C3C-CAC	3.33	1.54	1.47
3	B	602	U7P	C16-C14	-3.33	1.47	1.54
3	A	601	U7P	C23-C22	3.31	1.47	1.37
3	D	602	U7P	C19-C18	3.21	1.53	1.48
3	D	602	U7P	C17-C09	3.17	1.59	1.53
3	C	602	U7P	C22-N21	3.16	1.43	1.33
3	C	602	U7P	C12-C01	3.11	1.55	1.50
3	C	602	U7P	C23-C22	3.07	1.46	1.37
3	A	601	U7P	C12-C01	3.03	1.55	1.50
2	C	601	HEM	FE-NB	3.02	2.11	1.96
3	B	602	U7P	C07-C09	-3.00	1.51	1.56
3	A	601	U7P	C06-C07	-2.99	1.48	1.54
2	A	600	HEM	C4B-NB	-2.87	1.32	1.38
2	B	601	HEM	CAB-C3B	2.87	1.55	1.47
2	D	601	HEM	C1D-ND	-2.87	1.32	1.38
2	D	601	HEM	FE-ND	-2.79	1.83	1.96
2	A	600	HEM	C3C-C2C	-2.78	1.36	1.40
3	D	602	U7P	C05-C03	2.78	1.56	1.49
3	A	601	U7P	C24-C19	2.75	1.44	1.39
3	D	602	U7P	C07-C09	-2.74	1.51	1.56
3	A	601	U7P	C23-C24	2.73	1.44	1.38
3	C	602	U7P	C11-C10	-2.72	1.48	1.53
3	B	602	U7P	C17-C09	2.71	1.58	1.53
2	C	601	HEM	C4B-NB	-2.61	1.33	1.38
3	B	602	U7P	C19-C18	2.54	1.52	1.48
2	D	601	HEM	C4A-CHB	-2.51	1.34	1.41
2	C	601	HEM	O2D-CGD	-2.47	1.22	1.30
3	B	602	U7P	C05-C03	2.46	1.55	1.49
3	A	601	U7P	C11-C10	-2.45	1.48	1.53
3	C	602	U7P	C23-C24	2.45	1.44	1.38
3	C	602	U7P	C24-C19	2.44	1.43	1.39
2	A	600	HEM	FE-ND	-2.43	1.84	1.96
2	A	600	HEM	C1B-C2B	-2.41	1.39	1.44
2	B	601	HEM	CAA-C2A	2.40	1.55	1.52
3	D	602	U7P	C10-C13	-2.39	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	HEM	O2A-CGA	-2.38	1.22	1.30
3	B	602	U7P	C10-C13	-2.37	1.49	1.53
2	C	601	HEM	C1D-ND	-2.33	1.34	1.38
2	A	600	HEM	O2D-CGD	-2.30	1.23	1.30
2	B	601	HEM	CMB-C2B	2.28	1.55	1.50
2	C	601	HEM	C3C-C2C	-2.26	1.37	1.40
2	C	601	HEM	FE-ND	-2.22	1.85	1.96
3	C	602	U7P	C06-C07	-2.20	1.50	1.54
2	D	601	HEM	CAA-C2A	-2.19	1.48	1.52
2	A	600	HEM	C1D-ND	-2.19	1.34	1.38
2	A	600	HEM	FE-NB	2.15	2.07	1.96
2	A	600	HEM	O2A-CGA	-2.08	1.23	1.30
2	D	601	HEM	C1A-CHA	-2.08	1.35	1.41
3	B	602	U7P	C11-C12	2.08	1.57	1.52
3	D	602	U7P	C08-C07	-2.03	1.51	1.54

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	U7P	C13-C14-C18	12.17	110.09	99.70
3	C	602	U7P	C13-C14-C18	10.91	109.01	99.70
3	A	601	U7P	C13-C14-C18	9.93	108.17	99.70
3	C	602	U7P	C26-C25-C18	-9.68	104.91	112.87
3	A	601	U7P	C26-C25-C18	-9.11	105.38	112.87
3	D	602	U7P	C26-C25-C18	-8.55	105.84	112.87
3	B	602	U7P	C26-C25-C18	-6.69	107.36	112.87
3	C	602	U7P	C01-C02-C03	-6.46	113.25	123.67
3	B	602	U7P	C13-C14-C18	6.23	105.01	99.70
3	B	602	U7P	C15-C14-C16	-6.16	103.89	111.13
3	A	601	U7P	C01-C02-C03	-5.65	114.55	123.67
2	D	601	HEM	CHC-C4B-NB	5.48	130.38	124.43
2	A	600	HEM	CHC-C4B-NB	5.35	130.25	124.43
3	B	602	U7P	C26-C13-C14	5.08	107.85	104.05
2	D	601	HEM	C4B-C3B-C2B	-4.99	103.16	107.11
3	D	602	U7P	C15-C14-C13	-4.81	105.88	112.98
2	A	600	HEM	CBA-CAA-C2A	4.55	120.38	112.62
3	A	601	U7P	C06-C07-C09	-4.52	102.42	108.73
2	A	600	HEM	CHD-C1D-ND	4.43	129.24	124.43
3	B	602	U7P	C14-C13-C10	-4.43	108.38	113.12
2	C	601	HEM	CHC-C4B-NB	4.41	129.22	124.43
2	C	601	HEM	C1B-NB-C4B	4.36	109.58	105.07
3	D	602	U7P	C07-C09-C10	4.35	119.27	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	HEM	CMB-C2B-C1B	-4.28	118.52	125.04
2	D	601	HEM	CHD-C1D-ND	4.25	129.05	124.43
3	A	601	U7P	C26-C13-C14	4.25	107.23	104.05
3	A	601	U7P	C19-C20-N21	-4.10	117.43	123.49
2	D	601	HEM	C1B-NB-C4B	4.02	109.23	105.07
2	D	601	HEM	CHA-C4D-ND	3.90	129.20	124.38
3	C	602	U7P	C15-C14-C13	-3.89	107.23	112.98
2	C	601	HEM	CHD-C1D-ND	3.87	128.64	124.43
3	C	602	U7P	C06-C07-C01	3.87	115.84	108.75
2	A	600	HEM	C1B-NB-C4B	3.83	109.03	105.07
2	D	601	HEM	CHA-C4D-C3D	-3.82	118.16	125.33
2	D	601	HEM	O2A-CGA-O1A	-3.78	113.89	123.30
2	A	600	HEM	CHB-C1B-NB	3.73	128.99	124.38
3	D	602	U7P	C26-C13-C10	3.72	126.03	121.57
2	D	601	HEM	O2D-CGD-O1D	-3.67	114.16	123.30
2	D	601	HEM	CHB-C1B-NB	3.65	128.89	124.38
3	A	601	U7P	C15-C14-C18	-3.60	100.41	108.00
3	C	602	U7P	C06-C07-C09	-3.55	103.77	108.73
3	D	602	U7P	C22-N21-C20	3.49	122.89	116.85
2	C	601	HEM	CHA-C4D-ND	3.43	128.62	124.38
2	A	600	HEM	CHA-C4D-ND	3.39	128.57	124.38
3	B	602	U7P	C11-C10-C09	3.38	114.68	110.49
3	A	601	U7P	C22-N21-C20	3.34	122.62	116.85
3	D	602	U7P	C13-C26-C25	3.29	106.68	101.39
3	A	601	U7P	C24-C19-C20	3.28	121.35	117.63
2	C	601	HEM	CBA-CAA-C2A	3.28	118.22	112.62
3	B	602	U7P	C06-C07-C01	3.14	114.50	108.75
3	B	602	U7P	C22-N21-C20	3.14	122.27	116.85
3	D	602	U7P	C15-C14-C16	-3.11	107.47	111.13
2	D	601	HEM	O2D-CGD-CBD	3.10	123.99	114.03
3	C	602	U7P	C26-C13-C14	3.10	106.37	104.05
3	B	602	U7P	C15-C14-C13	-3.09	108.41	112.98
2	B	601	HEM	CHC-C4B-NB	3.07	127.77	124.43
2	B	601	HEM	C1B-NB-C4B	3.07	108.24	105.07
3	C	602	U7P	C15-C14-C16	-3.06	107.53	111.13
2	C	601	HEM	CHB-C1B-NB	3.05	128.15	124.38
2	B	601	HEM	C4D-ND-C1D	3.03	108.21	105.07
2	D	601	HEM	CHC-C4B-C3B	-2.98	120.00	124.57
3	B	602	U7P	C09-C10-C13	2.94	113.03	109.09
2	D	601	HEM	CAB-C3B-C2B	2.94	138.28	128.60
2	A	600	HEM	CHD-C1D-C2D	-2.92	120.42	124.98
2	A	600	HEM	O2A-CGA-O1A	-2.91	116.04	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	U7P	C01-C02-C03	-2.91	118.97	123.67
3	A	601	U7P	C14-C13-C10	-2.87	110.05	113.12
2	A	600	HEM	CAA-CBA-CGA	-2.85	105.76	113.76
2	A	600	HEM	O2A-CGA-CBA	2.80	123.04	114.03
2	B	601	HEM	C4B-CHC-C1C	2.80	126.25	122.56
3	B	602	U7P	C08-C07-C01	-2.77	103.86	108.34
3	C	602	U7P	C05-C03-C02	2.76	121.00	116.74
3	D	602	U7P	C01-C02-C03	-2.73	119.26	123.67
3	B	602	U7P	C19-C20-N21	-2.73	119.46	123.49
2	D	601	HEM	CMD-C2D-C1D	2.68	129.12	125.04
3	B	602	U7P	C05-C03-C02	2.64	120.81	116.74
2	D	601	HEM	C3B-C2B-C1B	2.61	108.42	106.49
3	D	602	U7P	C11-C10-C13	-2.61	107.63	112.08
3	C	602	U7P	C14-C13-C10	-2.58	110.36	113.12
2	B	601	HEM	CMA-C3A-C4A	-2.53	124.57	128.46
3	A	601	U7P	C06-C07-C01	2.52	113.37	108.75
3	A	601	U7P	C15-C14-C16	-2.52	108.17	111.13
2	D	601	HEM	C3C-C4C-NC	-2.49	106.24	110.94
3	D	602	U7P	C19-C20-N21	-2.46	119.85	123.49
2	B	601	HEM	C3D-C4D-ND	-2.45	107.44	110.17
2	D	601	HEM	CHD-C1D-C2D	-2.43	121.18	124.98
3	B	602	U7P	C26-C13-C10	2.42	124.48	121.57
2	D	601	HEM	CAD-C3D-C4D	2.42	128.89	124.66
2	C	601	HEM	CHA-C4D-C3D	-2.42	120.79	125.33
3	C	602	U7P	C11-C12-C01	-2.40	107.42	111.93
3	B	602	U7P	C07-C09-C10	2.39	116.31	112.73
3	D	602	U7P	C15-C14-C18	-2.38	102.99	108.00
3	A	601	U7P	C09-C07-C01	2.35	113.33	109.65
3	B	602	U7P	C17-C09-C07	-2.33	110.01	113.08
3	C	602	U7P	C15-C14-C18	-2.31	103.13	108.00
3	B	602	U7P	C16-C14-C13	2.31	112.63	108.99
3	A	601	U7P	C07-C09-C10	-2.28	109.32	112.73
2	A	600	HEM	CHA-C4D-C3D	-2.27	121.06	125.33
2	C	601	HEM	O2D-CGD-O1D	-2.27	117.64	123.30
2	C	601	HEM	CHD-C1D-C2D	-2.27	121.43	124.98
2	C	601	HEM	O2A-CGA-O1A	-2.26	117.66	123.30
2	A	600	HEM	O2D-CGD-O1D	-2.25	117.70	123.30
2	A	600	HEM	CHB-C1B-C2B	-2.24	120.54	126.72
2	D	601	HEM	C3D-C4D-ND	2.22	112.63	110.17
3	D	602	U7P	C14-C18-C25	-2.16	107.09	109.72
2	B	601	HEM	CMC-C2C-C3C	2.15	128.71	124.68
2	C	601	HEM	CAD-C3D-C4D	2.14	128.40	124.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	U7P	C06-C07-C09	-2.13	105.76	108.73
3	D	602	U7P	C05-C06-C07	2.12	117.44	113.45
2	B	601	HEM	C4C-CHD-C1D	2.09	125.32	122.56
3	C	602	U7P	O04-C03-C02	-2.09	117.67	121.68
2	D	601	HEM	O2A-CGA-CBA	2.08	120.70	114.03
3	C	602	U7P	C14-C18-C25	-2.07	107.20	109.72
3	D	602	U7P	C05-C03-C02	2.06	119.91	116.74
2	C	601	HEM	O2D-CGD-CBD	2.03	120.55	114.03
3	D	602	U7P	C06-C07-C01	2.03	112.46	108.75
2	C	601	HEM	O2A-CGA-CBA	2.02	120.52	114.03

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	HEM	C1A-C2A-CAA-CBA
2	D	601	HEM	C3A-C2A-CAA-CBA
3	A	601	U7P	C14-C18-C19-C20
3	C	602	U7P	C14-C18-C19-C20
3	A	601	U7P	C14-C18-C19-C24
2	C	601	HEM	C4B-C3B-CAB-CBB
3	C	602	U7P	C14-C18-C19-C24
3	B	602	U7P	C25-C18-C19-C24
3	B	602	U7P	C25-C18-C19-C20
2	A	600	HEM	C1A-C2A-CAA-CBA
2	B	601	HEM	CAD-CBD-CGD-O1D
2	B	601	HEM	CAD-CBD-CGD-O2D
2	C	601	HEM	CAD-CBD-CGD-O1D
2	D	601	HEM	CAD-CBD-CGD-O2D
2	D	601	HEM	CAA-CBA-CGA-O2A
2	C	601	HEM	CAD-CBD-CGD-O2D
2	D	601	HEM	CAA-CBA-CGA-O1A
2	D	601	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

6 monomers are involved in 27 short contacts:

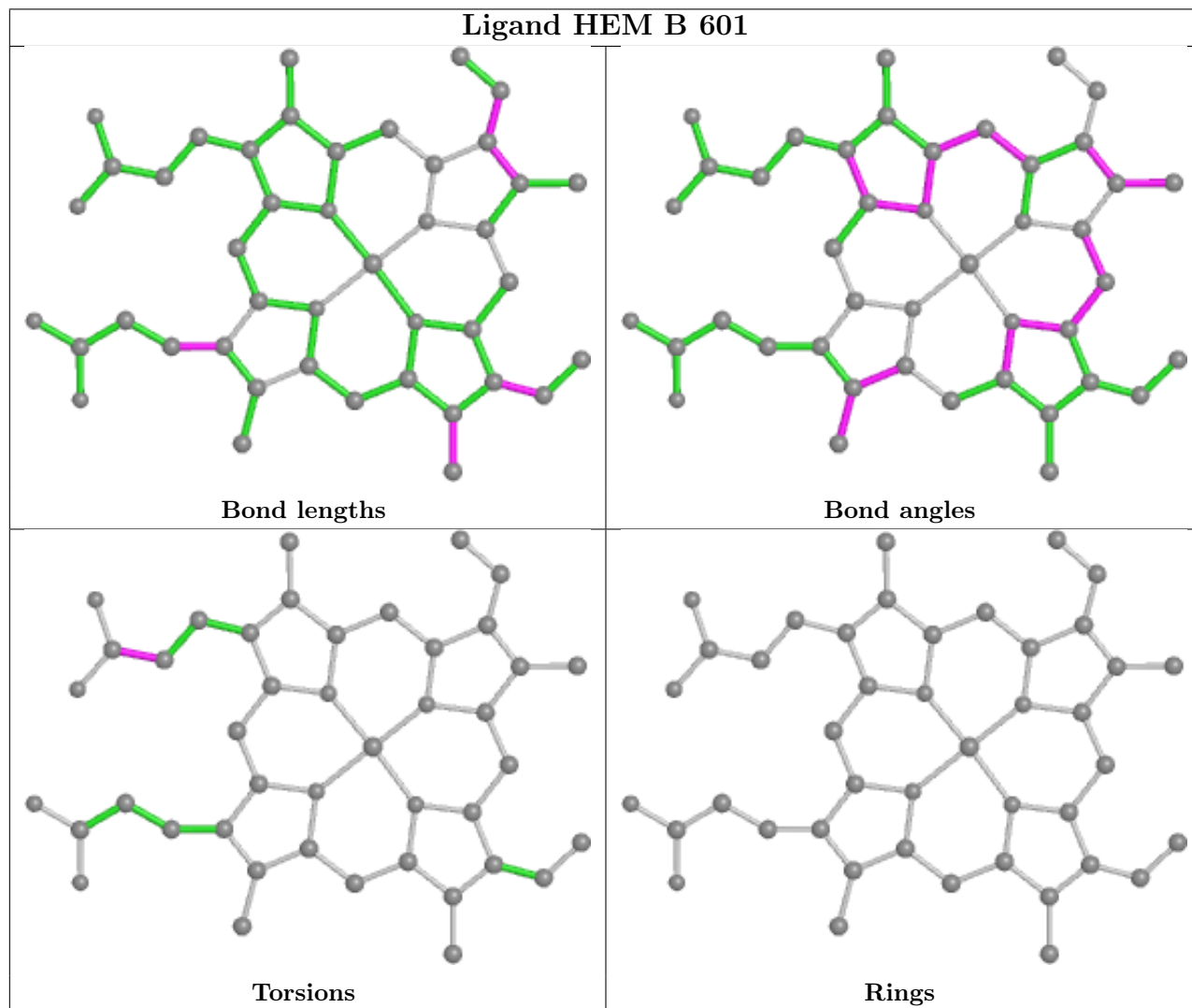
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	HEM	6	0
3	A	601	U7P	1	0
2	A	600	HEM	9	0

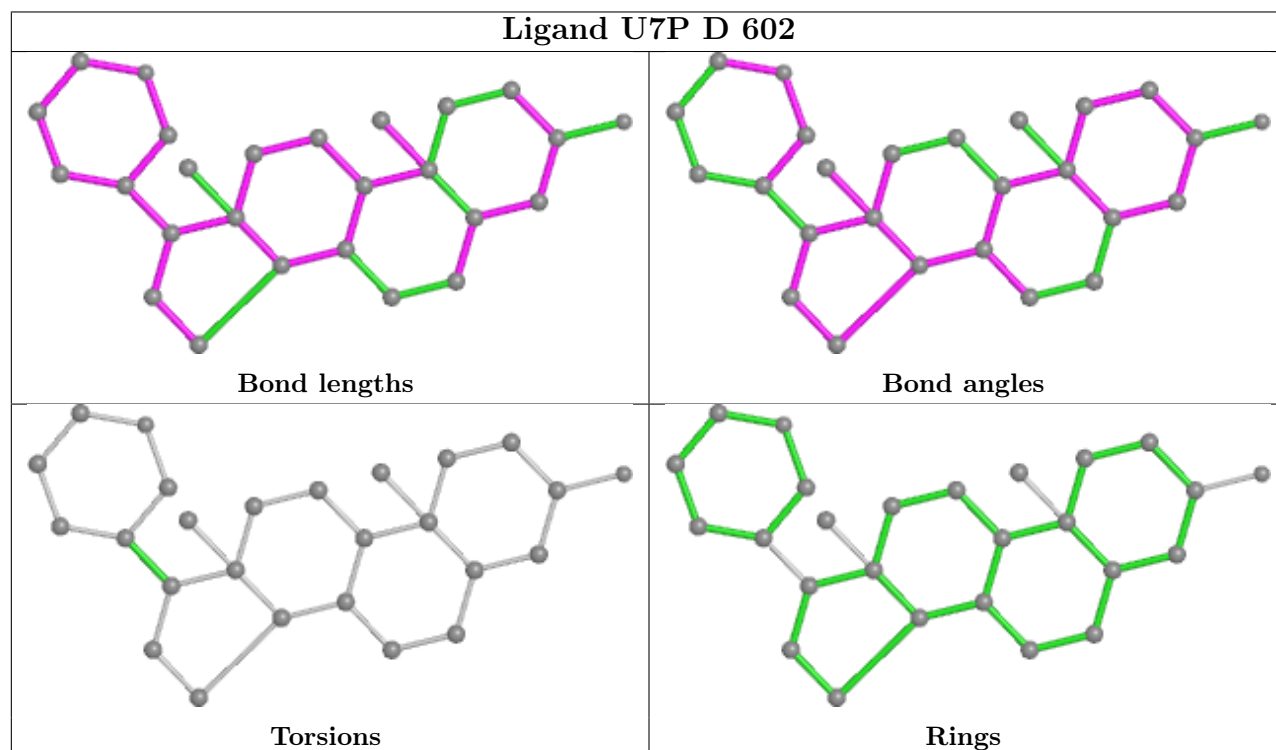
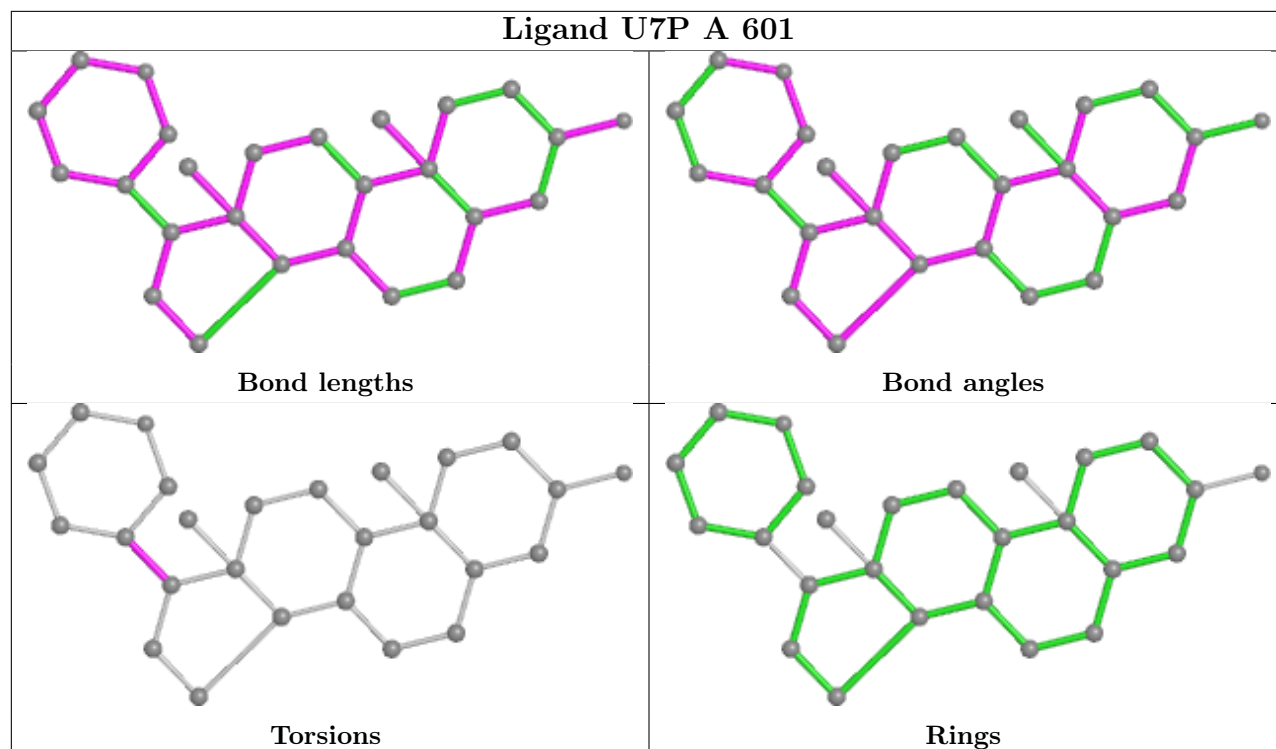
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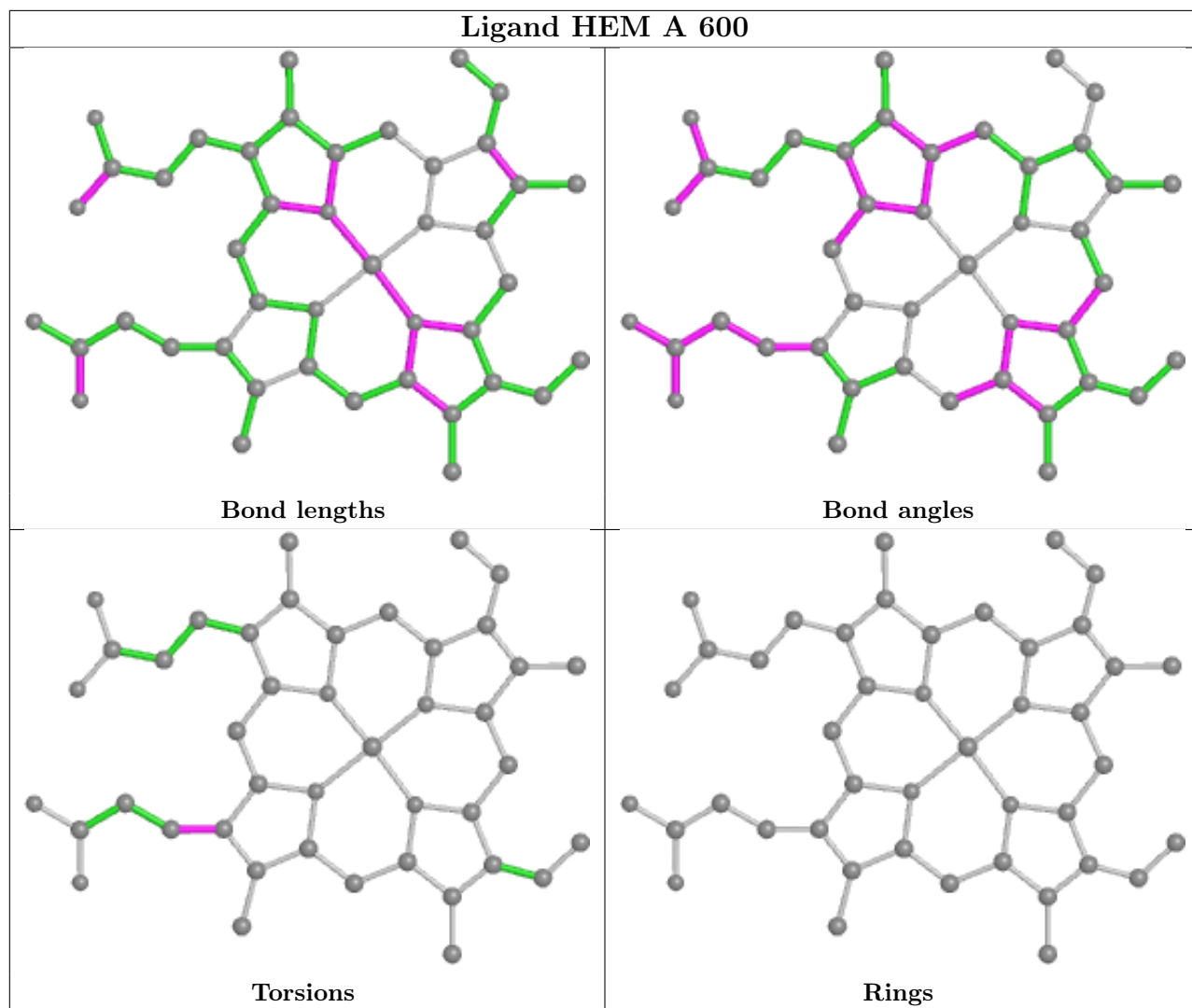
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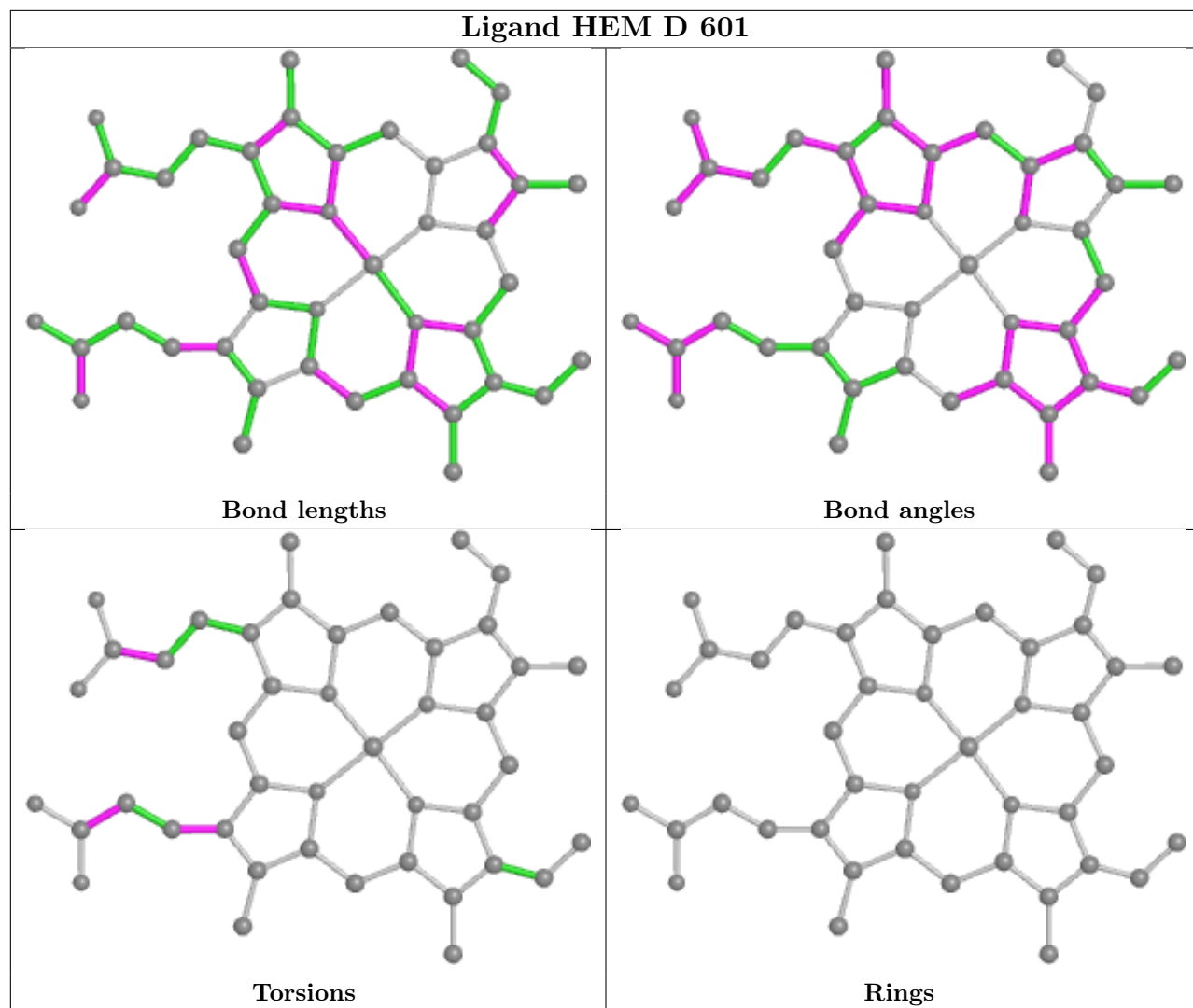
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	HEM	5	0
3	B	602	U7P	1	0
2	C	601	HEM	5	0

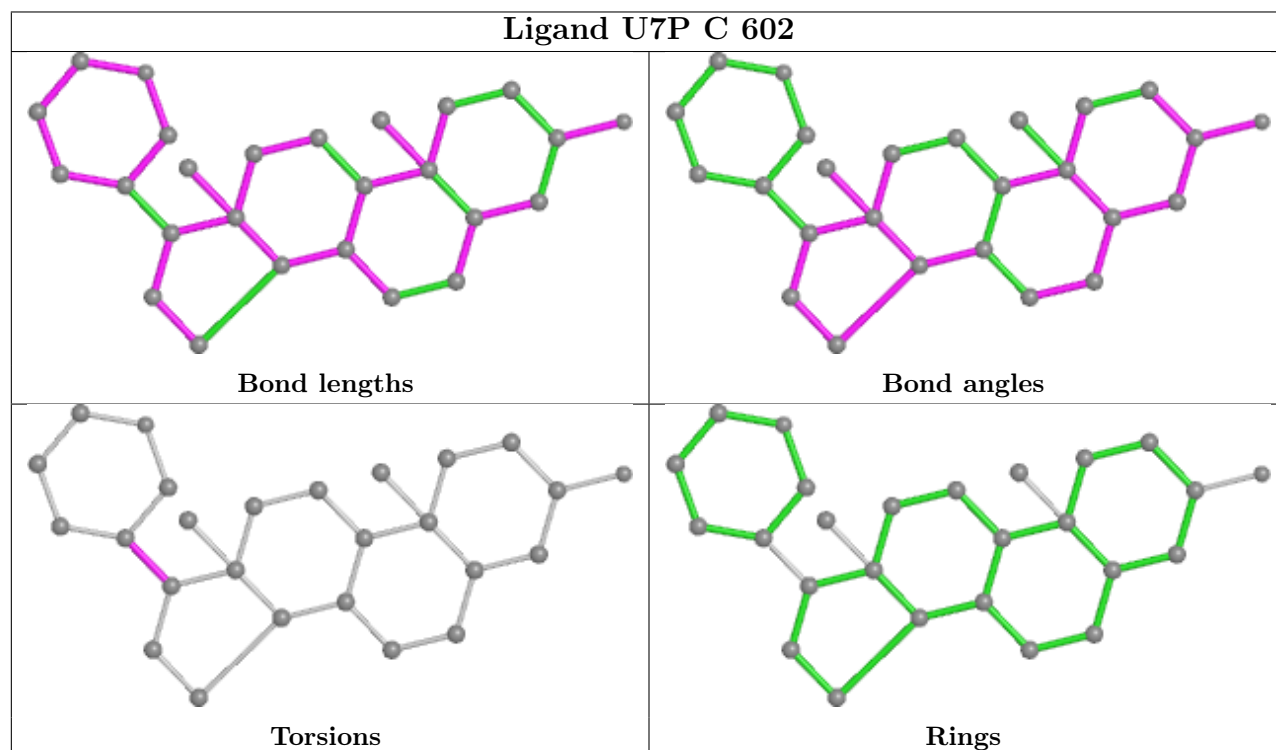
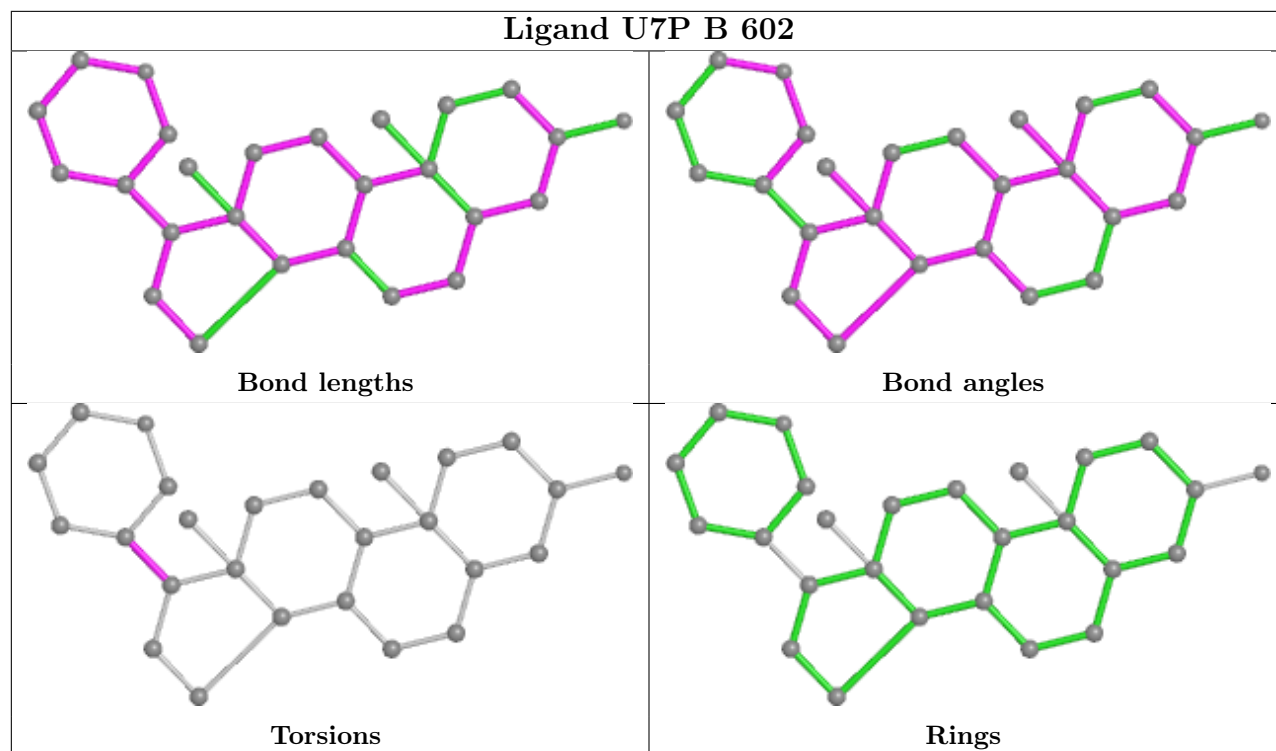
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

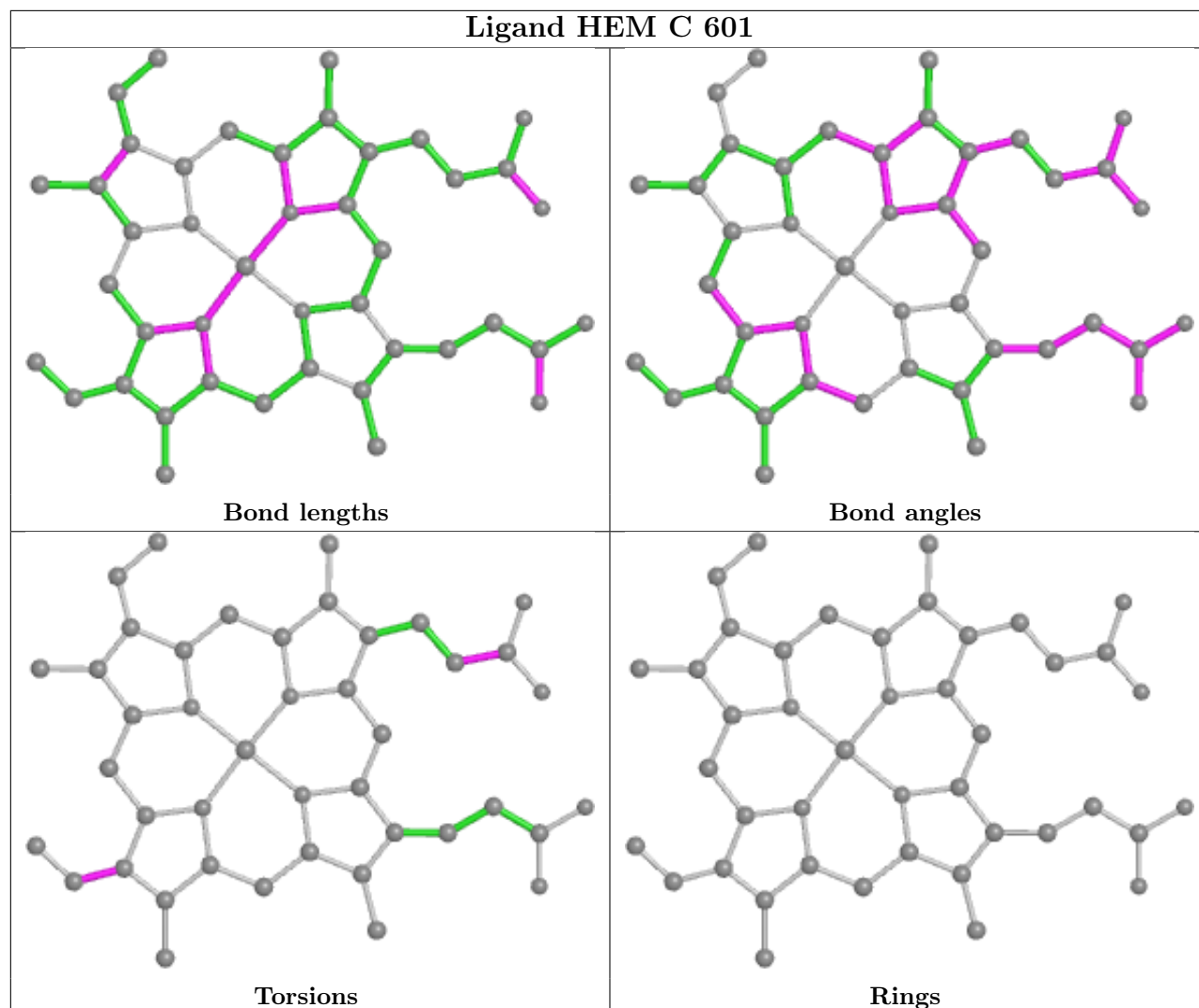












5.7 Other polymers [i](#)

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%)	0.31	13 (2%) 53 54	38, 52, 79, 108	0
1	B	465/494 (94%)	0.30	17 (3%) 41 41	37, 51, 77, 104	0
1	C	474/494 (95%)	0.47	35 (7%) 14 12	37, 52, 81, 96	0
1	D	466/494 (94%)	0.65	47 (10%) 7 5	39, 58, 94, 104	0
All	All	1871/1976 (94%)	0.43	112 (5%) 21 20	37, 53, 85, 108	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	ASP	6.2
1	A	504	ALA	5.4
1	C	139	ASP	5.2
1	D	271	MET	4.7
1	D	471	GLY	4.7
1	C	277	ASN	4.5
1	D	491	VAL	4.3
1	D	140	GLN	4.2
1	B	140	GLN	3.7
1	C	278	ALA	3.7
1	D	137	ASP	3.7
1	A	137	ASP	3.6
1	D	139	ASP	3.5
1	C	367	ALA	3.5
1	D	165	ILE	3.4
1	C	469	ASP	3.4
1	C	140	GLN	3.3
1	A	138	GLY	3.2
1	D	45	ARG	3.2
1	D	500	ARG	3.2
1	D	138	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	418	LEU	3.1
1	A	140	GLN	3.1
1	C	133	ALA	3.1
1	C	137	ASP	3.1
1	D	135	PHE	3.1
1	D	134	LEU	3.1
1	D	465	LEU	3.1
1	C	302	ALA	3.1
1	C	383	GLU	3.0
1	C	472	GLN	3.0
1	D	467	VAL	3.0
1	D	337	GLY	3.0
1	C	306	THR	3.0
1	D	470	ASP	3.0
1	D	459	LEU	2.9
1	B	252	GLU	2.9
1	D	306	THR	2.9
1	C	470	ASP	2.9
1	C	305	GLU	2.9
1	C	366	VAL	2.8
1	C	275	ASN	2.8
1	D	46	HIS	2.8
1	B	257	ASP	2.8
1	C	310	VAL	2.7
1	C	424	GLN	2.7
1	D	499	TRP	2.7
1	B	139	ASP	2.7
1	D	329	TYR	2.7
1	A	259	ILE	2.6
1	B	499	TRP	2.6
1	C	138	GLY	2.6
1	D	462	ARG	2.6
1	B	253	LYS	2.5
1	B	247	LEU	2.5
1	C	309	SER	2.5
1	D	159	THR	2.5
1	D	421	ALA	2.5
1	D	332	ILE	2.5
1	C	134	LEU	2.5
1	D	503	GLN	2.5
1	D	266	LEU	2.4
1	D	153	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	484	PHE	2.4
1	D	282	GLN	2.4
1	D	472	GLN	2.4
1	D	428	PRO	2.4
1	D	340	ARG	2.4
1	C	136	LYS	2.4
1	D	351	LEU	2.4
1	C	45	ARG	2.4
1	C	368	PRO	2.4
1	C	482	VAL	2.4
1	C	351	LEU	2.3
1	C	46	HIS	2.3
1	D	258	SER	2.3
1	B	500	ARG	2.3
1	D	442	CYS	2.3
1	A	349	ARG	2.3
1	C	120	HIS	2.3
1	D	164	SER	2.3
1	B	498	ALA	2.3
1	C	502	ALA	2.3
1	D	163	GLN	2.3
1	D	307	THR	2.3
1	B	424	GLN	2.2
1	A	274	ASP	2.2
1	C	279	GLY	2.2
1	D	494	LYS	2.2
1	D	436	GLY	2.2
1	C	483	VAL	2.2
1	B	135	PHE	2.2
1	D	338	PHE	2.2
1	D	349	ARG	2.2
1	B	255	ARG	2.1
1	C	308	THR	2.1
1	D	254	PHE	2.1
1	A	284	SER	2.1
1	D	460	LEU	2.1
1	B	307	THR	2.1
1	C	304	VAL	2.1
1	A	430	VAL	2.1
1	A	500	ARG	2.1
1	B	272	ASN	2.1
1	B	271	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	42	PHE	2.1
1	A	283	ASP	2.0
1	D	136	LYS	2.0
1	A	302	ALA	2.0
1	B	136	LYS	2.0
1	B	267	MET	2.0
1	D	287	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

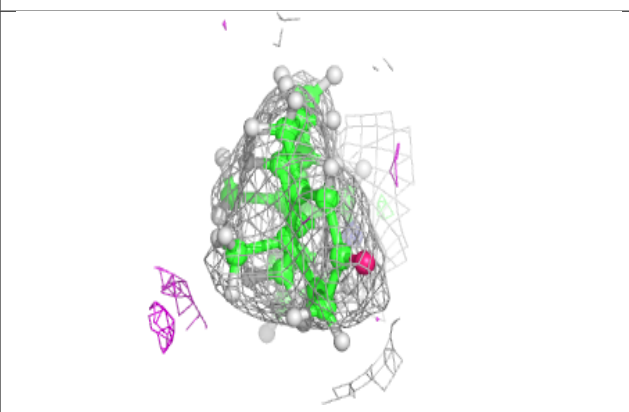
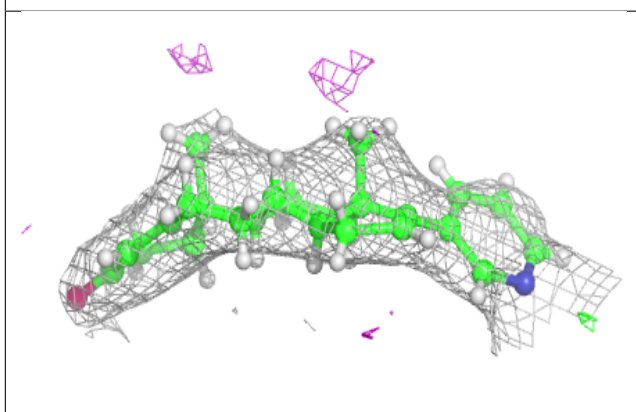
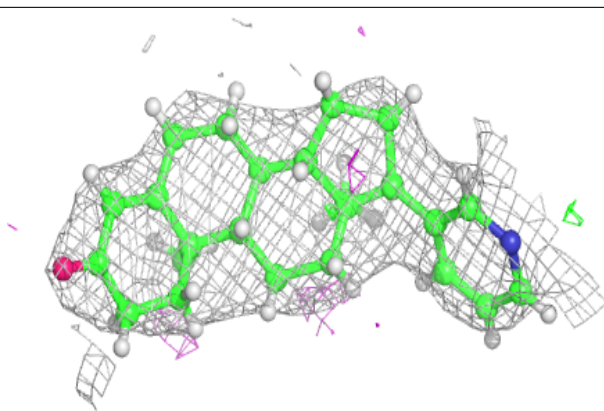
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	U7P	D	602	26/26	0.89	0.32	43,53,60,61	0
3	U7P	B	602	26/26	0.92	0.32	41,51,60,62	0
3	U7P	C	602	26/26	0.92	0.28	37,48,59,59	0
3	U7P	A	601	26/26	0.92	0.27	45,54,62,66	0
4	CL	D	603	1/1	0.92	0.09	49,49,49,49	0
4	CL	C	603	1/1	0.95	0.24	57,57,57,57	0
2	HEM	A	600	43/43	0.95	0.30	42,51,62,63	0
2	HEM	D	601	43/43	0.96	0.27	43,53,64,67	0
4	CL	B	603	1/1	0.96	0.13	60,60,60,60	0
2	HEM	B	601	43/43	0.97	0.27	39,44,54,56	0
2	HEM	C	601	43/43	0.97	0.29	35,43,52,54	0

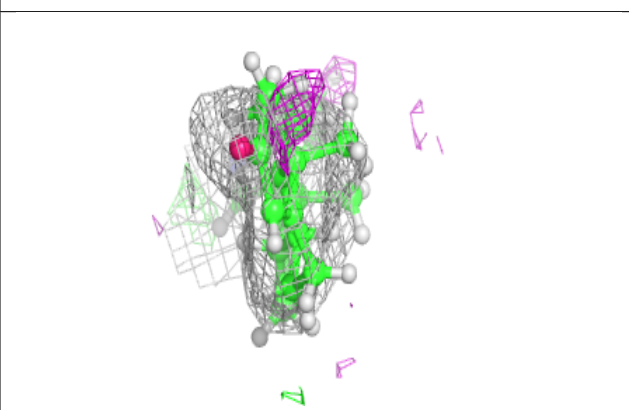
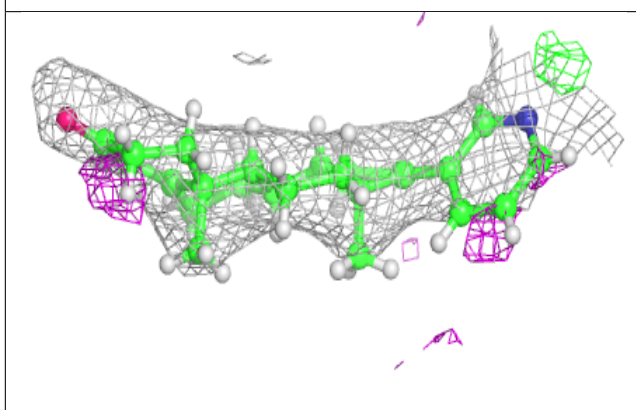
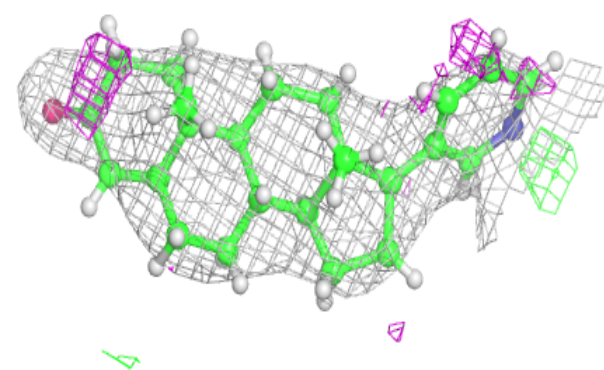
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around U7P D 602:

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

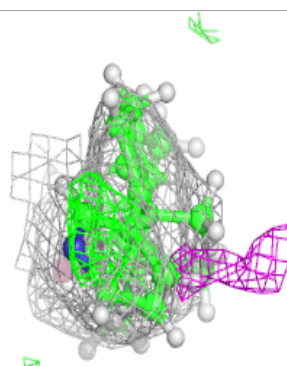
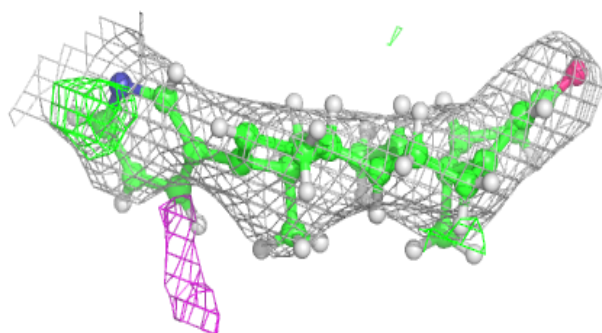
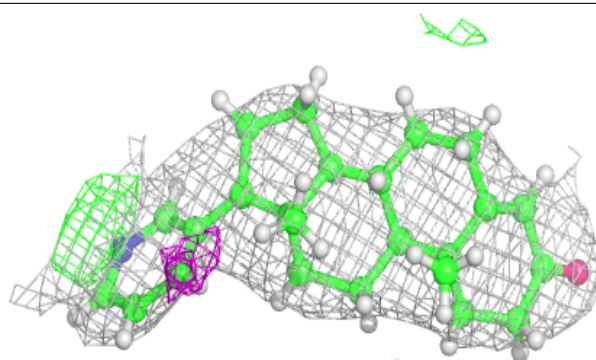
**Electron density around U7P B 602:**

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

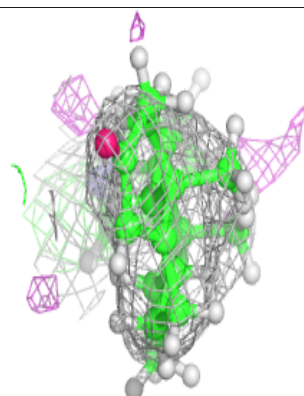
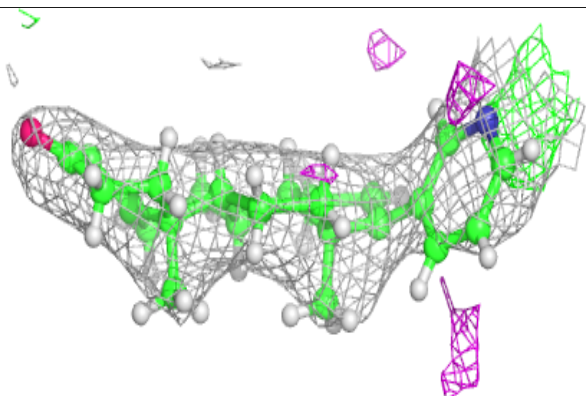
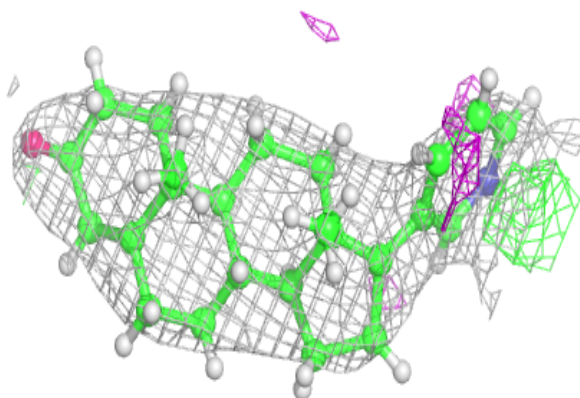


Electron density around U7P C 602:

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

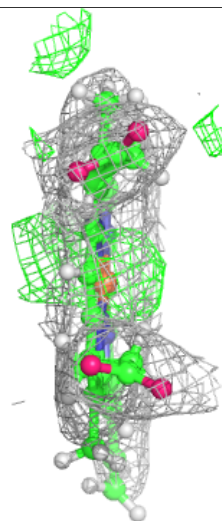
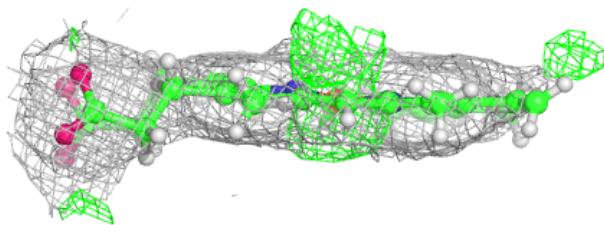
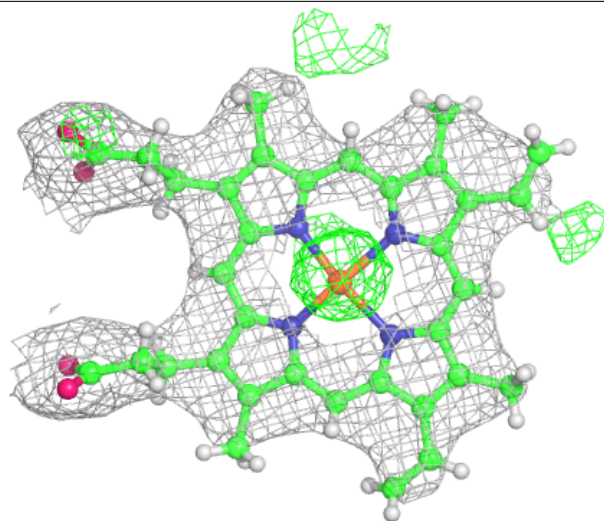
**Electron density around U7P A 601:**

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



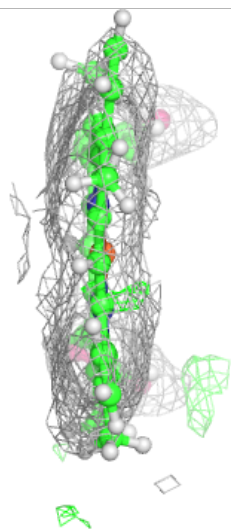
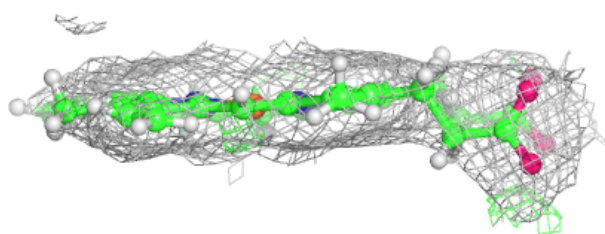
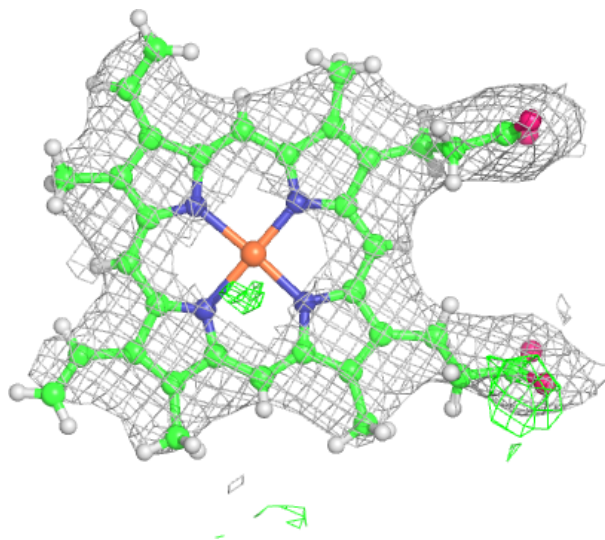
Electron density around HEM A 600:

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



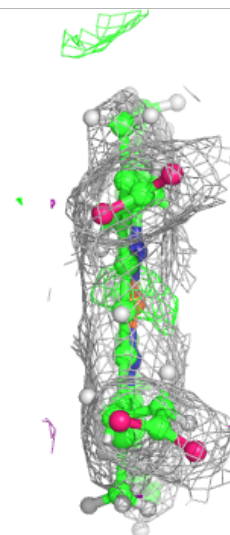
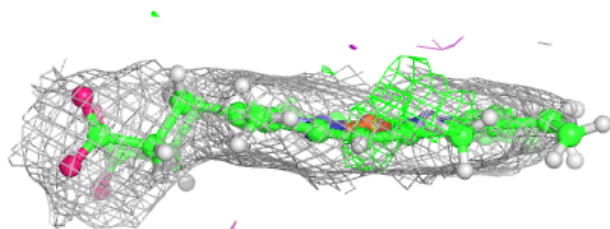
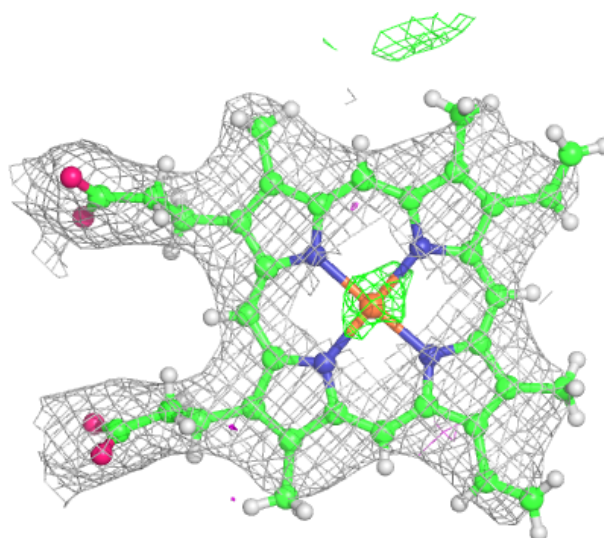
Electron density around HEM D 601:

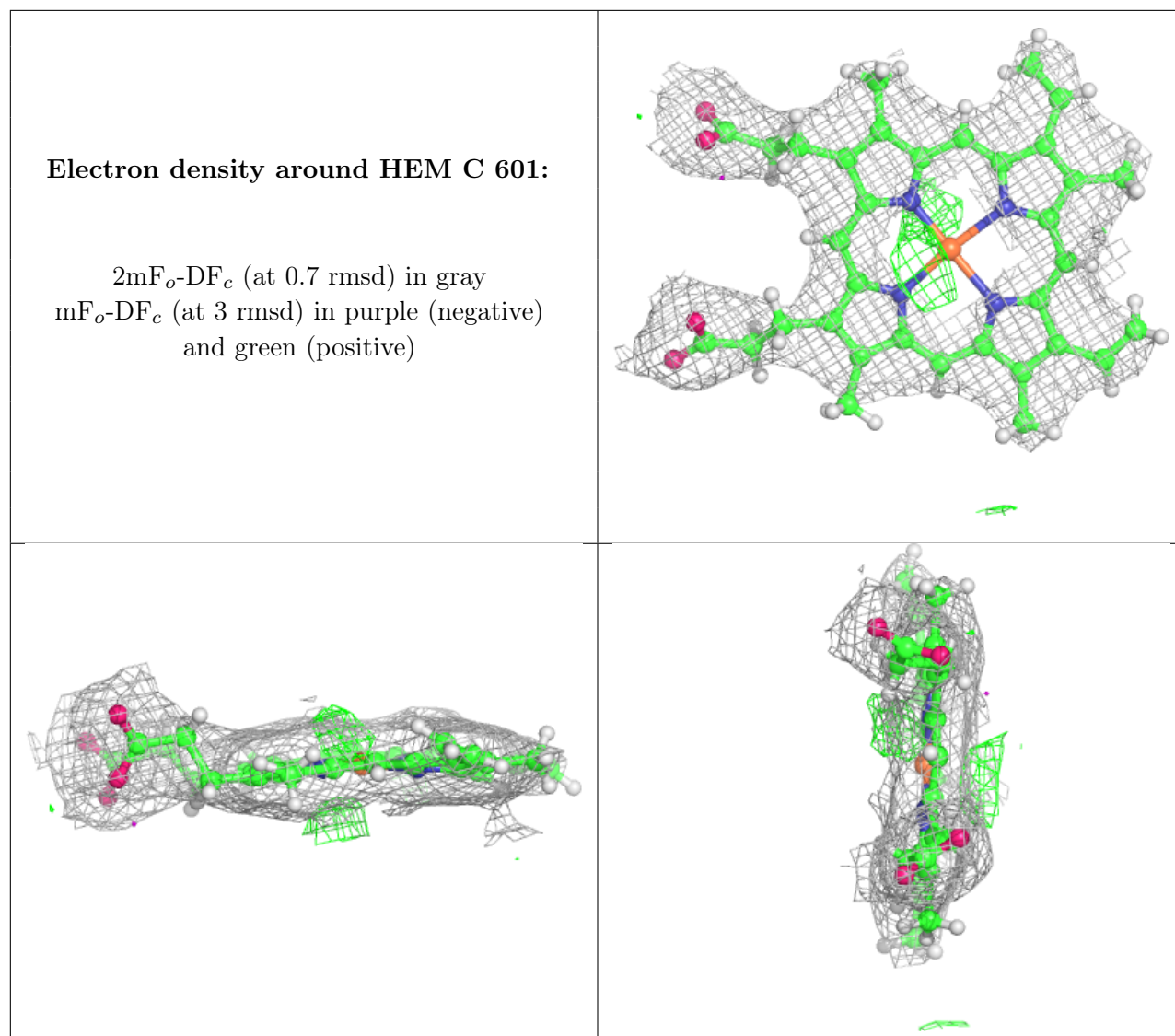
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.